Statistical Analysis and Bayesian Methods for Fatigue Life Prediction and Inverse Problems in Linear Time Dependent PDEs with Uncertainties

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ABSTRACT

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This work employs statistical and Bayesian techniques to analyze mathematical forward models with several sources of uncertainty. The forward models usually arise from phenomenological and physical phenomena and are expressed through regression-based models or partial differential equations (PDEs) associated with uncertain parameters and input data. One of the critical challenges in real-world applications is to quantify uncertainties of the unknown parameters using observations. To this purpose, methods based on the likelihood function, and Bayesian techniques constitute the two main statistical inferential approaches considered here.

Two problems are studied in this thesis. The first problem is the prediction of fatigue life of metallic specimens. The second part is related to inverse problems in linear PDEs. Both problems require the inference of unknown parameters given certain measurements. We first estimate the parameters by means of the maximum likelihood approach. Next, we seek a more comprehensive Bayesian inference using analytical asymptotic approximations or computational techniques.

In the fatigue life prediction, there are several plausible probabilistic stress-lifetime (S-N) models. These models are calibrated given uniaxial fatigue experiments. To generate accurate fatigue life predictions, competing S-N models are ranked according to several classical information-based measures. A different set of predictive information criteria is then used to compare the candidate Bayesian models. Moreover, we
propose a spatial stochastic model to generalize S-N models to fatigue crack initiation in general geometries. The model is based on a spatial Poisson process with an intensity function that combines the S-N curves with an averaged effective stress that is computed from the solution of the linear elasticity equations.

For the inverse problems in linear PDEs, we assume that, besides the unknown physical parameters, the boundary conditions are also unknown. However, noisy measurements of the boundary conditions are available. Here, we develop a novel marginalization method using a hierarchical Bayesian framework. This method accounts for uncertainties in the boundary conditions and therefore reduces the bias error in the estimated parameters. We apply the marginalization technique to the real-world problem of estimating thermal properties of building walls. Furthermore, we generalize the marginalization technique to a sequential framework by deriving an ensemble marginalized Kalman filter (EnMKF).
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Chapter 1

Statistical and Bayesian Inverse Problems

1.1 Motivation

It is a fundamental task in science and engineering to make accurate predictions and simulations of a physical phenomenon. Mathematical models are used to represent physical phenomena that take the abstract form:

\[ F(\theta, S; u(\theta, S)) = 0, \]  

(1.1)

where \( F \) is a collection of operators (algebraic, differential, partial-differential, integral, . . . ), \( \theta \) is a vector of model parameters, \( S \) is a scenario in which the problem is posed (domain, boundary and initial conditions, . . . ), and \( u(\theta, S) \) is the solution for specific \( \theta \) and \( S \) [1].

The task is then to solve the forward problem, that is to find \( u(\theta, S) \in U \) that satisfies (1.1) given \( \theta \in \Theta \subset \mathbb{R}^p \) and \( S \). The inverse problem, on the other hand, is to find \( \theta \in \Theta \subset \mathbb{R}^p \) given measurements of \( u(\theta, S) \) that satisfies (1.1) for a given \( S \).

In order to solve the forward problem, some information about \( \theta \) must be provided. However, \( \theta \) is usually unknown and cannot be observed directly. The only way to describe \( \theta \) is to solve the inverse problem given measurements of \( u(\theta, \cdot) \) under some scenarios \( S_1, S_2, \ldots \). It is important to keep in mind that the retrieved parameters will be used to make predictions under different scenarios. Therefore, confidence measures of the estimated parameters are also necessary.
1.2 Statistical inversion

Statistical inversion provides a set of methods to infer parameters and analyze uncertainties using measurements and prior knowledge. Unlike classical regularization methods, statistical inversion can provide more than a single estimate \cite{2}. The classical setup for inverse problems takes the form:

Given measurements \( y \in \mathcal{Y} \subset \mathbb{R}^m \), find \( \theta \in \Theta \subset \mathbb{R}^p \) such that

\[
y = H(u(\theta, S), \epsilon),
\]

where \( H \) is a map from the solution space \( \mathcal{U} \) to the measurement space \( \mathcal{Y} \) and \( \epsilon \in \mathbb{R}^m \) denotes the modeling error and measurement noise.

The statistical framework stands out naturally because measurements are usually noisy and probability theory is needed to model the noise. Also, \( y \) is viewed as a random vector which enlarges the measurement space and removes the ill-posedness of the problem \cite{2}.

Within the statistical framework, there are many theories, however, two approaches are usually distinguished \cite{3}: the classical/frequentist approach and the Bayesian approach. Although the Bayesian approach is superior, the classical approach can be more practical \cite{4}. The advantages of the Bayesian approach include the principled incorporation of prior knowledge by Bayes’ theorem, the full representation of uncertainty by the posterior distribution and the embedded concept of learning \cite{5, 6}. The classical/frequentist approach avoids the process of eliciting the prior distribution, which is a dividing subject between subjective and objective Bayesian statisticians \cite{7}. For a given problem, the two approaches share the same likelihood function and can complement each other \cite{8}.
1.3 Likelihood function

The likelihood function is the core of classical and Bayesian inferences [4]. It is based on the probability distribution and the type of observed data [9]. The likelihood function of $\theta$ is, in general, the probability mass/density function of the fully observed (non-censored) data, evaluated at the observed data points, denoted by $L(\theta)$ or $L(\theta|y)$ [8, 10]. If $y = (y_1, y_2, \ldots, y_m)$ are i.i.d (independent and identically distributed) observations, then the corresponding likelihood of $\theta$ is

$$L(\theta) = \rho(y|\theta) = \prod_{i=1}^{m} \rho(y_i|\theta),$$

(1.3)

where $\rho(y|\theta)$ is the assumed probability density function for the observation, $y$.

Contributions from censored data could be also included in the likelihood. Censored data are either left-censored, interval-censored or right-censored. The likelihood function must be constructed for each problem based on the available data.

1.4 Classical approach

In a classical/frequentist approach, estimated parameters depend only on the data through the likelihood function. No prior information about these parameters is included. Although this makes the classical approach more objective than the Bayesian approach, the use of non-informative priors maintains objectivity and the benefits of Bayesian analysis [11, 12]. Nevertheless, classical methods are very practical and it is reasonable to begin with these before applying the Bayesian tools.

1.4.1 Maximum likelihood estimate

The maximum likelihood estimator (MLE), $\hat{\theta}$, is the parameter vector where the maximum (over the parameter space $\Theta$) of $L(\theta)$ is achieved. It was first used by Ronald Fisher in 1912 [13] and is considered one of the most important methods for
point estimation in applied statistics. In practice, the MLE is obtained by maximizing
the log-likelihood function. In general, the MLE exists and is unique but there are
some exceptional cases [7, 14].

1.4.2 Profile likelihood

In many cases, the vector of unknown parameters may contain nuisance parameters
or parameters of little importance. These parameters can be replaced in the origi-
nal likelihood function by their estimated ML values, to obtain the so-called profile
likelihood function of the parameters of interest. The profile likelihood provides fur-
ther analysis on the relevant parameters or on one parameter in particular [15]. For
example, if $\theta = (\theta_0, \theta_1)$, then the profile likelihood of $\theta_1$ is

$$R(\theta_1) = \max_{\theta_0} \frac{L(\theta_0, \theta_1)}{L(\hat{\theta})},$$

where $R(\theta_1)$ is normalized by $L(\hat{\theta})$ to have a maximum of 1.

The profile likelihood functions can be used to construct confidence intervals of
certain parameters and the information induced from this is more accurate for the
relevant parameters [3].

1.4.3 Bootstrap

Bootstrap or bootstrapping is a simple computation-based method to estimate biases,
standard deviations and confidence intervals using resampling techniques [16, 14]. We
sample with replacement from the actual data and compute our quantity of interest
(QoI) using the resample dataset. By repeating this procedure, we generate several
bootstrap datasets and the corresponding values of the QoI. These values are then
used to estimate a sampling distribution of the QoI [17]. The QoI could be the MLE
or the full posterior distribution. Due to its simplicity, bootstrap is a very popular
non-parametric approach in many applications [18].

1.4.4 Model comparison

All the previous classical tools are used to analyze the assumed model using the data. In many applications, such as survival analysis, we may have several competing models that must be ranked to select the most superior model [8]. In a classical approach, these methods are called information criteria, such as Akaike information criterion (AIC) [19], Bayesian information criterion (BIC) [20, 21] and AIC with correction [22]. They take into account both the goodness of fit in terms of maximized log-likelihood value, $\log L(\hat{\theta})$, and the complexity of the model in terms of the number of parameters, $p$. Despite its name, the Bayesian information criterion is actually likelihood-based.

- **Akaike information criterion (AIC)**

$$\text{AIC} = -2 \log L(\hat{\theta}) + 2p.$$ 

- **Bayesian information criterion (BIC)**

$$\text{BIC} = -2 \log L(\hat{\theta}) + 2p \log(m).$$

- **AIC with correction (AICc)**

$$\text{AICc} = -2 \log L(\hat{\theta}) + \frac{2pm}{m - p - 1}.$$ 

1.5 Bayesian approach

In maximum likelihood inference, we seek a point estimation of the unknown vector of parameters, $\theta$ where we do not assume initially that $\theta$ is random. However, in a
Bayesian framework, \( \theta \) is assumed to be a random vector and it has a probability model that is independent of the data. This model is known as the prior distribution of \( \theta \). The posterior distribution is then the conditional density of \( \theta \) given the data \( y \) [8]. It is derived by Bayes’ theorem

\[
\rho(\theta|y) = \frac{L(\theta)\rho(\theta)}{\int_{\Theta} L(\theta)\rho(\theta)d\theta}.
\] (1.4)

Bayesian inference can be summarized by the three following steps:

1. Find a prior probability density \( \rho(\theta) \) that reflects prior experience,

2. Construct a likelihood function that connects the observations and \( \theta \),

3. Develop methods to explore the posterior probability density.

The construction of the likelihood is the same in classical and Bayesian methods, although the interpretation may differ. Choosing a prior density could be a difficult task because prior information is not usually described in terms of probability distributions [2]. There are standard classes of priors that can be used, such as conjugate priors, improper priors, and Jeffreys’ priors [8]. Each class serves a different purpose and may simplify or complicate the computation of the posterior. Recently, a new approach for constructing proper informative priors, called Penalised Complexity priors, has been introduced in [23]. These Penalised Complexity priors are designed to be default priors for many hierarchical models [23].

In practice, it is common to obtain a complicated posterior density that we cannot describe analytically or sample from. Therefore, approximations and sampling algorithms are needed to represent the posterior distribution.
1.5.1 Laplace method

When the posterior is unimodal and reasonably concentrated, the Laplace method provides a good approximation to the posterior moments, marginal posterior densities, predictive densities and Bayes factors [24, 25]. It is also the basis for approximate Bayesian inference with latent Gaussian models [26]. The idea of the Laplace method is to approximate the posterior density, $\rho(\theta|y)$, by utilizing the Gaussian density:

$$
\frac{1}{\sqrt{(2\pi)^p|\Sigma(\theta^*)|}} \exp \left\{ -\frac{1}{2} (\theta - \theta^*)' \Sigma(\theta^*)^{-1} (\theta - \theta^*) \right\}
$$

where $\theta^*$ is the maximum a posteriori (MAP) probability estimate of $\theta$ and $\Sigma(\theta^*)$ is the inverse Hessian matrix of the negative log posterior, evaluated at $\theta^*$ [10].

1.5.2 Markov chain Monte Carlo (MCMC)

Markov chain Monte Carlo (MCMC) simulation algorithms are used to generate samples from a target distribution using a proposal distribution that is simpler to sample from. The idea is to construct an irreducible, aperiodic Markov chain such that the target distribution is the stationary distribution of the chain [17]. MCMC algorithms can be divided into Gibbs samplers and Metropolis algorithms. To generate samples from a complicated posterior distribution, the Metropolis-Hastings algorithm could be the simplest and most efficient MCMC algorithm. There are many implementations of the Metropolis-Hastings algorithm based on the selected jumping rule [27, 28]. Algorithm 1 shows the Metropolis-Hastings algorithm with a random-walk jump and Gaussian proposal.

1.5.3 Model comparison

In a Bayesian approach, there are two types of criteria to compare Bayesian models. The first one integrates the likelihood with respect to the prior for each model and
Algorithm 1 Random walk Metropolis-Hastings algorithm

1: set an initial value for the chain: $\theta_c = \theta_0$ and choose $\delta > 0$
2: compute $a = \log L(\theta_c) + \log \rho(\theta_c)$
3: draw $\theta_p$ from $N(\theta_c, \text{diag}(\delta))$
4: compute $b = \log L(\theta_p) + \log \rho(\theta_p)$
5: let $H = \min(1, \exp(b - a))$ and draw $r$ from $U(0, 1)$
6: if $H > r$ then
7: $\theta_c = \theta_p$
8: $a = b$
9: else
10: go to step 3

yields the marginal likelihood. The second criterion measures the predictive accuracy and includes Bayesian equivalents of AIC and cross-validations [8, 29, 28].

1.5.3.1 Bayes factor

For two models, one can compute the Bayes factor that is the ratio of the two marginal likelihoods. Specifically, the Bayes factor of Model A against that of Model B is defined as

$$F_{B,A} := \frac{\int L_B(\theta_B; y)\rho_B(\theta_B)d\theta_B}{\int L_A(\theta_A; y)\rho_A(\theta_A)d\theta_A} = \frac{P_B(y)}{P_A(y)},$$

where $\rho_A(\theta_A)$ and $\rho_B(\theta_B)$ are the prior densities, and $P_A(y)$ and $P_B(y)$ are the marginal likelihoods [5].

Fast estimates of the log marginal likelihoods can be obtained by the Laplace method. Other methods combine the Laplace approximation with MCMC posterior samples such as the Laplace–Metropolis estimator [30, 31]. In both cases, the approximation of the log marginal likelihood $\log(P(y))$ is given by

$$\frac{p}{2} \log(2\pi) + \frac{1}{2} \log(|H^*|) + \log(\rho(\theta^*)) + \log(L(\theta^*|y)),$$

where $p$ is the number of parameters in the vector $\theta$, $\theta^*$ is the maximum posterior estimate and $H^*$ is the inverse Hessian of the negative log posterior. In the Laplace
estimator, $\theta^*$ and $H^*$ are approximated numerically. The Laplace–Metropolis estimator uses the MCMC posterior samples to find the maximum posterior estimate, $\theta^*$, and approximate, $H^*$, by the empirical covariance matrix.

### 1.5.3.2 Predictive Information Criteria

After inferring the parameters of a given model, the prediction accuracy of the model is computed by mean of the log predictive density, $\log \rho(y_{\text{new}}|\theta)$, where $y_{\text{new}}$ is a “new” observation. However, new observations are not always available. Therefore, approximate estimates and cross-validation methods are needed.

An overestimate of the log predictive density can be obtained by using the observed data, $\{y_i\}_{i=1}^m$. The log pointwise predictive density (lppd) estimate uses the observed data that were used to infer $\theta$ and the MCMC posterior samples, $\{\theta^j\}_{j=1}^S$. Predictive information criteria are then obtained from lppd by scaling and penalization [32]. Deviance information criterion (DIC) can be considered a Bayesian generalization of the AIC by replacing the maximum likelihood estimate by the posterior mean and computing the effective number of parameters [28]. Watanabe–Akaike information criterion, or widely applicable information criterion (WAIC), is another stable Bayesian criterion that also approximates the leave-one-out cross-validation [32, 33, 34].

- Log pointwise predictive density (lppd)

$$lppd = \sum_{i=1}^m \log \left( \frac{1}{S} \sum_{j=1}^S \rho(y_i|\theta^j) \right).$$

- Deviance information criterion (DIC)

$$\text{DIC} = -2 \left( \log L(\bar{\theta}) - p_{\text{DIC}} \right),$$
where $\bar{\theta}$ is the posterior mean and

$$p_{\text{DIC}} = 2 \left( \log L(\bar{\theta}) - \frac{1}{S} \sum_{j=1}^{S} \log \theta^j \right).$$

- Watanabe–Akaike information criterion or widely applicable information criterion (WAIC)

$$\text{WAIC} = -2(lppd - p_{\text{WAIC}}),$$

where

$$p_{\text{WAIC}} = 2 \sum_{i=1}^{m} \left( \log \left( \frac{1}{S} \sum_{j=1}^{S} \rho(y_i|\theta^j) \right) - \frac{1}{S} \sum_{j=1}^{S} \log \rho(y_i|\theta^j) \right),$$

Cross-validation is the most popular yet computationally expensive method to estimate the predictive accuracy. In leave-one-out cross-validation, we remove one observation from the data and use the rest to infer $\theta$. Then, we compute the log predictive density for the removed observation. In the K-fold cross-validation, the data are randomly partitioned into disjoint subsets, $\{y_k\}_{k=1}^{K}$. Subsequently, we define $\{y_{(-k)}\} = \{y_1, \ldots, y_{k-1}, y_{k+1}, \ldots, y_K\}$ to be a training set. For each training set, we compute the corresponding posterior distribution, $p(\theta|y_{(-k)})$. Following this, the log predictive density for $y_i \in y_k$ is computed using the training set $\{y_{(-k)}\}$, that is:

$$lpd_i = \log \left( \frac{1}{S} \sum_{j=1}^{S} \rho(y_i|\theta^{k,j}) \right), i \in k,$$

where $\{\theta^{k,j}\}_{j=1}^{S}$ are the MCMC samples of the posterior $p(\theta|y_{(-k)})$. Finally, we sum to obtain the expected log predictive density (elpd):

$$\text{elpd} = \sum_{i=1}^{m} lpd_i.$$
The K-fold cross-validation is usually used instead of the leave-one-out cross-validation [35, 33].

1.6 Bayesian experimental design

Designing an experiment is a decision problem where the expected utility must be maximized. The utility function depends on the problem, the mathematical model and the purpose of the experiment [36]. A comprehensive literature review and theoretical background based on decision theory can be found in [36] [37]. In Bayesian experimental design, the utility function is related to the Shannon information gain [38], which is the Kullback-Leibler divergence [39] between the prior density $\rho(\theta)$ and the posterior density function of $\theta$

$$D_{KL}(\mathbf{y}, \xi) := \int_{\Theta} \log \left( \frac{\rho(\theta|\mathbf{y}, \xi)}{\rho(\theta)} \right) \rho(\theta|\mathbf{y}, \xi) d\theta,$$

where $\xi$ is an experimental setup. The expected utility is then the integration of $D_{KL}$ over all possible observations

$$E[D_{KL}](\xi) := \int_{\mathbf{y}} \int_{\Theta} \log \left( \frac{\rho(\theta|\mathbf{y}, \xi)}{\rho(\theta)} \right) \rho(\theta|\mathbf{y}, \xi) d\theta \rho(\mathbf{y}, \xi) d\mathbf{y}. \quad (1.5)$$

The expected information gain (1.5) provides a criterion to determine which experimental design is the most informative to infer $\theta$ before executing the experiment. However, the computation cost to evaluate this quantity is very high. The Laplace method (1.5.1) provides a fast approximation of the information gain and the expected information gain. This approximation is accurate and robust [38, 10]. It has been tested in many applications such as seismic inversion [11], combustion kinetics [38], and survival analysis [12].
1.7 Data assimilation

Data assimilation refers to all methods for combining states of dynamical systems with partial noisy observations. As a special case, filtering is the sequential estimation of a state at some time, \( t \), given all observations up to time, \( t \). Filtering is also generalized to the joint estimation of the state and the unknown static parameters, \( \theta \). In Bayesian filtering, the goal is to find the joint posterior distribution of the state and the parameters. Sampling algorithms are then required to approximate the filtering distribution because the posterior cannot be obtained in a closed form. Sequential sampling algorithms include particle filters and ensemble Kalman filters. Particle filters converge to the true filtering distribution but they are impractical in high dimensions. The ensemble Kalman filter (EnKF), on the other hand, is the preferred method for nonlinear and high-dimensional models. The EnKF algorithms have been adopted in many real applications such as oceanography, weather prediction, tsunami prediction, reservoir engineering and hydrology. We now briefly introduce the Kalman filter, ensemble Kalman filter, and state-parameter estimation.

1.7.1 Kalman filter

Assume the following discrete state observation system:

\[
\begin{align*}
    u_k &= F u_{k-1} + v_k, \\
    y_k &= H u_k + w_k,
\end{align*}
\]

where \( u_k \) is the dynamic state of the system at time \( k \), \( y_k \) is the observational vector available at time \( k \), \( F \) is a linear dynamic operator and \( H \) is a linear observational operator. The vectors, \( v_k \) and \( w_k \), are centered Gaussian random vectors with covariance matrices \( V_k \) and \( W_k \), respectively. They represent the model error and the
measurement noise.

Under the above assumptions, the Kalman filter provides the exact Bayesian filtering of the above system \[51\]. The filtering distribution at time \(k\) is a Gaussian distribution with mean, \(u_{k|k}\), and covariance matrix, \(P_{k|k}\). The Kalman filter algorithm can be summarized by the two recursive steps:

- **Prediction step:**
  \[
  u_{k|k-1} = Fu_{k-1|k-1}, \\
  P_{k|k-1} = FP_{k-1|k-1}F' + W_k,
  \]

- **Analysis step:**
  \[
  K_k = P_{k|k-1}H'(HP_{k|k-1}H' + V_k)^{-1}, \\
  u_{k|k} = u_{k|k-1} + K_k (y_k - u_{k|k-1}), \\
  P_{k|k} = (I - K_k)P_{k|k-1},
  \]

where \(K_k\) is the Kalman gain matrix.

### 1.7.2 Ensemble Kalman filter (EnKF)

The basic idea of EnKF is to generate Monte Carlo samples of the prediction distribution and assume they are Gaussian and independent. Therefore, the analysis step will apply Kalman update formulas even for a nonlinear dynamic operator, \(F\). Several versions of EnKF algorithms are reviewed in the literature \[44, 46, 47\]. We describe below the stochastic EnKF algorithm.

- **Initialization:**
  \[
  \{u_0^i, i = 1, \ldots, M\},
  \]
• Prediction step:

\[ u_{i|k-1}^i = F(u_{i-1}^i), \quad i = 1, \ldots, M \]

\[ P_{k|k-1} = \frac{1}{M-1} \sum_{i=1}^{M} (u_{i|k-1}^i - \overline{u}_{k|k-1}) (u_{i|k-1}^i - \overline{u}_{k|k-1})', \]

where \( \overline{u}_{k|k-1} \) is the sample mean \( \overline{u}_{k|k-1} = \frac{1}{M} \sum_{i=1}^{M} u_{i|k-1}^i \).

• Analysis step:

\[ K_k = P_{k|k-1}H' (HP_{k|k-1}H' + V_k)^{-1}, \]

\[ u_{i|k}^i = u_{i|k-1}^i + K_k (y_k + v_k^i - u_{i|k-1}^i), \quad i = 1, \ldots, M, \]

where \( v_k^i \sim N(0, V_k) \) are random perturbations.

In practice, the full covariance matrix \( P_{k|k-1} \) cannot be computed. It is sufficient to compute the matrices \( P_{k|k-1}H' \) and \( HP_{k|k-1}H' \) directly as follows:

\[ P_{k|k-1}H' = \frac{1}{M-1} \sum_{i=1}^{M} (u_{i|k-1}^i - \overline{u}_{k|k-1}) (Hu_{i|k-1}^i - H\overline{u}_{k|k-1})' \]

\[ HP_{k|k-1}H' = \frac{1}{M-1} \sum_{i=1}^{M} (Hu_{i|k-1}^i - H\overline{u}_{k|k-1}) (Hu_{i|k-1}^i - H\overline{u}_{k|k-1})'. \]

In general, EnKF does not converge to the Bayesian posterior distribution, but to the mean-field EnKF (MFEnKF). A fixed bias error is always present due to the Gaussian assumption regardless of the ensemble size [52]. Therefore, the only way to improve EnKF is by reducing the Monte Carlo error. Multilevel techniques are currently been used with EnKF to reduce the Monte Carlo error using small ensemble sizes [53, 54].

1.7.3 EnKF for State-parameter estimation

As mentioned, model parameters are usually uncertain. In a filtering approach, EnKF can be generalized to address the joint state-parameter estimation problem. By as-
assuming trivial evolution of the static parameters, the analysis step of EnKF can be applied to the augmented vector of the parameters and the state \[53\]. The parameters are then updated using the state observations. The state-parameter estimation problems are naturally difficult and EnKF requires some adjustments by inflation \[56\], \[57\] and localization \[58\].
1.8 REFERENCES


Chapter 2

Overview of Articles

This chapter summarizes the work and the results of each paper in this thesis. Sections 2.1 and 2.2 are devoted to the problem of fatigue life prediction. Sections 2.3, 2.4 and 2.5 concern inverse problems in linear time-dependent PDEs and the application of estimating thermal properties of building walls.

2.1 Overview of Article I


In this article, we provide a systematic framework to calibrate and compare S-N models given uniaxial fatigue experiments. We consider fatigue-limit models and random fatigue-limit models and fit them to the data by maximum likelihood approach. The quantiles of the life distribution are computed and compared with the data visually. We also consider a Bayesian approach and estimate the posterior distribution for the model parameters for different a priori scenarios. Some S-N models are compared and ranked using classical information criteria, Bayes factor, predictive information criteria and cross-validation techniques.
2.1.1 Fatigue experiments data

Dogbone specimens are subjected to cyclic loadings until either the specimen breaks or the number of cycles is very high. For each experiment, recorded measurements are the maximum stress $S_{\text{max}}$, the stress ratio $R$, the number of cycles when the experiment is stopped and the binary variable $\delta$ that indicates whether the specimen is broken or not. If the specimen is not broken, then it is a right-censored observation or a run-out.

In order to obtain a general S-N model for different cycle ratios, we model the equivalent stress, $S_{eq}^{(q)} = S_{\text{max}} (1 - R)^q$, where $q$ is a fitting parameter. There are several possible ansatz functions for the equivalent stress in the literature.

2.1.2 S-N models

There are also several classes of S-N models that forecast the fatigue life, $N$ in terms of the stress $S$. The fatigue-limit models have in common a fatigue-limit parameter which defines a minimum stress threshold where the fatigue life is finite. If the stress is smaller than the fatigue-limit, then $N$ will be infinite. Let $A_3$ be the fatigue limit parameter. Given the equivalent stress $S_{eq} > A_3$, $\log_{10}(N)$ is a random variable with mean $\mu(S_{eq})$ and standard deviation $\sigma(S_{eq})$ where

- $\mu(S_{eq}) = A_1 + A_2 \log_{10}(S_{eq} - A_3)$, if $S_{eq} > A_3$
- $\sigma(S_{eq}) = \tau$.

In general, the standard deviation could be a function of $S_{eq}$ as well. Possible probability distributions for $N$ are lognormal, extreme value, Weibull and Birnbaum–Saunders.
Given the sample data, \( n = (n_1, \ldots, n_m) \) and assuming that the observations are independent, the likelihood function is given by

\[
L(A_1, A_2, A_3, \tau, q; n) = \prod_{i=1}^{m} \left[ \phi(\log_{10}(n_i); \mu(S_{eq}), \sigma(S_{eq})) \right]^{\delta_i} \left[ 1 - \Phi(\log_{10}(n_i); \mu(S_{eq}), \sigma(S_{eq})) \right]^{1-\delta_i},
\]

where \( \phi \) and \( \Phi \) is the probability density function (pdf) and cumulative density function of \( \log_{10}(N) \), respectively, and

\[
\delta_i = \begin{cases} 
1 & \text{if } n_i \text{ is a failure} \\
0 & \text{if } n_i \text{ is a run-out.} 
\end{cases}
\]

The class of fatigue-limit models can be extended to random fatigue-limit models where the fatigue-limit parameter, \( A_3 \) is modeled by a probability distribution with unknown hyper-parameters. In this case, we calibrate the hyper-parameters instead of \( A_3 \) and the likelihood function takes the form

\[
L(\theta; n) = \prod_{i=1}^{m} \left[ f_{\log_{10}(N)}(\log_{10}(n_i); \theta) \right]^{\delta_i} \left[ 1 - F_{\log_{10}(N)}(\log_{10}(n_i); \theta) \right]^{1-\delta_i},
\]

where \( \theta = (A_1, A_2, \mu_f, \sigma_f, q, \tau) \) and

\[
f_{\log_{10}(N)}(u; \theta) = \int_{0}^{S_{eq}} \phi(u; \mu(S_{eq}), \sigma(S_{eq})) \ell_{A_3}(w; \mu_f, \sigma_f) \, dw,
\]

\[
F_{\log_{10}(N)}(u; \theta) = \int_{0}^{S_{eq}} \Phi(u; \mu(S_{eq}), \sigma(S_{eq})) \ell_{A_3}(w; \mu_f, \sigma_f) \, dw,
\]

and \( \ell_{A_3} \) is the probability density function of \( A_3 \).

### 2.1.3 Model calibration

In a classical approach, we estimate the model parameters by maximizing the likelihood function. In fact, we minimize the negative log-likelihood function using MAT-
LAB built-in global optimization algorithms. The maximum likelihood estimates are validated visually by comparing the quantiles (S-N curves) with observations as in Figure 2.1. We develop a stratified bootstrap algorithm to generate confidence intervals for the ML estimates and confidence bands for the S-N curves.

![Figure 2.1: Quantiles of model Ia compared with observed failures (blue circles) and run-outs (red circles).](image)

In a Bayesian approach, we compute the maximum posterior estimate (analytically) using the Laplace method and implement a random walk Metropolis-Hastings algorithm to generate MCMC samples.

### 2.1.4 Model comparison

After calibrating the models by maximum likelihood approach, we compute some popular information criteria, such as Akaike information criterion (AIC), Bayesian information criterion (BIC) and AIC with correction. Despite its name, BIC is also a classical model comparison criterion. All these measures take into account the goodness of fit in terms of the maximum log-likelihood value and the complexity of the models in terms of the number of parameters.

In the Bayesian model comparison, we use Bayes factor, Deviance information...
criterion (DIC), Watanabe–Akaike information criterion (WAIC) and K-fold cross-validation. The Bayes factor is a traditional Bayesian method to compare hypothesis. It requires the computation of the log marginal likelihood that can be approximated using Laplace or Laplace–Metropolis methods. The other criteria measure the prediction accuracy of the models.

2.2 Overview of Article II


In this article, we propose a stochastic model for the number of crack initiations on the surface of metallic specimens in fatigue problems, which is applicable for a general class of loadings and geometries. The stochastic model is based on spatial Poisson processes with intensity function that combines the S-N model with the averaged effective stress, \( \sigma_{\text{eff}}^\Delta (x) \). Here, \( \Delta \) is a parameter that characterizes the local neighbor where we average the effective stress. The stress tensor is computed from the solution of the linear elasticity equations using finite element methods.

2.2.1 Fatigue experiments data

Data of fatigue experiments on notched and unnotched sheet specimens of 75S-T6 aluminum alloys are used to calibrate the model parameters. Figure 2.2 and Table 2.1 summarize the properties of each specimen. The thickness of the three different specimens is 0.09 (in) which is relatively small. We assume that crack propagation is instantaneous and therefore crack initiation is equivalent to failure in these experiments.
2.2.2 Averaged effective stress

We compute the stress tensor by solving a linear elastic boundary value problem and define the effective stress by the maximum principal stress. The averaged effective stress is then obtained by averaging the effective stress over \( B(x, \Delta) \cap D \)

\[
\sigma_{\text{eff}}^\Delta(x) = \frac{1}{|B(x, \Delta) \cap D|} \int_{B(x, \Delta) \cap D} \sigma_{\text{eff}}(y) dy.
\]
and as $\Delta$ converge to zero, the averaged effective stress converges to the effective stress.

### 2.2.3 Spatial Poisson process

To construct a spatial Poisson process for crack initiation in a domain $D$, we assume that

(a) The averaged effective stress at $x \in \partial D$ determines crack formation at $x$.

(b) Different cracks initiate independently.

The spatial Poisson process is governed by the intensity function, $\lambda(x, n) \geq 0$, that relates the spatial location and the number of cycles, $n$. This intensity function depends on the averaged effective stress, $\lambda(x, n) = \eta(n; \sigma_{\text{eff}}(x))$, where $\eta$ is a failure-rate function. For any surface region of $B \subset \partial D$, the number of cracks occurring inside this region can be modeled as a Poisson counting process with associated rate function $\lambda_B(n) = \int_B \lambda(x, n) dS(x)$. The number of crack initiations in the region $B$ after performing $n$ stress cycles is modeled as a Poisson random variable, $M_B(n)$, whose distribution is

$$P(M_B(n) = m) = \frac{(\Lambda_B(n))^m}{m!} \exp(-\Lambda_B(n)), m = 0, 1, \ldots$$

with $\Lambda_B(n) = \int_0^n \lambda_B(u) du \geq 0$.

We are interested in the number of load cycles, $N_{\partial D}$, when the first crack initiates on $\partial D$. The random variable $N_{\partial D}$ is related to the counting process $M_{\partial D}(n)$ by the equivalence relation $N_{\partial D} > n \iff M_{\partial D}(n) = 0$ which corresponds to the survival event. Similarly, the failure event, $N_{\partial D} \leq n$ is equivalent to $M_{\partial D}(n) \geq 1$.

To parameterize the function $\eta(n; s)$, we relate it to a given S-N model as following

$$\eta(n; s) = -\frac{1}{\gamma} \frac{\partial}{\partial n} \log \left(1 - F_{SN}(n; s, \theta)\right), \quad (2.1)$$
where $F_{SN}(n; s, \theta)$ is the cumulative distribution function of the S-N model and $\gamma$ is the size of the highly stressed volume.

### 2.2.4 The joint likelihood

The likelihood function consists of the survival and density function of $N_{\partial D}$. The survival probability after $n$ cycles is

$$P(N_{\partial D} > n; \sigma_{\text{eff}}) = \exp \left( - \int_0^n \int_{\partial D} \eta(\hat{n}; \sigma_{\text{eff}}(x))dS(x) \, d\hat{n} \right),$$

and the density function is

$$\rho^{\partial D}(n; \sigma_{\text{eff}}) = P(N_{\partial D} > n; \sigma_{\text{eff}}) \times \int_{\partial D} \eta(n; \sigma_{\text{eff}}(x))dS(x).$$

Under the assumption of independent experiments, the log-likelihood function is

$$\ell(\theta, \gamma, \Delta) = \sum_{i=1}^m \left[ (1 - \delta_i) \log(P(N_{\partial D} > n_i; \sigma_{\text{eff},i}^\Delta)) + \delta_i \log(\rho^{\partial D}(n_i; \sigma_{\text{eff},i}^\Delta)) \right]$$

The highly stressed volume (area), $\gamma$, depends on the specimen geometry. We re-parametrize the survival probability by defining the highly stressed volume.

**Definition 1. Highly stressed volume**

We let $A_\beta = \{ x \in \partial D : \sigma_{\text{eff}}^1(x) > \beta \}$, where $\sigma_{\text{eff}}^1(x)$ is the effective stress that corresponds to a unity traction and $\beta$ is an unknown parameter. The highly stressed volume is given by

$$\gamma(\beta) = \int_{\partial D} \mathbb{1}_{A_\beta}(x)dS(x). \quad (2.2)$$

We choose one of the S-N models presented in [1] to define the rate function (2.1). We obtain the ML estimates for two cases: $\Delta = 0$ and $\Delta > 0$ and compare them in
terms of Akaike information criterion. When $\Delta > 0$, the model provides a better fit to the combined data sets of the three specimens.

Table 2.2: Comparison between two different specifications of Model Ia using (4.10).

<table>
<thead>
<tr>
<th>Model Ia given data sets 1, 2 &amp; 3 (2D)</th>
<th>$\Delta = 0$</th>
<th>$\Delta &gt; 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum log-likelihood</td>
<td>-1650.05</td>
<td>-1648.50</td>
</tr>
<tr>
<td>Akaike information criterion (AIC)</td>
<td>3312.10</td>
<td>3311</td>
</tr>
</tbody>
</table>

We also consider a Bayesian inference of the model parameters under the two scenarios: $\Delta = 0$ and $\Delta = 0.0125$. We run MCMC algorithm to generate samples from the joint posterior distribution using the combined data sets. We plot the marginal and bivariate distributions and compare the results of the two scenarios using Bayes factor (log marginal likelihood) and the deviance information criterion (DIC).

Table 2.3: Bayesian comparison between two different specifications of Model Ia using (4.10).

<table>
<thead>
<tr>
<th>Model Ia given data sets 1, 2 &amp; 3 (2D)</th>
<th>$\Delta = 0$</th>
<th>$\Delta = 0.0125$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log marginal likelihood</td>
<td>-1660.24</td>
<td>-1658.48</td>
</tr>
<tr>
<td>Deviance information criterion (DIC)</td>
<td>3311.33</td>
<td>3308.27</td>
</tr>
</tbody>
</table>

2.3 Overview of Article III


In this article, we develop a Bayesian setting to infer unknown parameters in linear parabolic partial differential equations under the assumption that the boundary data are noisy. Given Gaussian priors for the time-dependent Dirichlet boundary values,
we analytically marginalize the joint likelihood using the linearity of the equation. Our hierarchical Bayesian approach is fully implemented in an example that involves the heat equation.

2.3.1 Statistical model

Consider the deterministic one-dimensional parabolic initial-boundary value problem:

\[
\begin{aligned}
\partial_t T + L_\theta T &= 0, \quad x \in (x_L, x_R), \quad 0 < t \leq t_N < \infty \\
T(x_L, t) &= T_L(t), \quad t \in [0, t_N] \\
T(x_R, t) &= T_R(t), \quad t \in [0, t_N] \\
T(x, 0) &= g(x), \quad x \in (x_L, x_R),
\end{aligned}
\]

where \( L_\theta \) is a linear second-order partial differential operator that takes the form

\[
L_\theta T = -\partial_x (a(x) \partial_x T) + b(x) \partial_x T + c(x) T.
\]

Our objective is to provide a Bayesian solution to the inverse problem for \( \theta \) given noisy measurements of \( T(x, t) \) at the locations, \( x_L = x_0, x_1, x_2, \ldots, x_{I-1}, x_I = x_R \) and the times \( t_1, t_2, \ldots, t_N \). We assume that the initial condition \( g \) is given and \( \theta \) can vary with space but it is time independent.

The vector of observed data at time \( t_n \) denoted by \( Y_n := (Y_{0,n}, \ldots, Y_{I,n})^T \) has an additive Gaussian noise \( \epsilon_n \):

\[
Y_n = \begin{bmatrix}
T_L(t_n) \\
T(x_1, t_n) \\
\vdots \\
T(x_{I-1}, t_n) \\
T_R(t_n)
\end{bmatrix} + \epsilon_n, \quad (2.3)
\]
where \( \epsilon_n \) \( \text{i.i.d.} \) \( \mathcal{N}(0_{I+1}, \sigma^2 I_{I+1}) \) for some noise variance \( \sigma^2 > 0 \).

The Dirichlet boundary condition, \( T_L(\cdot) \) and \( T_R(\cdot) \), are approximated by piecewise linear continuous functions in the time partition \( \{t_n\}_{n=1}^N \).

The joint likelihood function of \( \theta \) and the boundary parameters \( T_L = (T_{L,1}, \ldots, T_{L,N})^{tr} \), \( T_R = (T_{R,1}, \ldots, T_{R,N})^{tr} \) is given by

\[
\rho(Y_1, \ldots, Y_N|\theta, T_L, T_R) = \left( \sqrt{2\pi\sigma^2} \right)^{-N(I+1)} \exp \left( -\frac{1}{2\sigma^2} \sum_{n=1}^N \|R_{t_n}\|_{\ell^2}^2 \right) 
\times \exp \left( -\frac{1}{2\sigma^2} \left[ \|T_L - Y_L\|_{\ell^2}^2 + \|T_R - Y_R\|_{\ell^2}^2 \right] \right),
\]

where \( R_{t_n} := (T(x_1, t_n) - Y_{1,n}, \ldots, T(x_{I-1}, t_n) - Y_{I-1,n})^{tr} \), \( Y_L = (Y_{L,1}, \ldots, Y_{L,N})^{tr} \) and \( Y_R = (Y_{R,1}, \ldots, Y_{R,N})^{tr} \).

### 2.3.2 Numerical approximation

By using finite differences or finite elements (when \( \theta(x) \) is not constant), we obtain a discretized solution and the data residual vector \( R_{t_n} \) can be approximated by

\[
\tilde{R}_{t_n} = (B^n T_0 - Y_n^{tr}) + A_{L,n}(\theta) T_L + A_{R,n}(\theta) T_R.
\]

where the matrices \( B, A_{L,n}(\theta) \) and \( A_{R,n}(\theta) \) depend on the numerical approximation.

### 2.3.3 The marginal likelihood of \( \theta \)

In order to obtain a likelihood function of \( \theta \) only, we assume the independent Gaussian prior distributions for \( T_L \) and \( T_R \):

\[
T_L \sim \mathcal{N}(\mu_L, \sigma_L^2 I_N), \quad T_R \sim \mathcal{N}(\mu_R, \sigma_R^2 I_N),
\]
Then, using (2.4), the marginalized likelihood of $\theta$ is given by:

$$\rho(Y_1, \ldots, Y_N|\theta) = \left(\sqrt{2\pi\sigma}\right)^{-N(I+1)} \times \left(\sqrt{2\pi\sigma_p}\right)^{-2N} \int_{T_R} \int_{T_L} \exp \left(-\frac{1}{2\sigma^2} \sum_{n=1}^{N} \| R_{tn} \|^2 \right)$$

$$\times \exp \left(-\frac{1}{2\sigma^2} (T_L - Y_L)^{tr}(T_L - Y_L) - \frac{1}{2\sigma^2} (T_R - Y_R)^{tr}(T_R - Y_R) \right)$$

$$\times \exp \left(-\frac{1}{2\sigma_p^2} (T_L - \mu_L)^{tr}(T_L - \mu_L) - \frac{1}{2\sigma_p^2} (T_R - \mu_R)^{tr}(T_R - \mu_R) \right) dT_L dT_R.$$

Analytical integration is carried out to provide the following theorem:

**Theorem 2.3.1.** The marginal likelihood of $\theta$ is given by:

$$\rho(Y_1, \ldots, Y_N|\theta) = \left(\sqrt{2\pi\sigma}\right)^{-N(I+1)} \left(\sqrt{2\pi\sigma_p}\right)^{-2N} (2\pi)^N/2 |\Lambda_0|^{1/2} (2\pi)^N/2 |\Lambda_1|^{1/2}$$

$$\times \exp \left\{ -\frac{1}{2\sigma^2} \left[ Y_{L}^{tr}Y_L + Y_{R}^{tr}Y_R + \sum_{i=1}^{N} (Y_i^{I} - B^nT_0)^{tr}(Y_i^{I} - B^nT_0) \right] \right\}$$

$$-\frac{1}{2\sigma_p^2} \left[\mu_L^{tr}\mu_L + \mu_R^{tr}\mu_R\right] + \frac{1}{2} (\mu_L^{tr}D_{\sigma^2} + Y_{L}^{tr}D_{\sigma^2} + \Delta_{2,L}^{tr}D_{\sigma^2}) \Lambda_0 (D_{\sigma^2}\mu_L + D_{\sigma^2}Y_L + D_{\sigma^2}\Delta_{2,L})$$

$$+ \frac{1}{2} \left[ t_{R,2}^{tr}\Lambda_1 t_{R,2} + 2t_{R,3}^{tr}\Lambda_1 t_{R,2} + t_{R,3}^{tr}\Lambda_1 t_{R,3} \right],$$

where $\Lambda_0, \Lambda_1, t_{R,2}$ and $t_{R,3}$ are independent of $T_L$ and $T_R$.

### 2.4 Overview of Article IV


In this article, we improve the methodology developed in [2] to an experimental study conducted in an environmental chamber, with measurements recorded every minute from temperature probes and heat flux sensors placed on both sides of a
solid brick wall over a five-day period. The observed time series are locally averaged, according to a smoothing procedure determined by the solution of a criterion function optimization problem, to fit the required set of noise model assumptions. Therefore, after preprocessing, we can reasonably assume that the temperature and the heat flux measurements have stationary Gaussian noise and we can avoid working with full covariance matrices. The results show that our technique reduces the bias error of the estimated parameters when compared to other approaches.

2.4.1 Mathematical model

Since the wall thickness is much smaller than the wall length and height, we can assume that the wall temperature varies only along the thickness dimension:

\[
\rho C \frac{\partial T}{\partial t} = \frac{1}{R} \left( \frac{x_0 \partial T}{\partial x} \right), \quad x \in (0, x_0), \quad t \in [0, t_N]
\]

\[
T(0, t) = T_{\text{int}}(t), \quad t \in [0, t_N]
\]

\[
T(x_0, t) = T_{\text{ext}}(t), \quad t \in [0, t_N]
\]

\[
T(x, 0) = g(x), \quad x \in (0, x_0).
\]

and the heat flux functions are given by

\[
F_{\text{int}} = -x_0 \frac{\partial T}{\partial x} \bigg|_{x=0}, \quad F_{\text{ext}} = -\frac{x_0}{R} \frac{\partial T}{\partial x} \bigg|_{x=x_0}
\]

where \( R, \rho C \) are the thermal resistance and the volumetric heat capacity. We assume that the initial condition, \( T_0(x) \) is well approximated by the piecewise linear function

\[
\begin{align*}
T_{\text{int}}(0) + 2 \tau_0 \frac{x}{L} \quad & \text{if } 0 < x \leq \frac{L}{2} \\
\tau_0 + 2 \frac{T_{\text{ext}}(0) - \tau_0}{L} (x - \frac{L}{2}) \quad & \text{if } \frac{L}{2} < x < L,
\end{align*}
\]

(2.5)

where \( \tau_0 \) is an unknown constant parameter.
2.4.2 Experimental data

Figure 2.3 shows the temperature and heat flux time series, each consisting of 6,900 measurements, with a recording interval of one measurement per minute. Clearly, these raw measurements are contaminated by unknown noise. To analyze this noise, we use a smoothing spline method to fit a curve to each time series. This approach is based on the reasonable assumption that the real temperature and heat flux vary smoothly over time. The noise is then approximated by the difference between the raw measurements and the smooth values.

