Non-linear Bayesian update of PCE coefficients

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Abstract

Given: a physical system modeled by a PDE or ODE with uncertain coefficient $q(\omega)$, a measurement operator $Y(u(q), q)$, where $u(q, \omega)$ uncertain solution.
Aim: to identify $q(\omega)$. The mapping from parameters to observations is usually not invertible, hence this inverse identification problem is generally ill-posed. To identify $q(\omega)$ we derived non-linear Bayesian update from the variational problem associated with conditional expectation. To reduce cost of the Bayesian update we offer a *functional approximation*, e.g. polynomial chaos expansion (PCE).
New: We apply Bayesian update to the PCE coefficients of the random coefficient $q(\omega)$ (not to the probability density function of q).

1. Bayesian Updating and conditional expectation

Let measurement operator

$$Y : \mathcal{Q} \times \mathcal{U} \ni (q, u(t_k)) \mapsto y_k = Y(q; u(t_k)) \in \mathcal{Y},$$

Observation $z(\omega) = \hat{y} + \varepsilon(\omega)$, random measurement error ε, 'truth' $\hat{y}$.
Bayes's theorem may be formulated as (Tarantola2004 Ch. 1.5)

$$\pi_q(q|z) = \frac{p(z|q)}{Z_s} p_q(q), \tag{1}$$

where p_q is the pdf of q, $p(z|q)$ is the likelihood.
The Bayesian update as conditional expectation is:

$$\mathbb{E}(q|\mathfrak{S}) := P_{\mathscr{Q}_\infty}(q) := \text{arg min}_{\tilde{q}\in\mathscr{Q}_\infty} \|q - \tilde{q}\|^2_{\mathscr{Q}}, \tag{2}$$

where $\mathscr{Q} := \mathcal{Q} \otimes \mathcal{S}$, $\mathfrak{S}$ a sub-σ-algebra.

Proposition 1 *There is a unique minimiser to the problem in 2, denoted by $\mathbb{E}(q|\mathfrak{S}) = P_{\mathscr{Q}_\infty}(q) \in \mathscr{Q}_\infty$, and it is characterised by the* orthogonality condition

$$\forall \tilde{q} \in \mathscr{Q}_\infty : \quad \langle q - \mathbb{E}(q|\mathfrak{S}), \tilde{q}\rangle_{\mathscr{Q}} = 0. \tag{3}$$

Proposition 2 *The subspace $\mathscr{Q}_\infty = \mathcal{Q} \otimes \mathcal{S}_\infty$ is given by*

$$\mathscr{Q}_\infty = \overline{\text{span}}\{\varphi \mid \varphi(\phi, q) := \phi(Y(q)+\varepsilon);\ \phi \in L_0(\mathscr{Y};\mathscr{Q}) \quad s.t.\ \varphi \in \mathscr{Q}\}.$$

Finding the conditional expectation may be seen as rephrasing 2 *as:*

$$q_a := \mathbb{E}(q|\sigma(Y)) := P_{\mathscr{Q}_\infty}(q) = \text{arg min}_{\phi\in L_0(\mathscr{Y};\mathscr{Q})} \|q - \varphi(\phi, q)\|^2_{\mathscr{Q}}.$$

Approximation of the conditional expectation

Assume that $L_0(\mathscr{Y};\mathscr{Q})$ in 2 is approximated by subspaces $L_{0,n} \subset L_0(\mathscr{Y};\mathscr{Q})$, where $n \in \mathbb{N}$ is a parameter describing the level of approximation and $L_{0,n} \subset L_{0,m}$ if $n < m$, such that the subspaces

$$\mathscr{Q}_n = \text{span}\{\varphi(\phi, q) \mid \phi \in L_{0,n} \subset L_0(\mathscr{Y};\mathscr{Q}) \quad s.t.\ \varphi \in \mathscr{Q}\} \subset \mathscr{Q}_\infty$$

are closed and their union is dense $\overline{\bigcup_n \mathscr{Q}_n} = \mathscr{Q}_\infty$,

Proposition 3 *Define*

$$P_{\mathscr{Q}_n}(q) := \text{arg min}_{\phi\in L_{0,n}} \|q - \varphi(\phi, q)\|^2_{\mathscr{Q}}.$$