![Figure 2.3: Raw temperature and heat flux measurements. Temperature in Room 2 imitates outdoor weather conditions.](image)

Figures 2.4 and 2.5 show the estimated noise of the raw temperature and heat flux measurements on both sides of the wall. We notice that the estimated noise, especially in Room 1, is not Gaussian. Also, the autocorrelation function of the noise shows strong correlations, requiring the estimation of dense covariance matrices. We, therefore, consider a non-overlapping moving average of the raw data by computing local averages for every five consecutive measurements, where 5 is the lag of the moving average. The lag 5 arises from the selection criterion that minimizes the total
Figure 2.4: Estimated noise of the raw temperature and heat flux measurements in Room 1.

Figure 2.5: Estimated noise of the raw temperature and heat flux measurements in Room 2.

The sum of the squared autocorrelation functions of the noise for the four time series. Figures 2.6 and 2.7 shows the estimated noise of the moving average temperature and heat flux, where we can see that the estimated noise looks Gaussian for all the time series. Moreover, the corresponding autocorrelations are considerably reduced. We replace the raw measurements shown in Figure 2.3 with the moving average series and henceforth refer to these series as the data. As a consequence, the number of observations is reduced from 6,900 to 1,380.
2.4.3 Numerical example

The goal here is to estimate the parameters $\theta = (R, \rho C, \tau_0)$ given the pre-processed data in 2.4.2. To do so, we consider a deterministic and a stochastic approximation of the boundary parameters $T_{int}$ and $T_{ext}$. In the deterministic case, we assume that the boundary conditions are equal to smoothing splines constructed from the boundary temperature data. In the other case, we assume that $T_{int}$ and $T_{ext}$, are modeled by the Gaussian distributions $N(\mu_{int}, C_{int,p})$ and $N(\mu_{ext}, C_{ext,p})$, where $\mu_{int}$ and $\mu_{ext}$ are
the smoothing splines constructed from the boundary temperature data and we let
\( C_{int,p} = C_{ext,p} = (0.01)^2 I \). Then, we apply our proposed hierarchical approach \cite{2} and marginalize \( T_{int} \) and \( T_{ext} \) from the joint likelihood. The moving averages, \( Q_{int} \) and \( Q_{ext} \), for heat flux are assumed to be Gaussian distributed and uncorrelated with \( \Sigma_{int} = \Sigma_{ext} = (0.66)^2 I \) and we consider the following uniform priors:

\[
R \sim U(0.17, 0.36), \rho C \sim U(234000, 431000), \tau_0 \sim U(5, 25).
\]

In Figure 2.8 we compare the marginal posteriors of the three parameters using the deterministic approach and the marginalization approach. The deterministic approach provides over-concentrated posteriors and relatively biased MAP estimates. On the other hand, the marginalization approach incorporates uncertainties into the nuisance boundary parameters, thereby producing realistic posterior densities.

![Figure 2.8: Comparison between the marginal posteriors obtained by the deterministic approach and the marginalization approach.](image)

**2.4.4 Information gain**

We first consider an experimental setup that describes the duration of the measurement campaign. We use the Laplace approximation to compute the information gain
for overlapping increasing time intervals. Figure 2.9 shows that the information gain increases over time as more observations are incorporated into the Bayesian inference. However, we observe that after 5000 minutes, the rate of increase of the information gain slows, indicating that the collected measurements provide reliable information on the thermal properties of the solid brick wall. We introduce another experimental setup by considering the external temperature oscillation. Figure 2.10 shows how data are partitioned on the basis of the detected external temperature cycles in Room 2. We estimate the information gain for each cycle, and the results are summarized in Table 2.4. Cycles 1 and 3 are ranked as the most informative in terms of the Kullback-Leibler divergence, while Cycle 2 is the least informative, although Cycle 4 has the shortest duration. From these results, we can deduce that larger temperature oscillations bring more knowledge to the inference about $\theta$, suggesting that steady state conditions cannot be used to infer the thermal properties of the wall.

![Figure 2.9: The estimated information gain with respect to time.](image)
Figure 2.10: Different temperature cycles.

<table>
<thead>
<tr>
<th>Cycle</th>
<th>Time (min)</th>
<th>$D_{KL}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1470</td>
<td>14.46</td>
</tr>
<tr>
<td>2</td>
<td>1470</td>
<td>13.68</td>
</tr>
<tr>
<td>3</td>
<td>1460</td>
<td>14.47</td>
</tr>
<tr>
<td>4</td>
<td>1370</td>
<td>13.98</td>
</tr>
</tbody>
</table>

Table 2.4: The estimated information gain from the detected external temperature oscillation cycles.

2.5 Overview of Article V


In this work, we present the ensemble-marginalized Kalman filter (EnMKF), a sequential algorithm analogous to our previously proposed approach [2, 3], for estimating the state and parameters of linear parabolic partial differential equations in initial-boundary value problems when the boundary data are noisy. We apply EnMKF to infer the thermal properties of building walls and to estimate the corresponding heat flux from real and synthetic data. According to our results, the marginalization technique in EnMKF is key to performance improvement with smaller ensembles at any fixed time.

2.5.1 Problem formulation

We study general partially-observed linear systems that could be obtained from the discretization of linear time-dependent PDEs [2]. Specifically, we consider the following discrete state observation system:
\[
\begin{align*}
T_k &= A_\theta T_{k-1} + B_\theta u_k + w_k, \\
y_k &= H T_k + v_k,
\end{align*}
\]

where \( T_k \) is a state vector, \( y_k \) corresponds to measurements of \( T_k \), \( A_\theta \) is the forward model operator that depends on the parameter \( \theta \), \( H \) is a linear observational map, \( B_\theta \) is the control matrix operator, and we assume that the control vector \( u_k \) follows another state observation system:

\[
\begin{align*}
u_k &= F u_{k-1} + q_k, \\
z_k &= u_k + c_k,
\end{align*}
\]

where \( F \) is a user-defined linear evolution operator and \( z_k \) is the observed control vector. We further assume that \( w_k, v_k, q_k, c_k \) are independent centered Gaussian random vectors with covariances \( W_k, V_k, Q_k, C_k \), respectively.

Such state observation systems could be obtained from linear time-dependent PDEs with unknown Dirichlet boundary conditions. The state vector, \( T_k \), is the discretized solution of the PDE at time \( k \), \( u_k \) is the discretized boundary condition at time \( k \) and the size of \( T_k \) depends on the spatial mesh. Precisely, given a linear time-dependent parabolic initial-boundary value problem on the domain \( D \times [0, t_N] \subset \mathbb{R}^{d+1} \):

\[
\begin{align*}
\frac{\partial T}{\partial t} + L_\theta T &= 0, \quad x \in D, \ t \in [0, t_N] \\
T(x, t) &= u(x, t), \quad x \in \partial D, \ t \in [0, t_N] \\
T(x, 0) &= T_0(x), \quad x \in D,
\end{align*}
\]

and the observations \( y_{1:N} = y_1, y_2, \ldots, y_N \) at times \( t_1, t_2, \ldots, t_N \), we can derive the state-space model (2.6) by discretizing (2.8) using finite differences or finite elements. Additionally, given the measurements \( z_{1:N} = z_1, z_2, \ldots, z_N \) of the boundary condition \( u \) at times \( t_1, t_2, \ldots, t_N \), we may assume an adequate state-space model for \( u_k \), such
as system (2.7).

The joint Bayesian estimation of $\theta$ and $T_k$, in a sequential filtering approach, as the observations $\{z_{1:k}, y_{1:k}\}$ become available can be now posed in terms of the computation of the conditional density $p(T_k, \theta | z_{1:k}, y_{1:k})$. Following the marginalization technique [2, 3], we exploit the linear structure of (2.6) and propose an ensemble-marginalized Kalman filter (EnMKF) that provides an approximation of $p(T_k, \theta | z_{1:k}, y_{1:k})$. From (2.6), it is easy to approximate the conditional distribution $p(T_k, \theta | u_k, y_{1:k})$. In order to incorporate the error of the boundary conditions, we use the tractability of the distribution $p(u_k | z_{1:k})$. In other words, by noticing from (2.7) that $u_k$ follows a linear dynamic system independent of (2.6), and under further Gaussian assumptions on $u_0$, it follows that the distribution $p(u_k | z_{1:k})$ can be expressed in closed form by using the Kalman filter. The desired joint distribution $p(T_k, \theta | z_{1:k}, y_{1:k})$ is then approximated by integrating out $u_k$ from the fully joint distribution $p(T_k, \theta, u_k | z_{1:k}, y_{1:k}) = p(T_k, \theta | u_k, y_{1:k})p(u_k | z_{1:k})$.

### 2.5.2 EnMKF for $\theta$ and $T_k$

We now derive a filtering algorithm to estimate the joint state-parameter vector, $X_k = [\theta \ T_k]'$, given the observations $(z_{1:k}, y_{1:k})$ up to time $k$. We assume a trivial evolution of the static parameters and the samples from $p(\theta | y_{1:k-1})$ are denoted by $\theta_{j_{k-1}}^i$. Then, the predicted state, $T_{k-1|k-1}^i = E[T_{k-1}^i | \theta_{j_{k-1}}^i, z_{1:k}, y_{1:k-1}]$, is computed for each $i = 1, \ldots, M$ as

$$T_{k|k-1}^i = A_{\theta_{j_{k-1}}^i} T_{k-1|k-1}^i + B_{\theta_{j_{k-1}}^i} u_k.$$  \hspace{1cm} (2.9)$$

The prediction covariance matrix, $P_{k|k-1}$, is usually approximated by the sample covariance matrix of $X_{k|k-1}$.
where \( \bar{X}_{k|k-1} = \frac{1}{M} \sum_{i=1}^{M} X^i_{k|k-1} \). Instead, we derive the covariance matrix of \( X_{k|k-1} \) using the law of total covariance by conditioning on \( \theta_{|k-1} \):

\[
P_{k|k-1} = \text{Cov}(X_k|z_{1:k}, y_{1:k-1}) \\
= \text{Cov}(E[X_k|\theta_{|k-1}, z_{1:k}, y_{1:k-1}]) + \text{Cov}(\text{Cov}(X_k|\theta_{|k-1}, z_{1:k}, y_{1:k-1}))
\]

\[
= \text{Cov}(\theta_{|k-1}) + E_{\theta}[\text{Cov}(\theta_{|k-1}, z_{1:k}, y_{1:k-1})] + E_{\theta} E_{\theta}[\text{Cov}(\theta_{|k-1}, z_{1:k}, y_{1:k-1}, z_{1:k}, y_{1:k-1})]
\]

\[
\approx \frac{1}{M-1} \sum_{i=1}^{M} \begin{bmatrix}
(\theta^i_{|k-1} - \bar{\theta}_{|k-1})(\theta^i_{|k-1} - \bar{\theta}_{|k-1})' \\
(T^i_{k|k-1} - \bar{T}_{k|k-1})(\theta^i_{|k-1} - \bar{\theta}_{|k-1})'
\end{bmatrix}
\]

\[
+ \frac{1}{M} \sum_{i=1}^{M} \begin{bmatrix}
0 \\
0 A_{\theta|k-1} P_{k-1|k-1} A'_{\theta|k-1} + B_{\theta|k-1} P_{k|k} B'_{\theta|k-1} + W_k
\end{bmatrix}
\]

where \( \bar{\theta}_{|k-1} = \frac{1}{M} \sum_{i=1}^{M} \theta^i_{|k-1} \), and \( P^i_{k-1|k-1} \) must be computed using the Kalman update equation,

\[
P^i_{k|k} = (I - P^i_{k|k-1} H'(H P^i_{k|k-1} H + V_k)^{-1} H) P^i_{k|k-1}.
\]

Computing and storing these covariance matrices \( P^i_{k|k} \) for each \( i = 1, \ldots, M \) may be burdensome, especially when \( \text{dim}(T_k) \) is large. Therefore, we consider the following approximation of the prediction covariance matrix:
\[ P_{k|k-1} \approx \frac{1}{M-1} \sum_{i=1}^{M} (X^i_{k|k-1} - \bar{x}_{k|k-1})(X^i_{k|k-1} - \bar{x}_{k|k-1})' + \frac{1}{M} \sum_{i=1}^{M} \begin{bmatrix} 0 & 0 \\ B^i_{\theta|k-1} P_{k|k-1} B'^i_{\theta|k-1} + W_k \end{bmatrix}, \]

which requires the computation of \( B^i_{\theta|k-1} P_{k|k-1} B'^i_{\theta|k-1} \) for each \( i = 1, \ldots, M \) in addition to the standard prediction covariance of EnKF. The additional term can be interpreted as inflation with respect to \( u_k \) and \( w_k \), which are fixed in (2.9). In the next section, we introduce another algorithm where we sample \( u_k \); therefore, the inflation is not needed.

After applying the prediction step in (2.9) and (2.10), the analysis step for \( X_k \) is computed by

\[ K_k = P_{k|k-1} H' \left( H P_{k|k-1} H' + V_k \right)^{-1}, \]
\[ X^i_{k|k} = X^i_{k|k-1} + K_k \left( y_k + v^i_k - HX^i_{k|k-1} \right), \]

where \( H = \begin{bmatrix} 0 & H \end{bmatrix} \) is the observation operator that maps the augmented vector \( X_k \) to the corresponding observation space and \( v^i_k \sim N(0, V_k) \) is used to perturb the observations.

### 2.5.3 Heat transfer across a solid brick wall

We implement the EnMKF method to deal with the state and parameter estimation problem in a real-world heat-transfer application, which is summarized in Subsection 2.4.

The first step in implementing EnMKF is to run a Kalman filter for the control vector \( u_k \) in (2.7), which in this case, consists of the boundary conditions \( T_{\text{int},k} \) and \( T_{\text{ext},k} \). The forward-evolution operator for the boundary conditions is unknown but noisy measurements are available. We consider the two autoregressive models \( AR(1) \)
and $AR(2)$ and use them with the measurements to apply the Kalman filter. Figures 2.11 and 2.12 show the results from the Kalman filter with each model and the real temperature measurements.

![Figure 2.11](image1)

Figure 2.11: Internal temperature measurements (red dots) and Kalman filter with $AR(1)$ and $AR(2)$.

![Figure 2.12](image2)

Figure 2.12: External temperature measurements (red dots) and Kalman filter with $AR(1)$ and $AR(2)$.

We run EnMKF Algorithm with $M = 100$ and using the complete experimental data set, $N = 6,900$. We initially sample $R^i$ and $\rho C^i$ from the uniform priors, $U(0.17, 0.36)$ and $U(234000, 431000)$, and sample $T_0^i$ from the normal prior distribution, $N(T_0, 0.01I_n)$. The observation noise covariance matrix, $V_k$, is assumed to be
time-invariant and is approximated by

\[
V_k = \begin{bmatrix}
20 & 0 \\
0 & 5
\end{bmatrix}.
\]

Figure 2.13: Convergence of the thermal resistance \( R \) (left) and heat capacity per unit area \( \rho C \) (right) ensemble with respect to time using EnMKF with ensemble size \( M = 100 \).

Figure 2.13 shows the convergence of the ensemble parameters \( R \) and \( \rho C \) with respect to time as more observations are incorporated. The thermal-resistance mean converges to \( 0.31 m^2K/W \) and the mean of the heat capacity per unit area converges to \( 3.11 \times 10^5 J/m^2K \). As we increase the ensemble size, we obtain results that are more accurate and consistent with the MCMC results in [3].
2.6 REFERENCES


Chapter 3

Bayesian inference and model comparison for metallic fatigue data

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Abstract

In this work, we present a statistical treatment of stress-life (S-N) data drawn from a collection of records of fatigue experiments that were performed on 75S-T6 aluminum alloys. Our main objective is to predict the fatigue life of materials by providing a systematic approach to model calibration, model selection and model ranking with reference to S-N data. To this purpose, we consider fatigue-limit models and random fatigue-limit models that are specially designed to allow the treatment of the run-outs (right-censored data). We first fit the models to the data by maximum likelihood methods and estimate the quantiles of the life distribution of the alloy specimen. To assess the robustness of the estimation of the quantile functions, we obtain bootstrap confidence bands by stratified resampling with respect to the cycle ratio. We then compare and rank the models by classical measures of fit based on information criteria. We also consider a Bayesian approach that provides, under the prior distribution of the model parameters selected by the user, their simulation-based posterior distributions. We implement and apply Bayesian model comparison methods, such as Bayes factor ranking and predictive information criteria based on cross-validation techniques under


3.1 Introduction

Mechanical and structural components subjected to cyclic loading are susceptible to cumulative damage and eventual failure through an irreversible process called metal fatigue. Prediction of such fatigue through the expected service life of mechanical parts and assemblies is an important objective of numerical simulations used in mechanical and structural engineering practice. Based on such predictions, inspection intervals can be established. The frequency of these inspection intervals bears on the safety and costs of operation \([1, 2, 3]\).

The fatigue characteristics of materials are established through fatigue tests performed on coupons, also called dogbone specimens, made of round bars or flat plates. The coupons are designed such that the stress is highest in the gauge section and that it remains substantially constant when the coupon is loaded in the axial direction. In bending and torsion tests, the stress varies linearly over the cross section and is constant in the axial direction, for any fixed point in the cross section.

The number of cycles to failure, the peak stress and the cycle ratio are recorded for each experiment. The cycle ratio is defined as the minimum stress to maximum stress ratio. When an experiment is stopped before the specimen fails, then the test record is marked as a run-out. In some experiments, the specimen may buckle or fail outside of the gauge section. Such experiments are disregarded. State-of-the-art reviews on mechanical fatigue are presented in \([1]\) and \([3]\). Here, we focus on high-cycle (stress-life) fatigue.

The set of data pairs \((S_i, N_i)\), where \(S_i\) is the stress and \(N_i\) is the corresponding number of cycles at failure in the \(i\)th test, exhibits substantial statistical dispersion. Interpretation and generalization of test data are essential for making risk-informed design decisions. The goal is to find a probability distribution for the fatigue life given
data and underlying assumptions. There are many possible phenomenological models which will lead to different results. These results can be derived by different statistical frameworks, among them the frequentist and the Bayesian approaches. Furthermore, there are several ways to judge the results obtained by the use of different models. Various statistical models such as lognormal, extreme value, Weibull and Birnbaum–Saunders distributions have been used for this purpose.

We consider different types of models that contain fatigue limit parameters. Although such models have been widely used (see, for example, [4, 5, 6, 7]), there is an ongoing debate concerning the existence of the fatigue limit [8, 9]. Some authors use the terms “endurance limit” or “fatigue strength” instead of “fatigue limit” [1, 6]. We distinguish between the fatigue limit, which is a physical notion, and the fatigue limit parameter, which is an unknown parameter, expressed in the same scale as the equivalent stress and calibrated for different models. Usually, data support curve fitting up to a certain number of cycles to failure only. Extrapolation beyond that number substantially increases uncertainty. For example, aluminum does not have a fatigue limit, since it will always fail if tested to a sufficient number of cycles. Therefore, the fatigue limit (fatigue strength) of aluminum is reported as the stress level at which the material can survive after a large number of cycles. For the purposes of this paper, the number of cycles can be fixed at $2 \times 10^7$, since the available data do not contain substantially larger cycle values.

We employ a classical (likelihood-based) approach to fit and compare the proposed models using the 75S-T6 aluminum sheet specimen data set described in Section 2. Ultimately, we provide an analog Bayesian approach to fit and compare the models. The classical approach provides a point estimation (Maximum Likelihood estimate) for the model parameter $\theta$ that lies in the 90% confidence interval if it were repeatedly used with random data from the model for fixed $\theta$. In the Bayesian formulation, no repetition is required and the interval estimation is based on the posterior distribution.
Although Ryan used a Bayesian approach to find an optimal design for the random fatigue-limit model [7], we are, to our knowledge, the first to use Bayesian methods to analyze and compare fatigue models.

The remainder of this paper is organized as follows. Section 3.2 introduces the main characteristics of the fatigue tests conducted at the Battelle Memorial Institute on 85 75S-T6 aluminum sheet specimens by means of a Krouse direct repeated-stress testing machine. The data set with the fatigue test results is available as a csv file in the supplemental material to this paper. This data set contains run-outs. Section 3.3 presents classical statistical models of fatigue test results. In Subsection 3.3.1, we first consider a classical statistical fitting technique, called logarithmic fit, for illustration purposes only, that does not take into account the presence of run-outs. Subsequently, we introduce fatigue-limit models and random fatigue-limit models, which are both specially designed to fit data in the presence of run-outs. We fit two fatigue-limit models, whose mean value function is same as in the logarithmic fit, with constant and non-constant variance functions, by constructing the corresponding likelihood functions and estimating all the unknown parameters that define the S-N curves by means of the maximum likelihood method. The fatigue limit parameter assessment under both models can be done by computing numerically tailored functions from their joint likelihoods, usually called profile likelihoods [10]. Later, we extend these models by assuming that the fatigue limit parameter is a random variable. To clarify the fitting procedure that provides estimates for S-N curves and predictions of fatigue life, we consider two random fatigue-limit models and their extensions, where a non-constant variance function is used. The assessment of the fatigue limit parameter is then summarized by comparing the estimated probability density functions of the four fitted models. Subsection 3.3.2 includes the computation of bootstrap confidence bands for the S-N curves and bootstrap confidence intervals for the maximum likelihood estimates. Subsection 3.3.3 is dedicated to comparison of the models by
some widely used information criteria. Section 3.4 focuses on the Bayesian analysis of some of the models. In Subsection 3.4.1, three of the models analyzed using the likelihood approach are embedded in a Bayesian framework that we characterize based on informative priors and on non-informative priors. We use Bayesian computational techniques to estimate the posterior probability density function of each individual parameter of the six fitted models as well as the bivariate posterior probability functions of all the combinations of two parameters out of the total number of parameters for any of the six fitted models. Subsection 3.4.2 presents the Bayesian model comparison approach, which includes the Bayes factor and predictive information criteria. The Bayes factor is approximated by means of the Laplace method and the Laplace–Metropolis method. The Bayes factor is used to evaluate the fit of Bayesian models while the predictive information criteria are used to compare models based on their predictive accuracy.

3.2 The 75S-T6 aluminum sheet specimens data set

Data are available from 85 fatigue experiments that applied constant amplitude cyclic loading to unnotched sheet specimens of 75S-T6 aluminum alloys [11, table 3, pp.22–24]. The following data are recorded for each specimen:

- the maximum stress, \( S_{\text{max}} \), measured in ksi units.
- the cycle ratio, \( R \), defined as the minimum to maximum stress ratio.
- the fatigue life, \( N \), defined as the number of load cycles at which fatigue failure occurred.
- a binary variable (0/1) to denote whether or not the test had been stopped prior to the occurrence of failure (run-out).

In 12 of the 85 experiments, the specimens remained unbroken when the tests were stopped. The recorded number of load cycles for these 12 experiments is the lower
bound of an interval in which failure would have occurred had the test been continued. If specimens buckled or failed outside the test section, they are not included in the data set.

3.3 Classical approach

3.3.1 Model calibration

There are many linear and nonlinear models (S-N curves) that have been used to predict fatigue life, \( N \), in terms of the stress, \( S \). A good list of these models can be found in [12]. In this section, we consider relevant nonlinear regression models used with the 75S-T6 data set. For the sake of completeness, we first show how the fitting procedure works for a model that does not take into account the run-out feature of some observations. This so-called “equivalent stress equation model” was used in [4]. Secondly, we introduce some fatigue-limit models that are tailored to work well in the presence of run-out observations, similar to [5] and [6], and we calibrate each of these models by using the maximum likelihood method.

In all the proposed models, the quantities of interest are the prediction of fatigue life, given the test stress and the cycle ratio, and the estimation of the fatigue limit parameter. The fatigue life predictions are summarized by means of the quantile functions. We plot the median (S-N curve), the 0.95 quantile and the 0.05 quantile.

Prior to the fitting of any statistical model, the fatigue data obtained for particular cycle ratios need to be generalized to arbitrary cycle ratios. For this purpose, the equivalent stress, \( S_{eq} \), is then defined as \( S_{eq}^{(q)} = S_{max} (1 - R)^q \), where \( q \) is a fitting parameter. This definition is also used in [4] and [13].

We first consider the logarithmic fit as defined in [14] and [4]; that is,

\[
\mu(S_{eq}^{(lg)}) = A_1 + A_2 \log_{10}(S_{eq}^{(lg)} - A_3),
\]

(3.1)
using the objective function proposed in (14),

\[ e_{std} = \left( \frac{\sum_{i=1}^{n} (\log_{10}(n_i) - \mu(S_{eq}^{(lg)}))^2}{n - p} \right)^{1/2}, \tag{3.2} \]

where \( n \) is the number of data points and \( p \) is the number of fitting parameters (namely \( A_1, A_2, A_3 \) and \( q \)).

The resulting estimated mean value function is given by

\[ \mu(S_{eq}^{(lg)}) = 10.07 - 3.54 \log_{10}(S_{eq}^{(lg)} - 25.41), \]

where \( S_{eq}^{(lg)} = S_{max}(1-R)^{0.5147} \) and the value of the objective function is \( e_{std} = 0.5195 \).

Remark. Run-outs will introduce a bias error in the estimate when this approach is used. The resulting estimated mean value function, without the run-outs, is given by

\[ \mu(S_{eq}^{(lg)}) = 7.71 - 2.17 \log_{10}(S_{eq}^{(lg)} - 31.53), \]

where \( S_{eq}^{(lg)} = S_{max}(1-R)^{0.4633} \) and the value of the objective function is \( e_{std} = 0.3673 \). Clearly, removing the run-outs increases the value of the fatigue limit. Figure 3.1 shows the estimated quantile functions for the logarithmic fit, with the estimated fatigue limit parameter equal to 31.53 ksi. We point out that the estimated fatigue limit is equal to 31.53/(2^{0.4633}) = 22.87 ksi, since the fatigue limit is the value of the maximum stress when the cycle ratio, \( R \), is equal to \(-1\) (the “fully reversed” condition).

### 3.3.1.1 Model Ia

Let \( A_3 \) be the fatigue limit parameter. At each equivalent stress with \( S_{eq} > A_3 \), the fatigue life, \( N \), is modeled by means of a lognormal distribution. This implies
that $\log_{10}(N)$ is modeled with a normal distribution with mean $\mu(S_{eq})$ and standard deviation $\sigma(S_{eq})$. We generalize the logarithmic fit by assuming that

- $\mu(S_{eq}) = A_1 + A_2 \log_{10}(S_{eq} - A_3)$, if $S_{eq} > A_3$
- $\sigma(S_{eq}) = \tau$.

Moreover, the model is now properly tailored to include the available censored fatigue data (run-outs). Given the sample data, $n = (n_1, \ldots, n_m)$ and assuming that the observations are independent, the likelihood function is therefore given by

$$L(A_1, A_2, A_3, \tau, q; n) = \prod_{i=1}^{m} \left[ \frac{1}{n_i \log(10)} g(\log_{10}(n_i); \mu(S_{eq}), \sigma(S_{eq})) \right]^{\delta_i} \times \left[ 1 - \Phi \left( \frac{\log_{10}(n_i) - \mu(S_{eq})}{\sigma(S_{eq})} \right) \right]^{1-\delta_i},$$
where \( g(t; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left\{ -\frac{(t-\mu)^2}{2\sigma^2} \right\} \), \( \Phi \) is the cumulative distribution function of the standard normal distribution, and

\[
\delta_i = \begin{cases} 
1 & \text{if } n_i \text{ is a failure} \\
0 & \text{if } n_i \text{ is a run-out}.
\end{cases}
\]

Figure 3.2: Model Ia fit of the 75S-T6 data set. Under the assumption that \( \log_{10}(N) \) has constant variance, the addition of the run-outs (red circles) and fitting a model designed to handle right-censored data has the effect of enlarging the gap between the median and the 0.95 quantile (in the upper range of values of \( S_{eq} \), the number of cycles to attain failure has substantially increased with respect to the logarithmic fit) and between the median and the 0.05 quantile (in the lower range of values of \( S_{eq} \), the number of cycles to attain failure has decreased with respect to the logarithmic fit). The fatigue limit parameter estimate (purple line) is closer to the observed failures (blue circles) with smallest values of \( S_{eq} \) than the same estimate using the logarithmic fit (Figure 3.1).

This model is characterized by five parameters: \( \theta = (A_1, A_2, A_3, q, \tau) \), whose maximum likelihood (ML) estimate, obtained by calibrating the model with the data, is

\[
\mu(S_{eq}) = 7.38 - 2.01 \log_{10}(S_{eq} - 35.04) ,
\]

where \( S_{eq} = S_{max} (1 - R)^{0.5628} \) and \( \tau = 0.5274 \). The maximum likelihood estimates are summarized in Table 3.1. The corresponding fit is shown in Figure 3.2 (blue
circles = observed failures; red circles = run-outs). The difference between Model Ia and the logarithmic fit shows the importance of including the run-outs especially in the estimation of the fatigue limit. Run-outs that correspond to equivalent stress levels greater than the fatigue limit parameter are called significant run-outs. Only significant run-outs contribute to estimating the parameters. In this case, eight of the 12 run-outs were significant.

Table 3.1: Maximum likelihood estimates for Model Ia

<table>
<thead>
<tr>
<th>Model</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ia</td>
<td>7.38</td>
<td>-2.01</td>
<td>35.04</td>
<td>0.5628</td>
<td>0.5274</td>
</tr>
</tbody>
</table>

### 3.3.1.2 Model Ib

We extend the model proposed in Subsection 3.3.1.1 by allowing a non-constant standard deviation as in [5]:

- $\mu(S_{eq}) = A_1 + A_2 \log_{10}(S_{eq} - A_3)$, if $S_{eq} > A_3$
- $\sigma(S_{eq}) = 10^{(B_1 + B_2 \log_{10}(S_{eq}))}$, if $S_{eq} > A_3$

In this model, there are six parameters: $\theta = (A_1, A_2, A_3, q, B_1, B_2)$, and their ML estimates are

$$\mu(S_{eq}) = 6.72 - 1.57 \log_{10}(S_{eq} - 36.21),$$
$$\sigma(S_{eq}) = 10^{(4.55 - 2.89 \log_{10}(S_{eq}))},$$

where $S_{eq} = S_{max} (1 - R)^{0.5510}$. The maximum likelihood estimates are summarized in Table 3.2. The corresponding fit is shown in Figure 3.3 (blue circles = observed failures; red circles = run-outs). Figure 3.3 shows that the uncertainty in predicting fatigue life decreases with high values of the equivalent stress when compared to
Figure 3.3: Model Ib fit of the 75S-T6 data set. Allowing non-constant variance in a censored data model has the effect of reducing the gap between the median and both the 0.95 and 0.05 quantiles along the upper range of values of $S_{eq}$. In the case of the lower range of values of $S_{eq}$, the gap between the median and the 0.05 quantile has increased with respect to the Model Ia fit (Figure 2). The estimate of the fatigue limit parameter is very close to the minimum value of $S_{eq}$ that leads to failure. The estimated fatigue limit is 24.71 ksi.

Model Ia. However, the uncertainty increases for values of the equivalent stress that are close to the estimated fatigue limit parameter. In Model Ib, there are seven significant run-outs because the fatigue limit parameter has increased to 36.21 ksi. When $A_3 < S_{eq} < 100$, the estimated standard deviation ranges between 1.11 and 0.059, supporting the assumption of a non-constant standard deviation.

Table 3.2: Maximum likelihood estimates for Model Ib

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model Ib</td>
<td>6.72</td>
<td>-1.57</td>
<td>36.21</td>
<td>0.5510</td>
<td>4.55</td>
<td>-2.89</td>
</tr>
</tbody>
</table>

Remark (Profile likelihoods). To assess the plausibility of a range of values of the fatigue limit parameter, $A_3$, we construct the profile likelihood [5, p. 294]:

$$R(A_3) = \max_{\theta_0} \left[ \frac{L(\theta_0, A_3)}{L(\hat{\theta})} \right],$$

(3.3)
where \( \theta_0 \) denotes all parameters except for the fatigue limit parameter, \( A_3 \), and \( \hat{\theta} \) is the ML estimate of \( \theta \).

Figure 3.4 shows the profile likelihood functions for \( A_3 \) corresponding to the models in Subsections 3.3.1.1 and 3.3.1.2. As in [3], approximate 100(1 – \( \alpha \))% confidence intervals for \( A_3 \) based on the calibrated profile likelihoods are given by: 
\[
\{ A_3 : -2 \log(R(A_3)) \leq \chi^2_{1,1-\alpha} \}, \text{ where } \chi^2_{1,1-\alpha} \text{ is the 100}(1 - \alpha) \text{ percentile of a chi-square distribution with 1 degree of freedom.}
\]
The approximate 95% confidence intervals for \( A_3 \) are (32.45, 36.28) and (34.36, 36.88) for Models Ia and Ib, respectively. We can see that each model suggests a different range for the fatigue limit parameter, \( A_3 \). We therefore need to systematically choose which model is better to assess the value of \( A_3 \).

![Figure 3.4: Profile likelihood estimates for the fatigue limit parameter, \( A_3 \), with Model Ia fit (blue curve) and Model Ib fit (red curve). The two fitted fatigue-limit models display different ranges for the most plausible values of the fatigue limit parameter, \( A_3 \), a feature that is amplified by the left-skewed profile likelihood under Model Ib.](image)

### 3.3.1.3 Model IIa

We now extend the model proposed in Subsection 3.3.1.1 to allow a random fatigue limit parameter as in [6]:
\[ \mu(S_{eq}) = A_1 + A_2 \log_{10}(S_{eq} - A_3), \text{ if } S_{eq} > A_3. \]

\[ \sigma(S_{eq}) = \tau. \]

\[ \log_{10}(A_3) \sim N(\mu_f, \sigma_f). \]

Here, we assume that \( \log_{10}(N) \) given \( A_3 < S_{eq} \) is modeled with a normal distribution with mean \( \mu(S_{eq}) \) and standard deviation \( \sigma(S_{eq}) \). In this case, the probability density function (pdf) of \( \log_{10}(N) \) is obtained by marginalizing \( A_3 \):

\[
 f_{\log_{10}(N)}(u; \theta) = \int_0^{S_{eq}} h(u; \mu(S_{eq}), \sigma(S_{eq})) \ell_{A_3}(w; \mu_f, \sigma_f) \, dw,
\]

where \( \theta = (A_1, A_2, \mu_f, \sigma_f, q, \tau) \), \( h(u; \mu(S_{eq}), \sigma(S_{eq})) \) is the conditional density of \( \log_{10}(N) \) given \( A_3 \), and \( \ell_{A_3}(w; \mu_f, \sigma_f) \) is the marginal density of \( A_3 \). Similarly, the marginal cumulative distribution function (cdf) of \( \log_{10}(N) \) is given by

\[
 F_{\log_{10}(N)}(u; \theta) = \int_0^{S_{eq}} \Phi \left( \frac{u - \mu(S_{eq})}{\sigma(S_{eq})} \right) \ell_{A_3}(w; \mu_f, \sigma_f) \, dw,
\]

where \( \Phi \) is the conditional cumulative distribution function of \( \log_{10}(N) \) given \( A_3 \).

The functions \( f_{\log_{10}(N)} \) and \( F_{\log_{10}(N)} \) no longer have closed forms and must be numerically evaluated. Global adaptive quadrature is used to approximate the integrations (see [15]). Assuming independent observations, the likelihood function of \( \theta = (A_1, A_2, \mu_f, \sigma_f, q, \tau) \) is therefore given by

\[
 L(\theta; \{\log_{10}(n_1), \ldots, \log_{10}(n_m)\}) = \prod_{i=1}^{m} \left[ f_{\log_{10}(N)}(\log_{10}(n_i); \theta) \right]^{\delta_i} \times [1 - F_{\log_{10}(N)}(\log_{10}(n_i); \theta)]^{1-\delta_i}, \quad (3.4)
\]

where

\[
 \delta_i = \begin{cases} 
 1 & \text{if } n_i \text{ is a failure} \\
 0 & \text{if } n_i \text{ is a run-out}.
\end{cases}
\]
3.3.1.4 Model IIb

We can also consider a random fatigue-limit model with the smallest extreme value (sev) distribution as in [6]:

- \( \mu(S_{eq}) = A_1 + A_2 \log_{10}(S_{eq} - A_3) \), if \( S_{eq} > A_3 \).
- \( \sigma(S_{eq}) = \tau \).
- the density of \( \log_{10}(A_3) \) is \( \phi(t; \mu_f, \sigma_f) \).
- the conditional density of \( \log_{10}(N) \) given \( A_3 < S_{eq} \) is \( \phi(t; \mu(S_{eq}), \sigma(S_{eq})) \),

where \( \phi(t; \mu, \sigma) = \frac{1}{\sigma} \exp \left\{ \left( \frac{t-\mu}{\sigma} \right) - \exp \left( \frac{t-\mu}{\sigma} \right) \right\} \) is the sev probability density function with location parameter \( \mu \) and scale parameter \( \sigma \) [16, Chapter 4]. The likelihood function has the same form as in equation (3.4). In other words, the conditional fatigue life, \( N \), and the fatigue limit parameter, \( A_3 \), are modeled by a Weibull distribution.

![Figure 3.5: Model IIb fit of the 75S-T6 data set. The fitting of a random fatigue-limit model for censored data has the effect that the estimated quantiles converge fast to a horizontal asymptote. Unlike fatigue-limit models, the random fatigue-limit model has the property that each estimated quantile approaches a different horizontal asymptote.](image)

Table 3.3 shows the maximum likelihood estimates and the maximum likelihood values obtained for Model IIa and Model IIb. The estimated parameters for both
models are similar except for the parameters, $\sigma_f$ and $\tau$, which have smaller values with Model IIb. As a consequence, Model IIb has a smaller maximum likelihood value. Since Models IIa and IIb have the same number of parameters, we can conclude that Model IIb is better than Model IIa. It is thus sufficient to present the corresponding fit of Model IIb (Figure 3.5).

Table 3.3: Maximum likelihood estimates for Model IIa and Model IIb.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\log(L^*)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model IIa</td>
<td>6.53</td>
<td>-1.51</td>
<td>1.58</td>
<td>0.0473</td>
<td>0.4888</td>
<td>0.1447</td>
<td>-913.42</td>
</tr>
<tr>
<td>Model IIb</td>
<td>6.51</td>
<td>-1.47</td>
<td>1.60</td>
<td>0.0385</td>
<td>0.4886</td>
<td>0.0852</td>
<td>-907.31</td>
</tr>
</tbody>
</table>

### 3.3.1.5 Model IIc

The random fatigue-limit model proposed in Subsection 3.3.1.3 is extended by allowing non-constant standard deviation:

- $\sigma(S_{eq}) = 10^{(B_1 + B_2 \log_{10}(S_{eq}))}$.

### 3.3.1.6 Model IIId

The random fatigue-limit model proposed in Subsection 3.3.1.4 is extended by allowing non-constant standard deviation:

- $\sigma(S_{eq}) = 10^{(B_1 + B_2 \log_{10}(S_{eq}))}$.

Table 3.4 shows the maximum likelihood estimates and the maximum likelihood values obtained for Models IIc and IIId. Again, the random fatigue-limit model with the sev distribution (Model IIId) performs slightly better than the random fatigue-limit model with the lognormal distribution (Model IIc). The corresponding fit of Model IIId in Figure 3.6 is very similar to the one obtained by Model IIb in Figure 3.5.
Figure 3.6: Model IIId fit of the 75S-T6 data set. Allowing non-constant variance in a random fatigue-limit model for censored data has the effect of slightly reducing the gap between the median and the 0.95 and 0.05 quantiles for the highest values of $S_{eq}$.

Table 3.4: Maximum likelihood estimates for Model IIc and Model IIId.

<table>
<thead>
<tr>
<th>Model</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
<th>$B_1$</th>
<th>$B_2$</th>
<th>$\log(L^*)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model IIc</td>
<td>6.43</td>
<td>-1.44</td>
<td>1.58</td>
<td>0.0408</td>
<td>0.4923</td>
<td>2.68</td>
<td>-1.97</td>
<td>-908.15</td>
</tr>
<tr>
<td>Model IIId</td>
<td>6.49</td>
<td>-1.46</td>
<td>1.60</td>
<td>0.0366</td>
<td>0.4904</td>
<td>0.66</td>
<td>-0.94</td>
<td>-906.73</td>
</tr>
</tbody>
</table>

Figures 3.7 and 3.8 show the probability density function for $A_3$ corresponding to Models IIa, IIb, IIc and IIId.

Figure 3.7: Estimated probability density functions of the fatigue limit parameter, $A_3$, for models IIa and IIc.
In the next subsections, our goal is to compare the relative performances of the proposed models that include an adequate formulation in terms of run-outs. As an initial step, we explore the consistency of the fitted models by looking at the variability in the confidence bands of the quantile functions of fatigue life.

3.3.2 Bootstrap confidence bands and confidence intervals

We obtain bootstrap confidence bands for the model fittings Ia, Ib, IIb and IId, as illustrated in Figures 3.2, 3.3, 3.5 and 3.6 respectively. Stratified bootstrap algorithm 2 is implemented with censored data. First, the data set is stratified on the basis of the cycle ratio, \( R \). Then, we sample independently from each stratum where each sample contains \( S_{max}, R, N \) and the binary variable \( \delta \) (See [17]). By repetition, we generate \( M = 200 \) bootstrap data sets. For each data set, we obtain the maximum likelihood estimate and compute the corresponding quantiles.

Figure 3.9 shows the median functions (blue curves) and the bootstrapped 95% confidence bands (black curves) for Models Ia, Ib, IIb and IId. Figure 3.10 shows the 0.05 quantiles (blue curves) and the bootstrapped 95% confidence bands (black curves). Table 3.5 provides the bootstrap confidence intervals for the maximum like-
Algorithm 2 Stratified bootstrap algorithm for censored data

1: set data = [data_1, data_2, ..., data_n]
2: for i = 1 : n do
3: draw |data_i| samples with replacement from data_i
4: let data*_i be the bootstrap stratum.
5: let data* = [data*_1, data*_2, ..., data*_n] be the bootstrap data set.
6: find the maximum likelihood estimate \( \theta^* \) given data*
7: compute the bootstrap quantiles
8: repeat steps (2 to 7) \( M \) times.

Figure 3.9: 95% bootstrap confidence bands for the median of fatigue life.

likelihood estimates for these models. Clearly, the random fatigue-limit models (Model IIb and Model IIId) provide the narrowest confidence intervals for \( A_1, A_2 \) and \( q \).

3.3.3 Model comparison

Using a classical approach, we compute some popular information criteria, such as Akaike information criterion (AIC) [18], Bayesian information criterion (BIC) [19, 20] and AIC with correction [21], which are based on the maximized log-likelihood values. Such measures take into account both the goodness of fit and the complexity of the models in terms of the number of parameters.

Table 3.6 contains the maximum log-likelihood values that correspond to the mod-
Figure 3.10: 95% bootstrap confidence bands for the 0.05 quantile of fatigue life. The 0.05 quantile is not as robust as the median, especially for Model Ib.

Table 3.5: 95% bootstrap confidence intervals for the maximum likelihood estimates.

<table>
<thead>
<tr>
<th>Model Ia</th>
<th>A₁</th>
<th>A₂</th>
<th>A₃</th>
<th>q</th>
<th>τ</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(6.19, 8.79)</td>
<td>(-2.88, -1.22)</td>
<td>(31.01, 38.46)</td>
<td>(0.487, 0.613)</td>
<td>(0.355, 0.646)</td>
</tr>
<tr>
<td>Model Ib</td>
<td>A₁</td>
<td>A₂</td>
<td>A₃</td>
<td>q</td>
<td>B₁</td>
</tr>
<tr>
<td></td>
<td>(6.28, 7.45)</td>
<td>(-2.05, -1.31)</td>
<td>(33.66, 38.33)</td>
<td>(0.460, 0.595)</td>
<td>(3.48, 6.25)</td>
</tr>
<tr>
<td>Model IIb</td>
<td>A₁</td>
<td>A₂</td>
<td>μₖ</td>
<td>σₖ</td>
<td>q</td>
</tr>
<tr>
<td></td>
<td>(6.23, 6.87)</td>
<td>(-1.70, -1.30)</td>
<td>(1.58, 1.62)</td>
<td>(0.0275, 0.0497)</td>
<td>(0.451, 0.515)</td>
</tr>
<tr>
<td>Model IId</td>
<td>A₁</td>
<td>A₂</td>
<td>μₖ</td>
<td>σₖ</td>
<td>q</td>
</tr>
<tr>
<td></td>
<td>(6.21, 6.89)</td>
<td>(-1.71, -1.29)</td>
<td>(1.58, 1.62)</td>
<td>(0.0240, 0.0476)</td>
<td>(0.456, 0.519)</td>
</tr>
</tbody>
</table>

els introduced in Subsections 3.3.1.1 – 3.3.1.6 together with the classical information criteria computations. These classical evaluations of model uncertainty indicate that, despite its complexity, Model IIb is preferable.
Table 3.6: Classical information criteria show that Model IIb provides the best fit to
the 75S-T6 data set.

<table>
<thead>
<tr>
<th>Models</th>
<th>Ia</th>
<th>Ib</th>
<th>IIa</th>
<th>IIb</th>
<th>IIc</th>
<th>IIId</th>
</tr>
</thead>
<tbody>
<tr>
<td>maximum log-likelihood</td>
<td>-950.16</td>
<td>-920.51</td>
<td>-913.42</td>
<td>-907.31</td>
<td>-908.15</td>
<td>-906.73</td>
</tr>
<tr>
<td>Akaike Information Criterion (AIC)</td>
<td>1910.3</td>
<td>1853.0</td>
<td>1838.8</td>
<td>1826.6</td>
<td>1830.3</td>
<td>1827.5</td>
</tr>
<tr>
<td>Bayesian Information Criterion (BIC)</td>
<td>1922.5</td>
<td>1867.7</td>
<td>1853.5</td>
<td>1841.3</td>
<td>1847.4</td>
<td>1844.6</td>
</tr>
<tr>
<td>Akaike Information Criterion with correction</td>
<td>1911.1</td>
<td>1854.1</td>
<td>1839.9</td>
<td>1827.7</td>
<td>1831.8</td>
<td>1828.9</td>
</tr>
</tbody>
</table>

3.4 Bayesian approach

3.4.1 Model calibration

We consider now a Bayesian approach to study Models Ia, Ib and IIb under two differ-
ent scenarios. For each scenario, we compute the maximum posterior estimate (ana-
lytically) using the Laplace method and provide Markov chain Monte Carlo (MCMC)
posterior samples. The random walk Metropolis-Hastings algorithm is used to gen-
erate MCMC samples. We use a normal proposal distribution to perturb the current
simulated vector, \( \theta_c \), and generate a new perturbed vector, \( \theta_p \sim N(\theta_c, \text{diag}(\delta)) \), where
\( \delta \) is a vector of parameters that controls the acceptance rate of the algorithm. After
several attempts, we chose \( \delta \) such that we could obtain a reasonable acceptance rate
(see [22, Chapter 6]).

**Algorithm 3** Random walk Metropolis-Hastings algorithm

1: set an initial value for the chain: \( \theta_c = \theta_0 \) and choose \( \delta \)
2: compute \( a = \text{loglikelihood}(\theta_c) + \text{logprior}(\theta_c) \)
3: draw \( \theta_p \) from \( N(\theta_c, \text{diag}(\delta)) \)
4: compute \( b = \text{loglikelihood}(\theta_p) + \text{logprior}(\theta_p) \)
5: let \( H = \min(1, \exp(b - a)) \) and draw \( r \) from \( U(0, 1) \)
6: if \( H > r \) then
7: \( \theta_c = \theta_p \)
8: \( a = b \)
9: repeat steps (3 to 8) until \( L \) posterior samples are attained.

For both scenarios, the algorithm is initialized as follows:

- Model Ia: \( \theta_0 = (7.4, -2, 35, 0.56, 0.5) \) and \( \delta = (0.1, 0.1, 0.1, 0.01, 0.05) \).
- Model Ib: $\theta_0 = (6.7, -1.6, 36.2, 0.55, 4.6, -2.9)$ and $\delta = (0.1, 0.1, 0.1, 0.01, 0.1, 0.1)$.

- Model IIb: $\theta_0 = (6.5, -1.5, 1.6, 0.04, 0.49, 0.085)$ and $\delta = (0.1, 0.1, 0.005, 0.001, 0.01, 0.01)$.

Each chain was run for 1,010,000 times, with a 10,000 iterations burn-in period and every 50th draw of the chain kept. The MCMC posterior samples were summarized by the Laplace–Metropolis estimator (see [23]), the empirical mean and standard deviation and the estimated marginal densities. The marginal densities were obtained by kernel density estimation (KDE) with a normal kernel function. The bandwidth was chosen to be optimal for normal densities.

In attempting to provide an objective Bayesian analysis, we considered two different scenarios. For both scenarios, we chose data-dependent proper priors [24]. In the first scenario, normal priors centered around the maximum likelihood estimates with arbitrary variance were considered for all the parameters except the standard deviations that were assigned inverse-gamma priors. The second scenario adopted less informative uniform priors for all the parameters. The uniform priors were chosen by spreading the range of the likelihood function then tuning these priors until we obtained proper untruncated posterior distributions.

### 3.4.1.1 Scenario 1 (informative priors)

In scenario 1, we considered the following informative priors that were induced from the maximum likelihood estimates as explained previously.

- Model Ia: $A_1 \sim \mathcal{N}(7.4, 2)$, $A_2 \sim \mathcal{N}(-2, 2)$, $A_3 \sim \mathcal{N}(35, 2)$, $q \sim \mathcal{N}(0.56, 0.5)$, $\tau \sim \mathcal{IG}(0.5, 0.25)$.

- Model Ib: $A_1 \sim \mathcal{N}(6.7, 2)$, $A_2 \sim \mathcal{N}(-1.6, 2)$, $A_3 \sim \mathcal{N}(36.2, 2)$, $q \sim \mathcal{N}(0.55, 0.5)$, $B_1 \sim \mathcal{N}(4.6, 2)$, $B_2 \sim \mathcal{N}(-2.9, 2)$.

- Model IIIb: $A_1 \sim \mathcal{N}(6.5, 2)$, $A_2 \sim \mathcal{N}(-1.5, 2)$, $\mu_f \sim \mathcal{N}(1.6, 0.1)$, $\sigma_f \sim \mathcal{IG}(2, 0.1)$, $q \sim \mathcal{N}(0.49, 0.5)$, $\tau \sim \mathcal{IG}(1, 0.1)$. 
Figure 3.11: Prior densities (red line) and approximate marginal posterior densities (blue line) for $A_1$, $A_2$, $q$, $\tau$ and $A_3$. The marginal posterior densities for all parameters are highly concentrated around their unique mode, suggesting that the observed data, given the assumed model, considerably increase our degree of belief about the range of the parameters. The high concentrations of $q$ and $\tau$ are especially noticeable. The estimated marginal posterior of the fatigue limit parameter, $A_3$, is left-skewed although the prior was assumed to be a normal distribution.

Table 3.7: Maximum posterior estimates for Model Ia.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>7.39</td>
<td>-2.01</td>
<td>35.03</td>
<td>0.563</td>
<td>0.523</td>
</tr>
<tr>
<td>Laplace–Metropolis</td>
<td>7.46</td>
<td>-2.07</td>
<td>34.92</td>
<td>0.561</td>
<td>0.524</td>
</tr>
</tbody>
</table>

Table 3.8: MCMC posterior empirical mean estimates with their standard deviations for Model Ia.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>7.57</td>
<td>-2.13</td>
<td>34.53</td>
<td>0.559</td>
<td>0.544</td>
</tr>
<tr>
<td>SD</td>
<td>0.41</td>
<td>0.28</td>
<td>0.88</td>
<td>0.020</td>
<td>0.048</td>
</tr>
</tbody>
</table>
Maximum posterior estimates shown in Table 3.7 are similar to the maximum likelihood estimates obtained for Model Ia (Table 3.1). Figure 4.19 and empirical standard deviations given in Table 3.8 show that the fatigue limit parameter, $A_3$, is the most uncertain parameter whereas $q$ is the least uncertain parameter. Figure 4.19 also shows that the data are informative for all the parameters because there is a contraction between the prior densities and the posterior densities. Correlation coefficients presented in Table 3.9 and Figure 3.12 show that $A_1$ and $A_2$ are approximately linear dependent. We can therefore reduce the number of parameters in Model Ia by one parameter. These parameters are also highly correlated with the fatigue limit parameter, $A_3$. On the other hand, there is a weak linear relationship between $q$ and the parameters $A_1$, $A_2$ and $A_3$. Moreover, the standard deviation, $\tau$, has no notable correlation with any parameter.

Table 3.9: Correlation coefficients for each pair of parameters in Model Ia.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.980</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$A_3$</td>
<td>-0.860</td>
<td>0.799</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$q$</td>
<td>-0.385</td>
<td>0.365</td>
<td>0.384</td>
<td>—</td>
</tr>
<tr>
<td>$\tau$</td>
<td>-0.005</td>
<td>0.003</td>
<td>0.050</td>
<td>0.073</td>
</tr>
</tbody>
</table>
Figure 3.12: Contour plots of the estimated bivariate densities for each pair of parameters in Model Ia. A strong correlation appears between $A_1$ and $A_2$ and they also appear to be linearly dependent. The fatigue limit parameter, $A_3$, is highly correlated with $A_1$ and $A_2$.

**Numerical Results - Model Ib**

Table 3.10: Maximum posterior estimates for Model Ib.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>6.72</td>
<td>-1.57</td>
<td>36.21</td>
<td>0.551</td>
<td>4.56</td>
<td>-2.89</td>
</tr>
<tr>
<td>Laplace–Metropolis</td>
<td>6.78</td>
<td>-1.61</td>
<td>36.20</td>
<td>0.552</td>
<td>4.43</td>
<td>-2.83</td>
</tr>
</tbody>
</table>

Table 3.11: MCMC posterior empirical mean estimates with their standard deviations for Model Ib.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>6.87</td>
<td>-1.66</td>
<td>35.63</td>
<td>0.544</td>
<td>4.44</td>
<td>-2.81</td>
</tr>
<tr>
<td>SD</td>
<td>0.23</td>
<td>0.14</td>
<td>0.60</td>
<td>0.022</td>
<td>0.53</td>
<td>0.31</td>
</tr>
</tbody>
</table>
Figure 3.13: Prior densities (red line) and approximate marginal posterior densities (blue line) for $A_1, A_2, q, B_1, B_2$ and $A_3$. The estimated posterior densities for all parameters are more concentrated than the prior densities, which means that the data are informative. Again, the estimated posterior of $q$ is highly concentrated. Allowing a non-constant variance has the effect of reducing the uncertainties of $A_1, A_2$ and the fatigue limit parameter, $A_3$. The estimated marginal posterior of the fatigue limit parameter is left-skewed although the prior was assumed to be a normal distribution.

Maximum posterior estimates given in Table 3.10 are similar to the maximum likelihood estimates obtained for Model Ib (Table 3.2). Similarly to Model Ia, Figure 3.13 and Table 3.11 show that the fatigue limit parameter, $A_3$, is the most uncertain parameter whereas $q$ is the least uncertain parameter. However, the uncertainties have been reduced for $A_1, A_2$ and $A_3$ when compared with Model Ia. Figure 3.13 shows again that the data are informative for all the parameters as previously explained. The marginal posterior of the fatigue limit parameter, $A_3$ is left-skewed similar to the profile likelihood estimate. Correlation coefficients shown in Table 3.12 and Figure 3.14 show that $A_1$ and $B_1$ are almost perfectly correlated with $A_2$ and $B_2$, respectively. Thus, we can consider a fatigue limit model with non-constant variance with only four parameters, which is the same number of parameters in the logarithmic fit. The
fatigue limit parameter in Model Ib has a moderate linear relationship with $A_1$, $A_2$ and $q$ whereas the fatigue limit parameter in Model Ia has a strong linear relationship with $A_1$ and $A_2$ and a weak linear relationship with $q$.

Figure 3.14: Contour plots of the approximate bivariate densities for each pair of parameters in Model Ib. There are two strong correlations between $A_1$ and $A_2$ and between $B_1$ and $B_2$. Such strong correlation suggests linear dependence; it is therefore possible to remove two parameters from Model Ib. The fatigue limit parameter, $A_3$, shows a moderate correlation with $A_1$, $A_2$ and $q$. Allowing a non-constant variance has the effect of increasing the correlation between $q$ and the fatigue limit parameter, $A_3$.

Table 3.12: Correlation coefficients for each pair of parameters in Model Ib.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.993</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_3$</td>
<td>-0.610</td>
<td>0.592</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$q$</td>
<td>-0.384</td>
<td>0.396</td>
<td>0.658</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B_1$</td>
<td>-0.301</td>
<td>0.308</td>
<td>0.017</td>
<td>-0.177</td>
<td></td>
</tr>
<tr>
<td>$B_2$</td>
<td>0.300</td>
<td>-0.306</td>
<td>-0.011</td>
<td>0.188</td>
<td>-0.997</td>
</tr>
</tbody>
</table>
Figure 3.15: Prior densities (red line) and approximate marginal posterior densities (blue line) for $A_1, A_2, q, \tau, \mu_f$ and $\sigma_f$. The posterior densities for all parameters are more concentrated than the prior densities, which means the data are informative. The high concentrations of the location and scale parameters, $\mu_f$ and $\sigma_f$, are particularly noticeable. The random fatigue-limit model has the effect of considerably reducing the uncertainties of $A_1, A_2$ and $\tau$.

Table 3.13: Maximum posterior estimates for Model IIb.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>6.51</td>
<td>-1.47</td>
<td>1.60</td>
<td>0.0387</td>
<td>0.488</td>
<td>0.082</td>
</tr>
<tr>
<td>Laplace–Metropolis</td>
<td>6.53</td>
<td>-1.49</td>
<td>1.60</td>
<td>0.0386</td>
<td>0.485</td>
<td>0.080</td>
</tr>
</tbody>
</table>

Table 3.14: MCMC posterior empirical mean estimates with their standard deviations for Model IIb.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>6.58</td>
<td>-1.52</td>
<td>1.60</td>
<td>0.0424</td>
<td>0.488</td>
<td>0.087</td>
</tr>
<tr>
<td>SD</td>
<td>0.20</td>
<td>0.12</td>
<td>0.012</td>
<td>0.007</td>
<td>0.018</td>
<td>0.023</td>
</tr>
</tbody>
</table>

Maximum posterior estimates presented in Table 3.13 are similar to the maximum likelihood estimates obtained for Model IIb (Table 3.3). Figure 3.15 and Table
show that the location and scale parameters, $\mu_f$ and $\sigma_f$, are the least uncertain parameters. Moreover, the uncertainties have been reduced for $A_1, A_2$ and $q$ when compared with Model Ia and Model Ib. Figure 3.15 shows that the data are very informative for all the parameters because there is a strong contraction between the prior densities and the posterior densities. Similarly to Model Ia, Table 3.15 and Figure 3.16 show that $A_1$ and $A_2$ are approximately linear dependent, and therefore we can reduce the number of parameters for Model IIb by one parameter. The location parameter, $\mu_f$, is strongly correlated with $A_1$ and $A_2$ whereas $\sigma_f$ is moderately correlated with $A_1, A_2$ and $\mu_f$. There is a weak negative correlation between $\tau$ and $\sigma_f$ and a weak positive correlation between $\tau$ and $q$.

Figure 3.16: Contour plots of the approximate bivariate densities for each pair of parameters in Model IIb. Again, a strong correlation appears between $A_1$ and $A_2$. Also, the parameter $\mu_f$ has a relatively strong correlation with $A_1$ and $A_2$. The random fatigue-limit model has the effect of reducing the correlations between $q$ and the parameters $A_1$ and $A_2$. 
Table 3.15: Correlation coefficients for each pair of parameters in Model IIb.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.986</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$\mu_f$</td>
<td>-0.777</td>
<td>0.708</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$\sigma_f$</td>
<td>0.447</td>
<td>-0.404</td>
<td>-0.526</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$q$</td>
<td>-0.045</td>
<td>0.090</td>
<td>-0.062</td>
<td>-0.145</td>
<td>—</td>
</tr>
<tr>
<td>$\tau$</td>
<td>0.034</td>
<td>-0.022</td>
<td>0.042</td>
<td>-0.396</td>
<td>0.321</td>
</tr>
</tbody>
</table>

### 3.4.1.2 Scenario 2 (uninformative priors)

Now, we provide the same results but for prescribed uninformative priors as follows:

- Model Ia: $A_1 \sim U(5, 13), A_2 \sim U(-5, 0), A_3 \sim U(24, 40), q \sim U(0.1, 0.9), \tau \sim U(0.1, 1.5)$.

- Model Ib: $A_1 \sim U(4, 10), A_2 \sim U(-4, 0), A_3 \sim U(30, 40), q \sim U(0.1, 0.9), B_1 \sim U(2, 7), B_2 \sim U(-5, -1)$.

- Model IIb: $A_1 \sim U(4, 10), A_2 \sim U(-4, 0), \mu_f \sim U(1.4, 1.8), \sigma_f \sim U(0, 0.1), q \sim U(0.1, 0.9), \tau \sim U(0, 0.25)$.

#### Numerical Results - Model Ia

Table 3.16: Maximum posterior estimates for Model Ia.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>7.38</td>
<td>-2.01</td>
<td>35.04</td>
<td>0.563</td>
<td>0.527</td>
</tr>
<tr>
<td>Laplace–Metropolis</td>
<td>7.39</td>
<td>-2.02</td>
<td>35.07</td>
<td>0.563</td>
<td>0.517</td>
</tr>
</tbody>
</table>

Table 3.17: MCMC posterior empirical mean estimates with their standard deviations for Model Ia.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>7.66</td>
<td>-2.18</td>
<td>34.31</td>
<td>0.557</td>
<td>0.549</td>
</tr>
<tr>
<td>SD</td>
<td>0.51</td>
<td>0.35</td>
<td>1.18</td>
<td>0.021</td>
<td>0.049</td>
</tr>
</tbody>
</table>
Figure 3.17: Prior densities (red line) and approximate marginal posterior densities (blue line) for $A_1, A_2, q, \tau$ and $A_3$. The estimated posterior densities for all parameters are concentrated around the corresponding modes. Again, we notice the high concentrations of $q$ and $\tau$ as in Scenario 1. The estimated marginal posteriors of $A_1, A_2$ and $A_3$ show greater variability in comparison with Figure 4.19.

Maximum posterior estimates presented in Table 3.16 are similar to the maximum posterior estimates obtained for Model Ia and reported in Table 3.7. Table 3.17 shows that the MCMC posterior samples obtained for Model Ia with uniform priors have more variability than the posterior samples obtained for Model Ia under Scenario 1. However, Figure 3.17 shows that the data are informative for all the parameters. The marginal posterior of the fatigue limit parameter is again left-skewed but with larger variance. Correlation coefficients given in Table 3.18 and Figure 3.18 show that $A_1$ and $A_2$ are again linearly dependent and the number of parameters for Model Ia can be reduced by one parameter. In general, the correlations among the parameters of Model Ia under Scenario 2 have increased when compared with those under Scenario 1 (Table 3.9).
Figure 3.18: Contour plots of the approximate bivariate densities of each pair of parameters in Model Ia. Similar to Figure 3.12, there is a strong correlation between $A_1$ and $A_2$. In addition, the fatigue limit parameter, $A_3$, is highly correlated with $A_1$ and $A_2$.

Table 3.18: Correlation coefficients between each pair of parameters in Model Ia.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.986</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$A_3$</td>
<td>-0.908</td>
<td>0.863</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$q$</td>
<td>-0.447</td>
<td>0.430</td>
<td>0.448</td>
<td>—</td>
</tr>
<tr>
<td>$\tau$</td>
<td>-0.017</td>
<td>-0.018</td>
<td>0.018</td>
<td>0.060</td>
</tr>
</tbody>
</table>

Numerical Results - Model Ib

Table 3.19: Maximum posterior estimates for Model Ib.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>6.72</td>
<td>-1.57</td>
<td>36.21</td>
<td>0.551</td>
<td>4.55</td>
<td>-2.89</td>
</tr>
<tr>
<td>Laplace–Metropolis</td>
<td>6.69</td>
<td>-1.55</td>
<td>36.19</td>
<td>0.551</td>
<td>4.76</td>
<td>-3.00</td>
</tr>
</tbody>
</table>
Figure 3.19: Prior densities (red line) and approximate marginal posterior densities (blue line) for $A_1, A_2, q, B_1, B_2$ and $A_3$. The estimated posterior densities for all parameters are concentrated around the corresponding modes but they show greater variability in comparison with Figure 3.13.

Table 3.20: MCMC posterior empirical mean estimates with their standard deviations for Model Ib.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
<th>$B_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>6.90</td>
<td>-1.67</td>
<td>35.50</td>
<td>0.541</td>
<td>4.46</td>
<td>-2.83</td>
</tr>
<tr>
<td>SD</td>
<td>0.26</td>
<td>0.16</td>
<td>0.69</td>
<td>0.024</td>
<td>0.55</td>
<td>0.32</td>
</tr>
</tbody>
</table>

Maximum posterior estimates presented in Table 3.19 are similar to the maximum posterior estimates obtained for Model Ib and given in Table 3.10. Similar to Scenario 1, Figure 3.19 and Table 3.20 show that the fatigue limit parameter, $A_3$, is again the most uncertain parameter whereas $q$ is the least uncertain parameter. However, the MCMC posterior samples obtained with uniform priors have more variability than do the posterior samples in Scenario 1 (Table 3.11). The marginal posterior of the fatigue limit parameter is again left-skewed but with larger variance. Correlation coefficients in Table 3.21 and Figure 3.20 show that $A_1$ and $B_1$ are almost perfectly correlated.
with $A_2$ and $B_2$, respectively. The correlations among the $A_1, A_2, A_3$ and $q$ parameters under Scenario 2 have increased when compared with those under Scenario 1 (Table 3.12).

Figure 3.20: Contour plots of the approximate bivariate densities of each pair of parameters in Model Ib. Similar to Figure 3.14, there are two strong correlations between $A_1$ and $A_2$ and between $B_1$ and $B_2$. The fatigue limit parameter, $A_3$, has a moderate correlation with $A_1, A_2$ and $q$. Allowing a non-constant variance has the effect of increasing the correlation between $q$ and the fatigue limit parameter, $A_3$.

Table 3.21: Correlation coefficients between each pair of parameters in Model Ib.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$B_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.995</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$A_3$</td>
<td>-0.671</td>
<td>0.653</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$q$</td>
<td>-0.428</td>
<td>0.436</td>
<td>0.664</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$B_1$</td>
<td>-0.272</td>
<td>0.279</td>
<td>0.001</td>
<td>-0.226</td>
<td>—</td>
</tr>
<tr>
<td>$B_2$</td>
<td>0.271</td>
<td>-0.278</td>
<td>0.004</td>
<td>0.235</td>
<td>-0.998</td>
</tr>
</tbody>
</table>
Numerical Results - Model IIb

![Graphs of prior and marginal posterior densities for Model IIb parameters.](image)

Figure 3.21: Prior densities (red line) and approximate marginal posterior densities (blue line) for $A_1, A_2, q, \tau, \mu_f$ and $\sigma_f$. The estimated posterior densities for all parameters are concentrated around the corresponding modes but they show slightly greater variability in comparison with Figure 3.15.

Table 3.22: Maximum posterior estimates for Model IIb.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>6.51</td>
<td>-1.48</td>
<td>1.60</td>
<td>0.0386</td>
<td>0.489</td>
<td>0.0853</td>
</tr>
<tr>
<td>Laplace–Metropolis</td>
<td>6.57</td>
<td>-1.51</td>
<td>1.60</td>
<td>0.0398</td>
<td>0.490</td>
<td>0.0856</td>
</tr>
</tbody>
</table>

Table 3.23: MCMC posterior empirical mean estimates with their standard deviations for Model IIb.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>6.60</td>
<td>-1.52</td>
<td>1.60</td>
<td>0.0428</td>
<td>0.489</td>
<td>0.0901</td>
</tr>
<tr>
<td>SD</td>
<td>0.21</td>
<td>0.13</td>
<td>0.012</td>
<td>0.008</td>
<td>0.019</td>
<td>0.025</td>
</tr>
</tbody>
</table>

Maximum posterior estimates given in Table 3.22 are similar to the maximum posterior estimates obtained for Model IIb under Scenario 1 and presented in Table...
3.13. Similar to Scenario 1, Figure 3.21 and Table 3.23 show that the location and scale parameters, \( \mu_f \) and \( \sigma_f \), are the least uncertain parameters. The MCMC posterior samples obtained with uniform priors have slightly greater variability than do the posterior samples in Scenario 1 (Table 3.14). Figure 3.21 shows that the data are very informative for all the parameters because there is a strong contraction between the prior densities and the posterior densities. Table 3.24 and Figure 3.22 show that \( A_1 \) and \( A_2 \) can be considered linear dependent, and therefore we can reduce the number of parameters for Model IIb by one parameter. In general, the correlations among the parameters of Model IIb under Scenario 2 are greater than those correlations under Scenario 1 (Table 3.15).

Figure 3.22: Contour plots of the approximate bivariate densities of each pair of parameters in Model IIb. Similar to Figure 3.16, the parameter \( \mu_f \) shows a strong correlation with \( A_1 \) and \( A_2 \). The random fatigue-limit model has the effect of reducing the correlations between \( q \) and the parameters \( A_1 \) and \( A_2 \).
Table 3.24: Correlation coefficients between each pair of parameters in Model IIb.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$\mu_f$</th>
<th>$\sigma_f$</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.987</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$\mu_f$</td>
<td>-0.788</td>
<td>0.722</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$\sigma_f$</td>
<td>0.494</td>
<td>-0.452</td>
<td>-0.566</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$q$</td>
<td>-0.067</td>
<td>0.111</td>
<td>-0.037</td>
<td>-0.158</td>
<td>—</td>
</tr>
<tr>
<td>$\tau$</td>
<td>-0.019</td>
<td>0.031</td>
<td>0.080</td>
<td>-0.412</td>
<td>0.326</td>
</tr>
</tbody>
</table>

3.4.2 Model comparison

We now analyze more closely comparisons among Models Ia, Ib and IIb.

3.4.2.1 Bayes Factor

We adopt a traditional Bayesian approach by estimating the Bayes factor of Model A against that of Model B, which is defined as

$$F_{B,A} := \frac{\int L_B(\theta_B; y)\rho_B(\theta_B)d\theta_B}{\int L_A(\theta_A; y)\rho_A(\theta_A)d\theta_A} = \frac{p_B(y)}{p_A(y)},$$

where $\rho_A(\theta_A)$ and $\rho_B(\theta_B)$ are the prior densities, and $p_A(y)$ and $p_B(y)$ are the marginal likelihoods [25, Chapter 2].

Common methods to estimate Bayes factors [26, 23] are applied to compare the fitted models and to rank their plausibility. Fast preliminary estimates of the log marginal likelihoods were obtained through the application of the Laplace approximation. Then, the log marginal likelihoods were computed using the Laplace–Metropolis estimator, which is based on the MCMC posterior samples together with the Laplace approximation.

In both cases, the approximation of the log marginal likelihood $\log(p(y))$ is given by

$$\frac{P}{2} \log(2\pi) + \frac{1}{2} \log(|H^*|) + \log(\rho(\theta^*)) + \log(L(\theta^*|y)),$$
where $P$ is the dimension of the vector $\theta$, $\theta^*$ is the maximum posterior estimate and $H^*$ is the inverse Hessian of the negative log posterior.

In the Laplace estimator, $\theta^*$ and $H^*$ are numerically approximated by means of the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm. The Laplace–Metropolis estimator uses the MCMC posterior samples to find the maximum posterior estimate, $\theta^*$, and approximate, $H^*$, by the empirical covariance matrix.

### 3.4.2.2 Predictive Information Criteria for Bayesian Models

In this section, we compare models by measuring their prediction accuracy. We estimate the prediction accuracy using deviance and Watanabe–Akaike information criteria as well as cross-validation.

- **Log pointwise predictive density (lppd)**

  The general method to estimate the prediction accuracy of a certain model is through the log predictive density, $\log \rho(y|\theta) = \log L(\theta; y)$, where $y$ is a new observation. An overestimate of the log predictive density can be obtained by using the observed data, $\{y_i\}_{i=1}^n$. It is an overestimate because the observed data were used first to infer $\theta$. In our Bayesian approach, $\theta$ is summarized by the MCMC posterior samples, $\{\theta^m\}_{m=1}^S$, and therefore the log pointwise predictive density estimate is given by

  \[
  lppd = \sum_{i=1}^n \log \left( \frac{1}{S} \sum_{m=1}^S \rho(y_i|\theta^m) \right),
  \]

  \[(3.5)\]

  where $S$ should be “large enough” [27][28].

- **Deviance information criterion (DIC)**

  DIC can be considered as a Bayesian generalization of the AIC by replacing the maximum likelihood estimate by the posterior mean and computing the
effective number of parameters, $p_{\text{DIC}}$, as follows:

$$p_{\text{DIC}} = 2 \left( \log L(\tilde{\theta}) - \frac{1}{S} \sum_{m=1}^{S} \log L(\theta^m) \right),$$

where $\tilde{\theta}$ is the posterior mean \cite{27}. Then, the deviance information criterion is given by

$$\text{DIC} = -2 \left( \log L(\tilde{\theta}) - p_{\text{DIC}} \right).$$

- **Watanabe–Akaike information criterion (WAIC)**

WAIC or widely applicable information criterion is a stable Bayesian predictive measure that approximates the leave-one-out cross-validation (see \cite{27, 28, 29}) and is defined by

$$p_{\text{WAIC}} = 2 \sum_{i=1}^{n} \left( \log \left( \frac{1}{S} \sum_{m=1}^{S} \rho(y_i|\theta^m) \right) - \frac{1}{S} \sum_{m=1}^{S} \log \rho(y_i|\theta^m) \right),$$

$$\text{WAIC} = -2(lppd - p_{\text{WAIC}}).$$

- **K-fold cross-validation**

Cross-validation is the most popular yet computationally expensive method to estimate a model’s predictive accuracy. We consider the K-fold cross-validation where the data are randomly partitioned into K disjoint subsets, $\{y_k\}_{k=1}^{K}$. Then, we define $\{y_{(-k)}\} = \{y_1, \ldots, y_{k-1}, y_{k+1}, \ldots, y_K\}$ to be a training set. For each training set, we compute the corresponding posterior distribution, $p(\theta|y_{(-k)})$. Then, the log predictive density for $y_i \in y_k$ is computed using the training set $\{y_{(-k)}\}$, that is:

$$lpd_i = \log \left( \frac{1}{S} \sum_{m=1}^{S} \rho(y_i|\theta^{k,m}) \right), \ i \in k,$$

where $\{\theta^{k,m}\}_{m=1}^{S}$ are the MCMC samples of the posterior $p(\theta|y_{(-k)})$. Finally,
we sum to obtain the expected log predictive density (elpd):

\[
elpd = \sum_{i=1}^{n} lpd_i.
\]

The K-fold cross-validation (with \( K = 5 \) or 10) is usually used instead of the leave-one-out cross-validation, which is the most computationally exhaustive type of cross-validation (see [30, Chapter 5] and [28]).

In the next Subsection, we present the main numerical results from applying the techniques described in Subsections 3.4.2.1 and 3.4.2.2 for Models Ia, Ib and IIb under the two predefined scenarios.

### 3.4.2.3 Numerical Results (Scenario 1)

Table 3.25: Log marginal likelihoods (Bayes factors) show very strong evidence that Model Ib is better than Model Ia and that Model IIb is better than Model Ib. The predictive information criteria and the 5-fold cross-validation show that Model IIb also has better predictive accuracy than do Model Ia and Model Ib.

<table>
<thead>
<tr>
<th>Models</th>
<th>Model Ia</th>
<th>Model Ib</th>
<th>Model IIb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log marginal likelihood (Laplace)</td>
<td>-963.07</td>
<td>-940.18</td>
<td>-932.55</td>
</tr>
<tr>
<td>Log marginal likelihood (Laplace–Metropolis)</td>
<td>-963.16</td>
<td>-937.06</td>
<td>-923.68</td>
</tr>
<tr>
<td>Log pointwise predictive density (lppd)</td>
<td>-949.56</td>
<td>-920.51</td>
<td>-907.85</td>
</tr>
<tr>
<td>Deviance information criterion (DIC)</td>
<td>1909.6</td>
<td>1851.8</td>
<td>1826.5</td>
</tr>
<tr>
<td>Watanabe-Akaike information criterion (WAIC)</td>
<td>1911.3</td>
<td>1853.1</td>
<td>1825.9</td>
</tr>
<tr>
<td>5-fold cross-validation elpd</td>
<td>-955.42</td>
<td>-927.07</td>
<td>-913.80</td>
</tr>
</tbody>
</table>

Table 3.25 shows that Model IIb under Scenario 1 is preferable by the log marginal likelihood and the predictive information criteria. The Laplace method appears to underestimate the log marginal likelihood for Model IIb. This is expected because of the complex likelihood function of Model IIb and because the Gaussian approximation does not always provide a good estimation. Table 3.25 also shows consistency with the classical information criterion presented in Table 3.6.
3.4.2.4 Numerical Results (Scenario 2)

Table 3.26 shows that Model IIb under Scenario 2 is preferable by the log marginal likelihood and the predictive information criteria. In general, the estimated values in Table 3.26 are slightly higher in magnitude than are the results in Table 3.25. This is reasonable because Bayesian models with proper informative priors should be preferable.

Table 3.26: Log marginal likelihoods (Bayes factors) indicate that Model Ib is better than Model Ia and that Model IIb is better than Model Ib. The predictive information criteria and the 5-fold cross-validation show that Model IIb also has better predictive accuracy than do Model Ia and Model Ib.

<table>
<thead>
<tr>
<th>Models</th>
<th>Model Ia</th>
<th>Model Ib</th>
<th>Model IIb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log marginal likelihood (Laplace)</td>
<td>-963.36</td>
<td>-940.25</td>
<td>-923.91</td>
</tr>
<tr>
<td>Log marginal likelihood (Laplace–Metropolis)</td>
<td>-963.51</td>
<td>-938.17</td>
<td>-923.76</td>
</tr>
<tr>
<td>Log pointwise predictive density (lppd)</td>
<td>-949.70</td>
<td>-920.52</td>
<td>-908.01</td>
</tr>
<tr>
<td>Deviance information criterion (DIC)</td>
<td>1910.4</td>
<td>1852.4</td>
<td>1827.1</td>
</tr>
<tr>
<td>Watanabe-Akaike information criterion (WAIC)</td>
<td>1912.1</td>
<td>1853.9</td>
<td>1826.4</td>
</tr>
<tr>
<td>5-fold cross-validation elpd</td>
<td>-955.70</td>
<td>-927.80</td>
<td>-914.07</td>
</tr>
</tbody>
</table>

3.5 Conclusions

We calibrated models of various complexity that were designed to account for right-censored data by means of the maximum likelihood method. We used a data set described in Section 2 for this purpose. The robustness of the estimation of the quantile functions has been assessed by computing bootstrap confidence intervals for samples stratified with respect to the cycle ratio.

We then considerably enlarged the scope of our study by considering a Bayesian approach. Any prior distribution, which is suitable to describe the available knowledge on the physical parameters, can be easily incorporated into our Bayesian computational framework that provides a simulation-based posterior distribution.

To decide which model could be considered more reliable for deployment, first we
computed classical measures of fit based on information criteria. Then, the Bayesian approach for model comparison was applied to determine which model would be preferred under different a priori scenarios. This approach included very different techniques ranging from those based on the estimation of the marginal likelihood to those based on predictive information criteria, whose implementation requires the use of cross-validation techniques.

The classical approach and the Bayesian approach for model comparison have provided evidence in favor of Model IIb given the 75S-T6 data set described in Section 2. Model IIb assumes that both fatigue life and the fatigue limit parameter follow a Weibull distribution and the expected value of the fatigue limit parameter, $A_3$, is 39.88 ksi.

An integrated set of computational tools has been developed for model calibration, cross-validation, consistency and model comparison, allowing the user to rank alternative statistical models based on objective criteria.

**Acknowledgement**

Z. Sawlan, M. Scavino and R. Tempone are members of King Abdullah University of Science and Technology (KAUST) SRI Center for Uncertainty Quantification in Computational Science and Engineering.
3.6 REFERENCES


and 75S-T6 Aluminum Alloys and of SAE 4130 Steel NACA TN 2324, National Advisory Committee on Aeronautics, March 1951.


Chapter 4

Spatial Poisson processes for fatigue crack initiation

Ivo Babuška, Zaid Sawlan, Marco Scavino, Barna Szabó and Raúl Tempone

Abstract

In this work we propose a stochastic model for estimating the occurrence of crack initiations on the surface of metallic specimens in fatigue problems that can be applied to a general class of geometries. The stochastic model is based on spatial Poisson processes with intensity function that combines stress-life (S-N) curves with averaged effective stress, \( \sigma_{\text{eff}}^{\Delta}(x) \), which is computed after solving numerically the linear elasticity equations on the specimen domains using finite element methods. Here, \( \Delta \) is a parameter that characterizes the size of the neighbors covering the domain boundary. The averaged effective stress, parameterized by \( \Delta \), maps the stress tensor to a scalar field upon the specimen domain. Data from fatigue experiments on notched and unnotched sheet specimens of 75S-T6 aluminum alloys are used to calibrate the model parameters for the individual data sets and their combination. Bayesian and classical approaches are applied to estimate the survival-probability function for any specimen tested under a prescribed fatigue experimental setup. Our proposed model can predict the initiation of cracks in specimens made from the same material with new geometries.

4.1 Introduction

Predicting fatigue in mechanical components is extremely important for preventing hazardous situations. Fatigue starts with crack initiation, then the small crack propagates to become a complete fracture. To model the fatigue of real mechanical objects, the geometry of the objects must be considered in the mathematical formulation to compute the stress or strain field. In this work, we are only concerned with crack initiation and use survival analysis to model the time until the first crack occurs. As such, survival means that no cracks are initiated and failure means the initiation of cracks. We focus only on stress-based approaches that model fatigue crack initiation under high cycle fatigue.

Our goal is to construct a stochastic model that can estimate the survival probability of any mechanical component given data of fatigue experiments on specimens made of the same material. Statistical S-N models are usually used for survival prediction in uniaxial-fatigue experiments with cyclic loadings [1, 2]. There are also several generalizations of S-N models for fatigue of notched specimens (see [3] and the references therein). In these generalizations, the stress tensor field is computed around the notch and mapped into a stress predictor characterized by some parameters. Instead, we consider an effective stress field over the full domain and assume the existence of a material parameter $\Delta$ that define a local neighbor to average the effective stress locally following the theory of critical distances (TCD). There are many versions of the TCD involving additional material parameters [4, 5, 6]. Considering the limited amount of available data and the goal of this study, the most simple TCD using only the averages was used and calibrated.

In this work, we develop a general approach, following the ideas in [7], to modeling crack initiation on the surface of metallic specimens based on simple assumptions. Our model transforms the stress tensor field into a spatial stress function named the averaged effective stress function, $\sigma_{\text{eff}}^\Delta(x)$. We combine $\sigma_{\text{eff}}^\Delta(x)$ with a chosen S-N
model to build a rate function for the spatial Poisson process. The rate function is scaled by the highly stressed volume that is parameterized by a threshold parameter, \( \beta \). The choices of \( \sigma_{\text{eff}}^{\Delta}(x) \), the S-N model and the parameterization of the highly stressed volume are subject to user preference. The resulting model is independent of the shape of the specimen and can fit fatigue data from both notched and unnotched specimens. The Poisson process has been used similarly with a local strain field for low cycle fatigue with unnotched specimens in [8] and recently with notched specimens in [9]. We underline that references [8] and [9] are concerned with low cycle fatigue whereas the present paper is concerned with high cycle fatigue.

Following our previous work [1], we first calibrate the model parameters by means of the maximum likelihood (ML) method, and we consider Bayesian analysis to provide a better understanding of the results obtained by classical methods. The Bayesian analysis has become a primary part of studying fatigue life prediction. For example, Bayesian methods were used to analyze a new S-N model with fatigue tests on welded cover-plate steel-beam specimens [2] and low-cycle fatigue models for turbine disks [10]. In [11], the Bayesian framework was used to assess the uncertainty of a continuum damage model. A hierarchical Bayesian approach was also used in [12], which allowed general prior models to be considered.

The rest of the paper is organized as follows. In Section 4.2, we analyze available data from fatigue experiments to determine their utility in calibrating crack-initiation models. Section 4.3 includes a description of the linear elasticity equations used to compute the stress tensor. Then, we consider a map that transforms the stress tensor into a real-valued spatial function (the averaged effective stress). In Section 4.4, we recall a simple S-N model and calibrate it to the data introduced in Section 4.2 by assuming that the first crack will initiate at the spatial position with the highest effective stress. We introduce our novel spatial Poisson model in Section 4.5 and derive the exact form of the log-likelihood function. This new model is extensively
applied to estimate the survival-probability for each specimen in the data. Finally, we analyze our Poisson model via a Bayesian framework in Section 4.6 where the survival functions computed by posterior estimates for the entire set of data (hereafter referred to as pooled posterior estimates) are compared with the reference ML estimate of each data set.

4.2 Data sets from experiments on aluminum-sheet specimens

We extract three data sets from the National Advisory Committee for Aeronautics (NACA) technical notes 2324 [13], 2639 [14] and 2390 [15], which correspond to fatigue experiments conducted on three sheets of 75S-T6 aluminum (Figure 4.1). Specimen 1 is an unnotched, dogbone-shaped specimen, while specimens 2 and 3 are notched with blunt and sharp notches, respectively.

The first data set consists of fatigue experiments applied to specimen 1 [13, table 3, pp.22–24]. In each experiment, the following data are recorded:

- The maximum stress, $S_{\text{max}}$, measured in ksi units.
- The cycle ratio, $R$, defined as the minimum to maximum stress ratio.
- The number of load/stress cycles at which fatigue failure occurred.
- A binary variable (0/1) denoting whether or not the experiment was stopped prior to failure (run-out).

The other data sets contain fatigue experiments applied to the notched specimens (see [14, table 3, p.9] and [15, table 3, p.8]). We consider only experiments with high cycle fatigue; that is, $N > 8800$. In these data sets, the following data are recorded:

- The nominal maximum stress $S_{\text{max}}$, defined as the maximum applied force divided by the smallest cross-sectional area of the test specimen.
Figure 4.1: Three different types of 75S-T6 aluminum specimens ([13, 14, 15]).

- the nominal mean stress, $S_{\text{mean}}$, the stress ratio is then given by $R = 2 \frac{S_{\text{mean}}}{S_{\text{max}}} - 1$.
- The number of load cycles at which fatigue failure occurred.
- A binary variable (0/1) denoting whether or not the experiment was stopped prior to failure (run-out).

Remark. The fatigue data obtained for particular cycle ratios must be generalized to arbitrary cycle ratios. For this purpose, the equivalent stress is defined as

$$S_{eq}^{(q)} = S_{\text{max}} (1 - R)^q,$$

where $q$ is a fitting parameter [1, 16, 17]. The load force, or normal traction, is then given by $T = \frac{W_{\text{min}}}{W_{\text{max}}} S_{eq}^{(q)}$, where $W_{\text{max}}$ is the maximum width of the specimen and $W_{\text{min}}$ is the minimum width.
Table 4.1: Fatigue data for 75S-T6 aluminum alloys.

<table>
<thead>
<tr>
<th>Data set</th>
<th>Specimen</th>
<th>Source</th>
<th>Radius (in)</th>
<th>Number of experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 (Unnotched)</td>
<td>NACA TN 2324 [13]</td>
<td>12</td>
<td>85 (73)</td>
</tr>
<tr>
<td>2</td>
<td>2 (Blunt edge notch)</td>
<td>NACA TN 2639 [14]</td>
<td>0.76</td>
<td>31 (29)</td>
</tr>
<tr>
<td>3</td>
<td>3 (Sharp edge notch)</td>
<td>NACA TN 2390 [15]</td>
<td>0.03125</td>
<td>28 (22)</td>
</tr>
</tbody>
</table>

Table 4.1 summarizes the properties of each specimen shown in Figure 4.1. The total number of experiments is also given with the number of observed failures provided in parentheses. The thickness of all three specimens is 0.09 in, which is relatively small. Therefore, we can reduce the dimension of the problem to two. However, we note that for specimen 3, the radius of the notch is smaller than the specimen thickness; therefore, the three-dimensional (3D) model might not be sufficiently approximated by a two-dimensional (2D) model.

**Remark.** In the aforementioned experimental data, we assume that crack propagation is instantaneous as crack initiation occurs; that is, crack initiation is equivalent to fatigue failure. We validate this assumption by Paris law for some experiments. The number of cycles spent on crack propagation is negligible compared with the number of cycles until crack initiation. The life of the specimen is thus defined as the number of stress cycles until the first crack initiates. This assumption allows us to calibrate fatigue crack-initiation models to the available data. In general, we would need the number of stress cycles when the first crack appears.

### 4.3 Numerical computation of $\sigma_{\text{eff}}^\Delta(x)$

#### 4.3.1 Linear elasticity

The stress field in the specimens is defined by the linear elasticity theory. The mathematical model of linear elasticity is based on strain-displacement equations, stress-strain equations, and equilibrium equations [18]. We let $D$ be the domain shown
in Figure 4.2. Then, the displacement field \( \mathbf{u} = [u_x(x, y) \quad u_y(x, y)] \) satisfies the equations of two-dimensional elasticity (plane stress) [19]:

\[
\begin{align*}
\frac{E}{2(1-\nu)} \frac{\partial}{\partial x} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right) + G \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} \right) &= 0 \\
\frac{E}{2(1-\nu)} \frac{\partial}{\partial y} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right) + G \left( \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} \right) &= 0
\end{align*}
\]

where \( E > 0 \) is the modulus of elasticity, \( \nu \) is Poisson’s ratio, and \( G = \frac{E}{2(1+\nu)} \) is the shear modulus. Equivalently, the two-dimensional elasticity equations can be written in terms of the stress as follows:

\[
\begin{cases}
\frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} = 0 \\
\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} = 0
\end{cases}
\]

(4.2)

where the normal stresses in the x-axis and y-axis, \( \sigma_x \) and \( \sigma_y \), respectively, and the shear stress, \( \tau_{xy} \), are given by:

\[
\begin{align*}
\sigma_x &= \frac{E}{1-\nu^2} \left( \frac{\partial u_x}{\partial x} + \nu \frac{\partial u_y}{\partial y} \right) \\
\sigma_y &= \frac{E}{1-\nu^2} \left( \nu \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right) \\
\tau_{xy} &= G \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right)
\end{align*}
\]

The boundary conditions for the domain \( D \) shown in Figure 4.2 are \( \sigma_x = 1, \tau_{xy} = 0 \) on boundary segment \( B_1 \), free boundary condition are prescribed on \( B_2 \) and \( B_3 \), and symmetry boundary conditions are prescribed on \( B_4 \) and \( B_5 \).

The numerical solution for the system (4.2) was obtained by the Finite Element Method [18]. Figures 4.3 and 4.4 show the computed values of \( \sigma_x \) over the right upper quarter of specimens 1 and 2, respectively. The mesh of the right upper quarter of specimen 3 is shown in Figure 4.5. The adaptive PDE solver ADAPTMESH in
MATLAB was used. For specimen 3, we also computed three-dimensional stress field using the MATLAB function SOLVEPDE with unstructured mesh generated by COMSOL. The stress $\sigma_x$ is shown in Figure 4.6. We refer the reader to [18, Chapter 3] for the details of the three-dimensional elasticity equations.

**Remark.** Due to the linearity of the problem, it is sufficient to compute the stress tensor with a unit load force, denoted by $\sigma^1(y)$, $y \in D$, for a given specimen. Then, the stress tensor that corresponds to a specific experiment is given by

$$
\sigma(y) = T \times \sigma^1(y) = \frac{W_{min}}{W_{max}} S_{max} (1 - R)^q \times \sigma^1(y),
$$

(4.3)
Figure 4.4: Distribution of $\sigma_x$ for the notched specimen used in NACA TN 2639 (specimen 2).

Figure 4.5: Distribution of $\sigma_x$ in the plane of symmetry of the notched specimen used in NACA TN 2390 (specimen 3).

Figure 4.6: Three-dimensional $\sigma_x$ of specimen 3; the bottom plane is the plane of symmetry displayed in Figure 4.5.
where $S_{\text{max}}(1 - R)^q$ is the equivalent stress that characterizes the stress cycle of the experiment as defined in (4.1). Thus, we need to run a MATLAB PDE solver only once for each specimen.

In the rest of this section, we will denote the stress tensor at $y \in D$ by $\sigma(y)$, where $\sigma(y)$ depends on the stress ratio $R$ and the parameter $q$ through equation (4.3).

### 4.3.2 Averaged effective stress $\sigma_{\text{eff}}^\Delta(x)$

There are several proposals for the definition of effective stress [3, 7]. In this work, we define the effective stress by the maximum principal stress. The two-dimensional maximum principal stress is given by [20]:

$$
\sigma_{\text{eff}}(x, y) = \frac{1}{2}(\sigma_x + \sigma_y) + \sqrt{\left(\frac{\sigma_x - \sigma_y}{2}\right)^2 + \tau_{xy}^2}, \forall (x, y) \in D.
$$

Then, we obtain the averaged effective stress by averaging the effective stress locally:

$$
\sigma_{\text{eff}}^\Delta(x) = \frac{1}{|B(x, \Delta) \cap D|} \int_{B(x, \Delta) \cap D} \sigma_{\text{eff}}(y) dy. \quad (4.4)
$$

where $B(x, \Delta)$ is a cube (square) of length $\Delta$ centered at $x$ [7] in the 3D (2D) model. In general, there are different ways to define $B(x, \Delta)$, as in the theory of critical distances [5]. As $\Delta$ converges to zero, the averaged effective stress converges to the effective stress.

### 4.4 Preliminary calibration

In our initial attempt to model fatigue crack initiation, we assume that the crack formation is determined by $\sigma_{\text{eff}}^\Delta = \max_{x \in \partial D} \sigma_{\text{eff}}^\Delta(x)$. This assumption reduces the stress field to a scalar value that can be used with S-N models. We consider the fatigue-limit model (Model Ia) from [1]. The fatigue life, $N$, is modeled by means of
a lognormal distribution with mean $\mu(\sigma_{\text{eff}}^{\Delta})$ and standard deviation $\tau$, where

$$\mu(\sigma_{\text{eff}}^{\Delta}) = \begin{cases} A_1 + A_2 \log_{10}(\sigma_{\text{eff}}^{\Delta} - A_3), & \text{if } \sigma_{\text{eff}}^{\Delta} > A_3 \\ +\infty, & \text{otherwise} \end{cases}$$

and $A_3$ is the fatigue-limit parameter. When $\mu = +\infty$, we assume cracks will never initiate and the survival probability will be constant equals 1. The likelihood function for the S-N curve based on $m$ experiments is given by

$$L(\theta, \Delta; n) = \prod_{i=1}^{m} \left[ \frac{1}{n_i \log(10)} g(\log_{10}(n_i); \mu(\sigma_{\text{eff},i}^{\Delta}), \tau) \right]^{\delta_i} \left[ 1 - \Phi \left( \frac{\log_{10}(n_i) - \mu(\sigma_{\text{eff},i}^{\Delta})}{\tau} \right) \right]^{1-\delta_i},$$

where $\theta = (A_1, A_2, A_3, q, \tau)$, $n = (n_1, \ldots, n_m)$, $g(t; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left\{ -\frac{(t-\mu)^2}{2\sigma^2} \right\}$, $\Phi$ is the cumulative distribution function of the standard normal distribution, and

$$\delta_i = \begin{cases} 1 & \text{if } n_i \text{ is a failure} \\ 0 & \text{if } n_i \text{ is a run-out}. \end{cases}$$

Table 4.2: ML estimates of $\theta$ from Model Ia using (4.5) where $\Delta = 0$.

<table>
<thead>
<tr>
<th>Data set</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>Maximum log-likelihood</th>
<th>AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.40</td>
<td>-2.01</td>
<td>35.91</td>
<td>0.5627</td>
<td>0.5274</td>
<td>-950.16</td>
<td>1910.32</td>
</tr>
<tr>
<td>2</td>
<td>8.24</td>
<td>-2.39</td>
<td>38.98</td>
<td>0.5790</td>
<td>0.4216</td>
<td>-396.55</td>
<td>803.10</td>
</tr>
<tr>
<td>3 (2D)</td>
<td>8.78</td>
<td>-2.46</td>
<td>46.41</td>
<td>0.6470</td>
<td>0.5441</td>
<td>-303.44</td>
<td>616.88</td>
</tr>
<tr>
<td>3 (3D)</td>
<td>8.86</td>
<td>-2.47</td>
<td>48.94</td>
<td>0.6470</td>
<td>0.5439</td>
<td>-303.44</td>
<td>616.88</td>
</tr>
<tr>
<td>1, 2 &amp; 3 (2D)</td>
<td>7.77</td>
<td>-1.96</td>
<td>35.58</td>
<td>0.5780</td>
<td>0.7909</td>
<td>-1710.68</td>
<td>3431.36</td>
</tr>
<tr>
<td>1, 2 &amp; 3 (3D)</td>
<td>7.50</td>
<td>-1.75</td>
<td>36.11</td>
<td>0.5755</td>
<td>0.8199</td>
<td>-1715.12</td>
<td>3440.24</td>
</tr>
</tbody>
</table>

Before calibrating $\Delta$, we estimate $\theta = (A_1, A_2, A_3, q, \tau)$ under the restriction that $\Delta = 0$. Table 4.2 shows the corresponding ML estimates of $\theta$ obtained using each data set individually and the pooled ML estimates that are obtained from the combined data set. Figures 4.7 and 4.8 show the corresponding quantile functions with the
data used to fit the model. In these figures, the observations are plotted with respect to the maximum effective stress in the y-axis not the applied traction. The notched specimens are subjected to much smaller traction forces but the effective stress will include the notch effect. We notice that the ML estimates of $\theta$ differ considerably with each data set and the variance is increased when fitting the same S-N model to the combined data set. To reduce the variance, more parameters need to be introduced. However, for predicting the life of new specimens, it is preferable to have large variability in the model.

Figure 4.7: Fitting Model Ia to data set 1 (upper panel) and data set 2 (bottom panel) where $\Delta = 0$.

For specimen 3, we consider both 2D and 3D models and show the calibrated parameters for each case in Table 4.2. When calibrating the specimen 3 data set
Figure 4.8: Fitting Model Ia to data set 3 (2D) (upper panel) and the combined data set (bottom panel) where ∆ = 0.

only, the 2D and 3D models produce the same fit with only a small change in the fatigue-limit parameter. Moreover, the pooled estimates for the combined data sets are very similar, though the 2D model provides a better fit by underestimating the maximum effective stress, which makes it more similar to the maximum effective stress of specimens 1 and 2.

Table 4.3: ML estimate of $\theta$ and $\Delta$ from Model Ia using (4.5).

<table>
<thead>
<tr>
<th>Data set</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\Delta$ (in)</th>
<th>Maximum log-likelihood</th>
<th>AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 2 &amp; 3 (2D)</td>
<td>8.16</td>
<td>-2.38</td>
<td>34.65</td>
<td>0.5774</td>
<td>0.6006</td>
<td>0.025</td>
<td>-1673.56</td>
<td>3359.12</td>
</tr>
</tbody>
</table>

Now, we incorporate the parameter $\Delta$ to average the effective stress locally. By
maximizing the likelihood function (4.5) using the combined data, we obtain a pooled ML estimate of $\theta$ and $\Delta$ in Table 4.3. We present this fitting in Figure 4.9. The incorporation of $\Delta$ unifies the range of $\sigma_{\text{eff}}^{\Delta}$ for the three specimens, and therefore, improves the fitting of the data.

Figure 4.9: Fitting Model Ia to the combined data set where $\Delta > 0$.

Figure 4.10 shows the log of the profile likelihood function for $\Delta$ where the 95% confidence interval is approximately $(0.021, 0.03)$. We compare the fitting of the combined data set when $\Delta = 0$ and $\Delta > 0$ by means of the Akaike information criterion (AIC) in Table 4.4. We recall that the AIC is defined as $2(p - \log L^*)$ where $p$ is the number of parameters and $L^*$ is the maximum likelihood value. The smaller AIC value corresponds to the better fit. In the rest of the paper, we will use AIC to compare different models with different number of parameters.

Table 4.4: Comparison between two different specifications of Model Ia using (4.5).

<table>
<thead>
<tr>
<th>Model Ia given data sets 1, 2 &amp; 3 (2D)</th>
<th>$\Delta = 0$</th>
<th>$\Delta &gt; 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum log-likelihood</td>
<td>-1710.68</td>
<td>-1673.56</td>
</tr>
<tr>
<td>Akaike information criterion (AIC)</td>
<td>3431.36</td>
<td>3359.12</td>
</tr>
</tbody>
</table>

Remark. The parameter $\Delta$ smooths the effective stress locally and acts as a scaling.
parameter for a given non-uniform stress field. Therefore, $\Delta$ must be calibrated using combined data from fatigue experiments on specimens with different geometries.

Because it was experimentally observed that the crack was not always at the point where the notch is deepest, in the next section, we introduce a tailored stochastic model for the occurrence of crack initiations.

### 4.5 Spatial Poisson process to model crack initiation

For a given S-N model that depends on parameters $\theta$, we consider the following notations:

- The failure density function is denoted by $f_{SN}(n; s, \theta)$,
- The cumulative distribution function is denoted by $F_{SN}(n; s, \theta)$,
- The failure/hazard rate function is denoted by $h_{SN}(n; s, \theta)$,

where $s$ is a generic symbol for the stress. To construct a spatial Poisson process for crack initiation in a domain $D$, we assume that

(a) The (averaged) effective stress at $x \in \partial D$ determines the crack formation at $x$. 

![Log profile likelihood](image)
(b) Different cracks initiate independently.

The spatial Poisson process is governed by the intensity function $\lambda(x, n) \geq 0$, which relates the spatial location to the number of cycles, $n$. This intensity function depends on the effective stress, $\lambda(x, n) = \eta(n; \sigma_{\text{eff}}^\Delta(x))$, where $\eta$ is a failure-rate function. The number of cracks occurring inside any surface region, $B \subset \partial D$, can be modeled as a Poisson counting process with the associated rate function $\lambda_B(n) = \int_B \lambda(x, n) dS(x)$. Then, the number of crack initiations in the region $B$ after performing $n$ stress cycles is modeled as a Poisson random variable, $M_B(n)$, whose distribution is

$$P(M_B(n) = m) = \frac{(\Lambda_B(n))^m}{m!} \exp(-\Lambda_B(n)), \quad m = 0, 1, \ldots$$

with $\Lambda_B(n) = \int_0^n \lambda_B(u) du \geq 0$.

We are interested in the number of stress cycles, $N_{\partial D}$, when the first crack initiates on $\partial D$. The random variable $N_{\partial D}$ is related to the counting process $M_{\partial D}(n)$ by the equivalence relation $N_{\partial D} > n \iff M_{\partial D}(n) = 0$, which corresponds to the survival event. Similarly, the failure event, $N_{\partial D} \leq n$, is equivalent to $M_{\partial D}(n) \geq 1$. Therefore, the survival probability after $n$ cycles is

$$P(N_{\partial D} > n; \sigma_{\text{eff}}^\Delta) = P(M_{\partial D}(n) = 0) = \exp(-\Lambda_{\partial D}(n))$$

$$= \exp \left( - \int_0^n \int_{\partial D} \eta(\hat{n}; \sigma_{\text{eff}}^\Delta(x)) dS(x) \, d\hat{n} \right), \quad (4.6)$$
and the density function of $N_{\partial D}$ is

$$
\rho_{\partial D}(n; \sigma_{\text{eff}}^\Delta) = \frac{\partial}{\partial n} P(N_{\partial D} \leq n; \sigma_{\text{eff}}^\Delta) \\
= \frac{\partial}{\partial n} \left(1 - P(N_{\partial D} > n; \sigma_{\text{eff}}^\Delta)\right) \\
= \frac{\partial}{\partial n} \left(1 - \exp \left(- \int_0^n \int_{\partial D} \eta(\hat{n}; \sigma_{\text{eff}}^\Delta(x))dS(x) d\hat{n}\right)\right) \quad \text{(from (4.6))} \\
= - \exp \left(- \int_0^n \int_{\partial D} \eta(\hat{n}; \sigma_{\text{eff}}^\Delta(x))dS(x) d\hat{n}\right) \times \frac{\partial}{\partial n} \left( - \int_0^n \int_{\partial D} \eta(\hat{n}; \sigma_{\text{eff}}^\Delta(x))dS(x) d\hat{n}\right) \\
= - P(N_{\partial D} > n; \sigma_{\text{eff}}^\Delta) \times \frac{\partial}{\partial n} \left( - \int_0^n \int_{\partial D} \eta(\hat{n}; \sigma_{\text{eff}}^\Delta(x))dS(x) d\hat{n}\right) \\
= P(N_{\partial D} > n; \sigma_{\text{eff}}^\Delta) \times \int_{\partial D} \eta(n; \sigma_{\text{eff}}^\Delta(x))dS(x).
$$

To parameterize the rate function $\eta(n; s)$, we relate it to a given S-N model as follows:

$$
\eta(n; s) = - \frac{1}{\gamma} \frac{\partial}{\partial n} \log (1 - F_{SN}(n; s, \theta)) = \frac{1}{\gamma} \frac{f_{SN}(n; s, \theta)}{1 - F_{SN}(n; s, \theta)} = \frac{1}{\gamma} h_{SN}(n; s, \theta), \quad (4.7)
$$

where $\gamma$ is the size of the highly stressed volume. Thus, the spatial Poisson model is fully characterized by $\theta, \gamma, \Delta$, where $\theta$ depends on the selected S-N model.

From (4.7), the survival probability can be simplified to

$$
P(N_{\partial D} > n; \sigma_{\text{eff}}^\Delta) = \exp \left( \frac{1}{\gamma} \int_{\partial D} \log(1 - F_{SN}(n; \sigma_{\text{eff}}^\Delta(x), \theta))dS(x) \right). \quad (4.8)
$$

**Remark.** In the case of uniform stress, $\sigma_{\text{eff}}^\Delta(x) \equiv \sigma_{eq}$ and $\gamma = |\partial D|$. Thus, the survival probability (4.8) becomes

$$
P(N_{\partial D} > n; \sigma_{\text{eff}}^\Delta) = 1 - F_{SN}(n; \sigma_{eq}, \theta),
$$

which means that the parameterization of $\eta(n; s)$ in (4.7) ensures the consistency of the model for uniform and non-uniform stresses.
The highly stressed volume (area), $\gamma$, depends on the specimen geometry. We re-parametrize the survival probability by defining the highly stressed volume.

**Definition 2. Highly stressed volume**

We let $A_\beta = \{x \in \partial D : \sigma^{1}_{\text{eff}}(x) > \beta\}$, where $\sigma^{1}_{\text{eff}}(x)$ is the effective stress that corresponds to a unity traction and $\beta$ is an unknown parameter. The highly stressed volume is given by

$$\gamma(\beta) = \int_{\partial D} 1_{A_\beta}(x) dS(x). \quad (4.9)$$

Under the assumption of independent experiments, the log-likelihood function is

$$\ell(\theta, \beta, \Delta) = \sum_{i=1}^{m} \left[ (1 - \delta_i) \log(P(N_{\partial D} > n_i; \sigma^{\Delta}_{\text{eff}, i})) + \delta_i \log(\rho_{\partial D}(n_i; \sigma^{\Delta}_{\text{eff}, i})) \right]$$

$$= \sum_{i=1}^{m} \left\{ (\delta_i - 1) \int_{0}^{n_i} \eta(n; \sigma^{\Delta}_{\text{eff}, i}(x)) dS(x) dn + \delta_i \log\left(\int_{\partial D} \eta(n_i; \sigma^{\Delta}_{\text{eff}, i}(x)) dS(x)\right) \right. \right.$$}

$$\left. - \delta_i \int_{0}^{n_i} \int_{\partial D} \eta(n; \sigma^{\Delta}_{\text{eff}, i}(x)) dS(x) dn \right\}$$

$$= \sum_{i=1}^{m} \left\{ (1 - \delta_i) \frac{1}{\gamma(\beta)} \int_{\partial D} \log(1 - F_{SN}(n_i; \sigma^{\Delta}_{\text{eff}, i}(x), \theta)) dS(x) \right.$$

$$+ \delta_i \log\left(\frac{1}{\gamma(\beta)} \int_{\partial D} h_{SN}(n_i, \sigma^{\Delta}_{\text{eff}, i}(x), \theta) dS(x)\right) \right.$$}

$$\left. + \delta_i \frac{1}{\gamma(\beta)} \int_{\partial D} \log(1 - F_{SN}(n_i; \sigma^{\Delta}_{\text{eff}, i}(x), \theta)) dS(x) \right\}$$

$$= \sum_{i=1}^{m} \left\{ \frac{1}{\gamma(\beta)} \int_{\partial D} \log(1 - F_{SN}(n_i; \sigma^{\Delta}_{\text{eff}, i}(x), \theta)) dS(x) + \delta_i \log\left(\frac{1}{\gamma(\beta)} \int_{\partial D} h_{SN}(n_i, \sigma^{\Delta}_{\text{eff}, i}(x), \theta) dS(x)\right) \right. \right.$$}

$$\left. \left(4.10\right) \right.$$
4.5.1 Calibration of the spatial Poisson model

Again, we consider Model Ia and calibrate the likelihood (4.10) under the assumption that $\Delta = 0$. We replace the averaged effective stress, $\sigma_{\text{eff}}^\Delta(x)$ in the log-likelihood function (4.10) with the effective stress, $\sigma_{\text{eff}}(x)$. The results of the maximization of the log-likelihood with respect to $\theta$ and $\beta$ are summarized in Table 4.5. The overall fit in Table 4.5 is better than the fit in Table 4.2. When moving from 2D to 3D modeling, we did not obtain any significant gain concerning the goodness of fit (therefore, at this stage, 2D modeling is recommended). We still notice variations in the estimated parameters with each data set as in Table 4.2. However, the standard deviation $\tau$ is reduced considerably in all cases. Also, the difference between the calibrated fatigue-limit parameters from the 2D and 3D models of specimen 3 is small in this case. Therefore, we use only the 2D model for all three specimens from now on. We try to improve the fitting by incorporating $\Delta$.

Table 4.5: ML estimates of $\theta$ and $\beta$ from Model Ia using (4.10) where $\Delta = 0$.

<table>
<thead>
<tr>
<th>Data set</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\beta$</th>
<th>Maximum log-likelihood</th>
<th>AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.88</td>
<td>-1.32</td>
<td>35.88</td>
<td>0.5640</td>
<td>0.3011</td>
<td>1.16</td>
<td>-938.90</td>
<td>1889.80</td>
</tr>
<tr>
<td>2</td>
<td>6.00</td>
<td>-1.22</td>
<td>40.98</td>
<td>0.5965</td>
<td>0.2299</td>
<td>1.95</td>
<td>-391.45</td>
<td>794.90</td>
</tr>
<tr>
<td>3 (2D)</td>
<td>7.62</td>
<td>-2.18</td>
<td>45.35</td>
<td>0.6504</td>
<td>0.2692</td>
<td>2.54</td>
<td>-301.82</td>
<td>615.64</td>
</tr>
<tr>
<td>3 (3D)</td>
<td>7.62</td>
<td>-2.16</td>
<td>44.62</td>
<td>0.6504</td>
<td>0.2903</td>
<td>2.90</td>
<td>-302.03</td>
<td>616.06</td>
</tr>
<tr>
<td>1, 2 &amp; 3 (2D)</td>
<td>6.28</td>
<td>-1.47</td>
<td>35.99</td>
<td>0.5676</td>
<td>0.3804</td>
<td>1.83</td>
<td>-1650.05</td>
<td>3312.10</td>
</tr>
<tr>
<td>1, 2 &amp; 3 (3D)</td>
<td>6.30</td>
<td>-1.47</td>
<td>35.78</td>
<td>0.5646</td>
<td>0.3718</td>
<td>1.83</td>
<td>-1649.97</td>
<td>3311.94</td>
</tr>
</tbody>
</table>

Table 4.6: ML estimate of $\theta$, $\beta$, and $\Delta$ from Model Ia using (4.10).

<table>
<thead>
<tr>
<th>Data set</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\beta$</th>
<th>$\Delta$</th>
<th>Maximum log-likelihood</th>
<th>AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 2 &amp; 3 (2D)</td>
<td>6.29</td>
<td>-1.47</td>
<td>35.99</td>
<td>0.5664</td>
<td>0.3453</td>
<td>1.83</td>
<td>0.0125</td>
<td>-1648.16</td>
<td>3310.32</td>
</tr>
</tbody>
</table>

The pooled ML estimates of $\theta$, $\beta$, and $\Delta$ is presented in Table 4.6. Figure 4.11 shows the log profile likelihood function for $\Delta$. We compare the case when $\Delta$ is ne-
glected with the case when $\Delta$ is incorporated in terms of their AIC in Table 4.7. Slight preference is given to Model Ia when $\Delta > 0$ is calibrated with the other parameters. This slight preference may not justify the extra computations needed to estimate $\Delta$. However, it should pointed out that for specimens with diverse geometries, it is expected that $\Delta$ will play a role in the fitting process. Therefore, $\Delta$ must be calibrated given the available data to take into account the microstructural features. We further study this comparison using a Bayesian framework in the next section.

![Log profile likelihood](image)

**Figure 4.11:** The estimated log profile likelihood function for the parameter $\Delta$ derived from (4.10) and the combined data sets.

Comparing AIC in Tables 4.4 and 4.7, we see that the spatial Poisson process provides much better fit than the model introduced in 4.4 whether $\Delta = 0$ or $\Delta > 0$. Although both models are generalizations using simple assumptions of the same S-N model (Model Ia), the spatial Poisson model incorporates the complete stress field and accounts for the highly stressed volume. We emphasize that we adopted the same resolution for both models in sections 4.4 and 4.5. A detailed mesh sensitivity analysis for the Poisson model is provided in Subsection 4.5.3.
Table 4.7: Comparison between two different specifications of Model Ia using (4.10).

<table>
<thead>
<tr>
<th>Model Ia given data sets 1, 2 &amp; 3 (2D)</th>
<th>$\Delta = 0$</th>
<th>$\Delta &gt; 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum log-likelihood</td>
<td>-1650.05</td>
<td>-1648.16</td>
</tr>
<tr>
<td>Akaike information criterion (AIC)</td>
<td>3312.10</td>
<td>3310.32</td>
</tr>
</tbody>
</table>

4.5.2 Survival functions

We compare the survival-probability functions for each specimen using model parameters estimated from each of their individual data sets as well as using the combined data set. The pooled ML estimates can be used to predict the survival probability of new specimens but with larger variability. The ML estimates obtained from the three data sets and the combined data set are provided in Table 4.5. The survival-probability could be expressed as a function of the traction $T = \frac{W_{\min}}{W_{\max}} S_{\max} (1 - R)^q$ and the number of cycles $n$. We plot the contour lines of the survival-probability surface for each specimen together with its fatigue experiment data. Figures 4.12, 4.13, and 4.14 provide analog representations of the S-N curves computed using the Poisson model with the individual data sets estimates and the pooled estimates. In this case, the survival probability depends on the complete stress field of the specimen, and therefore, there are no unique S-N curves for the three specimens jointly.

![Figure 4.12: Contour plots of the survival-probability functions for specimen 1 computed using (4.8) with data set 1 ML estimates (dashed line) and pooled ML estimates (solid line); yellow is 0.95 probability, green is 0.5, and blue is 0.05.](image)

In Figure 4.12 we observe that the survival-probability functions computed from
Figure 4.13: Contour plots of the survival-probability functions for specimen 2 computed using (4.8) with data set 2 ML estimates (dashed line) and pooled ML estimates (solid line); yellow is 0.95 probability, green is 0.5, and blue is 0.05.

Figure 4.14: Contour plots of the survival-probability functions for specimen 3 computed using (4.8) with data set 3 ML estimates (dashed line) and pooled ML estimates (solid line); yellow is 0.95 probability, green is 0.5, and blue is 0.05.

data set 1 estimates and the pooled estimates are similar. In Figure 4.13, we notice a small increase in variability of the survival-probability function obtained by the pooled estimates compared. This variability increases considerably for specimen 3 in Figure 4.14. However, the variability introduced by the pooled estimates provide more conservative survival functions that could be used for predictions and making design rules [22]. The variability increased with the pooled estimates because we assume spatial independence. In a single data set case, the spatial correlation influences all the estimated parameters, and therefore, the variance is reduced. We also compare the survival-probability functions for specific values of $S_{max}$ with $R = 0.1$ and $R = -0.1$.
in Figures 4.15, 4.16 and 4.17.

Figure 4.15: Survival-probability functions for specimen 1 obtained using different ML estimates; \( S_{max} = 45 \) ksi.

Figure 4.16: Survival-probability functions for specimen 2 obtained using different ML estimates; \( S_{max} = 30 \) ksi.

Figure 4.17: Survival-probability functions for specimen 3 obtained using different ML estimates; \( S_{max} = 12 \) ksi.

Figure 4.15 shows the survival-probability functions for specimen 1, assuming
\( S_{\text{max}} = 45 \text{ ksi} \). The survival-probability functions produced by the pooled estimates are very similar to the ones produced from estimates obtained using only the dataset 1. Including fatigue data from the notched specimens has only a small effect on the survival probability of the unnotched specimen. Figures 4.16 and 4.17 show the survival-probability functions for specimens 2 and 3 using \( S_{\text{max}} = 30 \text{ ksi} \) and \( S_{\text{max}} = 12 \text{ ksi} \), respectively. The estimated survival of specimen 2 computed using the pooled estimates is more pessimistic than the estimated survival of specimen 2 using the data set 2 estimates. For specimen 3, the survival functions using the pooled estimates are initially smaller (more pessimistic) than the survival functions using the data set 3 estimates. However, the estimated survival functions from the data set 3 decay much faster with the number of cycles than those of the pooled estimates. Thus, the effect of pooling data sets is substantial for specimens 2 and 3. One possible reason is that data sets 2 and 3 are much smaller than data set 1.

### 4.5.3 Convergence analysis

In this subsection, we study the effect of finite element triangulation on the estimated parameters and analyze the convergence of the ML estimates with respect to the mesh. To simplify the analysis, we consider the case of \( \Delta = 0 \). In Tables 4.8, 4.9 and 4.10, we present the ML estimates of \( \theta \) and \( \beta \) for specimens 1, 2 and 3, respectively, under different meshes.

Table 4.8: ML estimates for Model Ia given data set 1 with different meshes for specimen 1.

<table>
<thead>
<tr>
<th># triangles</th>
<th>( A_1 )</th>
<th>( A_2 )</th>
<th>( A_3 )</th>
<th>( q )</th>
<th>( \tau )</th>
<th>( \beta )</th>
<th>Maximum log-likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>5.77</td>
<td>-1.23</td>
<td>35.54</td>
<td>0.5611</td>
<td>0.3112</td>
<td>1.16</td>
<td>-939.07</td>
</tr>
<tr>
<td>593</td>
<td>5.88</td>
<td>-1.32</td>
<td>35.84</td>
<td>0.5631</td>
<td>0.2975</td>
<td>1.14</td>
<td>-939.08</td>
</tr>
<tr>
<td>1275</td>
<td>5.88</td>
<td>-1.31</td>
<td>35.87</td>
<td>0.5636</td>
<td>0.3004</td>
<td>1.16</td>
<td>-938.90</td>
</tr>
<tr>
<td>2852</td>
<td>5.88</td>
<td>-1.32</td>
<td>35.87</td>
<td>0.5646</td>
<td>0.3020</td>
<td>1.16</td>
<td>-938.92</td>
</tr>
<tr>
<td>9948</td>
<td>5.88</td>
<td>-1.32</td>
<td>35.88</td>
<td>0.5640</td>
<td>0.3011</td>
<td>1.16</td>
<td>-938.90</td>
</tr>
</tbody>
</table>
Table 4.9: ML estimates for Model Ia given data set 2 with different meshes for specimen 2.

<table>
<thead>
<tr>
<th># triangles</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\beta$</th>
<th>Maximum log-likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td>74</td>
<td>5.39</td>
<td>-0.0514</td>
<td>24.98</td>
<td>0.5496</td>
<td>0.5640</td>
<td>1.7</td>
<td>-395.50</td>
</tr>
<tr>
<td>611</td>
<td>6.00</td>
<td>-1.25</td>
<td>39.48</td>
<td>0.5890</td>
<td>0.2395</td>
<td>1.83</td>
<td>-391.62</td>
</tr>
<tr>
<td>1294</td>
<td>6.00</td>
<td>-1.21</td>
<td>40.54</td>
<td>0.5994</td>
<td>0.2358</td>
<td>1.98</td>
<td>-391.62</td>
</tr>
<tr>
<td>2580</td>
<td>6.00</td>
<td>-1.23</td>
<td>40.79</td>
<td>0.5926</td>
<td>0.2241</td>
<td>1.91</td>
<td>-391.24</td>
</tr>
<tr>
<td>6508</td>
<td>6.00</td>
<td>-1.22</td>
<td>40.98</td>
<td>0.5965</td>
<td>0.2299</td>
<td>1.95</td>
<td>-391.45</td>
</tr>
</tbody>
</table>

Table 4.10: ML estimates for Model Ia given data set 3 with different meshes for specimen 3 (2D).

<table>
<thead>
<tr>
<th># triangles</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\beta$</th>
<th>Maximum log-likelihood</th>
</tr>
</thead>
<tbody>
<tr>
<td>352</td>
<td>7.14</td>
<td>-1.83</td>
<td>37.15</td>
<td>0.6445</td>
<td>0.4134</td>
<td>3.66</td>
<td>-301.50</td>
</tr>
<tr>
<td>3840</td>
<td>7.40</td>
<td>-2.04</td>
<td>44.60</td>
<td>0.6538</td>
<td>0.2797</td>
<td>2.62</td>
<td>-302.03</td>
</tr>
<tr>
<td>6664</td>
<td>7.5</td>
<td>-2.10</td>
<td>45.11</td>
<td>0.6504</td>
<td>0.2680</td>
<td>2.53</td>
<td>-301.83</td>
</tr>
<tr>
<td>15649</td>
<td>7.62</td>
<td>-2.18</td>
<td>45.41</td>
<td>0.6524</td>
<td>0.2729</td>
<td>2.59</td>
<td>-301.87</td>
</tr>
<tr>
<td>26544</td>
<td>7.62</td>
<td>-2.18</td>
<td>45.35</td>
<td>0.6504</td>
<td>0.2692</td>
<td>2.54</td>
<td>-301.82</td>
</tr>
</tbody>
</table>

Figure 4.18: Convergence of the ML estimates of the fatigue-limit parameter $A_3$ with the number of triangles used for specimen 1 (left panel), specimen 2 (middle panel), and specimen 3 (right panel).

Figure 4.18 shows the convergence of the estimated fatigue-limit parameter, $A_3$ with respect to the number of triangles used in the finite element triangulation. The other estimated parameters exhibit similar behavior. This analysis also ensures the robustness of the estimated survival functions in 4.5.2.
4.6 Bayesian analysis

So far, we have analyzed the spatial Poisson model following a classical statistical approach. Now, we consider a Bayesian framework and infer the Model Ia parameters under the two scenarios of $\Delta = 0$ and $\Delta = 0.0125$. We assume the following uniform priors:

\[
A_1 \sim U(2, 13), \ A_2 \sim U(-7, 0), \ A_3 \sim U(20, 40), \ q \sim U(0.9, 1), \ \tau \sim U(0.01, 1.5), \ \beta \sim U(0.01, 5)
\]

We run Markov chain Monte Carlo (MCMC) algorithm to generate samples from the joint posterior distribution using the combined data sets. We plot the marginal posterior distributions and compare the results of the two scenarios using the Bayes factor (log marginal likelihood) and the deviance information criterion (DIC). We refer the reader to [1] for the details of the MCMC algorithm and the Bayesian comparison tools.

Figure 4.19: The estimated marginal posteriors for the parameters $A_1, A_2, A_3, q, \tau, \beta$, where $\Delta = 0$.
Table 4.11: The estimated correlation coefficients of each pair of the parameters $A_1, A_2, A_3, q, \tau, \beta$, where $\Delta = 0$.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td></td>
<td>-0.98</td>
<td></td>
<td>-0.43</td>
<td>0.27</td>
</tr>
<tr>
<td>$A_2$</td>
<td>-0.85</td>
<td></td>
<td>0.82</td>
<td>0.42</td>
<td>-0.23</td>
</tr>
<tr>
<td>$q$</td>
<td></td>
<td></td>
<td></td>
<td>0.41</td>
<td>-0.25</td>
</tr>
<tr>
<td>$\tau$</td>
<td></td>
<td></td>
<td></td>
<td>-0.17</td>
<td>-0.19</td>
</tr>
<tr>
<td>$\beta$</td>
<td></td>
<td>-0.30</td>
<td></td>
<td>-0.20</td>
<td>0.51</td>
</tr>
</tbody>
</table>

Ia parameters using the combined data sets and assuming $\Delta = 0$. We see that the data sets used are informative for all the parameters. The correlation coefficients are presented in Table 4.11. The parameters $A_1$ and $A_2$ are highly correlated, and both are also correlated with the fatigue-limit parameter $A_3$. In general, the results obtained here are similar to the results obtained in [1] using only the simple uniaxial Model Ia and data set 1.

Figure 4.20: The estimated marginal posteriors for the parameters $A_1, A_2, A_3, q, \tau, \beta$ where $\Delta = 0$.

Figure 4.20 and Table 4.12 show the estimated marginal posterior distributions and the correlation coefficients, respectively, when $\Delta = 0.0125$. The results are almost identical to the previous case, except for the parameter $\tau$, which now has a
Table 4.12: The estimated correlation coefficients of each pair of the parameters $A_1, A_2, A_3, q, \tau, \beta$, where $\Delta = 0.0125$.

<table>
<thead>
<tr>
<th></th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$q$</th>
<th>$\tau$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_2$</td>
<td>-0.97</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$A_3$</td>
<td>-0.86</td>
<td>0.84</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$q$</td>
<td>-0.44</td>
<td>0.44</td>
<td>0.41</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$\tau$</td>
<td>0.16</td>
<td>-0.08</td>
<td>-0.16</td>
<td>-0.06</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$\beta$</td>
<td>0.37</td>
<td>-0.22</td>
<td>-0.14</td>
<td>-0.10</td>
<td>0.57</td>
<td>—</td>
</tr>
</tbody>
</table>

Table 4.13: Bayesian comparison between two different specifications of Model Ia using (4.10).

<table>
<thead>
<tr>
<th>Model Ia given data sets 1, 2 &amp; 3 (2D)</th>
<th>$\Delta = 0$</th>
<th>$\Delta = 0.0125$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Log marginal likelihood</td>
<td>-1660.24</td>
<td>-1658.48</td>
</tr>
<tr>
<td>Deviance information criterion (DIC)</td>
<td>3311.33</td>
<td>3308.27</td>
</tr>
</tbody>
</table>

slightly smaller mode. We approximate the log marginal likelihood by the Laplace-Metropolis estimator [23] and compute DIC using the MCMC posterior samples. Table 4.13 shows that Model Ia performs better with $\Delta = 0.0125$ than with $\Delta = 0$. However, the small difference between the two cases suggests that conclusions cannot be generalized to other S-N models.

### 4.6.1 Survival functions

In this subsection, we compute some of the survival functions presented in [4.5.2] this time using the MCMC posterior samples of the model parameters obtained in the previous section with $\Delta = 0$, instead of the pooled ML estimates. Also, we consider a “reference” survival function that is obtained from the ML estimate of each data set.

Figures 4.21 and 4.22 show the survival functions for specimen 1 when $R = 0.1$ and $R = -0.1$, respectively, and $S_{max} = 45$. The reference survival function falls within the cloud of survival functions obtained from the pooled posterior samples. Figures 4.23 and 4.24 show the survival functions for specimen 2 when $S_{max} = 30$. 
Figure 4.21: Survival-probability functions for specimen 1 when \( S_{\text{max}} = 45 \text{ ksi} \) and \( R = 0.1 \), given different posterior samples of the parameters \( A_1, A_2, A_3, q, \tau, \beta \).

Figure 4.22: Survival-probability functions for specimen 1 when \( S_{\text{max}} = 45 \text{ ksi} \) and \( R = -0.1 \), given different posterior samples of the parameters \( A_1, A_2, A_3, q, \tau, \beta \).

The pooled posterior samples produce more conservative survival functions than the reference function. However, the difference between the survival functions cloud and the reference function is not significant.

For specimen 3, we show the survival functions when \( S_{\text{max}} = 12 \) in Figures 4.25 and 4.26. For \( R = 0.1 \), the pooled posterior samples provide more conservative survival probability than the reference function, especially when \( n < 2.5 \times 10^5 \). For \( R = -0.1 \), the survival functions from the pooled sample are more optimistic than the reference function when \( n > 10^5 \). In general, we notice that the survival functions are concentrated at high probability levels and that the dispersion increases at low probability levels.
Figure 4.23: Survival-probability functions for specimen 2 when $S_{\text{max}} = 30$ ksi and $R = 0.1$, given different posterior samples of the parameters $A_1, A_2, A_3, q, \tau, \beta$.

Figure 4.24: Survival-probability functions for specimen 2 when $S_{\text{max}} = 30$ ksi and $R = -0.1$, given different posterior samples of the parameters $A_1, A_2, A_3, q, \tau, \beta$.

Figure 4.25: Survival-probability functions for specimen 3 when $S_{\text{max}} = 12$ ksi and $R = 0.1$, given different posterior samples of the parameters $A_1, A_2, A_3, q, \tau, \beta$. 
Figure 4.26: Survival-probability functions for specimen 3 when $S_{max} = 12$ ksi and $R = -0.1$, given different posterior samples of the parameters $A_1, A_2, A_3, q, \tau, \beta$.

4.7 Summary and conclusions

The stress tensor is computed from the solution of the linear elasticity equations. A spatial stress function, $\sigma_{\text{eff}}^\Delta(x)$, is defined by the maximum principal stress (where $\Delta = 0$) or by the local average of the maximum principal stress. The stress function can be combined with any statistical S-N curve without prior knowledge of the spatial correlation, under two “extreme” assumptions. The first assumption is the full spatial dependence on the global maximum value of the effective stress. Implicitly, this assumption means that the first crack will initiate at the position with the highest stress. The second assumption is complete spatial independence, which is modeled by the spatial Poisson process. For both assumptions, we calibrate the model parameters using the ML approach, given the data from the fatigue experiments. The simplifying assumptions are needed because we lack information about the spatial correlation. It is expected then to increase the variance when calibrating different data sets.

For simplicity, we first fit the models to the fatigue experiments on each specimen separately, assuming $\Delta = 0$. Then, we fit the models to the combined data set when $\Delta = 0$ and $\Delta > 0$. When calibrating $\Delta$, specimens with different geometries must be used for the parameter $\Delta$ to be identifiable. With the available data, the effect of $\Delta$ was limited. However, $\Delta$ is a fundamental parameter that must be calibrated. For
specimen 3, we compare the effects of using biaxial stress (2D) and triaxial stress (3D) on fitting data set 3. When the likelihood function is given by (4.10) and the highly stressed volume is given by (4.9), the difference is negligible. For more complicated geometries such as v-notched specimens, the 3D effect might be more prominent.

By classical model comparison tools, the spatial Poisson model is superior to the full spatial dependence assumption. Also, we find that the spatial Poisson model with $\Delta > 0$ provides the best fit for the combined data sets. In the Bayesian framework, the estimated posteriors of the parameters are similar to the results obtained in [1] with data set 1 except for the variance parameter $\tau$ that is reduced because we improved the model and added the new threshold parameter $\beta$ in the highly stressed volume. The deviance information criterion suggests that non-zero $\Delta$ improves slightly the fit of the combined data sets for Model Ia. To draw general conclusions, several S-N models must be studied and compared.

The spatial Poisson process provides a systematic approach to generalize uniaxial S-N models and calibrate fatigue experiments on different specimens without special treatments for notches. Given a sufficient number of fatigue experiments for specimens with diverse geometries, our proposed approach could be used to predict the life of any mechanical component made from the same material and having the same surface finish.

Acknowledgements

Z. Sawlan, M. Scavino and R. Tempone are members of the KAUST SRI Center for Uncertainty Quantification in Computational Science and Engineering. R. Tempone received support from the KAUST CRG3 Award Ref: 2281 and the KAUST CRG4 Award Ref: 2584.
4.8 Appendix

4.8.1 Matlab PDE solver

The MATLAB function ADAPTMESH is used to solve the elliptic system PDE problem in 2D:

\[-\nabla \cdot (c \otimes \nabla u) + au = f,\]

with user-supplied boundary conditions.

In our case, \(a = f = 0\), and the coefficient tensor \(c = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}\) where

\[
c_{11} = \begin{bmatrix} \frac{E}{1-\nu^2} & 0 \\ 0 & \frac{E}{2(1+\nu)} \end{bmatrix}, \quad c_{12} = \begin{bmatrix} 0 & \frac{\nu E}{1-\nu^2} \\ \frac{\nu E}{2(1+\nu)} & 0 \end{bmatrix}, \quad c_{21} = \begin{bmatrix} 0 & \frac{E}{2(1+\nu)} \\ \nu E & 0 \end{bmatrix}, \quad c_{22} = \begin{bmatrix} \frac{E}{2(1+\nu)} & 0 \\ 0 & \frac{E}{1-\nu^2} \end{bmatrix}.
\]

4.8.2 Numerical computations

In this appendix, we show how to approximate the integrals that appear in (4.10). The averaged effective stress is computed in two-dimensional domain and assumed constant along the thickness dimension. Let \(C \subset \mathbb{R}^2\) be the curve boundary of the specimen and \(D_1 \subset \mathbb{R}^2\) be the projection of the specimen domain \(D\) into \(\mathbb{R}^2\). Then, the integral \(\int_{\partial D} F(n, \sigma_{\text{eff}}^\Delta(x))dS(x)\) is given by

\[
\int_{\partial D} F(n, \sigma_{\text{eff}}^\Delta(x))dS(x) = \ell_0 \int_C F(n, \sigma_{\text{eff}}^\Delta(s))ds + 2 \int_{D_1} F(n, \sigma_{\text{eff}}^\Delta(z))dz,
\]

where \(\ell_0\) is the specimen thickness. We use the trapezoidal rule to approximate the line integral \(\int_C F(n, \sigma(s))ds\) where the discretization of \(C\) is induced from the adaptive PDE solver. The second integral, \(\int_{D_1} F(n, \sigma(z))dz\) is also approximated.
by trapezoidal rule using the FEM triangulation. In this case, the integral over the triangle $t$ with nodes $p_1, p_2$ and $p_3$ is simply

$$\frac{1}{3} \times \text{Area}(t) \times \left[ F(n, \sigma_{\text{eff}}^\Delta(p_1)) + F(n, \sigma_{\text{eff}}^\Delta(p_2)) + F(n, \sigma_{\text{eff}}^\Delta(p_3)) \right].$$
4.9 REFERENCES


Chapter 5

A hierarchical Bayesian setting for an inverse problem in linear parabolic PDEs with noisy boundary conditions

Fabrizio Ruggeri, Zaid Sawlan, Marco Scavino and Raúl Tempone

Abstract

In this work we develop a Bayesian setting to infer unknown parameters in initial-boundary value problems related to linear parabolic partial differential equations. We realistically assume that the boundary data are noisy, for a given prescribed initial condition. We show how to derive the joint likelihood function for the forward problem, given some measurements of the solution field subject to Gaussian noise. Given Gaussian priors for the time-dependent Dirichlet boundary values, we analytically marginalize the joint likelihood using the linearity of the equation. Our hierarchical Bayesian approach is fully implemented in an example that involves the heat equation. In this example, the thermal diffusivity is the unknown parameter. We assume that the thermal diffusivity parameter can be modeled a priori through a lognormal random variable or by means of a space-dependent stationary lognormal random field. Synthetic data are used to test the inference. We exploit the behavior of the non-normalized log posterior distribution of the thermal diffusivity. Then, we use the Laplace method to obtain an approximated Gaussian posterior and therefore avoid costly Markov Chain Monte Carlo computations. Expected information gains

and predictive posterior densities for observable quantities are numerically estimated using Laplace approximation for different experimental setups.

5.1 Introduction

Parabolic partial differential equations model various important physical phenomena such as diffusion and heat transport. The solution of such equations propagates forward in time from an initial condition given boundary conditions and equation coefficients. In applications, some equation coefficients can be unknown quantities that need to be estimated. In addition, exact initial and boundary conditions might not be known. One possible approach to estimate these unknowns is to solve the inverse problem given some information about the solution. Classical inversion methods for parabolic partial differential equations are introduced by [1] in Chapter 8 of their book.

Several approaches on parameter estimation for PDE models are available in the literature. For example, [2] have modeled the unknown PDEs as multivariate polynomials of the independent variables, then choose the best fit by computation of the nullclines of the fitted PDEs. [3] have applied a two-stage generalization of the multiple shooting method to deal with the parameter estimation for nonlinear PDEs with noisy and partially observed data. A generalized smoothing approach for a system of nonlinear ordinary differential equations has been provided by [4]. Recently, [5] have developed two methods to estimate parameters in PDE models: a parameter cascading method and a Bayesian method. In both approaches, the unknown dynamic process is represented by a linear combination of B-spline basis functions that, in the Bayesian approach, is estimated by the Bayesian P-spline method. Markov Chain Monte Carlo procedures have been used to sample from the posterior distributions of the PDE parameters and the B-spline coefficients. It is worth mentioning that most of such works address problems with nonlinear PDEs. These works do not exploit the
linear structure for the efficient treatment of noisy initial and boundary conditions. Motivated by this fact, our goal in this work is to develop an efficient parameter estimation method that exploits the particular structure of linear time dependent PDEs. This extremely important class of PDEs includes, among others, the heat equation, the wave equation and the transport equation. Moreover, this class is broad enough to cover many crucial engineering applications and therefore deserves its own very efficient computational approach.

In this work, we consider a Bayesian inversion problem to determine the coefficients of linear parabolic partial differential equations, as an example of linear time dependent PDEs, under the assumption that noisy measurements are available in the interior of a domain of interest and for the unknown boundary conditions. A main novelty of our approach to solve the inverse problem relies on the assumption that the boundary parameters are unknown and modeled by means of adequate probability distributions. Subsequently, the contribution of the boundary parameters is marginalized out from the joint law with the unknown equation coefficients we want to infer, allowing the characterization of their posterior distribution. There are many advantages to a Bayesian approach. For example, it provides a solution along with a comprehensive measure of uncertainty given by the posterior distribution. Moreover, the prior available information can be easily incorporated in terms of elicited prior distributions [6]. An important issue in this work is that Bayesian inversion is posed as a hierarchical process. Boundary conditions can therefore be treated as unknown parameters [7]. Since we are only interested in estimating the equation coefficients, we eliminate those extra parameters by analytic marginalization. We show how to perform such analytical marginalization for a linear parabolic PDE in Section 5.4. This marginalization step allows us to compute the marginal likelihood very efficiently, yielding thus via numerical optimization posterior estimates of our unknown parameters, such as the maximum a posteriori estimate. We note in passing that for
the case of nonlinear PDEs, our analytic marginalization does not apply and more costly simulation-based schemes such as MCMC will be needed, as described in [5].

Bayesian inversion techniques for the heat equation have been discussed and implemented in some previous works. [7] provided a general Bayesian framework for inverse problems in heat transfer, classified according to the dominant mode in heat transfer. The authors address many issues regarding forward problems and their statistical analysis. The prior modeling is extensively discussed, as well as how to deal, in particular, with different sources of uncertainties. Heat flux reconstruction problems have been studied by [8, 9]. When referring to the problem of parameter estimation in inverse heat conduction problems, Wang and Zabaras showed how to infer the thermal conductivity using a hierarchical Bayesian framework, on the basis of temperature readings within a conducting solid, assuming that the heat flux on the boundary and the heat source are known. They also explored the high dimensional posterior state space by means of Markov Chain Monte Carlo simulation. [10] estimated the thermal conductivity of a polymer, transforming the heat equation into a stochastic differential equation and considering the Euler-Maruyama approximation to get the likelihood, introducing latent observations in space and then using a relatively cumbersome Markov Chain Monte Carlo method. [11] and [12] addressed the estimation problem of the thermal diffusivity, as in the present work, which is a parameter that describes thermophysical property of materials. In their works a large number of temperature measurements is made by an infrared camera, with fine spatial resolution and high frequency. They solved one and two-dimensional forward problems for transient heat conduction, with spatially varying thermal conductivity and volumetric heat capacity, by finite differences, according to a nodal strategy. The parameter vector at each node is then estimated either by minimizing an a posteriori objective function when prior Gaussian distributions are assumed for the parameters, or by means of Markov Chain Monte Carlo methods for different prior distributions.
This work is organized as follows. In Section 5.2, we introduce the statistical setting and we derive the explicit form of the joint law of the unknown equation coefficients and the boundary parameters. In Section 5.3, we use a finite element scheme in order to write the solution of the forward problem as a linear function of the boundary conditions. We demonstrate in Section 5.4 that, under certain conditions, an exact marginalization can be carried out, yielding a closed formula for the marginal likelihood of the equation coefficients. In Section 5.5, we apply our marginalization technique to estimating thermal diffusivity in the one-dimensional heat equation in two cases given temperature simulated data. Numerical results are obtained for the non-normalized log posterior distribution of the thermal diffusivity. We model prior knowledge about the thermal diffusivity first as a lognormal random variable and then using a lognormal random field with a squared exponential (SE) covariance function. In the first case, we use the Laplace method to provide an approximated Gaussian posterior distribution for the thermal diffusivity. Such method is then applied to obtain fast estimations of the information gain and the expected information gain under three experimental setups, and the predictive posterior mean of the temperature is also derived using the inferred thermal diffusivity. In the second case, where the thermal diffusivity is allowed to depend on the spatial variable, the Laplace approximation is used to obtain the posterior distribution of the hyperparameters that characterize the prior distribution for the thermal diffusivity.

5.2 Statistical setting and preliminary results

In this section we introduce the statistical model associated to the forward initial-boundary value problems for linear parabolic partial differential equations. We then derive, under mild assumptions, the exact expression for the joint likelihood function of the unknown parameters in the parabolic equation and the unknown boundary parameters.
Consider the deterministic one-dimensional parabolic initial-boundary value problem:

\[
\begin{aligned}
\partial_t T + \mathcal{L}_\mathbf{\theta} T &= 0, \quad x \in (x_L, x_R), \ 0 < t \leq t_N < \infty \\
T(x_L, t) &= T_L(t), \quad t \in [0, t_N] \\
T(x_R, t) &= T_R(t), \quad t \in [0, t_N] \\
T(x, 0) &= g(x), \quad x \in (x_L, x_R),
\end{aligned}
\]  

(5.1)

where \( \mathcal{L}_\mathbf{\theta} \) is a linear second-order partial differential operator that takes the form

\[
\mathcal{L}_\mathbf{\theta} T = -\partial_x(a(x)\partial_x T) + b(x)\partial_x T + c(x)T,
\]

\( \mathbf{\theta}(x) = (a(x), b(x), c(x))^{tr} \), and the partial differential operator \( \partial_t + \mathcal{L}_\mathbf{\theta} \) is parabolic, because ((14), [p.372]) there exists \( \epsilon \) such that \( a(x) \geq \epsilon > 0 \) for all \( x \in (x_L, x_R) \). We also assume that

P1 \( a, b \) and \( c \) are bounded functions.

P2 \( T_L, T_R \) and \( g \) are square integrable functions.

P3 The initial condition, \( g \), is consistent with the boundary functions, namely \( g(x_L) = T_L(0) \) and \( g(x_R) = T_R(0) \).

Then, under the assumptions P1-P3, there exists a unique weak solution of \( (5.1) \) ((14), [pp.375-377]).

Our main objective is to provide a Bayesian solution to an inverse problem for \( \mathbf{\theta} \), where we assume that

i. \( \mathbf{\theta} \) is unknown, while the initial condition \( g \) in the initial-boundary value problem is known;

ii. \( \mathbf{\theta} \) is allowed to vary with the spatial variable \( x \).
Remark. In our Bayesian approach, we will assume later that the coefficient \(a(x)\) is a lognormal random variable or lognormal random field. Therefore, \(a(x)\) will not be bounded as assumed in P1. However, it can be proved that there exists a unique solution of the stochastic parabolic initial-boundary value problem in the space \(L^2(\Omega, H^1)\). Such proof can be found in [12] for elliptic boundary value problems but it can be also extended to parabolic initial-boundary value problems.

Given noisy readings of the function \(T(x, t)\) at the \(I+1\) spatial locations, including the boundaries, \(x_L = x_0, x_1, x_2, \ldots, x_{I-1}, x_I = x_R\), at each of the \(N\) times \(t_1, t_2, \ldots, t_N\), we want to infer \(\theta\) using a Bayesian approach. To determine the posterior distribution for \(\theta\), we need first to obtain the likelihood function of \(\theta\). The remainder of this section derives the joint likelihood function of \(\theta\) and the boundary parameters. Let us introduce some convenient notation and assumptions: let \(Y_n := (Y_{0,n}, \ldots, Y_{I,n})^{tr}\) denote the vector of observed readings at time \(t_n\), and assume a statistical model with an additive Gaussian experimental noise \(\epsilon_n\); that is:

\[
Y_n \sim N(0_{I+1}, \sigma^2 I_{I+1}),
\]

where \(\epsilon_n \sim i.i.d. N(0, \sigma^2 I)\) for some measurement error variance \(\sigma^2 > 0\). The covariance matrix of \(\epsilon_n\) is assumed equal to \(\sigma^2 I\) for simplicity, a general covariance matrix \(\Sigma_{\epsilon_n}\) could be used as well provided that the boundary measurement errors are independent from the interior measurement errors. Also denote by \(Y_n^I := (Y_{1,n}, \ldots, Y_{I-1,n})^{tr}\) the vector of observed data at the interior locations \(x_1, x_2, \ldots, x_{I-1}\) and let \(Y_n^B := (Y_{L,n}, Y_{R,n})^{tr}\) be the vector of observed data at the boundary locations \(x_0, x_I\) at time \(t_n\). The density of \(Y_n^I\) is derived as it follows. First
consider the time local problem, defined between consecutive measurement times, i.e.

\[
\begin{align*}
\partial_t T + L_\theta T &= 0, & x \in (x_L, x_R), \ t_{n-1} < t < t_n, \\
T(x_L, t) &= T_L(t), & t \in [t_{n-1}, t_n], \\
T(x_R, t) &= T_R(t), & t \in [t_{n-1}, t_n], \\
T(x, t_{n-1}) &= \hat{T}(x, t_{n-1}), & x \in (x_L, x_R),
\end{align*}
\]

(5.3)

whose exact solution, denoted by \(\hat{T}(\cdot, t_n)\), depends only on \(\theta, \hat{T}(\cdot, t_{n-1})\) and the boundary values \(\{T_L(t), T_R(t)\}_{t \in (t_{n-1}, t_n)}\). Finally, use the form of the statistical model (5.2) to obtain the form of the density of \(Y^I_n\).

**Lemma 5.2.1.** Given the model (5.2), the probability density function of \(Y^I_n\) is expressed as

\[
\rho(Y^I_n|\theta, \hat{T}(\cdot, t_{n-1}), \{T_L(t), T_R(t)\}_{t \in (t_{n-1}, t_n)}) = \frac{1}{(\sqrt{2\pi\sigma})^{I-1}} \exp \left(-\frac{1}{2\sigma^2} \|R_{t_n}\|^2 \right),
\]

(5.4)

where \(R_{t_n} \triangleq (\hat{T}(x_1, t_n) - Y_{1,n}, \ldots, \hat{T}(x_{I-1}, t_n) - Y_{I-1,n})^\text{tr} \) denotes the data residual vector at time \(t = t_n\).

For illustration purposes and without loss of generality, assume now that the Dirichlet boundary condition functions, \(T_L(\cdot)\) and \(T_R(\cdot)\), are well approximated by piecewise linear continuous functions in the time partition \(\{t_n\}_{n=1,\ldots,N}\).

In this way, only \(2N\) parameters, say \(T_L(t_n) = T_{L,n}, T_R(t_n) = T_{R,n}, n = 1, 2, \ldots, N\), suffice to determine the boundary conditions that are, in principle, infinite dimensional parameters. Let \(LBC_n\) denote the time nodes that determine the local boundary conditions \(\{T_{L,n}, T_{L,n-1}, T_{R,n-1}, T_{R,n}\}\). Other interpolation schemes may be used as well.

**Remark.** Given the discretized Dirichlet boundary conditions introduced above, we can say that \(\hat{T}(\cdot, t_n)\) depends only on \(\theta, T(\cdot, t_{n-1})\) and the boundary parameters \(LBC_n\).
Similarly, $\hat{T}(\cdot, t_{n-1})$ depends on $\theta, T(\cdot, t_{n-2})$ and the boundary parameters $LBC_{n-1}$.

From this recursion, we can obtain

$$
\rho(Y_n^I|\theta, g, \{LBC_j\}_{j=1,\ldots,n}) = \rho(Y_n^I|\theta, \hat{T}(\cdot, t_{n-1}), LBC_n).
$$

(5.5)

Since the initial condition, $g$, is assumed to be known, it will be omitted in the rest of the paper.

**Lemma 5.2.2.** Given the model (5.2) and Lemma 5.2.1, the joint likelihood function of $\theta$ and the boundary parameters $\{LBC_n\}_{n=1,\ldots,N}$ is given by

$$
\rho(Y_1, \ldots, Y_N|\theta, \{LBC_n\}_{n=1,\ldots,N}) = \prod_{n=1}^{N} \frac{1}{(\sqrt{2\pi\sigma})^{T-1}} \exp\left(-\frac{1}{2\sigma^2}\|R_n\|^2\right) \times \frac{1}{2\pi\sigma^2} \exp\left(-\frac{1}{2\sigma^2}(T_{L,n} - Y_{L,n})^2 - \frac{1}{2\sigma^2}(T_{R,n} - Y_{R,n})^2\right).
$$

(5.6)

**Proof.** Observe that $Y_n^I, Y_n^B$ are conditionally independent given $\theta, \hat{T}(\cdot, t_{n-1}), LBC_n$.

Thus, we have

\[
\rho(Y_n|\theta, \hat{T}(\cdot, t_{n-1}), LBC_n) = \rho(Y_n^I|\theta, \hat{T}(\cdot, t_{n-1}), LBC_n) \times \rho(Y_n^B|\theta, \hat{T}(\cdot, t_{n-1}), LBC_n),
\]

since $Y_n^B|LBC_n$ does not depend on either $\theta$ nor $\hat{T}(\cdot, t_{n-1})$.

The joint likelihood function can then be written as

\[
\rho(Y_1, \ldots, Y_N|\theta, \{LBC_n\}_{n=1,\ldots,N}) = \rho(Y_N|\theta, \{LBC_n\}_{n=1,\ldots,N}, Y_{N-1}, \ldots, Y_1) \times \rho(Y_1, \ldots, Y_{N-1}|\theta, \{LBC_n\}_{n=1,\ldots,N-1})
\]
(since \( Y_N | \theta, \{ LBC_n \}_{n=1}^{N} \) is independent from \( Y_1, \ldots, Y_{N-1} \))

\[
= \rho(Y_N | \theta, \{ LBC_n \}_{n=1}^{N}) \times \rho(Y_1, \ldots, Y_{N-1} | \theta, \{ LBC_n \}_{n=1}^{N-1})
\]

(using equation (5.5))

\[
= \rho(Y_N | \theta, \hat{T}(\cdot, t_{N-1}), LBC_N) \times \rho(Y_1, \ldots, Y_{N-1} | \theta, \{ LBC_n \}_{n=1}^{N-1})
\]

(iterating the previous arguments)

\[
= \prod_{n=1}^{N} \rho(Y_n | \theta, \hat{T}(\cdot, t_{n-1}), LBC_n) = \prod_{n=1}^{N} \rho(Y_n^I | \theta, \hat{T}(\cdot, t_{n-1}), LBC_n) \times \rho(Y_n^B | LBC_n)
\]

and finally, using (5.4), the expression (5.6) is obtained.

Remark. A generalization of the joint likelihood can be obtained given serial correlations, that is, \( \{ \epsilon_n \}_{n=1}^{N} \) are time correlated.

Using the notation \( T_L = (T_{L,1}, \ldots, T_{L,N})^{tr} \), \( T_R = (T_{R,1}, \ldots, T_{R,N})^{tr} \), \( Y_L = (Y_{L,1}, \ldots, Y_{L,N})^{tr} \) and \( Y_R = (Y_{R,1}, \ldots, Y_{R,N})^{tr} \), the joint likelihood function (5.6) can be written as

\[
\rho(Y_1, \ldots, Y_N | \theta, T_L, T_R) = (\sqrt{2\pi\sigma})^{-N(I+1)} \exp \left( -\frac{1}{2\sigma^2} \sum_{n=1}^{N} \| R_{tn} \|_{\ell^2}^2 \right) \\
\times \exp \left( -\frac{1}{2\sigma^2} \left[ \| T_L - Y_L \|_{\ell^2}^2 + \| T_R - Y_R \|_{\ell^2}^2 \right] \right),
\]

which is a suitable expression to derive later the marginal likelihood of \( \theta \). The prior distributions for \( \theta \) and the boundary parameters \( T_L, T_R \) can be specified in different ways. Generally speaking, the prior distribution for \( \theta \) should be proposed according to the physical properties described by the unknown parameters and taking into account available prior knowledge about the observed phenomena. As an example, it is known that the thermal conductivity of polymethyl methacrylate (plexiglas) is in the
range 0.167-0.25 W/(mK). A uniform prior distribution for the thermal conductivity could be chosen if there is no preference among the values of the interval.

As per the boundary parameters, we assume independent Gaussian models \( T_{L,n} \sim \mathcal{N}(\mu_{L,n}, \sigma^2_{\mu}) \), \( T_{R,n} \sim \mathcal{N}(\mu_{R,n}, \sigma^2_{\mu}) \), \( n = 1, \ldots, N \), with means \( \mu_L = (\mu_{L,1}, \ldots, \mu_{L,N})^{tr} \), \( \mu_R = (\mu_{R,1}, \ldots, \mu_{R,N})^{tr} \), and variance \( \sigma^2 \) > 0. The mean vectors \( \mu_L \) and \( \mu_R \) can be either known beforehand or constructed from a subsample of the boundary data \( Y_L \) and \( Y_R \). In the latter case, the likelihood function \( (5.7) \) should be modified accordingly. For simplicity, hereafter we assume that \( \mu_L \) and \( \mu_L \) are known beforehand.

We claim that the data residual vector \( R_t \) can be written as a linear function of \( T_L \) and \( T_R \). The next section is devoted to the proof of this basic result. This proof allows for the exact marginalization of the contribution of the nuisance boundary parameters from the joint likelihood function \( (5.7) \).

### 5.3 Numerical approximation

In this section, our goal is to approximate the residual vector \( R_t \) as a linear function of the boundary conditions. After reformulating the main problem \( (5.1) \), as described in the next lemma, we will introduce its weak form and finite element method will be then applied to provide a numerical approximation of the solution of the weak problem.

**Lemma 5.3.1.** The solution of \( (5.1) \) can be written in the form

\[
T(x, t) = T_L(t) \frac{x_R - x}{x_R - x_L} + T_R(t) \frac{x - x_L}{x_R - x_L} + u(x, t),
\]

where \( u \) solves a new initial-boundary value problem with homogeneous Dirichlet
boundary conditions:

\[
\begin{aligned}
\partial_t u + L_\theta u &= f(x,t), \quad x \in (x_L, x_R), 0 < t \leq t_N < \infty \\
u(x_L, t) &= 0, \quad t \in [0, t_N] \\
u(x_R, t) &= 0, \quad t \in [0, t_N] \\
u(x, 0) &= g^0(x), \quad x \in (x_L, x_R)
\end{aligned}
\]

and

\[
f(x, t) = - (\partial_t + L_\theta) T_L(t) \frac{x_R - x}{x_R - x_L} - (\partial_t + L_\theta) T_R(t) \frac{x - x_L}{x_R - x_L}.
\]

\[
g^0(x) = g(x) - T_L(0) \frac{x_R - x}{x_R - x_L} - T_R(0) \frac{x - x_L}{x_R - x_L}.
\]

We now introduce the weak formulation of problem (5.9).

Find \( u(t) \in V = H_0^1(x_L, x_R), \ t \in (0, t_N) \) such that:

\[
\begin{aligned}
\int_{x_L}^{x_R} \partial_t u(t)vdx + B(u(t), v) &= \int_{x_L}^{x_R} f(t)vdx, \forall v \in V, \ t \in (0, t_N), \\
u(0) &= g^0, \ x \in (x_L, x_R),
\end{aligned}
\]

where \( B(u, v) = \int_{x_L}^{x_R} [a(x)\partial_x u\partial_x v + b(x)\partial_x uv + c(x)uv] \, dx \) and \( H_0^1(x_L, x_R) \) is the closure of the space \( C_c^1(x_L, x_R) \) of continuously differentiable functions with compact support on \( (x_L, x_R) \) with respect to the \( H^1 \)-norm ([16], [p.149]).

Given a mesh \( x_L = x_0 < \ldots < k\Delta x = x_k < \ldots < I\Delta x = x_I = x_R \) of the spatial domain \( (x_L, x_R) \), we apply the finite element method with piecewise linear functions (hat functions) \( \{\phi_k\}_{k=1}^{I-1} \) to approximate the weak solution \( u(x, t) \) of (5.9) as linear combinations of the basis functions:

\[
u(x, t) \approx u_{\Delta x}(x, t) = \sum_{k=1}^{I-1} u_k(t)\phi_k(x), \quad 0 < t \leq t_N.
\]
and we get
\[
\sum_{k=1}^{I-1} \partial_t u_k(t) \int_{x_L}^{x_R} \phi_k \phi_j \, dx + \sum_{k=1}^{I-1} u_k(t) B(\phi_k, \phi_j) = \int_{x_L}^{x_R} f(t) \phi_j \, dx, \quad j = 1, \ldots, I-1, \quad t \in (0, t_N).
\] (5.11)

Let \( \mathbf{u}(t) = (u_1(t), \ldots, u_{I-1}(t))^T \), then we can write the linear system of ODEs (5.11) in a matrix form as:
\[
M \partial_t \mathbf{u}(t) + S_\theta \mathbf{u}(t) = \mathbf{f}(t), \quad 0 < t \leq t_N,
\] (5.12)
where \( M \) is the mass matrix, \( S_\theta \) is the stiffness matrix and \( \mathbf{f}(t) \) is the load vector.

We consider now a uniform time discretization of \((0, t_N)\) such that \( t_0 = 0 < \ldots < n \Delta t = t_n < \ldots < N \Delta t = t_N \) and denote \( \mathbf{u}(t_n) = \mathbf{u}_n \) and \( \mathbf{f}(t_n) = \mathbf{f}_n \). We apply the backward Euler method on equation (5.12) to obtain the fully discrete analogue of (5.10) that takes the form
\[
\begin{cases}
(M + \Delta t S_\theta) \mathbf{u}_{n+1} = M \mathbf{u}_n + \Delta t \mathbf{f}_{n+1}, & n = 0, \ldots, N-1, \\
M \mathbf{u}_0 = g^0,
\end{cases}
\] (5.13)
where \( g^0 = (\int_{x_L}^{x_R} g^0 \phi_1 \, dx, \ldots, \int_{x_L}^{x_R} g^0 \phi_{I-1} \, dx)^T \).

**Theorem 5.3.2.** The approximation of the weak solution of (5.9) can be written as a linear function of the initial and boundary conditions:
\[
\mathbf{u}_n = A_n(\theta) \mathbf{u}_0 + \tilde{A}_{L,n}(\theta) \mathbf{T}_L + \tilde{A}_{R,n}(\theta) \mathbf{T}_R,
\] (5.14)
where \( \mathbf{u}_n = (u_{1,n}, \ldots, u_{I-1,n})^T \), \( \mathbf{T}_L = (T_{L,1}, \ldots, T_{L,N})^T \), \( \mathbf{T}_R = (T_{R,1}, \ldots, T_{R,N})^T \), and the matrices \( A_n(\theta), \tilde{A}_{L,n}(\theta) \) and \( \tilde{A}_{R,n}(\theta) \) are explicitly constructed in the proof.

**Proof.** See Appendix 5.7.1. \(\boxright\)
Theorem 5.3.3. The approximation of the weak solution of (5.1) can be written as a linear function of the initial and boundary conditions:

\[ T_n = B^nT_0 + A_{L,n}(\theta)T_L + A_{R,n}(\theta)T_R. \]  

(5.15)

where \( T_n \) is defined similarly to \( u_n \) and the matrices \( B, A_{L,n}(\theta) \) and \( A_{R,n}(\theta) \) are explicitly constructed in the proof.

Proof. See Appendix 5.7.2.

Remark. The weak solution of two-dimensional and higher dimensional linear parabolic PDEs can be written in a similar form of equation (5.15) (see [16], [pp.149–156]).

Corollary 5.3.4. The data residual vector \( R_{t_n} = (\hat{T}(x_1,t_n) - Y_{1,n}, \ldots, \hat{T}(x_{I-1},t_n) - Y_{I-1,n})^{tr} \) is approximated by

\[ \tilde{R}_{t_n} = (B^nT_0 - Y_n^I) + A_{L,n}(\theta)T_L + A_{R,n}(\theta)T_R. \]  

(5.16)

5.4 The marginal likelihood of \( \theta \)

Given the observations \( Y_1, \ldots, Y_N \), we showed, in the Section 5.2, how to obtain the joint likelihood function of \( \theta \) and the boundary parameters \( T_L, T_R \).

In the present section, we derive a convenient expression for the marginal likelihood of \( \theta \), under the assumption that the prior distributions for \( T_L \) and \( T_R \) are independent Gaussian:

\[ T_L \sim \mathcal{N}(\mu_L, \sigma_p^2I_N), \quad T_R \sim \mathcal{N}(\mu_R, \sigma_p^2I_N), \]  

(5.17)
Then, using (5.7), the marginal likelihood of $\theta$ is given by:

$$
\rho(Y_1, \ldots, Y_N|\theta) = (\sqrt{2\pi}\sigma)^{-N(I+1)} \times (\sqrt{2\pi}\sigma_p)^{-2N} \int_{T_L} \int_{T_R} \exp \left( -\frac{1}{2\sigma^2} \sum_{n=1}^N \| R_{t_n} \|^2 \right) \\
\times \exp \left( -\frac{1}{2\sigma^2} (T_L - Y_L)^T (T_L - Y_L) - \frac{1}{2\sigma^2} (T_R - Y_R)^T (T_R - Y_R) \right) \\
\times \exp \left( -\frac{1}{2\sigma_p^2} (T_L - \mu_L)^T (T_L - \mu_L) - \frac{1}{2\sigma_p^2} (T_R - \mu_R)^T (T_R - \mu_R) \right) dT_L dT_R.
$$

(5.18)

To provide the exact expression of the marginal likelihood of the linear parabolic equation coefficients $\theta$, which has been implemented in the computational examples presented in Section 5.5, it is convenient to introduce the following notation:

$$
\Delta_L = \sum_{n=1}^N A_{L,n}(\theta)^T A_{L,n}(\theta), \quad \Delta_R = \sum_{n=1}^N A_{R,n}(\theta)^T A_{R,n}(\theta),
$$

$$
\Delta_{2,L} = \sum_{n=1}^N A_{L,n}(\theta)^T (Y_n^T - B^\alpha T_0), \quad \Delta_{2,R} = \sum_{n=1}^N A_{R,n}(\theta)^T (Y_n^T - B^\alpha T_0),
$$

$$
A_{LR} = \sum_{n=1}^N A_{L,n}(\theta)^T A_{R,n}(\theta), \quad D_{\sigma^2} = \frac{1}{\sigma^2} I_N, \quad D_{\sigma_p^2} = \frac{1}{\sigma_p^2} I_N.
$$

Theorem 5.4.1. The marginal likelihood of $\theta$ is given by:

$$
\rho(Y_1, \ldots, Y_N|\theta) = (\sqrt{2\pi}\sigma)^{-N(I+1)} (\sqrt{2\pi}\sigma_p)^{-2N} (2\pi)^{N/2} |\Lambda_0|^{1/2} (2\pi)^{N/2} |\Lambda_1|^{1/2} \\
\times \exp \left\{ -\frac{1}{2\sigma^2} \left[ Y_L^T Y_L + Y_R^T Y_R + \sum_{i=1}^N (Y_n^I - B^\alpha T_0)^T (Y_n^I - B^\alpha T_0) \right] \\
- \frac{1}{2\sigma_p^2} \left[ \mu_L^T \mu_L + \mu_R^T \mu_R \right] + \frac{1}{2} \left( \mu_L^T D_{\sigma^2} + Y_L^T D_{\sigma^2} + \Delta_{2,L}^T D_{\sigma^2} \right) \Lambda_0 (D_{\sigma^2} \mu_L + D_{\sigma^2} Y_L + D_{\sigma^2} \Delta_{2,L}) \right\}.
$$

(5.19)

where $\Lambda_0, \Lambda_1, t_{R,2}$ and $t_{R,3}$ are independent of $T_L$ and $T_R$. 
Proof. First, we observe that (5.18) can be written as:

\[
(\sqrt{2\pi}\sigma)^{-N(I+1)} \times (\sqrt{2\pi}\sigma_p)^{-2N} \times \exp \left\{ -\frac{1}{2\sigma_p^2} \left[ \mu_L^t \mu_L + \mu_R^t \mu_R - \frac{1}{\sigma^2} \left[ Y_L^t Y_L + Y_R^t Y_R \right. \right. \right. \\
+ \sum_{n=1}^{N} (Y_n^I - B_n^T T_0)^t (Y_n^I - B_n^T T_0) \right] \times \int_{T_R} \int_{T_L} \exp \left\{ -\frac{1}{2} \left[ T_L^t (D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_L) T_L + 2 \sigma^2 T_R^t A_{LR}^t T_L + T_R^t (D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_R) T_R \right. \right. \right. \\
- 2(\mu_L^t D_{\sigma_p^2} + Y_L^t D_{\sigma^2} + \Delta_{2,L}^t D_{\sigma^2}) T_L + \int_{T_R} \int_{T_L} \exp \left\{ -\frac{1}{2} \left[ T_L^t (D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_L) T_L \right. \right. \right. \\
\left. \left. \left. - 2(\mu_R^t D_{\sigma_p^2} + Y_R^t D_{\sigma^2} + \Delta_{2,R}^t D_{\sigma^2}) T_R \right] dT_L dT_R \right. \left. \right. \left. \right. \right. \right. \right. \\
\left. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right.
\]

To marginalize \( T_L \) and \( T_R \), we assume that they are independent Gaussian random vectors. We can then use the following standard result: if \( X \sim N_p(\mu, \Sigma) \), then

\[
E(\exp(t^T X)) = \exp(t^T \mu + \frac{1}{2} t^T \Sigma t).
\]

Therefore, by integrating first with respect to \( T_L \), the marginal likelihood of \( \theta \) and \( T_R \) is proportional to the product of a factor that is independent of \( T_L \) and the following term

\[
\int_{T_L} \exp \left\{ -\frac{1}{2} T_L^t \left( D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_L \right) T_L \right\} \exp(t_{L,1}^T T_L) dT_L,
\]

where

\[
t_{L,1}^T = (\mu_L^t D_{\sigma_p^2} + Y_L^t D_{\sigma^2} + \Delta_{2,L}^t D_{\sigma^2}) - \frac{1}{\sigma^2} T_R^t A_{LR}^t.
\]

It is now convenient to define \( \Lambda_0^{-1} := (D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_L) \). The marginal likelihood of \( \theta \) and \( T_R \) is proportional to the product of a factor that is independent of \( T_L \) and the term \((2\pi)^{N/2}|\Lambda_0|^{1/2} \exp \left\{ \frac{1}{2} t_{L,1}^T \Lambda_0 t_{L,1} \right\} \).
Therefore, the marginal likelihood of $\theta$ can be explicitly written as

\[
(\sqrt{2\pi}\sigma)^{-N(I+1)} \times (\sqrt{2\pi}\sigma_p)^{-2N} \times (2\pi)^{N/2} |\Lambda_0|^{1/2} \times \exp \left\{ -\frac{1}{2\sigma_p^2} (\mu_L^{tr} \mu_L + \mu_R^{tr} \mu_R) \right\}
\]

\[
- \frac{1}{2\sigma^2} \left[ Y_L^{tr} Y_L + Y_R^{tr} Y_R + \sum_{i=1}^N (Y_I^{n} - B^u T_0)^{tr} (Y_I^{n} - B^u T_0) \right] \right\} \times \int_{T_R} \exp \left\{ \frac{1}{2} t_{R,1}^{tr} \Lambda_0 t_{R,1} \right\} \times \int_{T_R} \exp \left\{ \frac{1}{2} t_{R,1}^{tr} \Lambda_0 t_{R,1} \right\} dT_R.
\]

The entire last expression is equal to the product of a term that is independent of $T_R$ and the following term:

\[
\int_{T_R} \exp \left\{ -\frac{1}{2} t_{R}^{tr} \left[ (D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_R) T_R - 2(\mu_R^{tr} D_{\sigma_p^2} + Y_R^{tr} D_{\sigma^2} + \Delta_{2R}^{tr} D_{\sigma^2}) T_R \right] \right\} \exp \left\{ t_{R,1}^{tr} T_R \right\} dT_R,
\]

where

\[
t_{R,1}^{tr} = \left( \mu_R^{tr} D_{\sigma_p^2} + Y_R^{tr} D_{\sigma^2} + \Delta_{2R}^{tr} D_{\sigma^2} \right) \Lambda_0 A_{LR}.
\]

If we now define $\Lambda_1^{-1} := (D_{\sigma^2} + D_{\sigma_p^2} + \frac{1}{\sigma^2} \Delta_R) - (\frac{1}{\sigma^2})^2 A_{LR}^{tr} \Lambda_0 A_{LR}$ and integrate with respect to $T_R$, we have

\[
\int_{T_R} \exp \left\{ -\frac{1}{2} T_R^{tr} \Lambda_1^{-1} T_R \right\} \exp(t_{R,1}^{tr} T_R) dT_R = (2\pi)^{N/2} |\Lambda_1|^{1/2} \exp \left\{ \frac{1}{2} t_{R,1}^{tr} \Lambda_1 t_{R,1} \right\}
\]

\[
= (2\pi)^{N/2} |\Lambda_1|^{1/2} \exp \left\{ \frac{1}{2} (t_{R,2}^{tr} + t_{R,3}^{tr}) \Lambda_1 (t_{R,2} + t_{R,3}) \right\},
\]

after evaluating the integral. We finally obtain (5.19).

Remark. If the initial condition is unknown, our approach allows the incorporation of its random modeling and the corresponding marginalization step.

Remark. The marginal likelihood (5.19) is actually valid for any linear evolution.
model given by (5.15). In fact, this framework can be extended to time dependent linear PDEs and the marginalization procedure is independent from the dimension of the PDE.

5.5 A Bayesian inference for thermal diffusivity

In this section, we implement our Bayesian approach to infer the thermal diffusivity $\theta$, an unknown parameter that appears in the heat equation and measures the rapidity of the heat propagation through a material [17].

Synthetic data are used to simulate as close as possible the experimental measurements of heat conduction properties by [10] that, although unavailable for public use, have inspired the present work. Those authors considered the thermal properties of a polymethyl methacrylate specimen when submitted to heating and cooling cycles in a range of temperatures between 25 and 90 °C, measured by thermocouples in 5 inner, equispaced points and 2 outer ones. In particular, comparison of our Figure 5.1 with the cooling phase of Experiment B in Figure 4 of [10] presents a similar behavior.

Consider the heat equation (one-dimensional diffusion equation for $T(x,t)$):

\[
\begin{cases}
\partial_t T - \partial_x (\theta(x)\partial_x T) = 0, & x \in (x_L, x_R), \ 0 < t \leq t_N < \infty \\
T(0, t) = T_L(t), & t \in [0, t_N] \\
T(1, t) = T_R(t), & t \in [0, t_N] \\
T(x, 0) = g(x), & x \in (x_L, x_R).
\end{cases}
\] (5.20)

We want to infer the thermal diffusivity, $\theta(x)$, using a Bayesian approach when the temperature is measured at $I + 1$ locations, $x_0 = x_L, x_1, x_2, \ldots, x_{I-1}, x_I = x_R$, at each of the $N$ times, $t_1, t_2, \ldots, t_N$. Clearly, this problem is a special case of (5.1) where $L_\theta = -\partial_x (\theta(x)\partial_x T)$ and $\theta(x) > 0$. We can therefore immediately obtain the non-normalized posterior distribution of $\theta$ using the marginal likelihood (5.19).
The prior distributions for $\theta$ can be specified in different ways. In this section we will consider two cases, when $\theta$ is a lognormal random variable and when $\theta$ depends on the space variable $x$ and is modeled by means of a lognormal random field. We focus on the second case in Subsection 5.5.4. We start by discussing the case where the thermal diffusivity prior is independent of $x$.

If we consider a lognormal prior $\log \theta \sim \mathcal{N}(\nu, \tau)$, where $\nu \in \mathbb{R}$ and $\tau > 0$, then the non-normalized posterior distribution of $\theta$ is given by

$$
\rho_{\nu,\tau}(\theta|Y_1, \ldots, Y_N) \propto \frac{1}{\sqrt{2\pi\theta\tau}} \exp \left( -\frac{(\log \theta - \nu)^2}{2\tau^2} \right) \rho(Y_1, \ldots, Y_N|\theta). \quad (5.21)
$$

The posterior distribution of $\theta$ can be approximated by Laplace’s method ([6], [Chapter 4]) to obtain a Gaussian posterior

$$
\rho_{\nu,\tau}(\theta|Y_1, \ldots, Y_N) \approx \frac{1}{\sqrt{2\pi|H(\hat{\theta})|}} \exp \left\{ -\frac{1}{2}(\theta - \hat{\theta})^trH(\hat{\theta})^{-1}(\theta - \hat{\theta}) \right\}
$$

where $\hat{\theta}$ is the maximum a posteriori (MAP) probability estimate of $\theta$ and $H(\hat{\theta})$ is the inverse Hessian matrix of the negative log posterior evaluated at $\hat{\theta}$.

To assess the behavior of our method, we introduce a synthetic dataset generated with constant $\theta$. Let us assume, without loss of generality, that the interval time $[0, t_N]$ is equal to $[0, 1]$, $x_L = 0$ and $x_R = 1$.

### 5.5.1 Dataset A

In order to generate data, we solve the initial-boundary value problem for the heat equation with Robin boundary conditions:

$$
\begin{align*}
\partial_x T(x_L, t) &= \frac{h}{\kappa}(T(x_L, t) - T_{out}), \quad t \in [0, 1], \\
\partial_x T(x_R, t) &= \frac{h}{\kappa}(T_{out} - T(x_R, t)), \quad t \in [0, 1].
\end{align*}
$$
and the initial condition $T(x, 0) = T_0$, $x \in (0, 1)$, where $\theta(x) = 1 \times 10^{-7} \text{ m}^2/\text{s}$, $h$ is the convective heat transfer coefficient, $\kappa$ denotes the thermal conductivity, $\frac{h}{\kappa} = 1 \text{ (1/m)}$, $T_{out} = 20^\circ \text{C}$ and $T_0 = 100^\circ \text{C}$ (see Figure 5.1).

Figure 5.1: Exact solution of the initial-boundary value problem for the heat equation, $\theta = 1 \times 10^{-7} \text{ m}^2/\text{s}$.

A synthetic dataset (hereafter named dataset A) is generated, with a measurement standard error noise of $\sigma_d = 0.56$.

Before presenting the implementation of our novel technique, we will show how the Bayesian method works, using the joint likelihood (5.7), under the very restrictive assumption that the temperature values at the boundaries are exactly known.

### 5.5.2 Example 1

Suppose that the thermal diffusivity, $\theta$, is a random variable with a lognormal prior, $\log \theta \sim \mathcal{N}(\nu, \tau)$. In this case, the non-normalized posterior density for $\theta$ is given by

$$
\rho_{\nu, \tau}(\theta | Y_1, \ldots, Y_N) \propto \frac{1}{\sqrt{2\pi \theta \tau}} \exp \left( -\frac{(\log \theta - \nu)^2}{2\tau^2} \right) \exp \left( -\frac{1}{2\sigma^2} \sum_{n=1}^N \| R_{t_n} \|_2^2 \right),
$$

where $R_{t_n}$ is used here because the boundary data are known exactly.

Given that $\theta$ is a lognormal random variable with $\nu = \tau = 0.1$, the resulting
posterior will depend on $\sigma$ and the number of observations $N$ that are used to compute the log-likelihood. Figure 5.2 shows the behavior of the log-likelihood and the log-posterior for $\theta$ using different values for $\sigma$ and $N$.

We then use the Laplace approximation to derive the Gaussian posterior approximated density for $\theta$. The prior and posterior densities for $\theta$ are presented in Figure 5.3 where it can be appreciated that we obtained a Gaussian posterior, with mean 1.0025 and standard deviation 0.0044, which is concentrated around the true value of the parameter, $\theta$, despite having a very broad prior. We are now in the position to extend our implementation to embrace the case where the temperature values at the boundaries are unknown parameters as well.

![Figure 5.2: Example 1: Comparison between log-likelihoods (on the left) and log-posteriors (on the right) for $\theta$ using different numbers of observations, $N$, and different values of $\sigma$.](image)

5.5.3 Example 2

In this example, we consider again $\theta$ as a random variable with a lognormal prior, $\log \theta \sim \mathcal{N}(\nu, \tau)$. Unlike Example 1, we assume noisy boundary measurements and a Gaussian prior distribution for the boundary parameters as in (5.17). Therefore, the non-normalized posterior density for $\theta$ is given by

$$
\rho_{\nu, \tau}(\theta|Y_1, \ldots, Y_N) \propto \frac{1}{\sqrt{2\pi\theta\tau}} \exp \left( - \frac{(\log \theta - \nu)^2}{2\tau^2} \right) \rho(Y_1, \ldots, Y_N|\theta),
$$
Figure 5.3: Example 1: Lognormal prior and approximated Gaussian posterior densities for \( \theta \), where \( \sigma_p = \sigma = 0.5 \) and \( N = 60 \).

where \( \rho(Y_1, \ldots, Y_N|\theta) \) is the marginal likelihood of \( \theta \) defined in Theorem 5.4.1.

\textbf{Remark.} Since \( \theta(x) \) is supposed to be constant, we can obtain equation (5.15) alternatively by solving the heat equation using finite differences (see Appendix 5.7.3).

Figure 5.4: Example 2: Comparison between log-likelihoods (on the left) and log-posteriors (on the right) for \( \theta \) using different values of \( N \) and different values of \( \sigma \).

Numerical results are now presented using the synthetic dataset A and assuming that \( \theta \) is a lognormal random variable with \( \nu = \tau = 0.1 \). Figure 5.4 shows the behavior of the log-likelihood and the log-posterior for \( \theta \) using different values of \( N \) and \( \sigma \). Clearly, the accuracy of the estimated \( \theta \) depends on the size of the dataset, \( N \), and the reliability of measurement devices, \( \sigma \).
Figure 5.5: Example 2: Comparison between log-likelihoods (on the left) and log-posteriors (on the right) for $\theta$ using different values of $\sigma$ and $\sigma_p$, with $N = 60$.

Figure 5.5 shows the relationship between the prior distribution of the boundary conditions and their measurements. Although we notice different behaviors of the log-likelihood and the log-posterior, these functions exhibit the same argument of the maximum which is close to the true value of $\theta$.

Figure 5.6: Example 2: Lognormal prior and approximated Gaussian posterior densities for $\theta$ where $\sigma_p = \sigma = 0.5$ and $N = 60$.

Again, the Laplace approximation is used to derive the Gaussian posterior approximated density for $\theta$. The prior and posterior densities for $\theta$ are presented in Figure 5.6 in which the Gaussian posterior, with mean 0.9955 and standard deviation 0.0047, is concentrated around the true value of $\theta$ unlike the very broad prior.
5.5.3.1 Convergence of MAP estimates

When using numerical methods to approximate the dynamic process, it is important to control the discretization error because it produces a bias error in the statistical inference. Many methods are developed to assess the impact of the discretization error when PDEs are used in a statistical framework. In particular, very recently, [18] have introduced probability measures over the numerical solutions by randomizing the deterministic solvers.

Here, we show that MAP estimates have the same convergence rate as the numerical solver used to obtain the marginal likelihood (5.19). For this purpose, we present the results from basic convergence tests with respect to discretization space size, $\Delta x$, and discretization time step, $\Delta t$, to ensure that the discretization error is negligible in comparison with the statistical error.

The numerical solver is based on finite element method with piecewise linear functions to approximate the solution in space and backward Euler discretization in time (see Section 5.3). Equivalently, we can use centered difference in space and backward difference in time (see Appendix C of the Supplementary Material). Therefore, the convergence rate of our solver is quadratic in space and linear in time. MAP estimates are obtained by means of the MATLAB function fmincon, which is suitable to minimize the negative log-posterior with a prescribed tolerance equal to $1 \times 10^{-16}$.

Figures 5.7 and 5.8 show that the MAP estimates of $\theta$ converge quadratically with $\Delta x$ and linearly with $\Delta t$, which is consistent with the chosen solver. The above criteria aim to check that the discretization error is smaller than the statistical error, and they apply when the thermal diffusivity is modeled as a random field.
5.5.3.2 Information Divergence and Expected Information Gain

In the Bayesian setting that we adopted to infer the thermal diffusivity, $\theta$, the utility of the performed experiment, given an experimental setup $\xi$, can be conveniently measured by the so-called information divergence (or discrimination information as [19] called it), which is here defined as the Kullback-Leibler divergence [20] between the prior density function $p(\theta)$ and the posterior density function of $\theta$, $\rho(\theta|\mathbf{Y}_1, \ldots, \mathbf{Y}_N, \xi)$:

$$D_{KL}(\mathbf{Y}_1, \ldots, \mathbf{Y}_N, \xi) := \int_\Theta \log \left( \frac{\rho(\theta|\mathbf{Y}_1, \ldots, \mathbf{Y}_N, \xi)}{p(\theta)} \right) \rho(\theta|\mathbf{Y}_1, \ldots, \mathbf{Y}_N, \xi) d\theta. \quad (5.22)$$

The quantity in (5.22) is always non-negative; it is equal to zero when the prior and the posterior coincide; it provides a quantification of the relative discrimination between the prior and the posterior; and it depends on the observations $\mathbf{Y}_1, \ldots, \mathbf{Y}_N$. Therefore, given the synthetic dataset, $A$, we may introduce different experimental setups of interest by varying the interval time during which the temperature is measured. By choosing some specific thermocouples, we may evaluate the information divergence for any experimental setup. Moreover, under the same generating process used for the dataset $A$, we may obtain as many synthetic datasets as needed to explore the properties of the proposed simulated experiment. The utility of such
computer-based experiments can be adequately summarized by the so-called expected information gain [21], which is defined as the marginalization of $D_{KL}$ over all possible simulated data:

$$I(\xi) := \int_Y \int_{\Theta} \log \left( \frac{p(\theta|Y_1, \ldots, Y_N, \xi)}{p(\theta)} \right) \rho(\theta|Y_1, \ldots, Y_N, \xi)d\theta \rho(\{Y_i\}_{i=1}^N|\xi)d(\{Y_i\}_{i=1}^N).$$

(5.23)

This quantity (5.23) provides a criterion to determine which features of the setup, $\xi$, are, on average, most informative when inferring $\theta$. A larger value of $I(\xi)$ when, say, $\xi \in A$, suggests that, given the proposed statistical model, the inference on the unknown parameter will be more efficient, on average, when the features of the designed experiment take value in the set $A$.

Let us label as TC1, . . . , TC7 the thermocouples from the left boundary to the right boundary, respectively.

The numerical estimations of the information divergence for the synthetic dataset A and of the expected information gain, by using (5.21) to compute the approximated posterior in Example 1, are shown in Figures 5.9, 5.10 and 5.11, which refer to the following three experimental setups (es’s):

es1) $\xi$ consists of three non-overlapping time intervals, with the same length, which cover the entire observational period $[0, 1]$;

es2) $\xi$ consists of the five inner thermocouples;

es3) $\xi$ is the combination of the two previous experimental setups, es1 and es2.

From the values in Figure 5.9, which depicts the results from an experimental setup in which the temperature measurements are collected at different time intervals, we may conclude, by virtue of the interpretation of the expected information gain, that the second time interval is the most informative time interval from which to draw inferences on the thermal diffusivity, whereas the last time interval is the least
Figure 5.9: Example 2: The expected information gain compared with the information divergence for dataset A, for the three time intervals experimental setup (es1).

Figure 5.10: Example 2: The expected information gain compared with the information divergence for dataset A, for the five inner thermocouples experimental setup (es2).

informative one.

Figure 5.10 summarizes how the expected information gain behaves for the five inner thermocouples experimental setup (es2). Given the synthetic dataset A, the sixth thermocouple (TC6) is the one where the information divergence takes the smallest value. However, when we look at the expected information gain, we may appreciate the nearly symmetric informative content of the thermocouples with respect to the central thermocouple (TC4) and how the expected gain about the thermal diffusivity becomes larger near the central thermocouple.

Finally, we look for the best combination of the two previous experimental setups, and the corresponding results are displayed in Figure 5.11. We observe that the highest expected information gain is attained at the middle thermocouple (TC4) by using the information collected during the second time interval. Any indication provided by the numerical estimation of the expected information gain is very valuable to an experimentalist, since it suggests the most relevant features to be considered to build up an efficient experiment to infer the unknown parameters of the assumed statistical model.
Figure 5.11: Example 2: The expected information gain for the combination (es3) of the three time intervals and the five inner thermocouples experimental setups.

Figure 5.12: Example 2: The predictive posterior densities of the observable temperatures for the thermocouples TC2, TC3, TC4 at time $t = 0.52$.

5.5.3.3 Predictive Posterior Distribution

In this section, we examine the possibility of predicting the observable temperature at future time intervals after estimating the thermal diffusivity, $\theta$. More specifically, assume we have inferred $\theta$ using temperature measurements up to time $t_n$. Then, we want to predict the temperature in the next time step, $t_{n+1}$. Given our Bayesian model, it is necessary to assume the knowledge of the boundary temperature at time $t_{n+1}$. A typical situation could be given by an experiment in which there is interest in temperature values at inner points for different boundary values.

The predictive posterior distribution, $\rho(Y_{n+1} \mid \{Y_k\}_{k=1}^n, T_{L,n+1}, T_{R,n+1})$, is given by

$$\int_{\Theta} \rho(Y_{n+1} \mid \{Y_k\}_{k=1}^n, T_{L,n+1}, T_{R,n+1}, \theta) \rho(\theta \mid \{Y_k\}_{k=1}^n) \, d\theta, \quad (5.24)$$

and it is estimated by averaging

$$\frac{1}{M} \sum_{i=1}^M \rho(Y_{n+1} \mid \{Y_k\}_{k=1}^n, T_{L,n+1}, T_{R,n+1}, \theta_i),$$

where the $\theta_i$'s are sampled from the posterior distribution of $\theta$.

Figure 5.12 shows the one-step-ahead predictive posterior densities at three dif-
different inner thermocouples based on the observations until time $t = 0.5$, when the observed temperature at thermocouples TC2, TC3 and TC4 were 53.98, 55.53 and 57.84°C respectively.

We emphasize that this methodology allows us to obtain the k-step ahead predictive posterior density for any inner thermocouple, assuming boundary conditions subject to uncertainty that are adequate for the experiment.

5.5.4 Example 3

In this example, we consider the case where the thermal diffusivity depends on the space variable, $x$. The finite element method used to solve the heat equation under such an assumption was presented in Section 5.3.

5.5.4.1 Prior distribution of $\theta(x)$

Assume that the prior distribution of $\theta(x)$ is a lognormal random field with a squared exponential (SE) covariance function. Then, the prior distribution of $\log \theta(x)$ can be expressed using the joint multivariate Gaussian distribution:

$$(\log(\theta(x_1)), \ldots, \log(\theta(x_s))) \sim \mathcal{N}_s(\mu, K),$$

where $\mu = (\mu, \mu, \ldots, \mu)^{tr}$, $K_{ij} = \text{Cov}(\log(\theta(x_i)), \log(\theta(x_j))) = \eta^2 \exp\left(-\frac{|x_i - x_j|^2}{2\ell^2}\right)$, $i, j = 1, \ldots, s$, $\eta$ is the magnitude, and $\ell$ denotes the length scale.

We assume the following priors for the hyperparameters $\mu, \eta$ and $\ell$ (the prior density of $\mu$ and $\eta$ is displayed in Figure 5.13):

$$\mu \sim \mathcal{N}(0.1, 0.1), \quad \eta \sim \text{half-Cauchy}(0.1), \quad \ell \sim U(0.5, 5).$$

In this example, we choose a Gaussian prior for $\mu$ and uninformative uniform prior for $\ell$. The half-Cauchy prior for $\eta$ was chosen because it is a practical prior for scale
Figure 5.13: Example 3: Joint prior density for the hyperparameters $\mu$ and $\eta$, with $\mu \sim \mathcal{N}(0.1, 0.1)$ and $\eta \sim \text{half-Cauchy}(0.1)$.

parameters in hierarchical models \[22\], \[23\].

5.5.4.2 Joint posterior distribution of the hyperparameters $\mu, \eta, \ell$

Given $\theta := (\theta(x_1), \ldots, \theta(x_s))^\text{tr}$, let us consider the joint posterior density of the hyperparameters $(\mu, \eta, \ell)$ that characterize the distribution of $\log\theta(x)$.

$$
\rho(\mu, \eta, \ell|\mathbf{Y}_1, \ldots, \mathbf{Y}_N) \propto \rho(\mu, \eta, \ell) \int_{\Theta} \rho(\theta|\mu, \eta, \ell) \rho(\mathbf{Y}_1, \ldots, \mathbf{Y}_N|\theta) d\theta.
$$

Let us introduce the auxiliary variable $\mathbf{z} = (z_1, \ldots, z_s) \sim \mathcal{N}_s\left(0, C = \frac{1}{\eta^2}K\right)$ and consider the change of variables transformation: $\log(\theta_i) = \mu + \eta z_i$ where $\theta_i := \theta(x_i)$, $z_i := z(x_i)$, $i = 1, \ldots, s$. Then, the prior density of $\theta$ is given by

$$
\rho(\theta|\mu, \eta, \ell) = \frac{(\eta^2 2\pi)^{-\frac{s}{2}} |C|^{-\frac{1}{2}}}{\theta_1 \theta_2 \cdots \theta_s} \exp\left(-\frac{(\log \theta - \mu)^\text{tr} C (\log \theta - \mu)}{2\eta^2}\right)
$$

$$
= \frac{(2\pi)^{-\frac{s}{2}} |C|^{-\frac{1}{2}}}{\eta^se^{s\mu + \eta(z_1 + \ldots + z_s)}} \exp\left(-\frac{1}{2}z^\text{tr} C^{-1} z\right)
$$

$$
= \frac{\rho(\mathbf{z}|\ell)}{\eta^se^{s\mu + \eta(z_1 + \ldots + z_s)}}.
$$
The posterior density of the hyperparameters can be therefore written as

$$\rho(\mu, \ell, \eta | Y_1, \ldots, Y_N) \propto \rho(\mu, \ell, \eta) \int_{Z} \frac{\rho(z|\ell)}{\eta^s e^{\mu + \eta(z_1 + \ldots + z_s)}} |J| \rho(Y_1, \ldots, Y_N | \mu, \eta, z) dz,$$

where $J$ is the Jacobian matrix of the transformation.

By considering $\ell$ as a nuisance parameter, we obtain

$$\rho(\mu, \eta | Y_1, \ldots, Y_N) \propto \rho(\mu, \eta) \int_{\ell} \rho(\ell) \int_{Z} \rho(z|\ell) \rho(Y_1, \ldots, Y_N | \mu, \eta, z) dz d\ell \tag{5.26}$$

after $\ell$ is marginalized.

Figure 5.14: Example 3: Non-normalized joint posterior density of the hyperparameters $\mu$ and $\eta$.

Figure 5.15: Example 3: Laplace’s approximation of the posterior density of the hyperparameters $\mu$ and $\eta$.

To evaluate the posterior distribution of the hyperparameters, we need to compute the $s + 1$ dimensional integral in formula (5.26). Alternatively, Monte Carlo method can be used to approximate these integrals. First, we sample $\ell$ from its prior distribution, $\rho(\ell)$. Then, given $\ell$ we can sample $z$ and evaluate the joint likelihood function, $\rho(Y_1, \ldots, Y_N | \mu, \eta, z)$, for any pair $(\mu, \eta)$. Therefore, we approximate the
non-normalized posterior distribution using a double sum as follows:

\[
\int_{\ell} \int_{\mathbf{z}} \rho(\ell) \rho(\mathbf{z} | \ell; \mathbf{Y}_1, \ldots, \mathbf{Y}_N | \mu, \eta, \mathbf{z}) d\mathbf{z} d\ell \approx \frac{1}{M_\ell} \sum_{i=1}^{M_\ell} \int_{\mathbf{z}} \rho(\mathbf{z} | \ell_i) \rho(\mathbf{Y}_1, \ldots, \mathbf{Y}_N | \mu, \eta, \mathbf{z}) d\mathbf{z} \\
\approx \frac{1}{M_\ell M_z} \sum_{i=1}^{M_\ell} \sum_{j=1}^{M_z} \rho(\mathbf{Y}_1, \ldots, \mathbf{Y}_N | \mu, \eta, \mathbf{z}_j),
\]

where \( \mathbf{z}_j \sim \rho(\mathbf{z} | \ell_i) \).

Figure 5.14 shows that the non-normalized posterior of the hyperparameters \( \mu \) and \( \eta \) has a unique mode at \((-0.05, 0.025)\). We use then Laplace’s method to obtain a Gaussian posterior, using the synthetic dataset A, as shown in Figure 5.15.

A new dataset is now introduced to test our method when \( \theta \) depends on \( x \).

### 5.5.4.3 Dataset B

To analyze the performance of our inferential technique in the case where the thermal diffusivity parameter depends on the space variable, \( x \), we consider another synthetic dataset (hereafter named dataset B) that is generated similarly to the dataset A, except for the fact that \( \theta(x) \) is sampled randomly from the new prior (5.25) where \( \mu = 0, \eta = 0.1 \) and \( \ell = 5 \).

Again, we approximate the posterior distribution of the hyperparameters \( \mu \) and \( \eta \) using Laplace’s approximation given the following priors for the hyperparameters \( \mu, \eta \) and \( \ell \):

\[
\mu \sim \mathcal{N}(0, 0.25), \quad \eta \sim \text{half-Cauchy}(0.5), \quad \ell \sim U(4, 6),
\]

where we assume broad priors for \( \mu \) and \( \eta \) with a more informative uniform prior for \( \ell \).

From Figure 5.17, we find that the maximum a posteriori probability (MAP) estimate is \((0.05, 0.025)\) and Laplace’s approximation can be used. By comparing the
Figure 5.16: Example 3: Joint prior density for the hyperparameters $\mu$ and $\eta$, with $\mu \sim \mathcal{N}(0, 0.25)$ and $\eta \sim \text{half-Cauchy}(0.5)$.

Figure 5.17: Example 3: Non-normalized joint posterior density of the hyperparameters $\mu$ and $\eta$.

Figure 5.18: Example 3: Laplace’s approximation for the posterior density of the hyperparameters $\mu$ and $\eta$.

prior and posterior densities for $\mu$ and $\eta$ in Figures 5.16 and 5.18, we can say that the experiment is informative since the posterior concentrates around $(0.05, 0.025)$ which is close to the true value.

5.6 Conclusion

In this work, we developed a general Bayesian approach for one-dimensional linear parabolic partial differential equations with noisy boundary conditions. First, we derived the joint likelihood of the thermal diffusivity $\theta$ and the boundary parameters. Second, we approximated the solution of the forward problem, by showing that such solution can be written as a linear function of the boundary conditions. After that, we
marginalized out the boundary parameters, under the assumptions that they are well approximated by piecewise linear functions and that they are independent Gaussian random vectors. This approach can be generalized to any well-posed linear partial differential equation.

On the implementation side, we computed the log-posterior of the thermal diffusivity in different cases. Besides, we used the Laplace approximation to obtain a Gaussian posterior. In the first example, we used directly the joint likelihood of the thermal diffusivity $\theta$ and the boundary parameters, assuming that the boundary conditions were known. In the second example, we used the marginalized likelihood of $\theta$, assuming that $\theta$ is a lognormal random variable and, as in the previous example, we obtained an approximated Gaussian posterior distribution, showing that the unknown value of the thermal diffusivity is recovered almost exactly. Moreover, we explored two important advantages of using the Bayesian approach, by providing the estimation of the expected information gain for different experimental setups and the predictive posterior distribution of the temperature. We noticed that the temperature measurements from the middle thermocouple at the second time interval are, in general, the most informative measurements. Finally, assuming that $\theta$ is a lognormal random field with squared exponential covariance function, we evaluated the joint posterior distribution for the covariance hyperparameters by applying hierarchical Bayesian techniques.

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5.7 Appendix

5.7.1 Proof of Theorem 5.3.2

First, let us introduce the vectors

\[
F_{L,1}^{(I-1)\times 1} = \left[ \begin{array}{c} -\left( \int_{x_L}^{x_R} \frac{x_R - x}{x_R - x_L} \phi_j dx \right) \end{array} \right],
\]

\[
F_{L,2}^{(I-1)\times 1} = \left[ \begin{array}{c} \left( \int_{x_L}^{x_R} \left( \frac{x_R - x}{x_R - x_L} - \Delta t L \theta \frac{x_R - x}{x_R - x_L} \right) \phi_j dx \right) \end{array} \right],
\]

\[
F_{R,1}^{(I-1)\times 1} = \left[ \begin{array}{c} -\left( \int_{x_R}^{x_L} \frac{x - x_L}{x_R - x_L} \phi_j dx \right) \end{array} \right],
\]

\[
F_{R,2}^{(I-1)\times 1} = \left[ \begin{array}{c} \left( \int_{x_L}^{x_R} \left( \frac{x - x_L}{x_R - x_L} - \Delta t L \theta \frac{x - x_L}{x_R - x_L} \right) \phi_j dx \right) \end{array} \right],
\]

and the matrices

\[
B^{(I-1)\times(I-1)} = (M + \Delta t S \theta)^{-1} M,
\]

\[
F_{L,n}^{(I-1)\times N+1} = \begin{pmatrix} 0_{(I-1)\times(n-1)} & F_{L,1}^{(I-1)\times 1} & F_{L,2}^{(I-1)\times 1} & 0_{(I-1)\times(N-n)} \end{pmatrix}, \quad n = 2, \ldots, N - 1,
\]

\[
F_{R,n}^{(I-1)\times N+1} = \begin{pmatrix} 0_{(I-1)\times(n-1)} & F_{R,1}^{(I-1)\times 1} & F_{R,2}^{(I-1)\times 1} & 0_{(I-1)\times(N-n)} \end{pmatrix}, \quad n = 2, \ldots, N - 1,
\]

\[
F_{L,1}^{(I-1)\times N+1} = \begin{pmatrix} F_{L,1}^{(I-1)\times 1} & F_{L,2}^{(I-1)\times 1} & 0_{(I-1)\times(N-1)} \end{pmatrix},
\]

\[
F_{R,1}^{(I-1)\times N+1} = \begin{pmatrix} F_{R,1}^{(I-1)\times 1} & F_{R,2}^{(I-1)\times 1} & 0_{(I-1)\times(N-1)} \end{pmatrix},
\]

\[
F_{L,N}^{(I-1)\times N+1} = \begin{pmatrix} 0_{(I-1)\times(N-1)} & F_{L,1}^{(I-1)\times 1} & F_{L,2}^{(I-1)\times 1} \end{pmatrix},
\]

\[
F_{R,N}^{(I-1)\times N+1} = \begin{pmatrix} 0_{(I-1)\times(N-1)} & F_{R,1}^{(I-1)\times 1} & F_{R,2}^{(I-1)\times 1} \end{pmatrix}.
\]

Then, the solution of (9) is given by:

\[
u_{n+1} = Bu_n + (M + \Delta t S \theta)^{-1} \left( F_{L,n} T_L + F_{R,n} T_R \right).
\]
Applying recursively the previous relation we derive the discrete representation (Duhamel’s formula)

\[ u_n = B^n u_0 + \sum_{k=1}^{n} B^{n-k} (M + \Delta t S_{\theta})^{-1} (F_{L,k} T_L + F_{R,k} T_R). \]

Now we can build the matrices \( A_n(\theta), \tilde{A}_{L,n}(\theta) \) and \( \tilde{A}_{R,n}(\theta) \), \( n = 1, \ldots, N \), introduced in the expression (14), to recover the solution of the problem (9) as a linear function of the initial-boundary conditions, namely:

\[
\begin{align*}
A_n(\theta) &= B^n, \\
\tilde{A}_{L,n}(\theta) &= \sum_{k=1}^{n} B^{n-k} (M + \Delta t S_{\theta})^{-1} F_{L,k}, \text{ and} \\
\tilde{A}_{R,n}(\theta) &= \sum_{k=1}^{n} B^{n-k} (M + \Delta t S_{\theta})^{-1} F_{R,k}. \Box
\end{align*}
\]

5.7.2 Proof of Theorem 5.3.3

From equations (8) and (14), we can write:

\[ T_n = B^n u_0 + \tilde{A}_{L,n}(\theta) T_L + \tilde{A}_{R,n}(\theta) T_R - T_{L,n} F_{L,1} - T_{R,n} F_{R,1}, \]

Now, define \( A_{L,n}(\theta) \) and \( A_{R,n}(\theta) \) by:

\[
\begin{align*}
A_{L,n}(\theta) &= \tilde{A}_{L,n}(\theta) + \begin{pmatrix}
B^n F_{L,1} & 0 & -F_{L,1} & 0 \\
(I-1) \times 1 & (I-1) \times 1 & (I-1) \times 1 & (I-1) \times (N-n)
\end{pmatrix}, \\
A_{R,n}(\theta) &= \tilde{A}_{R,n}(\theta) + \begin{pmatrix}
B^n F_{R,1} & 0 & -F_{R,1} & 0 \\
(I-1) \times 1 & (I-1) \times 1 & (I-1) \times 1 & (I-1) \times (N-n)
\end{pmatrix}.
\end{align*}
\]

Therefore, we obtain equation (15). \Box
5.7.3 Proof of Remark 5.5.3

Consider the following backward Euler discretization of the local problem (3) in the interval time, \((t_n, t_{n+1}) = (n\Delta t, (n + 1)\Delta t)\):

\[
\left\{
\begin{aligned}
\frac{1}{\Delta t}(T_{i,n+1} - T_{i,n}) - \frac{\theta}{\Delta x^2}(T_{i+1,n+1} - 2T_{i,n+1} + T_{i-1,n+1}) &= 0, & i = 2, \ldots, I \\
T_{L,n} &= T_L(n\Delta t), \\
T_{R,n} &= T_R(n\Delta t).
\end{aligned}
\right.
\]

To write the discretization in a matrix form, let us introduce the vectors

\[T_n = (T_{2,n}, \ldots, T_{I,n})^{tr}, \quad n = 1, \ldots, N,\]

and the matrix

\[
A = \begin{pmatrix}
-2 & 1 & 0 & 0 & \ldots & 0 \\
1 & -2 & 1 & 0 & \ldots & 0 \\
0 & 1 & -2 & 1 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \ldots & 0 & 1 & -2 & 1 \\
0 & 0 & 0 & \ldots & 1 & -2
\end{pmatrix}.
\]

In this way, we may write

\[
\frac{1}{\Delta t}(T_{n+1} - T_n) - \frac{\theta}{\Delta x^2}AT_{n+1} = \frac{\theta}{\Delta x^2}(T_{L,n+1}v + T_{R,n+1}w), \quad (\star)
\]

where \(v = (1, 0, \ldots, 0)^{tr}\) and \(w = (0, \ldots, 0, 1)^{tr}\).

The expression (6.13) is equal to

\[
(I_{I-1} - \theta \frac{\Delta t}{\Delta x^2} A)T_{n+1} = T_n + \theta \frac{\Delta t}{\Delta x^2}(T_{L,n+1}v + T_{R,n+1}w).
\]
and letting $\frac{\Delta t}{\Delta x^2} = \lambda$ and $B = (I - \theta \lambda A)^{-1}$, we obtain

$$T_{n+1} = BT_n + \theta \lambda (T_L, n+1 B v + T_R, n+1 B w).$$

Applying recursively the previous relation, we derive

$$T_n = B^n T_0 + \theta \lambda \sum_{k=1}^{n} T_{L, k} B^{n-k+1} v + \theta \lambda \sum_{k=1}^{n} T_{R, k} B^{n-k+1} w,$$

whose compact matrix form is

$$T_n = B^n T_0 + C_n \tilde{T}_L + D_n \tilde{T}_R,$$

where

- $\tilde{T}_L = (T_{L,1}, \ldots, T_{L,n})^{tr} = (T_L(\Delta t), \ldots, T_L(n \Delta t))^{tr},$
- $\tilde{T}_R = (T_{R,1}, \ldots, T_{R,n})^{tr} = (T_R(\Delta t), \ldots, T_R(n \Delta t))^{tr},$
- the matrix $C_n$ has column vectors $c_k = \theta \lambda A^{n-k+1} v, k = 1, \ldots, n,$
- the matrix $D_n$ has column vectors $d_k = \theta \lambda A^{n-k+1} w, k = 1, \ldots, n.$

Now, we can build the matrices $A_{L, n}(\theta)$ and $A_{R, n}(\theta), n = 1, \ldots, N,$ introduced in the expression (16), to recover the solution of the problem (3) for each interval time, $(t_{n-1}, t_n), n = 1, \ldots, N,$ as a linear function of the initial-boundary conditions:

$$A_{L, n}(\theta) = \begin{pmatrix} C_n & 0 \\ (I-1) \times n & (I-1) \times (N-n) \end{pmatrix},$$

$$A_{R, n}(\theta) = \begin{pmatrix} C_n & 0 \\ (I-1) \times n & (I-1) \times (N-n) \end{pmatrix}.$$
5.8 REFERENCES


Chapter 6

Bayesian inferences of the thermal properties of a wall using temperature and heat flux measurements

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Abstract

The assessment of the thermal properties of walls is essential for accurate building energy simulations that are needed to make effective energy-saving policies. These properties are usually investigated through in-situ measurements of temperature and heat flux over extended time periods. The one-dimensional heat equation with unknown Dirichlet boundary conditions is used to model the heat transfer process through the wall. In [F. Ruggeri, Z. Sawlan, M. Scavino, R. Tempone, A hierarchical Bayesian setting for an inverse problem in linear parabolic PDEs with noisy boundary conditions, Bayesian Analysis 12 (2) (2017) 407–433], it was assessed the uncertainty about the thermal diffusivity parameter using different synthetic data sets. In this work, we adapt this methodology to an experimental study conducted in an environmental chamber, with measurements recorded every minute from temperature probes and heat flux sensors placed on both sides of a solid brick wall over a five-day period. The observed time series are locally averaged, according to a smoothing procedure determined by the solution of a criterion function optimization problem, to fit the required set of noise model assumptions. Therefore, after preprocessing, we can reasonably as-

sume that the temperature and the heat flux measurements have stationary Gaussian noise and we can avoid working with full covariance matrices. The results show that our technique reduces the bias error of the estimated parameters when compared to other approaches. Finally, we compute the information gain under two experimental setups to recommend how the user can efficiently determine the duration of the measurement campaign and the range of the external temperature oscillation.

6.1 Introduction

Concerns about climate change and the effects of greenhouse gases have led to international targets for reducing carbon emissions [1, 2]. One substantial source of carbon emissions is the built environment, which accounts for approximately one-third of global energy consumption [3]. For example, approximately 40% of national energy consumption in the UK is from the building sector. Reduction in carbon emissions from the built environment is, therefore, vital to meeting carbon reduction targets. Carbon emissions from buildings can be considerably reduced through large-scale policies that seek to limit energy demand for space heating and cooling [3]. Accurate predictions of building performance and energy demands are essential to the success of such policies. Specifically, computer simulations of heat loss from buildings are necessary to assess the effectiveness of energy-saving strategies such as retrofit interventions [4]. However, recent works [5, 6, 7] have shown that standard computer simulations of building performance may be unreliable due to inaccuracies from poorly characterized building structures including walls. Energy-saving measures based on inaccurate predictions of building performance may be economically ineffective.

Uncertainty in the thermal properties of walls is a primary source of inaccuracy in predictions of energy demand in buildings [7, 8]. The heat capacitance and thermal conductance (resistance) of walls are used in standard heat transfer models as
parameters for building performance simulations. Since these parameters of existing buildings are often unknown, the corresponding inputs in building simulations are typically obtained by visual inspection and tabulated values. In most cases, these values do not provide accurate characterizations of the walls of the building under consideration.

The thermal properties of walls can be inferred from in-situ measurements of temperature and heat flux \[9\ [10\ [7\]. More specifically, the surface temperatures of internal and external walls denoted as \(\{T_{\text{int}}^i\}_{i=1}^N\) and \(\{T_{\text{ext}}^i\}_{i=1}^N\), are measured at a specified location over time. In addition, the heat flux through the wall, \(\{q^i\}_{i=1}^N\), is also measured at \(N\) equispaced time points. ISO 9869:2014 \[11\] outlines a simple averaging procedure to determine the thermal transmittance (U-value) from in-situ measurements. With this approach, the R-value (i.e., the inverse of the U-value) is computed directly by

\[
R = \frac{\sum_{i=1}^N (T_{\text{int}}^i - T_{\text{ext}}^i)}{\sum_{i=1}^N q^i}.
\]

Since the averaging procedure assumes that the thermal mass of the wall is zero or almost zero, the accuracy of the estimate of the U-value will require measurements collected over an extended period of time (often longer than two weeks) \[9\ [11\]. More importantly, the averaging method does not provide a statistical framework that accounts for either the uncertainty in the thermal properties or errors in the measurements. As a result, this method fails to provide a proper quantification of the uncertainty in the estimated U-value of the wall.

Recent work has proposed the use of statistical approaches to infer thermal properties from in-situ measurements of temperature and heat flux with simplified heat transfer models. In particular, a standard Bayesian inference has recently been proposed \[9\] to estimate the thermal properties of walls under the assumption that the heat dynamics of the wall can be described with a simple lumped-mass resistance-capacitance (RC) model. In contrast to the averaging method, the approach in \[9\]
employs an RC network whose parameters include the thermal conductivity and the heat capacity. This standard Bayesian methodology suggests that these thermal properties can be inferred from in-situ measurements based on relatively shorter measurement campaigns than the ones required by the averaging method. While other non-Bayesian statistical methods for estimating thermal properties have been proposed [12], [9] provides substantial insight into the advantages of using Bayesian inference in building models and provides a motivation for further developments.

Our present work is a special application of parameter estimation for partial differential equations [13] [14]. In particular, we develop and implement the hierarchical Bayesian approach introduced in [15]. Related works on Bayesian inference used for different applications can be found in the literature (see, for example, [16] [17] [18]). A general Bayesian formulation of inverse problems in heat transfer is also available in [19] [20]. However, we address a problem where the boundary conditions cannot be assumed known and a Bayesian approach based on the full likelihood function will not be recommended. Instead, the strength of our approach is to construct data-driven Gaussian priors [15], treating the boundary conditions as nuisance parameters to be marginalized out, to develop a quick and applicable Bayesian assessment of the parameters of interest. In [15], this approach was implemented to infer the thermal diffusivity parameter using synthetic temperature measurements in the interior and boundary of the domain. Here, we adapt the methodology to deal with temperature and heat flux measurements that are only available on the boundaries. We provide the maximum likelihood estimate (MLE) and the posterior distributions of the unknown parameters. Under the specification of independent uniform priors for the parameters of interest, we first use the Laplace method to produce fast estimates of their posterior distributions [21] [22]. Then, we apply a Markov chain Monte Carlo (MCMC) sampling algorithm to assess the accuracy of the approximations obtained via Laplace method. The MCMC simulations, for this problem, support the employ-
ment of Laplace method to speed up the computations and estimate information gain values.

Most existing methodologies for inferring thermal properties [9] use forward models that can be derived from simplified coarse-grid approximations (often with 2 or 3 spatial nodes) of the heat equation that describes heat transfer through a wall. These simplified models are often used for the sake of computational expediency in the parameter identification process. However, such simplifications introduce intrinsic modeling errors that may, in turn, result in biased and potentially inaccurate estimated parameters. Alternatively, we use a heat equation with unknown Dirichlet boundary conditions to model the interior temperature of the wall, and we provide a convergence analysis to assess the effect of the discretization error in the Bayesian estimates of the thermal properties. We show that the proposed technique is robust under grid refinement and is, therefore, suitable for any discretization that we may choose according to the computational resources at hand.

In-situ temperature measurements of a wall are often used as boundary conditions for a forward heat transfer model of the wall. In the Bayesian approach in [9] the inference of the thermal properties is made by inverting heat flux observations while using measurements of temperatures for the forward heat transfer model. Only the heat flux measurements are used to construct the likelihood function. Temperature measurements are assumed “exact” and are utilized as boundary conditions for the forward RC model in the Bayesian framework for inferring thermal properties. In contrast, our hierarchical approach accounts for uncertainty in the temperature measurements by treating the nuisance boundary conditions as random functions modeled by Gaussian distributions. As we show in Section 6.3, failing to account for the uncertainty in these measurements can result in biased and inaccurate estimates of the inferred properties. We also compare our results with those obtained by applying a similar approach to the one in [9], in which smooth spline fits of the temperature
measurements are used as exact boundary conditions.

Standard protocols based on asymptotic assumptions \cite{11} require long measurement campaigns during winter to reduce the dynamic effect of the capacitance of the wall. However, \cite{9} suggests that shorter measurements campaigns may provide similar estimates of inferred parameters to the ones from longer measurement campaigns. Hence, we use the proposed hierarchical Bayesian framework to investigate the effects of the duration and the conditions (i.e., measurement cycle) of the measurement campaign. To this end, we estimate, by Laplace method, the information gain \cite{23, 24} to quantify the duration of the measurement campaign and the corresponding cycle. The proposed approach can then be used to design cost-effective measurement campaigns.

The rest of this paper is organized as follows. In Section 6.2, we derive a simulation model of the heat flow process through a wall using the heat equation. Based on simple assumptions, we reduce the model to a one-dimensional heat equation with unknown Dirichlet boundary conditions and write the modeled heat flux as a linear function of the boundary conditions. The Bayesian approach is then introduced; we construct the joint likelihood by assuming Gaussian noise in the heat flux measurements. We also assume that the nuisance boundary conditions are random functions modeled by Gaussian distributions. Under these assumptions, the marginalization of the boundary conditions can be performed analytically. Section 6.3 includes the description of the experiment conducted at the Nottingham University Innovation Park to collect temperature and heat flux measurements from both sides of a brick wall. Moreover, smoothing time series techniques are applied to the real data to assess the relevance of the measurement error. Example 1 shows how the thermal properties of the wall can be estimated when a deterministic approximation of the nuisance boundary conditions is used. The numerical results of the marginalization technique are then presented in Example 2, where we also study the convergence of the ML
estimates of the model parameters and estimate bivariate posterior distributions. In Subsection 6.3.6, we analyze the robustness of our Bayesian approach by means of bootstrap resampling methods. Finally, we compute the information gain about the model parameters under different experimental setups in Section 6.4.

6.2 Methodology

In this Section, we describe the forward and inverse methodologies used to characterize the thermal properties of walls. We also introduce the heat transfer (forward) model that we combine with the hierarchical Bayesian methodology introduced in Subsection 6.2.2.

6.2.1 The Forward model

The existing forward models used to infer the thermal properties of walls are based on simplified heat transfer models [9]. Inferring parameters (i.e., thermal properties) from such simplified models can be done in a computationally affordable fashion through standard identification/inference techniques. However, as we stated earlier, this oversimplification of the heat transfer process might lead to modeling errors that are often not incorporated into standard inference approaches. In this Section, we propose a realistic mathematical model to simulate the heat transfer process through a wall using an initial/boundary value formulation for the heat equation.

6.2.1.1 Heat equation

The heat transport process inside a wall is modeled, in general, by a three-dimensional heat equation on a rectangular prism, \( \Omega \). The initial/boundary value problem for the heat equation along the period \([0, t_N]\), with initial wall temperature \( T_0 \) and temperature profile \( T_s \) at the boundary \( \Gamma \), is given by:
\[ \rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k(x) \nabla T), \, x \in \Omega, \, t \in [0, t_N] \]

\[ T(x, t) = T_s(x, t), \, x \in \Gamma, \, t \in [0, t_N] \]

\[ T(x, 0) = T_0(x), \, x \in \Omega \]

where \( \rho, c_p \) and \( k \) denote the density of the material, the specific heat capacity and the thermal conductivity, respectively.

Here, we consider the specific situation where the wall is surrounded by insulation materials and its thickness is less than its length and width. We, therefore, assume that the wall temperature varies only along the thickness dimension denoted by \( x \).

Also, given that the wall is solid, the thermal conductivity is assumed to be constant, \( k(x) := k \). As a consequence, our simulation model consists of a one-dimensional heat equation with Dirichlet boundary conditions. From the solution of the heat equation, we then define the heat flux functions, \( F_{int} \) and \( F_{ext} \), which correspond to the model predictions of heat fluxes at the boundary. The model under consideration takes the following form:

\[
\begin{cases}
\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right), & x \in (0, L), \, t \in [0, t_N] \\
T(0, t) = T_{int}(t), \, T(L, t) = T_{ext}(t), & t \in [0, t_N] \\
T(x, 0) = T_0(x), & x \in (0, L), \tag{6.1}
\end{cases}
\]

where \( L \) is the wall thickness, \( T_{int} \) and \( T_{ext} \) are the internal and external wall surface temperatures, respectively. In our implementation, we replace the thermal conductivity, \( k \), with \( \frac{L}{R} \) and replace \( \rho c_p \), with \( \frac{\rho C}{L} \). Then, we estimate the thermal resistance,
and the heat capacity per unit area, \( \rho C \), which are properties of the wall.

### 6.2.1.2 Numerical approximation

In the numerical implementation of the forward heat transfer model, it is simple to show, upon discretization, that the heat flux can be written as a linear function of the initial condition, \( T_0 \), and the boundary conditions, \( T_{\text{int}} \) and \( T_{\text{ext}} \).

Consider the following uniform space-time discretization,

\[
x_0 = 0, x_1 = \Delta x, \ldots, x_m = m\Delta x, \ldots, x_M = M\Delta x = L,
\]

\[
t_0 = 0, t_1 = \Delta t, \ldots, t_n = n\Delta t, \ldots, t_N = N\Delta t,
\]

and define the vectors

\[
T_{\text{int}} = (T_{\text{int}}(t_0), \ldots, T_{\text{int}}(t_N))^\prime, T_{\text{ext}} = (T_{\text{ext}}(t_0), \ldots, T_{\text{ext}}(t_N))^\prime.
\]

\[
T_0 = (T_0(x_1), \ldots, T_0(x_{M-1}))^\prime,
\]

\[
F_{\text{int}} = (F_{\text{int}}(t_0), \ldots, F_{\text{int}}(t_N))^\prime, F_{\text{ext}} = (F_{\text{ext}}(t_0), \ldots, F_{\text{ext}}(t_N))^\prime.
\]

Then, the discretized heat flux can be approximated by a linear function of the initial condition, \( T_0 \), and the boundary conditions, \( T_{\text{int}} \) and \( T_{\text{ext}} \):

\[
F_{\text{int}} \approx H T_0 + H_{\text{int}} T_{\text{int}} + H_{\text{ext}} T_{\text{ext}}, \quad (6.2)
\]

\[
F_{\text{ext}} \approx G T_0 + G_{\text{int}} T_{\text{int}} + G_{\text{ext}} T_{\text{ext}}, \quad (6.3)
\]

where \( H, H_{\text{int}}, H_{\text{ext}}, G, G_{\text{int}} \) and \( G_{\text{ext}} \) are matrices that may depend nonlinearly on the parameters \( R \) and \( \rho C \), which, in turn, we infer in the next Subsection. Such matrices are explicitly defined in the Appendix \((6.6.1)\). In the case in which thermal conductivity is not constant, the previous result can be proved using the finite element
method instead of the finite difference method (see [15]).

In the subsequent analysis, we assume that the initial condition, \( T_0(x) \) (and its corresponding discretization \( T_0 \)), is well approximated by the piecewise linear function

\[
\begin{align*}
T_{\text{int}}(0) + 2\frac{T_{\text{int}}(0) - T_{\text{int}}(0)}{L} x & \quad \text{if } 0 < x \leq \frac{L}{2} \\
\tau_0 + 2\frac{T_{\text{ext}}(0) - \tau_0}{L} (x - \frac{L}{2}) & \quad \text{if } \frac{L}{2} < x < L,
\end{align*}
\]

(6.4)

where \( \tau_0 \) is an unknown constant parameter.

The discretized model (6.2)-(6.3) can be written as

\[
\begin{bmatrix}
F_{\text{int}} \\
F_{\text{ext}}
\end{bmatrix} = \mathcal{F}(R, \rho C, \tau_0, T_{\text{int}}, T_{\text{ext}}),
\]

(6.5)

where \( \mathcal{F} \) is a non-linear function that arises from the numerical discretization (6.2)-(6.3) and the modeling assumption (6.4).

6.2.2 The Bayesian inverse problem

Assume that we have noisy measurements of the heat fluxes, \( F_{\text{int}} \) and \( F_{\text{ext}} \), at the observation times, \( t_0, \ldots, t_N \). We denote these measurements as \( Q_{\text{int}} = \{Q_{\text{int}}^0, \ldots, Q_{\text{int}}^N\} \) and \( Q_{\text{ext}} = \{Q_{\text{ext}}^0, \ldots, Q_{\text{ext}}^N\} \), respectively. Similarly, we assume that noisy measurements of the boundary temperatures, \( T_{\text{int}} \) and \( T_{\text{ext}} \), are taken at those observation times. These observations are denoted by \( Y_{\text{int}} = \{Y_{\text{int}}^0, \ldots, Y_{\text{int}}^N\} \) and \( Y_{\text{ext}} = \{Y_{\text{ext}}^0, \ldots, Y_{\text{ext}}^N\} \), respectively. The objective of the proposed Bayesian methodology is to estimate \( \theta = (R, \rho C, \tau_0) \) given heat flux measurements \( (Q_{\text{int}}, Q_{\text{ext}}) \) and boundary temperature measurements \( (Y_{\text{int}}, Y_{\text{ext}}) \). Whereas the parameters \( R \) and \( \rho C \) are the unknown variables of interest that characterize the thermal properties of the wall, the initial temperature parameter, \( \tau_0 \), is also unknown. It must be inferred alongside \( R \) and \( \rho C \).
6.2.2.1 The Bayesian approach

We adopt the Bayesian approach in which the goal is to find the probability distribution of the unknown parameters, $\gamma$, given the data, namely the posterior distribution, $\pi(\gamma|data)$. From Bayes’ theorem, the posterior distribution of $\gamma$ is given by

$$
\pi(\gamma|data) \propto \pi(data|\gamma)\pi_p(\gamma),
$$

where $\pi(data|\gamma) = \mathcal{L}(\gamma|data)$ is the likelihood function of $\gamma$ and $\pi_p$ is the prior distribution of $\gamma$ [25]. In the context of the model defined by expression (6.5), we can see that the parameters of the model are $\theta \equiv (R, \rho C, \tau_0)$ as well as $T_{int}$ and $T_{ext}$. Once these parameters are prescribed, expressions (6.2)-(6.3) determine the model predictions of the heat fluxes. Therefore, the joint posterior distribution of all these parameters is given by

$$
\pi(\theta, T_{int}, T_{ext}|Q_{int}, Q_{ext}) \propto \pi(Q_{int}, Q_{ext}|\theta, T_{int}, T_{ext})\pi_p(\theta, T_{int}, T_{ext}).
$$

(6.6)

Note that $\theta$ is the unknown parameter of interest that contains the thermal properties of the wall.

In contrast, the boundary parameters, $T_{int}$ and $T_{ext}$, are related to noisy measurements. Therefore, these nuisance boundary parameters will be marginalized from the joint likelihood. The specification of the prior distributions of these nuisance parameters is driven by the data by means of the boundary temperature measurements ($Y_{int}, Y_{ext}$). As a result, the joint likelihood function will be based only on the heat flux measurements. Nevertheless, by incorporating $T_{int}$ and $T_{ext}$ as unknown parameters in this hierarchical fashion, we are effectively taking into account the uncertainty in the corresponding temperature measurements ($Y_{int}, Y_{ext}$). This is a new contribution relative to [9] where the noise in these observations is neglected.
6.2.2.2 Joint likelihood

To construct the joint likelihood \( \pi(Q_{\text{int}}, Q_{\text{ext}}|\theta, T_{\text{int}}, T_{\text{ext}}) \), we assume that the noises of the heat flux measurements are independent Gaussian:

\[
\begin{align*}
(Q_{\text{int}} - F_{\text{int}}) \mid \{\theta, T_{\text{int}}, T_{\text{ext}}\} & \sim N(0, \Sigma_{\text{int}}), \\
(Q_{\text{ext}} - F_{\text{ext}}) \mid \{\theta, T_{\text{int}}, T_{\text{ext}}\} & \sim N(0, \Sigma_{\text{ext}}).
\end{align*}
\]

The Gaussianity assumption will be satisfied by the data used in the Bayesian analysis in Section 6.3.

Under the aforementioned assumptions, the joint likelihood function of \( \theta, T_{\text{int}}, T_{\text{ext}} \) is given by

\[
\mathcal{L}(\theta, T_{\text{int}}, T_{\text{ext}} \mid Q_{\text{int}}, Q_{\text{ext}}) = \frac{1}{(2\pi)^N \sqrt{|\Sigma_{\text{int}}||\Sigma_{\text{ext}}|}} \exp \left\{ -\frac{1}{2} \left( \frac{||Q_{\text{int}} - F_{\text{int}}||_{\Sigma_{\text{int}}}^2 + ||Q_{\text{ext}} - F_{\text{ext}}||_{\Sigma_{\text{ext}}}^2}{2} \right) \right\}.
\] (6.7)

We emphasize that \( T_{\text{int}} \) and \( T_{\text{ext}} \) are nuisance parameters that appear in the formulation via the forward model (i.e., the heat equation). A direct approach to eliminating these parameters is to set \( T_{\text{int}} = Y_{\text{int}} \) and \( T_{\text{ext}} = Y_{\text{ext}} \) (recall that \( Y_{\text{int}} \) and \( Y_{\text{ext}} \) are noisy measurements of the boundary temperatures) or to set \( T_{\text{int}} = \mu_{\text{int}} \) and \( T_{\text{ext}} = \mu_{\text{ext}} \) where \( \mu_{\text{int}} \) and \( \mu_{\text{ext}} \) are smoothed versions of \( Y_{\text{int}} \) and \( Y_{\text{ext}} \), respectively. This approach is used in [9] where temperature measurements are considered to be deterministic boundary conditions of the RC model. Instead, we eliminate the aforementioned nuisance parameters by marginalizing them using data-driven priors [15]. This marginalization, which we conduct in the subsequent Subsection, enables us to account for the uncertainty in temperature measurements. As we demonstrate in Subsection 6.3.5, the marginalization process removes the bias in the inferred parameters, thereby providing accurate estimates and reliable quantification of their
uncertainty. Moreover, rather than the simple RC model used in [9], here we consider more advanced model given by the heat equation introduced earlier.

### 6.2.3 Marginal likelihood

In this Section, we use temperature measurements to construct the data-driven Gaussian priors. We perform analytical integration to marginalize out the boundary conditions and obtain a marginal likelihood for $\theta$. We assume that the errors related to the nuisance boundary parameters are independent Gaussian with covariances $C_{\text{int},p}$ and $C_{\text{ext},p}$ as follows:

$$
T_{\text{int}} - \mu_{\text{int}} \sim N(0, C_{\text{int},p}),
T_{\text{ext}} - \mu_{\text{ext}} \sim N(0, C_{\text{ext},p}),
$$

where $\mu_{\text{int}}$ and $\mu_{\text{ext}}$ are smoothing splines constructed from the boundary temperature measurements.

The marginal likelihood of $\theta$ is given by

$$
\mathcal{L}(\theta|Q_{\text{int}}, Q_{\text{ext}}) \propto |\Lambda_0|^{1/2}|\Lambda_1|^{1/2} \exp \left\{ -\frac{1}{2} U + \frac{1}{2} t_{\text{int},2}' \Lambda_0 t_{\text{int},2} + \frac{1}{2} t_{\text{ext},1}' \Lambda_1 t_{\text{ext},1} \right\},
$$

where $\Lambda_0, \Lambda_1, U, t_{\text{int},2}$ and $t_{\text{ext},1}$ are independent of $T_{\text{int}}$ and $T_{\text{ext}}$ and explicitly defined in the Appendix [6.6.2]. The marginal likelihood (6.9) can now be used in the Bayesian framework, summarized in Subsection [6.2.2.1] to compute the posterior distribution, $\pi(\theta|Q_{\text{int}}, Q_{\text{ext}})$.

### 6.3 Experimental data and numerical results

In this Section, we apply the proposed Bayesian approach to infer the thermal properties of a wall from in-situ measurements of heat flux and temperature collected under controlled conditions. In Subsection [6.3.1] we describe the experimental setup. The
results from the Bayesian analysis are presented in Subsections 6.3.4 and 6.3.5.

6.3.1 Experimental setup

Data were collected from an experiment conducted inside an environmental chamber in the Energy Technologies Building, Nottingham University Innovation Park. The chamber consisted of two rooms separated by a 215-mm thick partition wall. The two rooms had internal dimensions of $3.70 \times 3.50 \times 2.38$ m. The data were collected from a $970 \times 600 \times 215$-mm brick section of the partition wall. Heat flux sensors and temperature probes were placed on both sides of the bricks.

The heat flux sensors are Hukseflux (HFP01) sensors with an accuracy of $\pm 5\%$. The surface temperatures were measured with platinum resistance sensors (PT100) with an accuracy of $\pm 0.1^{\circ}C$. The surface temperature was taken directly on the wall next to the heat flux sensor. This instrumental setup was replicated on each side of the wall. All the sensors were connected to a DataTaker DT85 data logger and readings were recorded at 1 minute intervals.

According to CIBSE Guide A [26] (Tables 3.38, 3.47), reference values of $R$ and $\rho C$ for the wall under consideration should be in the range of $[0.279, 0.3839]$ ($m^2K/W$) and $[3.01 \times 10^5, 3.76 \times 10^5]$ ($J/m^2K$), respectively. The temperature in Room 2 fluctuated based on hourly weather data collected from Nottingham city during 8 to 15 February 2014.

Figure 6.1 shows the temperature and heat flux time series, each consisting of 6,900 measurements, with a recording interval of one measurement per minute. Clearly, these raw measurements are contaminated by unknown noise. To analyze this noise, we use a smoothing spline method to fit a curve to each time series. This approach is based on the reasonable assumption that the real temperature and heat flux, according to the characteristics of the conducted experiment, vary smoothly over time. The noise is then approximated by the difference between the raw measure-
ments and the smooth values.

Figure 6.1: Raw temperature and heat flux measurements. Temperature in Room 2 imitates outdoor weather conditions.

Figure 6.2: Estimated noise of the raw temperature and heat flux measurements in Room 1.

### 6.3.2 Smoothing spline method

We assume that the time series \( \mathbf{y} = (y_1, \ldots, y_N) \) follows the regression model

\[
y_i = g(t_i) + \epsilon_i, \quad i = 1, \ldots, N,
\]
where \( g(\cdot) \) is a smooth function that belongs to

\[
W_2^{(m)} = \{ f : f^{(j)} \text{ is absolutely continuous, } j = 0, 1, \ldots, m-1, \text{ and } f^{(m)} \text{ is square integrable} \}
\]

and that \( \epsilon_i \) are independent Gaussian random variables with zero mean and unknown variance, \( \sigma^2 \). We estimate \( g \) by fitting a function to \( y = (y_1, \ldots, y_N) \) and adding a penalty measure of roughness:

\[
\min_{f \in W_2^{(m)}} \frac{1}{N} \sum_{i=1}^{N} (f(t_i) - y_i)^2 + \lambda \int (f^{(m)}(u))^2 du,
\]

where \( \lambda \) is the smoothing parameter. There are several methods on how to choose the smoothing parameter, \( \lambda \) (see, for example, [27, 28]). Here, we consider a cubic smoothing spline estimator for \( g \) where \( m = 2 \), which is computed by a MATLAB function (CSAPS). We choose \( \lambda \) to minimize the autocorrelation function of the estimated noise.
6.3.3 Data analysis

Figures 6.2 and 6.3 show the estimated noise of the raw temperature and heat flux measurements on both sides of the wall. We notice that the estimated noise, especially in Room 1, is not Gaussian. Also, the autocorrelation function of the noise shows strong correlations, requiring the estimation of dense covariance matrices. We therefore consider a non-overlapping moving average of the raw data by computing local averages for every five consecutive measurements, where 5 is the lag of the moving average. The lag 5 arises from the selection criterion that minimizes the total sum of the squared autocorrelation functions of the noise for the four time series. Figures 6.4 and 6.5 show the estimated noise of the moving average temperature and heat flux, where we can see that the estimated noise looks Gaussian for all the time series. Moreover, the corresponding autocorrelations are considerably reduced. We replace the raw measurements shown in Figure 6.1 with the moving average series and henceforth refer to these series as the data. Meanwhile, the original time series will be referred as raw data.

We distinguish between the moving average series based on their usage. The heat flux moving averages are used in the likelihood functions (6.7) and (6.9) associated with noise covariance matrices. Figures 6.4 and 6.5 show that the heat flux noises are almost stationary. This property can be tested by using the Ljung-Box Q-test on the two residual series (see [29]). Test results show evidence to accept the null hypothesis that the residual series are not autocorrelated. Therefore, we need only to estimate the corresponding variance of each residual series which is approximated by the sample variance with zero mean. On the other hand, the temperature moving averages are used to obtain data-driven priors (6.8). In this case, we first approximate the mean functions, \( \mu_{\text{int}} \) and \( \mu_{\text{ext}} \) by means of smoothing splines. Then, we choose prior covariances that represent the uncertainties induced by the previous approximation. It is reasonable to assume that such uncertainties will be similar to the estimated
noises of the temperature moving averages.

By replacing the original raw time series with the moving average series, we avoid estimating full covariance matrices of long time series which can be a difficult task, fulfilling the assumptions governing the statistical models (6.7) and (6.8). As a consequence, the number of observations is reduced from 6,900 to 1,380.

Figure 6.4: Estimated noise of the moving average temperature and heat flux in Room 1.

Figure 6.5: Estimated noise of the moving average temperature and heat flux in Room 2.
6.3.4 Numerical Example 1

In this Subsection, we report a numerical example in which we use the Bayesian framework to infer the thermal properties of the wall by following a direct approach similar to the one in [9] in which the boundary conditions, $T_{\text{int}}$ and $T_{\text{ext}}$, are assumed to be exact. However, in contrast to [9] in which raw measurements are used, here $T_{\text{int}}$ and $T_{\text{ext}}$ are approximated by smoothing splines constructed from the boundary temperature measurements. The moving average heat fluxes, $Q_{\text{int}}$ and $Q_{\text{ext}}$, are assumed to be Gaussian distributed and uncorrelated. Moreover, $\Sigma_{\text{int}} = \sigma_{\text{int}}^2 I$, $\Sigma_{\text{ext}} = \sigma_{\text{ext}}^2 I$, where $\sigma_{\text{int}} = \sigma_{\text{ext}} = 0.66$, which is the empirical standard deviation of the two moving average heat flux series. In this example, to get a likelihood function of $\theta$, we modify the joint likelihood (6.7) by removing the dependency of $T_{\text{int}}$ and $T_{\text{ext}}$, which are assumed to be known. In other words, the likelihood is given by

$$
\mathcal{L}(\theta|Q_{\text{int}}, Q_{\text{ext}}) = \frac{1}{(2\pi \sigma_{\text{int}} \sigma_{\text{ext}})^N} \exp \left\{ - \frac{1}{2\sigma_{\text{int}}^2} ||Q_{\text{int}} - F_{\text{int}}||_2^2 + \frac{1}{2\sigma_{\text{ext}}^2} ||Q_{\text{ext}} - F_{\text{ext}}||_2^2 \right\} .
$$

(6.10)

Before applying Bayesian inference, we first compute the maximum likelihood estimate and validate the forward model with the raw measurements.

We maximize the likelihood function using a MATLAB function (FMINUNC) with several initial guess points. In the optimization algorithm, the heat equation is solved using $M = 60$ in the space mesh for each time step, $\Delta t = 60$ seconds. The heat flux functions are computed by equations (6.14)-(6.15) for every five time steps. Then, the maximum likelihood (ML) estimates of the model parameters are

$$
R = 0.3107, \quad \rho C = 3.17 \times 10^5, \quad \tau_0 = 16.11 .
$$

Note that the values of $R$ and $\rho C$ are well within the range provided by the tabulated values as described at the beginning of this section. We also assess the
consistency of such ML estimates by plugging them into the forward model to compare the simulated heat flux with the experimental measurements. Figures 6.6 and 6.7 show that the heat flux simulations, computed by using the above ML estimates of \( \theta \), are consistent with the data.

![Figure 6.6: Raw heat flux measurements (red dots) with a model prediction for Room 1.](image)

We now take the Bayesian approach by computing the posterior distribution of \( \theta \) associated with the likelihood (6.10):

\[
\pi(\theta|Q_{\text{int}}, Q_{\text{ext}}) \propto \mathcal{L}(\theta|Q_{\text{int}}, Q_{\text{ext}}) \pi_p(\theta).
\]

To specify the joint prior, \( \pi_p(\theta) = \pi_p(R, \rho C, \tau_0) \), we assume independence among the parameters and we consider the following uniform priors:

\[
R \sim U(0.17, 0.36), \rho C \sim U(234000, 431000), \tau_0 \sim U(5, 25).
\]
Figure 6.7: Raw heat flux raw measurements (red dots) with a model prediction for Room 2.

The marginal posterior densities of $R$, $\rho C$ and $\tau_0$ are obtained by using the Laplace method and a Markov chain Monte Carlo (MCMC) sampling algorithm. The Laplace method provides a Gaussian approximation of the posterior distribution of $\theta$ as follows:

$$
\pi(\theta|Q_{\text{int}}, Q_{\text{ext}}) \approx \frac{1}{\sqrt{(2\pi)^3|H(\hat{\theta})|}} \exp \left\{ -\frac{1}{2} (\theta - \hat{\theta})^T H(\hat{\theta})^{-1} (\theta - \hat{\theta}) \right\},
$$

where $\hat{\theta}$ is the maximum a posteriori (MAP) probability estimate of $\theta$ and $H(\hat{\theta})$ is the inverse Hessian matrix of the negative log posterior evaluated at $\hat{\theta}$ [21, Chapter 4].

We used the random-walk Metropolis-Hastings algorithm (4) to generate MCMC samples (see [30, Chapter 6] and [31]). We ran the MCMC chain 101,000 times, with a 1,000–iteration burn-in period and every twentieth draw of the chain kept. Figure 6.8 shows that the Laplace method provides a very accurate approximation of the three posterior densities when compared with the simulation-based posterior
densities. The marginal posterior densities of $R$ and $\tau_0$ are highly concentrated around their respective modes.

**Algorithm 4** Random-walk Metropolis-Hastings algorithm

1: set an initial value for the chain: $\theta_c = \theta_0$ and choose the covariance $\text{diag}(\delta)$
2: run the forward model at $\theta_c$ up to time $t_N$
3: compute $a = \text{loglikelihood}(\theta_c) + \text{logprior}(\theta_c)$
4: draw $\theta_p$ from $N(\theta_c, \text{diag}(\delta))$
5: run the forward model at $\theta_p$ up to time $t_N$
6: compute $b = \text{loglikelihood}(\theta_p) + \text{logprior}(\theta_p)$
7: let $H = \min(1, \exp(b - a))$ and draw $r$ from $U(0, 1)$
8: if $H > r$ then
9: $\theta_c = \theta_p$
10: $a = b$
11: repeat steps (2 to 10) until $S$ posterior samples are obtained.

Figure 6.8: Marginal posteriors of the model parameters $R, \rho C$ and $\tau_0$ approximated by the Laplace method (blue line) and the random-walk Metropolis-Hastings algorithm (red line).

### 6.3.5 Numerical Example 2

In this example, we incorporate uncertainty in the observations of $T_{\text{int}}$ and $T_{\text{ext}}$ and we apply our proposed hierarchical approach to characterize the posterior distribution of $\theta$ that arises from the marginalized likelihood (6.9). More precisely, we assume that the nuisance boundary conditions, $T_{\text{int}}$ and $T_{\text{ext}}$, are modeled by the Gaussian
distributions introduced in (6.8), where \( \mu_{\text{int}} \) and \( \mu_{\text{ext}} \) are the smoothing splines constructed from the boundary temperature data and we let \( C_{\text{int,p}} = C_{\text{ext,p}} = (0.01)^2 I \) using the estimated noises of the moving average temperature series. The initial condition is approximated by the piecewise linear function (6.4) using the initial surface temperature measurements. Similar to Example 6.3.4, the moving averages, \( Q_{\text{int}} \) and \( Q_{\text{ext}} \), for heat flux are assumed to be Gaussian distributed and uncorrelated with \( \Sigma_{\text{int}} = \Sigma_{\text{ext}} = (0.66)^2 I \).

The ML estimates of the components of \( \theta \) corresponding to the marginal likelihood (6.9) are

\[
R = 0.3106, \quad \rho C = 3.20 \times 10^5, \quad \tau_0 = 16.11.
\]

Given the ML estimates, we plot the predicted median heat flux with 95% confidence bands in Figures 6.9 and 6.10, where the boundary conditions are sampled from

\[
T_{\text{int}} \sim N(\mu_{\text{int}}, (0.01)^2 I), \quad T_{\text{ext}} \sim N(\mu_{\text{ext}}, (0.01)^2 I).
\]

Figure 6.9: Median prediction (blue line) and 95% confidence bands (black lines) for the heat flux in Room 1.
One of the main contributions of our work, relative to existing Bayesian approaches that infer the thermal properties of walls, is that we use the heat equation to describe heat transfer through the wall. Analysis of the effect of the space-time discretization ($\Delta x, \Delta t$) on ML estimates of the components of $\theta$ is, therefore, necessary. We determined that the convergence of the ML estimates is quadratic with respect to $\Delta x$ and linear with respect to $\Delta t$ as shown in Figures 6.11 and 6.12 respectively. We also study the effect of the initial condition approximation by estimating the thermal properties and comparing the corresponding Akaike information criterion (AIC) for different initial conditions. The smallest AIC value indicates the preferred model among possible models [32]. Table 6.1 shows that the piecewise linear approximation of the initial condition is better than linear and higher order approximations.

We now consider the Bayesian approach using the marginal likelihood defined in (6.9) with the following uniform priors:

$$R \sim U(0.17, 0.36), \rho C \sim U(234000, 431000), \tau_0 \sim U(5, 25).$$
We again obtain the corresponding marginal posterior densities by the Markov chain Monte Carlo (MCMC) sampling algorithm (Algorithm 4) and by using the Laplace method. Figure 6.13 shows the estimated marginal posteriors for $R$, $\rho C$ and $\tau_0$. The Laplace method and the MCMC technique provide very similar estimated marginal

<table>
<thead>
<tr>
<th>Initial condition</th>
<th>$R$</th>
<th>$\rho C \times 10^k$</th>
<th>AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>0.3106</td>
<td>3.197</td>
<td>-25020</td>
</tr>
<tr>
<td>Piecewise linear</td>
<td>0.3106</td>
<td>3.20</td>
<td>-25066</td>
</tr>
<tr>
<td>Quadratic</td>
<td>0.3106</td>
<td>3.20</td>
<td>-25056</td>
</tr>
<tr>
<td>Cubic</td>
<td>0.3105</td>
<td>3.196</td>
<td>-24973</td>
</tr>
</tbody>
</table>
posterior densities. Also, Figures 6.14 and 6.15 show the correlation between the thermal resistance, $R$, and the heat capacity, $\rho C$. In Figure 6.16, we compare these marginal posteriors with the ones obtained in Subsection 6.3.4 where the boundary parameters are assumed to be deterministic. The direct deterministic approach provides over-concentrated posteriors and relatively biased MAP estimates. On the other hand, the marginalization approach incorporates uncertainties into the nuisance boundary parameters, thereby producing realistic posterior densities.

We also analyze the effect of the initial condition approximation by comparing the marginal posteriors of the thermal properties. Figure 6.17 shows that the posteriors of $R$ and $\rho C$ are very similar under three different initial conditions.

![Figure 6.13: Marginal posteriors of $R$, $\rho C$ and $\tau_0$ approximated by the Laplace method (blue line) and the random-walk Metropolis-Hastings algorithm (red line).](image)

6.3.6 Robustness analysis

To assess the robustness of our Bayesian approach, we consider a subsampling method that generates variability intervals for $R$ and $\rho C$. First, the raw time series is divided into consecutive, non-overlapping subintervals of length $\ell$. Then, we resample the original time series in which subsamples of size $b$ are drawn from each subinterval. The local average is computed for each subsample to filter the sampled time series.
Figure 6.14: Approximated bivariate posterior distribution of $R$ and $\rho C$.

Figure 6.15: Contour plot of the approximated bivariate posterior distribution of $R$ and $\rho C$.

We use smoothing splines to model the boundary temperature parameters. We then use our Bayesian approach under the same uniform priors used in Examples 6.3.4 and 6.3.5. By repeating this procedure, we obtain several MAP estimates. We summarize the variability of these estimates by means of boxplots. The subsampling procedure
Figure 6.16: Comparison between the marginal posteriors obtained by the deterministic approach (Figure 6.8) and the marginalization approach (Figure 6.13).

Figure 6.17: Comparison between the marginal posteriors of $R$ and $\rho C$ obtained by the marginalization approach under different approximations of the initial condition.

is summarized in Algorithm 5

**Algorithm 5** Subsampling algorithm

1. **partition** the raw time series into subintervals $D_i$, $i = 1, \ldots, \ell$
2. **sample** $b$ observations from each $D_i$ without replacement
3. **compute** local averages for each subsample
4. **estimate** $\mu_{\text{int}}$ and $\mu_{\text{ext}}$ using smoothing spline fit of the averaged time series
5. **apply** the Bayesian inference given the averaged heat flux measurements
6. **repeat** steps (2 to 4) **until** $S$ MAP estimates are obtained.

Figures 6.18 and 6.19 show the variability intervals obtained for $R$ and $\rho C$ using
the subsampling algorithm that draws $b$ observations randomly from each subinterval of size $\ell$. In Figure 6.18, we use $\ell = 5$ and compare the variability between drawing 4 and 3 observations. Clearly, the uncertainty increases when small subsamples are used. Similarly, Figure 6.19 shows the difference in variability between sampling algorithms that randomly draw 8, 7 and 6 observations from each subinterval. In general, the variability intervals include our MAP estimate of $\theta$ obtained in Example 6.3.5. These intervals are within a reasonable range. Such results ensure the robustness of our Bayesian methodology in estimating the thermal properties of a wall.

Figure 6.18: The variability of $R$ and $\rho C$ using subsampling algorithms with subinterval length $\ell = 5$ and subsample sizes $b = 4$ and 3.

Figure 6.19: The variability of $R$ and $\rho C$ using subsampling algorithms with subinterval length $\ell = 10$ and subsample sizes $b = 8, 7$ and 6.
6.4 Information gain

In a Bayesian framework, the utility of an experiment can be measured by the so-called information gain (relative entropy) function, which is defined by the Kullback-Leibler divergence between the prior density function, \( \pi_p(\theta) \), and the posterior density function, \( \pi(\theta|Q_{\text{int}}, Q_{\text{ext}}, \xi) \):

\[
D_{KL}(Q_{\text{int}}, Q_{\text{ext}}, \xi) := \int_{\Theta} \log \left( \frac{\pi(\theta|Q_{\text{int}}, Q_{\text{ext}}, \xi)}{\pi_p(\theta)} \right) \pi(\theta|Q_{\text{int}}, Q_{\text{ext}}, \xi) d\theta ,
\]  

where \( \xi \) is the experimental setup [23, 24].

We first consider an experimental setup that describes the duration of the measurement campaign. We use the Laplace approximation to compute the information gain for overlapping increasing time intervals. Figure [6.20] shows that the information gain increases over time as more observations are incorporated into the Bayesian inference. However, we observe that after 5000 minutes, the rate of increase of the information gain slows, indicating that the collected measurements provide reliable information on the thermal properties of the solid brick wall. We introduce another experimental setup by considering the external temperature oscillation. Figure [6.21] shows how data are partitioned on the basis of the detected external temperature cycles in Room 2. We estimate the information gain for each cycle, and the results are summarized in Table [6.2]. Cycles 1 and 3 are ranked as the most informative in terms of the Kullback-Leibler divergence, while Cycle 2 is the least informative, although Cycle 4 has the shortest duration. From these results, we can deduce that larger temperature oscillations bring more knowledge to the inference about \( \theta \), suggesting that steady state conditions cannot be used to infer the thermal properties of the wall.
Figure 6.20: The estimated information gain with respect to time.

Figure 6.21: Different temperature cycles.

### 6.5 Summary and conclusions

Our goal is to advance the mathematical modeling of the thermal properties of walls through statistical inference when in-situ measurements of surface temperatures and heat flux are available. Existing approaches are based on simplified models [9]. Our approach uses the heat equation as a forward model to describe the heat dynamics of the wall. Moreover, our statistical methodology uses a marginalization technique that includes uncertainty in the temperature measurements, which are often incorporated as exact readings. We are thus able to achieve high error reduction and remove the bias due to the measurement error in the boundary temperature readings. Ex-
perimental data collected under controlled conditions demonstrate the utility of our method. To apply our methodology, we consider preprocessing techniques that are carefully chosen to fulfill convenient model assumptions. Consequently, we reduce the noise inherent in the experimental data and simplify the computations.

We considered two main numerical examples. In the first example, we explored a deterministic approach in which smoothed temperature measurements are used as exact boundary conditions. In the second example, we removed this deterministic constraint by modeling the nuisance boundary conditions as Gaussian random functions that are then marginalized analytically. In both examples, we derived the ML estimates of the thermal properties of the wall and the approximated posterior densities of such parameters by the Laplace method and the random-walk Metropolis-Hastings algorithm. We remark that, in both examples, the two techniques for the approximated Bayesian inference produce similar marginal posterior densities for the physical parameters of the wall. Based on that, one can use the Laplace method to obtain fast and efficient results and avoid costly MCMC simulations. We emphasize that the numerical results show that the utilization of our marginalization technique considerably reduces the bias error of the estimates of the model parameters, in contrast to when boundary conditions are assumed to be deterministic. Moreover, our estimates of the thermal resistance and the heat capacitance of the wall are consistent with the corresponding tabulated values for the wall under examination [26]. We carried out computationally intensive experiments to analyze the convergence of the MAP estimates, which are computed with the numerical solver when the space step, $\Delta x$, and the time step, $\Delta t$, are small. Besides, we have checked the robustness of our Bayesian inference in estimating parameters of the heat equation model, using the design and the application of subsampling algorithms with different subinterval lengths and subsample sizes.

Finally, in the Bayesian framework, we use the Laplace method again to estimate
the information gain when the experimental setup consists either of the duration of the measurement campaign or the amplitude of the external temperature oscillation cycle. In this way, we can make recommendations on how to plan an efficient experimental design. Our numerical results indicate that a period of about 3.5 days is sufficient to gather data that allow the physical parameters of interest to be inferred with a high degree of accuracy. Moreover, our analysis shows that data corresponding to the oscillation cycles, which are characterized by a considerable variation in the temperature range, are informative. Our approach allows us to determine the optimal duration of the measurement campaign and the temperature oscillation cycle, both of which are valuable to practitioners. On the contrary, standard methods have required that data should be collected for two weeks, during the winter, such that large oscillations in temperature be avoided [11]. The numerical examples reported in this work, applied to experimental data, indicate that our approach provides an accurate and robust methodology for inferring the thermal properties of solid brick walls, as well as for determining optimal experimental conditions for cost-effective measurement campaigns.

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6.6 Appendix

6.6.1 Numerical approximation of the heat flux

Let us introduce the following notation: \( T_{m,n} = T(m\Delta x, n\Delta t) \), \( T_{\text{int}}(n\Delta t) = T_{\text{int},n} \) and \( T_{\text{ext}}(n\Delta t) = T_{\text{ext},n} \). The backward Euler discretization of the heat equation in the interval, \( (n\Delta t, (n+1)\Delta t) \), is given by

\[
\begin{cases}
\frac{1}{\Delta t} (T_{m,n+1} - T_{m,n}) - \frac{\eta}{\Delta x^2} (T_{m+1,n+1} - 2T_{m,n+1} + T_{m-1,n+1}) = 0, \quad m = 1, \ldots, M - 1 \\
T_{0,n+1} = T_{\text{int},n+1}, \\
T_{M,n+1} = T_{\text{ext},n+1},
\end{cases}
\]

(6.12)

where \( \eta = \frac{k}{\rho c} \).

Let us consider the vectors \( \mathbf{T}_n = (T_{1,n}, \ldots, T_{M-1,n})', n = 0, \ldots, N \), and the matrix

\[
A_{(M-1)\times(I-1)} = \begin{pmatrix}
-2 & 1 & 0 & 0 & \cdots & 0 \\
1 & -2 & 1 & 0 & \cdots & 0 \\
0 & 1 & -2 & 1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & 1 & -2 & 1 \\
0 & 0 & 0 & \cdots & 1 & -2
\end{pmatrix}.
\]

The discretized system (6.12) can be written in a matrix form as

\[
\frac{1}{\Delta t} (\mathbf{T}_{n+1} - \mathbf{T}_n) - \frac{\eta}{\Delta x^2} \mathbf{A} \mathbf{T}_{n+1} = \frac{\eta}{\Delta x^2} (T_{\text{int},n+1} \mathbf{a} + T_{\text{ext},n+1} \mathbf{b}),
\]

(6.13)

where \( \mathbf{a}_{(M-1)\times 1} = (1, 0, \ldots, 0)' \) and \( \mathbf{b}_{(M-1)\times 1} = (0, \ldots, 0, 1)' \).
The expression (6.13) is equal to
\[(I_{t-1} - \eta \frac{\Delta t}{\Delta x^2} A)T_{n+1} = T_n + \eta \frac{\Delta t}{\Delta x^2} (T_{int,n+1}a + T_{ext,n+1}b). \]

By letting \( \frac{\Delta t}{\Delta x^2} = \lambda \) and \( B = (I_{M-1} - \eta \lambda A)^{-1}, \) we obtain
\[T_{n+1} = B T_n + \eta \lambda (T_{int,n+1}B a + T_{ext,n+1}B b). \]

Applying recursively the previous relation, we derive
\[T_n = B^n T_0 + \eta \lambda \sum_{k=1}^{n} T_{int,k} B^{n-k+1} a + \eta \lambda \sum_{k=1}^{n} T_{ext,k} B^{n-k+1} b. \]

Now, we approximate \( F_{int} \) and \( F_{ext} \) using forward and backward differences with second-order error:
\[F_{int}(t_n) \approx \frac{k}{2\Delta x} \left[ 3T_{int,n} - 4T_{1,n} + T_{2,n} \right], \quad (6.14)\]
\[F_{ext}(t_n) \approx \frac{k}{2\Delta x} \left[ 3T_{ext,n} - 4T_{M-1,n} + T_{M-2,n} \right]. \quad (6.15)\]

By defining the vectors \( \mathbf{c} = (-4, 1, 0, \ldots, 0)' \) and \( \mathbf{d} = (0, \ldots, 0, 1, -4)' \), we obtain
\[F_{int}(t_n) \approx \frac{k}{2\Delta x} \left[ \mathbf{c}' B^n T_0 + 3T_{int,n} + \eta \lambda \sum_{k=1}^{n} T_{int,k} \mathbf{c}' B^{n-k+1} a + \eta \lambda \sum_{k=1}^{n} T_{ext,k} \mathbf{c}' B^{n-k+1} b \right], \]
\[F_{ext}(t_n) \approx \frac{k}{2\Delta x} \left[ \mathbf{d}' B^n T_0 + \eta \lambda \sum_{k=1}^{n} T_{int,k} \mathbf{d}' B^{n-k+1} a + 3T_{ext,n} + \eta \lambda \sum_{k=1}^{n} T_{ext,k} \mathbf{d}' B^{n-k+1} b \right]. \]

Finally, we construct the matrices \( H^{(N+1) \times (M-1)} \), \( H_{int}^{(N+1) \times (N+1)} \) and \( H_{ext}^{(N+1) \times (N+1)} \) as follows:

- the matrix \( H \) has the row vectors \( \mathbf{H}^i = \frac{k}{2\Delta x} \mathbf{c}' B^{i-1}, \ i = 1, \ldots, N + 1; \)
• the matrix $H_{int}$ is lower triangular and is given by

$$
\begin{pmatrix}
\frac{3}{\eta \lambda} & 0 & 0 & \ldots & 0 \\
0 & \frac{3}{\eta \lambda} + c'Ba & 0 & \ldots & 0 \\
\frac{k\eta \lambda}{2\Delta x} & c'B^2a & \frac{3}{\eta \lambda} + c'Ba & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & c'B^N a & c'B^{N-1} a & \ldots & \frac{3}{\eta \lambda} + c'Ba
\end{pmatrix}
$$

• the matrix $H_{ext}$ is lower triangular and is given by

$$
\begin{pmatrix}
0 & 0 & 0 & \ldots & 0 \\
0 & c'Bb & 0 & \ldots & 0 \\
\frac{k\eta \lambda}{2\Delta x} & c'B^2b & \frac{3}{\eta \lambda} + c'Bb & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & c'B^N b & c'B^{N-1} b & \ldots & c'Bb
\end{pmatrix}
$$

Similarly, we can construct the matrices $G_{(N+1)\times(M-1)}$, $G_{int_{(N+1)\times(N+1)}}$ and $G_{ext_{(N+1)\times(N+1)}}$.

### 6.6.2 Marginal likelihood

From equations (6.6), (6.7) and (6.8), the joint likelihood kernel of $\theta$ is given by
\[
\exp \left\{ -\frac{1}{2} \left( Q_{\text{int}}' \Sigma^{-1}_{\text{int}} Q_{\text{int}} + (H T_0)' \Sigma^{-1}_{\text{int}} (H T_0) \right) - 2 Q_{\text{int}}' \Sigma^{-1}_{\text{int}} (H T_0) \right. \\
+ Q_{\text{ext}}' \Sigma^{-1}_{\text{ext}} Q_{\text{ext}} + (G T_0)' \Sigma^{-1}_{\text{ext}} (G T_0) - 2 Q_{\text{ext}}' \Sigma^{-1}_{\text{ext}} (G T_0) \right. \\
- \frac{1}{2} \left( (H_{\text{int}} T_{\text{int}})' \Sigma^{-1}_{\text{int}} (H_{\text{int}} T_{\text{int}}) + 2 (H_{\text{int}} T_{\text{int}})' \Sigma^{-1}_{\text{int}} (H T_0) \right. \\
+ 2 (H_{\text{int}} T_{\text{int}})' \Sigma^{-1}_{\text{ext}} (H_{\text{ext}} T_{\text{ext}}) - 2 Q_{\text{int}}' \Sigma^{-1}_{\text{int}} (H_{\text{int}} T_{\text{int}}) \right. \\
- \frac{1}{2} \left. \left( (G_{\text{int}} T_{\text{int}})' \Sigma^{-1}_{\text{ext}} (G_{\text{ext}} T_{\text{ext}}) + 2 (G_{\text{int}} T_{\text{int}})' \Sigma^{-1}_{\text{ext}} (G T_0) - 2 Q_{\text{ext}}' \Sigma^{-1}_{\text{ext}} (G_{\text{ext}} T_{\text{ext}}) \right) \right. \\
- \frac{1}{2} \left( \mu_{\text{int}}' C_{\text{int}, \mu} C_{\text{int}, \mu} - 2 \mu_{\text{int}}' C_{\text{int}, \mu} T_{\text{int}} + T_{\text{int}}' C_{\text{int}, \mu} T_{\text{int}} \right. \\
+ \mu_{\text{ext}}' C_{\text{ext}, \mu} C_{\text{ext}, \mu} T_{\text{ext}} + T_{\text{ext}}' C_{\text{ext}, \mu} T_{\text{ext}} \right) \right\}. 
\]

Let \( U \) include any term that is independent from \( T_{\text{int}} \) and \( T_{\text{ext}} \); that is:

\[
U = Q_{\text{int}}' \Sigma^{-1}_{\text{int}} Q_{\text{int}} + Q_{\text{ext}}' \Sigma^{-1}_{\text{ext}} Q_{\text{ext}} + (H T_0)' \Sigma^{-1}_{\text{int}} (H T_0) + (G T_0)' \Sigma^{-1}_{\text{ext}} (G T_0) \]

\[- 2 Q_{\text{int}}' \Sigma^{-1}_{\text{int}} (H T_0) - 2 Q_{\text{ext}}' \Sigma^{-1}_{\text{ext}} (G T_0) + \mu_{\text{int}}' C_{\text{int}, \mu} C_{\text{int}, \mu} T_{\text{int}} + \mu_{\text{ext}}' C_{\text{ext}, \mu} C_{\text{ext}, \mu} T_{\text{ext}}.\]

Define

\[
t_{\text{int}, 1}' = [Q_{\text{int}}' - (H T_0)' - (H_{\text{ext}} T_{\text{ext}})'] \Sigma^{-1}_{\text{int}} \Lambda_{\text{int}} \]

\[
+ [Q_{\text{ext}}' - (G T_0)' - (G_{\text{ext}} T_{\text{ext}})'] \Sigma^{-1}_{\text{ext}} \Lambda_{\text{int}} \]

\[
\Lambda_0 = (H_{\text{int}}' \Sigma_{\text{int}}^{-1} H_{\text{int}} + G_{\text{int}}' \Sigma_{\text{int}}^{-1} G_{\text{int}} + C_{\text{int}, \mu}^{-1})^{-1}.\]

By integrating first with respect to \( T_{\text{int}} \), the marginal likelihood of \( \theta \) and \( T_{\text{ext}} \) is proportional to the product of a factor that is independent of \( T_{\text{int}} \) and the term

\[
(2\pi)^{N/2} |\Lambda_0|^{1/2} \exp \left\{ \frac{1}{2} t_{\text{int}, 1}' \Lambda_0 t_{\text{int}, 1} \right\}.\]
Now, let

\[ t'_{\text{int},2} = (Q'_\text{int} - (HT_0)') \Sigma_{\text{int}}^{-1} H_{\text{int}} + (Q'_\text{ext} - (GT_0)') \Sigma_{\text{ext}}^{-1} G_{\text{int}} + \mu_{\text{int}}' C_{\text{int,p}}^{-1}, \]

\[ \Lambda_1^{-1} = H'_{\text{ext}} \Sigma_{\text{int}}^{-1} H_{\text{ext}} + G'_{\text{ext}} \Sigma_{\text{ext}}^{-1} G_{\text{ext}} + C_{\text{ext,p}}^{-1} \]

\[ t'_{\text{ext},1} = (Q'_\text{int} - (HT_0)') \Sigma_{\text{int}}^{-1} H_{\text{ext}} + (Q'_\text{ext} - (GT_0)') \Sigma_{\text{ext}}^{-1} G_{\text{ext}} + \mu_{\text{ext}}' C_{\text{ext,p}}^{-1} \]

By integrating with respect to \( T_{\text{ext}} \), the marginal likelihood of \( \theta \) is proportional to the product of a factor that is independent of \( T_{\text{ext}} \) and the term \((2\pi)^{N/2} |\Lambda_1|^{1/2} \exp \left\{ \frac{1}{2} t'_{\text{ext},1} \Lambda_1 t_{\text{ext},1} \right\} \).
6.7 REFERENCES


Chapter 7

Ensemble-marginalized Kalman filter for linear time-dependent PDEs with noisy boundary conditions: Application to heat transfer in building walls

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Abstract

In this work, we present the ensemble-marginalized Kalman filter (EnMKF), a sequential algorithm analogous to our previously proposed approach (Ruggeri et al 2017 Bayesian Anal. 12 407–433, Iglesias et al 2018 Int. J. Heat Mass Transfer 116 417–431), for estimating the state and parameters of linear parabolic partial differential equations in initial-boundary value problems when the boundary data are noisy. We apply EnMKF to infer the thermal properties of building walls and to estimate the corresponding heat flux from real and synthetic data. Compared with a modified ensemble Kalman filter (EnKF) that is not marginalized, EnMKF reduces the bias error, avoids the collapse of the ensemble without needing to add inflation, and converges to the mean field posterior using 50% or less of the ensemble size required by EnKF. According to our results, the marginalization technique in EnMKF is key to performance improvement with smaller ensembles at any fixed time.

7.1 Introduction

Uncertainty in the thermophysical properties of building envelopes has been recognized as one of the main sources of uncertainty when simulating the thermal performance of buildings [1, 2, 3, 4, 5]. Simulations of this kind are essential to the development of cost-effective retrofitting measures aimed at improving the energy efficiency of existing buildings. Moreover, accurate uncertainty analyses of the energy performance of the housing stock are vital for drafting policies to reduce global carbon emissions [6, 11]. Most existing approaches use simplified heat diffusion models to quantify uncertainty in the thermophysical properties of walls [6, 7]. However, recent works have suggested that a PDE-constrained data-assimilation approach is required to accurately estimate the thermophysical properties of walls [8, 9].

Most existing statistical approaches that infer thermophysical properties of walls [6, 7, 8] assume that the boundary temperatures, $T_{int}(t)$ and $T_{ext}(t)$, can be approximated by their corresponding measurements recorded on the internal and external surfaces of a wall by temperature sensors. Although these approaches ignore the uncertainty in those measurements, they enable the construction of a well-defined parameter-to-measurements map that can be inverted via existing frameworks [10]. However, we recently showed that ignoring the uncertainty in boundary temperatures can lead to biased estimates of the thermophysical properties and, thus, reduce the accuracy of uncertainty analyses in energy-performance evaluations of buildings [9].

In order to account for the uncertainty of boundary measurements within a PDE-constrained Bayesian framework, we developed a marginalization technique that assimilates the available data all at once. This approach was both (i) accurate in identifying thermophysical properties of walls, and (ii) useful for developing off-line experimental design strategies to reduce the measurement campaigns.

Following these recent advances, practitioners would substantially benefit from a data assimilation framework capable of updating the probabilistic knowledge of
thermophysical properties as new measurements become available. Such a framework could be used to assess in real time whether a specific level of accuracy or uncertainty has been achieved, in order to reduce the long measurement campaigns that often involve several weeks [3]. The objective of this work is to develop a sequential Bayesian approach to infer the thermal properties of walls and estimate the corresponding heat flux within a computationally tractable framework that accounts for the uncertainty in the measurements of the boundary temperatures.

Bayesian filtering [11, 12] can be used to compute the desired distribution for a joint state-parameter assimilation problem. However, sampling is required to approximate the desired distribution when the Bayesian posterior cannot be expressed in a closed form. For example, particle filters use importance sampling to represent the posterior distribution. Unfortunately, particle filters may become computationally prohibitive [13] and, thus, unsuitable for practical implementation in real-time data assimilation. As an alternative to fully Bayesian samplers, the ensemble Kalman filter (EnKF) is the preferred method for data assimilation in partially observed systems where the underlying dynamics are nonlinear and the state space is high-dimensional [14]. Initially proposed for state estimation [15], modified versions of EnKF have been proposed to address joint state-parameter estimation [16]. The EnKF methodology uses a Gaussian approximation for the predictive step in the Bayesian filtering framework; this enables the characterization of the Bayesian posterior within the analysis step as a Gaussian distribution with mean and covariance computed via standard Kalman-like formulas. Different approaches to characterize this Gaussian distribution have led to several EnKF algorithms including the stochastic EnKF and the ensemble square-root Kalman filter that are reviewed elsewhere [17, 14].

The Gaussian approximations within the EnKF framework do not lead to algorithms with asymptotic convergence to the desired posterior when the underlying dynamics of the state-parameter system are nonlinear [18]. Nevertheless, EnKF has been
successfully used in numerous applications, including oceanography, meteorology, sub-surface flow and engineering [19, 20]. In most of these studies, the success of EnKF was reliant on ad-hoc fixes such as covariance inflation and localization [21, 22, 19]. More recently, regularized versions of EnKF were proposed that merged ideas from particle filters with iterative regularization techniques [23, 24, 8]. For example, a regularizing EnKF was applied for parameter estimation of thermal properties of walls [8]. This approach, however, focused entirely on the Bayesian parameter estimation of the thermophysical properties and did not consider joint state-parameter estimation. Consequently, the resulting algorithm required that the heat transfer model was run from the initial start time until the current assimilation time to update the state of the system (i.e., the wall-temperature profile). A joint state-parameter estimation approach for the real-time assimilation of in-situ measurements that enabled sequential updating of both the parameters and the state would be much more efficient.

In this paper, we study the joint state-parameter estimation problem within a setting of linear PDEs with noisy boundary conditions motivated by the aforementioned application which involves the mathematical modeling of heat transfer through walls. More specifically, we are interested in the real-time uncertainty quantification of thermophysical properties of walls via the sequential assimilation of in-situ measurements of the wall’s surface temperature and heat flux. We propose an ensemble-marginalized Kalman filter (EnMKF) to approximate the joint state-parameter Bayesian estimation problem for a partially observed linear system that is obtained from the discretization of linear time-dependent PDEs. In this general setting, we obtain a linear forward operator that depends nonlinearly on a vector of parameters while the observation operator is linear and independent of all parameters. In our specific application, we also adapt EnMKF and EnKF to handle an observation operator that depends linearly on the thermal resistance parameter.

The remainder of the paper is organized as follows. In Section 7.2 we introduce
the state-space formulation that can be used to analyze a class of linear PDE problems. We present the filtering approach for estimating the unknown state-parameter vectors in Section 7.3. In particular, subsection 7.3.3 provides a Bayesian formulation for the proposed marginalized filtering algorithms. Subsection 7.3.4 contains our novel ensemble-marginalized Kalman filter (EnMKF). In subsection 7.3.5, we consider a slightly modified EnKBF where the boundary conditions are sampled from their filtered distribution, and we describe the primary differences between EnMKF and the modified EnKBF. The performances of the EnMKF and the modified EnKBF algorithms are compared using real and synthetic data in Section 7.4. Conclusions are summarized in Section 7.5.

7.2 General formulation

Consider the linear time-dependent parabolic initial-boundary value problem on the domain $D \times [0, t_N] \subset \mathbb{R}^{d+1}$:

\[
\begin{aligned}
&\frac{\partial T}{\partial t} + L_\theta T = 0, \ x \in D, \ t \in [0, t_N] \\
&T(x, t) = u(x, t), \ x \in \partial D, \ t \in [0, t_N] \\
&T(x, 0) = T_0(x), \ x \in D,
\end{aligned}
\]

(7.1)

where $L_\theta T = - \sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial^2 T}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_{i}(x) \frac{\partial T}{\partial x_i} + c(x)T$ and $\theta = (a_{11}, \ldots, a_{dd}, b_1, \ldots, b_d, c)$. Our goal is to estimate $\theta$ and $T$ sequentially in time given partial observations of $T(x, t)$ and measurements of $u(x, t)$. As a special case, we consider in Section 7.4 the heat equation to model the heat transfer process through building walls and, given real measurements, we estimate the thermal properties of a brick wall.

By discretizing (7.1) using finite differences or finite elements [25], we can derive the discrete state-space model
\[
\begin{aligned}
T_k &= A_\theta T_{k-1} + B_\theta u_k + w_k, \\
y_k &= H T_k + v_k,
\end{aligned}
\] (7.2)

where \( T_k \) is the state vector at time \( t_k \), \( y_k \) corresponds to measurements of \( T_k \), \( A_\theta \) is the forward model operator that depends on the parameter vector \( \theta \), \( H \) is a linear observational map, \( B_\theta \) is the control matrix operator, and we assume that the control vector \( u_k \) follows another state observation system:

\[
\begin{aligned}
\dot{u}_k &= F u_{k-1} + q_k, \\
\dot{z}_k &= u_k + c_k,
\end{aligned}
\] (7.3)

where \( F \) is a user-defined linear evolution operator (see subsection 7.3.1) and \( z_k \) is the observed control vector at time \( t_k \). We further assume that \( w_k, v_k, q_k, c_k \) are independent centered Gaussian random vectors with covariances \( W_k, V_k, Q_k, C_k \), respectively.

The joint Bayesian estimation of \( \theta \) and \( T_k \), in a sequential filtering approach, as the observations \( \{ z_{1:k}, y_{1:k} \} \) become available can be now posed in terms of the computation of the conditional density \( p(T_k, \theta | z_{1:k}, y_{1:k}) \). Following the marginalization technique \cite{25, 9} and ideas from marginalized particle filters \cite{26, 27, 28}, we exploit the linear structure of (7.2) and propose an ensemble-marginalized Kalman filter (EnMKF) that provides an approximation of \( p(T_k, \theta | z_{1:k}, y_{1:k}) \). From (7.2), it is easy to approximate the conditional distribution \( p(T_k, \theta | u_k, y_{1:k}) \). In order to incorporate the error of the boundary conditions, we use the tractability of the distribution \( p(u_k | z_{1:k}) \). In other words, by noticing from (7.3) that \( u_k \) follows a linear dynamic system independent of (7.2), and under further Gaussian assumptions on \( u_0 \), it follows that the distribution \( p(u_k | z_{1:k}) \) can be expressed in closed form by using the Kalman filter \cite{29}. The desired joint distribution \( p(T_k, \theta | z_{1:k}, y_{1:k}) \) is then approximated by integrating out \( u_k \) from the fully joint distribution \( p(T_k, \theta, u_k | z_{1:k}, y_{1:k}) = p(T_k, \theta | u_k, y_{1:k}) p(u_k | z_{1:k}) \).
7.3 Methodology

In this section, we introduce the ensemble-marginalized Kalman filter (EnMKF) as a state-parameter estimation algorithm for the partially observed linear system (7.2). The boundary conditions \( u_k \) are estimated first by applying the classical Kalman filter to (7.3). Next, we derive a marginalized Kalman filter for the state \( T_k \), assuming that \( \theta \) is known. Then, this intermediate result is generalized to develop a joint filter for the state \( T_k \) and parameter \( \theta \) based on the EnKF framework. EnMKF differs from EnKF in the prediction step; in EnMKF, the prediction covariance of \( T_k \) is inflated by the expectation of the analysis covariance matrix of \( u_k \) with respect to \( \theta \).

7.3.1 Kalman filtering for \( u_k \)

The state-space model for \( u_k \) in (7.3) is linear and independent from \( T_k \). Therefore, we can implement Kalman filter given the observation \( z_k \) as follows:

1. Prediction step:

\[
\begin{align*}
    u_{k|k-1} &=FU_{k-1|k-1}, \\
    P_{u_{k|k-1}} &= FP_{u_{k-1|k-1}}F' + Q_k,
\end{align*}
\]

(7.4)

2. Analysis step:

\[
\begin{align*}
    K^u_k &= P_{u_{k|k-1}} \left( P_{u_{k|k-1}} + C_k \right)^{-1}, \\
    u_{k|k} &= u_{k|k-1} + K_k \left( z_k - u_{k|k-1} \right), \\
    P_{u_{k|k}} &= (I - K_k) P_{u_{k|k-1}},
\end{align*}
\]

(7.5)

where \( K^u_k \) is the Kalman gain matrix of the state-space model for the control vector \( u_k \).

Assuming \( u_0 \) is Gaussian, the Kalman filter provides the exact filtering distribution as \( N(u_{k|k}, P_{u_{k|k}}) \).
In many applications, the forward operator $F$ is unknown and autoregressive models must be considered \[30\]. Some proposals for the autoregressive forward models are:

- Random walk model AR(1)

\[
 u_k = u_{k-1} + q_k,
\]

- Random increment model AR(2)

\[
 u_k = 2u_{k-1} - u_{k-2} + q_k,
\]

with $q_k \sim N(0, Q_k)$.

In subsection \[7.4.1.1\], we impose AR(1) and AR(2) on the boundary temperatures, $T_{\text{int}}(t)$ and $T_{\text{ext}}(t)$, and compare the filtered results with the real data.

**Remark.** Although the state-space model for $u_k$ is independent from $T_k$, we apply the Kalman filter within the time propagation of either EnMDF or EnKF.

### 7.3.2 Marginalized Kalman filter for $T_k|\theta$  

Before deriving the filtering algorithm for the joint state-parameter vector, we derive the marginalized Kalman filter for the conditional state $T_k|\theta$ given the observations $(z_{1:k}, y_{1:k})$. Assuming $T_0$ is Gaussian, the Kalman filter is sufficient to estimate the filtering distribution of $T_k$ given $\theta$. We derive the conditional mean and the conditional
covariance for $T_k|\theta$ given the observations $(z_{1:k}, y_{1:k-1})$:

\[
T_{k|k-1} = E[T_k|\theta, z_{1:k}, y_{1:k-1}] = E[A_\theta T_{k-1} + B_\theta u_k + w_k|\theta, z_{1:k}, y_{1:k-1}]
\]

\[
= A_\theta E[T_{k-1}|\theta, z_{1:k-1}, y_{1:k-1}] + B_\theta E[u_k|z_{1:k}]
\]

\[
= A_\theta T_{k-1|k-1} + B_\theta u_{k|k}.
\]  \hspace{1cm} (7.6)

\[
P_{k|k-1} = Cov[T_k|\theta, z_{1:k}, y_{1:k-1}]
\]

\[
= Cov[A_\theta T_{k-1} + B_\theta u_k + w_k|\theta, z_{1:k}, y_{1:k-1}]
\]

(\text{using the mutual independence of } T_{k-1}, u_k \text{ and } w_k)

\[
= Cov[A_\theta T_{k-1}|\theta, z_{1:k-1}, y_{1:k-1}] + Cov[B_\theta u_k|\theta, z_{1:k}] + Cov[w_k]
\]

\[
= A_\theta P_{k-1|k-1} A'_\theta + B_\theta P_{u|k} B'_\theta + W_k.
\]  \hspace{1cm} (7.7)

From (7.6) and (7.7), the marginalized Kalman filter for $T_k|\theta$ is summarized by

1. Prediction step:

\[
T_{k|k-1} = A_\theta T_{k-1|k-1} + B_\theta u_k,
\]

\[
P_{k|k-1} = A_\theta P_{k-1|k-1} A'_\theta + B_\theta P_{u|k} B'_\theta + W_k,
\]

where $T_{k|k-1}$ is the state prediction at time $k$, given $\theta$ and the observations $(z_{1:k}, y_{1:k-1})$, and $P_{k|k-1}$ is the corresponding covariance matrix.

2. Analysis step:

\[
K_k = P_{k|k-1} H' \left( HP_{k|k-1} H' + V_k \right)^{-1},
\]

\[
T_{k|k} = T_{k|k-1} + K_k \left( y_k - HT_{k|k-1} \right),
\]

\[
P_{k|k} = (I - K_k H) P_{k|k-1},
\]

where $T_{k|k}$ is the state estimation at time $k$, given $\theta$ and the observations.
(z_{1:k}, y_{1:k}), and $K_k$ is the Kalman gain.

**Remark.** The prediction step can be generalized under the Bayesian approach and corresponds to the following equation:

$$p(T_k|\theta, z_{1:k}, y_{1:k-1}) = \int p(T_k|\theta, z_{1:k}, T_{k-1}) p(T_{k-1}|\theta, z_{1:k-1}, y_{1:k-1}) \, dT_{k-1}$$

$$= \int \left( \int p(T_k|\theta, u_k, T_{k-1}) p(u_k|z_{1:k}) \, du_k \right) p(T_{k-1}|\theta, z_{1:k-1}, y_{1:k-1}) \, dT_{k-1},$$

where the marginalization of $u_k$ appears explicitly. The analysis step is generalized under the Bayesian approach as

$$p(T_k|\theta, z_{1:k}, y_{1:k}) = \frac{p(y_k|T_k)p(T_k|\theta, z_{1:k}, y_{1:k-1})}{\int p(y_k|T_k)p(T_k|\theta, z_{1:k}, y_{1:k-1}) \, dT_k} \propto p(y_k|T_k)p(T_k|\theta, z_{1:k}, y_{1:k-1}).$$

### 7.3.3 Marginalized Bayesian filtering for $T_k$ and $\theta$

We now derive filtering algorithms to estimate the joint state-parameter vector, $X_k = [\theta \ T_k]'$, given the observations $(z_{1:k}, y_{1:k})$ up to time $k$. In this case, the evolution of the joint vector, $X_k$, is nonlinear and approximate filtering algorithms are needed.

We derive first the underlying Bayesian formulation for the filtering algorithms. The static parameters, $\theta$, have a trivial evolution in the prediction step and therefore we neglect their time subscript.

1. Initialization:

$$\theta \sim \rho_\Theta(\theta),$$

$$T_0 \sim \rho_{T_0}(T_0),$$

where $\rho_\Theta(\cdot)$ and $\rho_{T_0}(\cdot)$ are the prior distributions of $\theta$ and $T_0$, respectively.
2. Prediction step:

\[
p(X_k|z_{1:k}, y_{1:k-1}) = p(T_k, \theta|z_{1:k}, y_{1:k-1}) = p(T_k|\theta, z_{1:k}, y_{1:k-1})p(\theta|z_{1:k}, y_{1:k-1})
\]

\[
= \left( \int p(T_k|\theta, z_{1:k}, T_{k-1})p(T_{k-1}|\theta, z_{1:k-1}, y_{1:k-1})dT_{k-1} \right) p(\theta|z_{1:k-1}, y_{1:k-1})
\]

\[
= \int p(T_k|\theta, z_{1:k}, T_{k-1})p(T_{k-1}|\theta, z_{1:k-1}, y_{1:k-1})dT_{k-1}
\]

\[
= \int \left( \int p(T_k|\theta, u_k, T_{k-1})p(u_k|z_{1:k})du_k \right) p(X_{k-1}|z_{1:k-1}, y_{1:k-1})dT_{k-1}.
\]

3. Analysis step:

\[
p(X_k|z_{1:k}, y_{1:k}) \propto p(y_k|X_k)p(X_k|z_{1:k}, y_{1:k-1})
\]

\[
= p(y_k|T_k)p(X_k|z_{1:k}, y_{1:k-1})
\]

7.3.4 EnMKF for $\theta$ and $T_k$

Here, the main idea is to consider an ensemble version of the marginalized Kalman filter introduced in 7.3.2 to approximate the Bayesian filter 7.3.3. We initialize the algorithm by drawing independently $M$ samples from the prior distributions of the parameters and the initial state, \(\{\theta^i\}_{i=1}^M\) and \(\{T_{0i}\}_{i=1}^M\). Then, in the prediction step, we evolve each state vector $T_{0i}$ in time given the parameters $\theta^i$ to obtain the state vectors at time $t_1$. The measurements at time $t_1$ are then utilized in the analysis step to update both states and parameters. We iterate the prediction and analysis steps until we use all measurements and reach the final time point $t_N$.

The evolution of the joint vector, $X_k$, is nonlinear because $T_k$ depends on $\theta$ nonlinearly. Therefore, we cannot use Kalman filter directly. The ensemble Kalman framework is introduced to handle the nonlinear dependence on $\theta$, and it uses a
Gaussian approximation to update the ensemble members in the analysis step. In our EnMKF algorithm, we exploit the conditional linearity of the joint vector to derive its prediction mean and covariance.

Following the stochastic EnKF scheme [19, 16], we assume a trivial evolution of the static parameters and denote the samples from $p(\theta|y_{1:k-1})$ by $\theta^i_{k-1}$. Given the ensemble size $M$, we compute the predicted state $T^i_{k|k-1} = E[T^i_k|\theta^i_{k-1}, z_{1:k}, y_{1:k-1}]$ for each $i = 1, \ldots, M$ as

$$T^i_{k|k-1} = A\theta^i_{k-1} T^i_{k-1|k-1} + B\theta^i_{k-1} u_{k|k}. \tag{7.8}$$

The prediction covariance matrix, $P_{k|k-1}$, is usually approximated by the sample covariance matrix of $X_{k|k-1}$:

$$\frac{1}{M-1} \sum_{i=1}^{M} (X^i_{k|k-1} - \bar{X}_{k|k-1})(X^i_{k|k-1} - \bar{X}_{k|k-1})', \tag{7.9}$$

where $\bar{X}_{k|k-1} = \frac{1}{M} \sum_{i=1}^{M} X^i_{k|k-1}$. This approximation is needed due to the nonlinearity. Instead, we derive the covariance matrix of $X_{k|k-1}$ using the law of total covariance.
by conditioning on $\theta_{|k-1}$:

$$P_{k|k-1} = \text{Cov}(X_k|z_{1:k}, y_{1:k-1})$$

$$= \text{Cov}(E[X_k|\theta_{|k-1}, z_{1:k}, y_{1:k-1}]) + E\text{Cov}(X_k|\theta_{|k-1}, z_{1:k}, y_{1:k-1})$$

$$= \text{Cov}(E \left[ \theta \left| \theta_{|k-1}, z_{1:k}, y_{1:k-1} \right. \right]) + E \text{Cov}(E \left[ \theta \left| \theta_{|k-1}, z_{1:k}, y_{1:k-1} \right. \right])$$

$$= \text{Cov}(E \left[ T_k \left| \theta_{|k-1}, z_{1:k}, y_{1:k-1} \right. \right]) + E \text{Cov}(E \left[ T_k \left| \theta_{|k-1}, z_{1:k}, y_{1:k-1} \right. \right])$$

$$= \text{Cov}(E \left[ T_k \left| \theta_{|k-1}, z_{1:k}, y_{1:k-1} \right. \right]) + E \text{Cov}(E \left[ T_k \left| \theta_{|k-1}, z_{1:k}, y_{1:k-1} \right. \right])$$

$$= \frac{1}{M - 1} \sum_{i=1}^{M} \left[ (\theta_{|k-1}^i - \bar{\theta}_{|k-1}^i)(\theta_{|k-1}^i - \bar{\theta}_{|k-1}^i)' \right] + \frac{1}{M} \sum_{i=1}^{M} \left[ 0 \begin{bmatrix} 0 & 0 \\ 0 & A_{\theta^i_{|k-1}} P_{k|k-1} A_{\theta^i_{|k-1}}' + B_{\theta^i_{|k-1}} P_{k|k} B_{\theta^i_{|k-1}}' + W_k \end{bmatrix} \right],$$

(7.10)

where $\bar{\theta}_{|k-1} = \frac{1}{M} \sum_{i=1}^{M} \theta_{|k-1}^i$, and $P_{k|k-1}$ must be computed using the Kalman update equations:

$$P_{k|k}^i = (I - P_{k|k-1} H'(H P_{k|k-1} H + V_k)^{-1} H) P_{k|k-1},$$

$$P_{k|k-1}^i = A_{\theta^i_{|k-1}} P_{k|k-1} A_{\theta^i_{|k-1}}'.$$

Computing and storing these covariance matrices $P_{k|k}^i$ and $P_{k|k-1}^i$ for each $i = 1, \ldots, M$ may be burdensome, especially when $\text{dim}(T_k)$ is large. Therefore, we consider the following approximation of the prediction covariance matrix:

$$P_{k|k-1} \approx \frac{1}{M - 1} \sum_{i=1}^{M} (X_{k|k-1}^i - \bar{X}_{k|k-1})(X_{k|k-1}^i - \bar{X}_{k|k-1})' + \frac{1}{M} \sum_{i=1}^{M} \left[ 0 \begin{bmatrix} 0 & 0 \\ 0 & B_{\theta^i_{|k-1}} P_{k|k} B_{\theta^i_{|k-1}}' + W_k \end{bmatrix} \right],$$

(7.11)
which requires the computation of $B_{\theta_i|k-1} P_{k|k}^u B_{\theta_i|k-1}'$ for each $i = 1, \ldots, M$ in addition to the standard prediction covariance of EnKF (7.9). The additional term in (7.11) can be interpreted as inflation with respect to $u_k$ and $w_k$. The full prediction covariance (7.10) provides an extra inflation with respect to $T_{k-1}$. However, it is computationally intractable except in very simple cases. The standard practice in EnKF is to consider the sample covariance (7.9) only. Our implementation (7.11) inflates the covariance in a tractable way. In the next section, we introduce another algorithm where we sample $u_k$; therefore, the inflation is not needed.

After applying the prediction step in (7.8) and (7.11), the analysis step for $X_k$ is computed by

$$K_k = P_{k|k-1} H' \left( HP_{k|k-1} H' + V_k \right)^{-1},$$
$$X_{k|k}^i = X_{k|k-1}^i + K_k \left( y_k + v_k^i - H X_{k|k-1}^i \right),$$

where $H = \begin{bmatrix} 0 & H \\ m \times (p+n) & m \times n \end{bmatrix}$ is the observation operator that maps the augmented vector $X_k$ to the corresponding observation space and $v_k^i \sim N(0, V_k)$ is used to perturb the observations.

A clear advantage of EnMKF is that it runs sequentially on time without the need to restart from the initial state. At a given time $t_k$, the static parameters are updated in the analysis step using measurements at time $t_k$. We summarize the complete algorithm of EnMKF in Algorithm 6.
Algorithm 6 Ensemble-marginalized Kalman filter (EnMKF)

1: draw an initial ensemble $\theta^i, i = 1, \ldots, M$ from the prior distribution $\rho_\Theta(\theta)$
2: draw independently an initial ensemble $T_0^i, i = 1, \ldots, M$ from a normal prior distribution $N(T_0, P_0)$
3: for $k = 1$ to number of time observation $N$ do
4: run the Kalman filter for $u_k$ (equations (7.4) and (7.5)) to obtain $u_{k|k}$ and $P_{u|k}$
5: run the prediction step for $i = 1, \ldots, M$
   
   $T_k^i_{k|k-1} = A_{\theta|k-1} T_{k-1|k-1}^i + B_{\theta|k-1} u_k^i$
6: compute the prediction covariance matrix $P_{k|k-1}$ using (7.11)
7: run the analysis step for each $X^i, i = 1, \ldots, M$
   
   $K_k = P_{k|k-1} H\left(H P_{k|k-1} H^T + V_k\right)^{-1}$
   $X_k^i = X_{k|k-1}^i + K_k \left(y_k + v_k^i - H X_{k|k-1}^i\right), v_k^i \sim N(0, V_k)$

In general, ensemble Kalman filters suffer from bias errors, especially with nonlinear systems. A common bias error is due to the Kalman formula that assumes Gaussianity. Nevertheless, the incorporation of the boundary temperature uncertainties will reduce the total bias error in the estimated parameters [9]. We show in subsection 7.4.5 that EnMKF admits smaller bias errors than the following EnKF algorithm.

7.3.5 Ensemble Kalman filter for $\theta$ and $T_k$

An alternative approach to solve our problem (7.2)–(7.3), is to apply an adequately modified EnKF to the joint vector $X_k = [\theta \ T_k]^T$. In this modified EnKF, the control vector $u_k$ is sampled from its distribution, which was determined during the prediction step. Thus, we sample $u_k^i$ from $N(u_{k|k}, P_{k|k}^u)$ for each $i = 1, \ldots, M$. Then, the prediction step differs from (7.8) and is given by

$$T_k^i_{k|k-1} = A_{\theta|k-1} T_{k-1|k-1}^i + B_{\theta|k-1} u_k^i.$$
In this case, the prediction covariance matrix is approximated by

\[
\frac{1}{M-1} \sum_{i=1}^{M} (X_{k|k-1}^i - \bar{X}_{k|k-1})(X_{k|k-1}^i - \bar{X}_{k|k-1})' + \begin{bmatrix} 0 & 0 \\ 0 & W_k \end{bmatrix}.
\] (7.14)

The analysis step is the same as the one that we developed for EnMKF, which is summarized by equations (7.12) and (7.13).

Both EnMKF and EnKF are Monte Carlo implementations of Bayesian filtering. The main difference appears in the prediction step, especially in the integration with respect to \( u_k \). In EnMKF, we use the fact that \( u_k|z_{1:k} \) and \( T_k|\theta, u_k, T_{k-1} \) have Gaussian distributions and, therefore, the resulting distribution is Gaussian with mean (7.6) and covariance (7.7). In EnKF (7.3.5) the same integral is approximated with the Monte Carlo method by sampling from \( p(u_k|z_{1:k}) \).

The modified EnKF approach avoids the computation of the matrices \( B_{\theta|k-1}^i \), \( P_{\theta|k} B_{\theta|k-1}^i \) that are needed in formula (7.11) of EnMKF. However, the additional term in EnMKF can be considered inflation induced from the law of total covariance by conditioning on the unknown parameters \( \theta \). Similarly, the joint distribution of the state and parameters can be split into the distribution of the conditional state and the marginal distribution of the parameters [31]. In our case, the linear evolution of the state and control vectors simplifies the conditional distribution to the conditional mean (7.6) and the conditional covariance (7.7).

### 7.4 Real-world application: Heat transfer across a solid brick wall

In this section, we show how to formulate and implement the EnMKF method to deal with the state and parameter estimation problem in a real-world heat-transfer application, which is summarized in subsection 7.4.1. Next, we compare the results obtained with the EnMKF Algorithm [6] to those obtained with the modified EnKF.
method from Section 7.3.5 using experimental and synthetic data. We also propose stopping criteria that indicate when the ensemble parameters are stationary with adequate non-zero variance.

We consider the problem of describing the thermal performance of a solid wall given in-situ measurements. This can be posed as a state and parameter estimation problem constrained by the heat equation. For simplicity, we consider the case of a single-layer wall with homogeneous density, thermal conductivity, and specific heat capacitance. Therefore, we characterize the thermophysical properties of the wall in terms of its heat capacity per unit area \( J/m^2K \) and thermal resistance \( m^2K/W \). These are denoted by \( \rho C \) and \( R \), respectively. Under the standard assumption of uni-directional heat flux across the wall’s thickness, the forward model is described by the internal temperature profile of the wall, denoted by \( T(x,t) \). This profile is the solution to the 1D heat equation \([32]\):

\[
\frac{\rho C}{L} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \frac{L}{R} \frac{\partial T}{\partial x} \right), \quad x \in (0,L), \quad t \in [0,t_N]
\]

\[
\begin{cases}
T(0,t) = T_{int}(t), \quad t \in [0,t_N] \\
T(L,t) = T_{ext}(t), \quad t \in [0,t_N] \\
T(x,0) = T_0(x), \quad x \in (0,L),
\end{cases}
\] (7.15)

where \( L \) is the wall thickness, \( T_{int} \) and \( T_{ext} \) are the internal and external wall surface temperatures, respectively, and \( T_0(x) \), is the initial temperature of the wall. The goal is to estimate the thermophysical properties \( \theta = (R, \rho C) \) given boundary temperature measurements \( T_{int} \) and \( T_{ext} \) as well as measurements of the internal and external boundary heat flux defined via:

\[
\begin{cases}
F_{int}(t) = -\frac{L}{R} \frac{\partial T}{\partial x} |_{x=0}, \\
F_{ext}(t) = -\frac{L}{R} \frac{\partial T}{\partial x} |_{x=L}.
\end{cases}
\] (7.16)
An experimental setting consistent with (7.15)-(7.16) can be designed by placing temperature sensors and heat flux meters on the internal and external surfaces of the wall [9, 8]. These quantities are then monitored for a period of time which often consists of at least two weeks. In order to reduce the effect of solar radiation (not considered in (7.15)), measurement campaigns are usually conducted on north-facing walls during the winter [33]. For simplicity, we also assume that the initial condition, \( T_0(x) \), is well-approximated by the piecewise linear function

\[
\begin{align*}
T_{\text{int}}(0) + 2\frac{\tau_0 - T_{\text{int}}(0)}{L}x & \quad \text{if } 0 < x \leq \frac{L}{2} \\
\tau_0 + 2\frac{T_{\text{ext}}(0) - \tau_0}{L}(x - \frac{L}{2}) & \quad \text{if } \frac{L}{2} < x < L,
\end{align*}
\]

where we assume \( \tau_0 = 16.1^\circ C \), according to the estimate we obtained in our previous study [9].

To formulate the discrete state observation system, we consider the following uniform space-time discretization:

\[
x_0 = 0, x_1 = \Delta x, \ldots, x_i = i\Delta x, \ldots, x_n = n\Delta x = L,
\]

\[
t_0 = 0, t_1 = \Delta t, \ldots, t_j = j\Delta t, \ldots, t_N = N\Delta t,
\]

and denote by \( \hat{T}_k = (T(\Delta x, k\Delta t), \ldots, T((n-1)\Delta x, k\Delta t)), T_{\text{int},k} = T_{\text{int}}(k\Delta t) \) and \( T_{\text{ext},k} = T_{\text{ext}}(k\Delta t) \) the inner, internal and external surface temperatures at time \( t_k \), respectively. The inner temperature vector \( \hat{T}_k \) can be written as a linear function of \( T_{\text{int},k} \) and \( T_{\text{ext},k} \) as follows [9]:

\[
\hat{T}_k = \tilde{A}_\theta \hat{T}_{k-1} + \tilde{B}_{\theta,int} T_{\text{int},k} + \tilde{B}_{\theta,ext} T_{\text{ext},k},
\]

where the matrices \( \tilde{A}_\theta, \tilde{B}_{\theta,int}, \) and \( \tilde{B}_{\theta,ext} \) are specified exactly (see [9]).

We let \( T_k = [ T_{\text{int},k} \ T_k' \ T_{\text{ext},k}]' \) be the temperature vector on the closed interval
Then, the time evolution equation of the state vector \( T_k \) is given by

\[
T_k = A_\theta T_{k-1} + B_{\theta,\text{int}} T_{\text{int},k} + B_{\theta,\text{ext}} T_{\text{ext},k}.
\]  

(7.18)

The heat-flux vector \( F_k = \begin{bmatrix} F_{\text{int},k} & F_{\text{ext},k} \end{bmatrix}' \) is approximated by the first difference

\[
F_{\text{int},k} = \frac{1}{R} \frac{1}{2\Delta x} (3T_{\text{int},k} - 4T_{1,k} + T_{2,k})
\]

\[
F_{\text{ext},k} = \frac{1}{R} \frac{1}{2\Delta x} (3T_{\text{ext},k} - 4T_{n-1,k} + T_{n-2,k}).
\]

Therefore, the observation matrix operator takes the form

\[
H = \frac{1}{2\Delta x} \begin{bmatrix} 3 & -4 & 1 & 0 & \ldots & 0 \\ 0 & \ldots & 0 & 1 & -4 & 3 \end{bmatrix}
\]

and the observation equation is

\[
y_k = \frac{1}{R} HT_k + v_k,
\]  

(7.19)

where \( v_k \sim N(0, V_k) \) is the measurements noise and \( H = \begin{bmatrix} 0 & H \end{bmatrix} \) is the observation operator that maps the augmented vector \( X_k \) to the observation space.

We define the observation matrix operator without \( R \) to avoid dependence of the Kalman gain on this unknown parameter. Instead, we keep the Kalman gain fixed in each iteration of the algorithm and modify the so-called innovation to be \( R y_k - HT_k \). We tailor the EnMKF in Algorithm 6 to the state observation system (7.18)-(7.19).
in Algorithm 7 by augmenting the state vector with log$(R)$ and log$(\rho C)$ to ensure that the physical parameters are positive.

The heat conduction problem described in (7.15) for a single-layer wall model is relevant for the experimental setting described in the following subsection. However, it is important to emphasize that the EnMKF algorithm introduced in subsection 7.3.4 can be used to infer thermophysical properties of a much wider class of walls. Multilayer walls, for example, can be described by suitable modifications to (7.15) that incorporate the thermophysical properties on each layer. Each of these properties can then be included in the unknown vector of parameters $\theta$ that is inferred within the EnMKF.

### 7.4.1 Experimental data set

We use real data from an experiment conducted inside an environmental chamber in the Energy Technologies Building at Nottingham University Innovation Park. The chamber was divided into two rooms by a 215–mm thick partition wall. The aim of the experiment was to estimate the thermal properties of a brick section of the partition wall. The temperature in both rooms was controlled to resemble internal conditions in Room 1 and external conditions in Room 2. The wall boundary temperature and heat-flux measurements were recorded every minute by sensors placed on the surface of the brick wall [9].

Figure 7.1 shows the time series of the temperature and heat flux measurements corresponding to the two sides of the brick wall, identified by internal and external measurements. The measurements contain noise that we can analyze, in a non-sequential framework, by using a smoothing spline method to fit a curve to each time series. Then, we approximate the noise by the difference between the measurements and the smooth curve values. The noise variance is estimated to be around 0.01 for the temperature measurements. The noise variances for the internal and external
Algorithm 7 EnMKF algorithm to estimate $R$, $\rho C$, $F_{int,k}$ and $F_{ext,k}$

1. **draw** an initial ensemble $\theta^i = (R^i, \rho C^i), i = 1, \ldots, M$ from a prior distribution $\rho_{\Theta}(\theta)$
2. **approximate** the initial condition $T_0$ using (7.17)
3. **draw** an initial ensemble $T^i_0, i = 1, \ldots, M$ from the normal prior distribution $N(T_0, P_0)$
4. **define** the augmented ensemble $X^i = \left[ \log(R^i) \quad \log(\rho C^i) \quad T^i \right]'$, $i = 1, \ldots, M$
5. **for** $k = 1$ **to** number of time observation **do**
6. **run** the Kalman filter for $T_{int,k}$ and $T_{ext,k}$ to obtain $T_{int,k|k}, T_{ext,k|k}, P_{int,k|k}$ and $P_{ext,k|k}$
7. **run** the prediction step for $i = 1, \ldots, M$
   \[ T^i_{k|k-1} = A_{q^i_{k-1}} T^i_{k-1|k-1} + B_{q^i_{k-1, int}} T_{int,k|k} + B_{q^i_{k-1, ext}} T_{ext,k|k} \]
8. **compute** the prediction covariance matrix
   \[ P_{k|k-1} \approx \frac{1}{M-1} \sum_{i=1}^{M} (X^i_{k|k-1} - \bar{X}_{k|k-1})(X^i_{k|k-1} - \bar{X}_{k|k-1})' \]
   \[ + \frac{1}{M} \sum_{i=1}^{M} \begin{bmatrix} 0 & 0 \\ 0 & B_{q^i_{k-1, int}} P_{int,k|k} B'_{q^i_{k-1, int}} + B_{q^i_{k-1, ext}} P_{ext,k|k} B'_{q^i_{k-1, ext}} \end{bmatrix} \]
9. **run** the analysis step for each $X^i, i = 1, \ldots, M$
   \[ K_k = P_{k|k-1} \mathcal{H}' (\mathcal{H} P_{k|k-1} \mathcal{H}' + V_k)^{-1} \]
   \[ X^i_{k|k} = X^i_{k|k-1} + K_k (R^i(y^i_k + v^i_k) - \mathcal{H} X^i_{k|k-1}) \]
   \[ v^i_k \sim N(0, V_k) \]
10. **estimate** the heat flux and its sample mean and sample covariance
    \[ F^i_k = \frac{1}{R^i_k} H T^i_{k|k} \]
    \[ \hat{F}_k = \frac{1}{M} \sum_{i=1}^{M} F^i_k \]
    \[ \hat{\Sigma}(F_k) = \frac{1}{M-1} \sum_{i=1}^{M} (F^i_k - \hat{F}_k)'(F^i_k - \hat{F}_k) \]

heat flux measurements are estimated to be 20 and 5, respectively. Therefore, the covariance matrix $V_k$ is approximated by
\[ V_k = \begin{bmatrix} 20 & 0 \\ 0 & 5 \end{bmatrix}. \]

Alternatively, we can approximate \( V_k \) by using prior knowledge on the accuracy of the measuring devices in different situations or by assuming a prior model with unknown hyper-parameters and estimate them sequentially along with the quantities of interest. Further statistical analyses and details about these experimental data are provided in [9].

![Figure 7.1: Raw temperature and heat-flux measurements. Temperature in Room 2 imitates outdoor weather conditions.](image)

### 7.4.1.1 Kalman filtering for \( u_k \)

The first step in implementing EnMKF is to run a Kalman filter for the control vector \( u_k \) in (7.3), which in this case, consists of the boundary conditions \( T_{\text{int},k} \) and \( T_{\text{ext},k} \). The forward-evolution operator for the boundary conditions is unknown but noisy measurements are available. We consider the two autoregressive models \( AR(1) \) and \( AR(2) \) from subsection 7.3.1 and use them with the measurements to apply the Kalman filter. Figures 7.2 and 7.3 show the results from the Kalman filter with each
model and the real temperature measurements. In the experiments with EnMKF and EnKF presented below, we use only the results from the Kalman filter with $AR(1)$.

Figure 7.2: Internal temperature measurements (red dots) and Kalman filter mean with AR(1) and AR(2).

Figure 7.3: External temperature measurements (red dots) and Kalman filter mean with AR(1) and AR(2).

We also estimate the variance for the boundary conditions $T_{int,k}$ and $T_{ext,k}$. For example, Figure 7.4 shows the estimated mean and confidence bands for the internal
temperature measurements using Kalman filter with AR(1). The estimated variances capture the variability of the data and therefore we can marginalize the uncertainty of the boundary conditions accurately.

![Temperature measurements](image)

Figure 7.4: Internal temperature measurements (red dots) and Kalman filter mean and 90% confidence bands with AR(1).

### 7.4.1.2 EnMKF results

We run EnMKF Algorithm 7 with $M = 100$ and using the complete experimental data set, $N = 6,900$. We initially sample $R^i$ and $\rho C^i$ from the uniform priors, $U(0.17, 0.36)$ and $U(234000, 431000)$, and sample $T_0^i$ from the normal prior distribution, $N(T_0, 0.01\mathcal{I}_n)$.

Figure 7.5 shows the convergence of the ensemble parameters $R$ and $\rho C$ with respect to time as more observations are incorporated. The thermal-resistance mean converges to 0.31 $m^2K/W$ and the mean of the heat capacity per unit area converges to $3.11 \times 10^5 J/m^2K$. As we increase the ensemble size, we obtain results that are more accurate and consistent with the MCMC results in [9]. We further analyze the convergence of EnMKF with respect to the ensemble size $M$ and compare it with the
Figure 7.5: Convergence of the thermal resistance $R$ (left) and heat capacity per unit area $\rho C$ (right) ensemble with respect to time using EnMKF with ensemble size $M = 100$.

convergence of the modified EnKF in subsection 7.4.3.

Figure 7.6: Estimated heat flux ensemble (solid lines) using EnMKF with ensemble size $M = 100$ compared with real raw measurements (red dots) in Room 1.

We also compute the heat flux from the estimated temperature and parameters by EnMKF. Figures 7.6 and 7.7 show that the estimated heat fluxes match the real measurements suitably. The corresponding variances for the estimated heat fluxes
Figure 7.7: Estimated heat flux ensemble (solid lines) using EnMKF with ensemble size $M = 100$ compared with real raw measurements (red dots) in Room 2.

converge to be smaller than 1. We recall that the heat flux measurements are very noisy and it would not be optimal to recover the measurements variance through the variance of the estimates. Figures 7.6 and 7.7 indicate that our estimates are unbiased and therefore smaller variances are preferable.

7.4.2 EnKF results

We apply the modified EnKF approach introduced in Section 7.3.5 with ensemble size $M = 100$, to infer the parameters $R$ and $\rho C$ as in the previous example. Figure 7.8 shows that the ensemble of $R$ and $\rho C$ collapse at time $t = 1734$ minutes. After this time, the parameters remain fixed at the biased estimates $R = 0.3 \, m^2 K/W$ and $\rho C = 3.42 \times 10^5 \, J/m^2 K$. Thus, the estimated heat fluxes do not match the measurements. In Figures 7.9 and 7.10, we show only the sample mean of the heat-flux ensemble because the variances of the internal and external heat fluxes are approximately 390 and 130, respectively. These values are much larger than the estimated variances produced by the EnMKF approach.

We can gradually increase the ensemble size $M$ to mitigate the ensemble collapse.
Figure 7.8: Propagation of the thermal resistance $R$ (left) and heat capacity $\rho C$ (right) ensemble with respect to time using EnKF with ensemble size $M = 100$.

Figure 7.9: Estimated heat-flux mean using EnKF with ensemble size $M = 100$ compared with real raw data measurements in Room 1.

and reduce the bias error in the estimated parameters. Figures 7.11, 7.12 and 7.13 show the estimated parameters and heat-flux mean when $M = 300$. Although the bias error of the estimated parameters is reduced, the corresponding variances still vanish as time increases, which is not a realistic feature. While the internal and external heat fluxes variances are reduced to 375 and 124, respectively, they are still
Figure 7.10: Estimated heat-flux mean using EnKF with ensemble size $M = 100$ compared with real raw data measurements in Room 2.

Figure 7.11: Propagation of the thermal resistance $R$ (left) and heat capacity $\rho C$ (right) ensemble with respect to time using EnKF with ensemble size $M = 300$. 
Figure 7.12: Estimated heat-flux mean using EnKF with ensemble size $M = 300$ compared with real raw data measurements in Room 1.

Figure 7.13: Estimated heat-flux mean using EnKF with ensemble size $M = 300$ compared with real raw data measurements in Room 2.

### 7.4.3 Comparing EnMKF and EnKF

Finally, we compare the EnMKF method and the modified EnKF method by analyzing the convergence of the estimated parameters at a fixed time with respect to the ensemble size $M$. Figures 7.14, 7.15, and 7.16 show the convergence of the parameters-ensemble mean and standard deviation with ensemble size $M$ at time
\[ t' = 3000 \text{ minutes}. \] The ensemble mean converges linearly for both methods but En-MKF has a better error constant and, therefore, is more reliable for small ensemble sizes. Moreover, due to the collapse of the ensemble, the convergence of the ensemble standard deviation for EnKF occurs only after \( M > 1000. \)

![Figure 7.14: Convergence of the ensemble mean of the estimated parameters \( R \) (left) and \( \rho C \) (right) at time \( t' = 3000 \) with respect to the ensemble size \( M. \)](image)

### 7.4.4 Stopping criteria

EnMKF solves the collapse problem that usually arises with EnKF algorithms for state-parameter estimation. Ideally, we want the ensemble of each parameter to converge with time to become samples from the posterior distribution. Assuming this posterior distribution is unimodal, the convergence of our algorithm can be confirmed by computing the ensemble mean and standard deviation for each parameter. The time convergence of these estimated values can be used to suggest stopping criteria for ongoing measurement campaigns. For example, when the difference between two consecutive means and two consecutive standard deviations are relatively small, then the measurement campaign should be stopped.
Figure 7.15: Convergence of the ensemble mean error of the estimated parameters $R$ (left) and $\rho C$ (right) at time $t' = 3000$ with respect to the ensemble size $M$.

Figure 7.16: Convergence of the ensemble standard deviation of the estimated parameters $R$ (left) and $\rho C$ (right) at time $t' = 3000$ with respect to the ensemble size $M$.

In Figures 7.17 and 7.18, we see that the ensemble mean and standard deviation for $R$ and $\rho C$ stabilize after 5000 minutes. This indicates that the measurements collected up to that time are sufficient and the experiment can be stopped.
Figure 7.17: Time convergence for the thermal resistance mean (left) and heat capacity mean (right) using EnMKF with ensemble size $M = 100$.

Figure 7.18: Time convergence for the thermal resistance standard deviation (left) and heat capacity standard deviation (right) using EnMKF with ensemble size $M = 100$.

7.4.5 Bias error analysis

We treat the boundary conditions as random variables that are marginalized in EnMKF and sampled in EnKF. In both EnKF and EnMKF, the bias error of the esti-
mated parameters and the variability of the estimated state are reduced by increasing the ensemble size. However, in EnKF, the bias error induced by the boundary conditions depends on the ensemble size, $M$; with EnMKF, that bias error is eliminated independently from $M$. Therefore, EnMKF reduces the total bias error in comparison with the EnKF. To strengthen this conclusion, we use a synthetic data set similar to the experimental data set from Nottingham University (Figure 7.1). The synthetic data are generated by assuming $R = 0.3106 \, m^2K/W$, $\rho C = 3.2 \times 10^5 \, J/m^2K$, smooth boundary conditions, and the initial condition given in (7.17). We solve the heat equation and compute the heat flux at the boundaries for each minute. The temperature and heat-flux time series are then perturbed by Gaussian white noise. The resulting synthetic data are presented in Figure 7.19.

![Figure 7.19: Synthetic data measurements of temperature and heat flux generated using $R = 0.3106$ and $\rho C = 3.2 \times 10^5$.](image)

We apply the Kalman filter to the perturbed temperature series and obtain the filtered mean temperatures and their corresponding variances. Then, we apply EnMKF and EnKF to estimate the parameters $R$ and $\rho C$ using the uniform priors:

$$R \sim U(0.28, 0.36), \quad \rho C \sim U(301000, 376000).$$
Figure 7.20: Convergence of the ensemble mean of the estimated parameters $R$ (left) and $\rho C$ (right) at time $t' = 2000$ with respect to the ensemble size $M$.

Figure 7.20 shows the convergence of the sample mean of the estimated parameters using EnMKF and EnKF at time 2000 with respect to the ensemble size. The total bias error obtained by EnMKF is smaller and more stable than the error produced by the modified EnKF. For large ensemble sizes, both methods provide similar results.

In this case, the synthetic data have Gaussian noise. In the previous sections, the real noise is not Gaussian. Nevertheless, the results show that the influence of Gaussianity assumption is not very significant when the sequential framework is applied to this heat-transfer problem.

### 7.5 Summary and conclusions

We studied the filtering problem for state observation system with random control vector and unknown static parameters. The control vectors may represent the boundary conditions or the source function of the underlying PDE model. By creating an artificial linear dynamic model for the control vector, we applied Kalman filter to obtain a Gaussian distribution of the random control vectors at each time step. The resulting
distributions were then incorporated to generate a marginalized Kalman filter for the conditional state. The ensemble-marginalized Kalman filter (EnMKF) was derived using conditional probability, in particular, the law of total covariance. The main feature of EnMKF appeared in the prediction covariance which is approximated by the sample covariance of the augmented vector inflated by $E_{\Theta} [\text{Cov} B_\theta u_k]$. Another sample-based EnKF algorithm was also proposed where the prediction covariance is only approximated by the sample covariance.

To deal with high-dimensional joint state-parameter estimation problems, fully Bayesian techniques such as particle filters are not computationally affordable. The two introduced algorithms are not fully Bayesian; thus, they may handle nonlinear state-parameter systems and high-dimensional problems. EnKF usually requires additional adjustments in order to provide better approximations to the desired posterior distribution. EnMKF, on the other hand, completely avoids the ensemble-collapse phenomenon.

We applied both algorithms to estimate the thermal properties of a solid brick wall from experimental data. We showed that EnMKF provides better results than the modified EnKF. Due to the marginalization technique in EnMKF, we prevented the collapse of the parameters ensemble without artificial inflation. EnMKF had other advantages as well, such as a reduced heat-flux variance and more accurate fit of the measurements. We also considered a synthetic data example and compared the bias error from the parameters estimated using EnMKF and EnKF. The results confirmed that EnMKF provides a smaller bias error when the ensemble size is not very large. Finally, we proposed stopping criteria to reduce the time and cost required for real experiments, based on the estimated parameters reaching a stationary period.

While the numerical results are focused on the heat-transfer application, the EnMKF can be used for a wider PDE-constrained data assimilation problems in which the boundary conditions are subject to uncertainty; these include, for example, flood
predictions via hydrological models [33].

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Chapter 8

Concluding Remarks

8.1 Summary

The problem of fatigue life prediction for metallic components is addressed in [1, 2]. In the first contribution [1], we provided a systematic approach to calibrate and rank stress-life (S-N) models given a collection of records of uniaxial fatigue experiments on unnotched dog bone specimens. An integrated set of computational tools was developed for model calibration, model comparison and cross-validation allowing the user to rank alternative statistical models based on objective criteria. Following that, we generalized the S-N models through spatial Poisson process to model multi-axial fatigue. The model was designed to be independent of the shape and size of the metallic component. New models were calibrated using fatigue experiments of notched specimens [2].

The second problem is concerned with inverse problems in linear time-dependent PDEs. A new approach to solve inverse problem with noisy boundary conditions was introduced in [3]. We showed that our method accounts for uncertainties in the boundary data and therefore reduces the bias error in the estimated parameters. The boundary conditions were modeled by means of adequate probability distributions then marginalized from the joint likelihood in a hierarchical Bayesian framework. We implemented the marginalization technique in the engineering application of inferring the thermal properties of building walls [4]. The methodology was also used to study the optimal design of experiments and minimize the duration of measurement
campaigns. Finally, a generalization of \cite{3} to a sequential framework was developed in \cite{5}. The novel ensemble marginalized Kalman filter (EnMKF) provides an instant estimation of the unknown parameters and states.

8.2 Future work

As a continuation of our work \cite{1, 2}, we study the problem of optimal design for fatigue experiments. This could save time and cost of such experiments and improve the quality of the data.
8.3 REFERENCES