Then the sequence $q_{a,n} := P_{\mathscr{Q}_n}(q)$ converges to $q_a := P_{\mathscr{Q}_\infty}(q)$:

$$\lim_{n\to\infty} \|q_a - q_{a,n}\|^2_{\mathscr{Q}} = 0. \tag{4}$$

Theorem 4 *With $q_{a,n}$ the condition* 3 *becomes for any $n \in \mathbb{N}_0$:*

$$\forall \ell = 0, \ldots, n : \quad \delta_{({}^{\ell}H)} \|q - q_a({}^{0}H, \ldots, {}^{n}H))\|^2_{\mathscr{Q}} = 0,$$

which determine the ${}^{k}H$ and may be written as

$$\begin{array}{llll}
{}^{0}H & \cdots + {}^{k}H\langle z^{\vee k}\rangle & \cdots + {}^{n}H\langle z^{\vee n}\rangle = & \langle q\rangle, \\
{}^{0}H\langle z\rangle & \cdots + {}^{k}H\langle z^{\vee(1+k)}\rangle & \cdots + {}^{n}H\langle z^{\vee(1+n)}\rangle = & \langle q \otimes z\rangle, \\
\vdots & \cdots & \vdots & \vdots \\
{}^{0}H\langle z^{\vee n}\rangle & \cdots + {}^{k}H\langle z^{\vee(n+k)}\rangle & \cdots + {}^{n}H\langle z^{\vee 2n}\rangle = & \langle q \otimes z^{\vee n}\rangle.
\end{array}$$

Example ($n = 1$): Linear Bayesian update

$$\begin{aligned}
{}^{0}H \quad + {}^{1}H\langle z\rangle &= \langle q\rangle \\
{}^{0}H\langle z\rangle + {}^{1}H\langle z \otimes z\rangle &= \langle q \otimes z\rangle.
\end{aligned}$$

Solving for ${}^{1}H$ and ${}^{0}H$, obtain

$$\begin{aligned}
{}^{1}H &= [\text{cov}_{qz}][\text{cov}_{zz}]^{-1} =: K \\
{}^{0}H &= \langle q\rangle - [\text{cov}_{qz}][\text{cov}_{zz}]^{-1}\langle z\rangle.
\end{aligned}$$

and linear BU will be

$$q_a = {}^{0}H + {}^{1}Hz = \langle q\rangle + K(z - \langle z\rangle).$$

Example ($n = 2$): Quadratic Bayesian update

$$\begin{aligned}
{}^{0}H \quad + {}^{1}H\langle z\rangle + {}^{2}H\langle z^{\otimes 2}\rangle &= \langle q\rangle \\
{}^{0}H\langle z\rangle + {}^{1}H\langle z^{\otimes 2}\rangle + {}^{2}H\langle z^{\otimes 3}\rangle &= \langle q \otimes z\rangle \\
{}^{0}H\langle z^{\otimes 2}\rangle + {}^{1}H\langle z^{\otimes 3}\rangle + {}^{2}H\langle z^{\otimes 4}\rangle &= \langle q \otimes z^{\otimes 2}\rangle.
\end{aligned}$$

solve for ${}^{0}H$, ${}^{1}H$, ${}^{2}H$ and $q_a = {}^{0}H + {}^{1}Hz + {}^{2}H(z, z)$.

2. Update of PCE coefficients

$$\begin{aligned}
\boldsymbol{q}_a &= \boldsymbol{q}_f + \boldsymbol{K}(\boldsymbol{z} - \boldsymbol{y}_f) \\
\sum_{\alpha\in\mathcal{J}} \boldsymbol{q}_a^{\alpha} H_{\alpha}(\boldsymbol{\theta}) &= \sum_{\alpha\in\mathcal{J}} \left(\boldsymbol{q}_f^{\alpha} + \boldsymbol{K}\left(\boldsymbol{z}^{\alpha} - \boldsymbol{y}_f^{\alpha}\right)\right) H_{\alpha}(\boldsymbol{\theta}).
\end{aligned}$$

$$\mathbf{q}_a = \mathbf{q}_f + \mathbf{K}(\mathbf{z} - \mathbf{y}_f), \quad \boldsymbol{K} = \boldsymbol{C}_{q,z}\boldsymbol{C}_{z,z}^{-1}$$

$$\boldsymbol{C}_{z,z} \approx \sum_{\alpha\in\mathcal{J},\alpha\neq 0} (\boldsymbol{\alpha}!)\, \boldsymbol{z}^{\alpha} \otimes \boldsymbol{z}^{\alpha}, \quad \boldsymbol{C}_{q,z} \approx \sum_{\alpha\in\mathcal{J},\alpha\neq 0} (\boldsymbol{\alpha}!)\, \boldsymbol{q}^{\alpha} \otimes \boldsymbol{z}^{\alpha},$$

and $\mathbf{q}_a$, $\mathbf{q}_f$, $\mathbf{z}$, $\mathbf{y}_f$ are matrices of corresponding PCE coefficients (column-wise).

3. Numerics with Lorenz-84

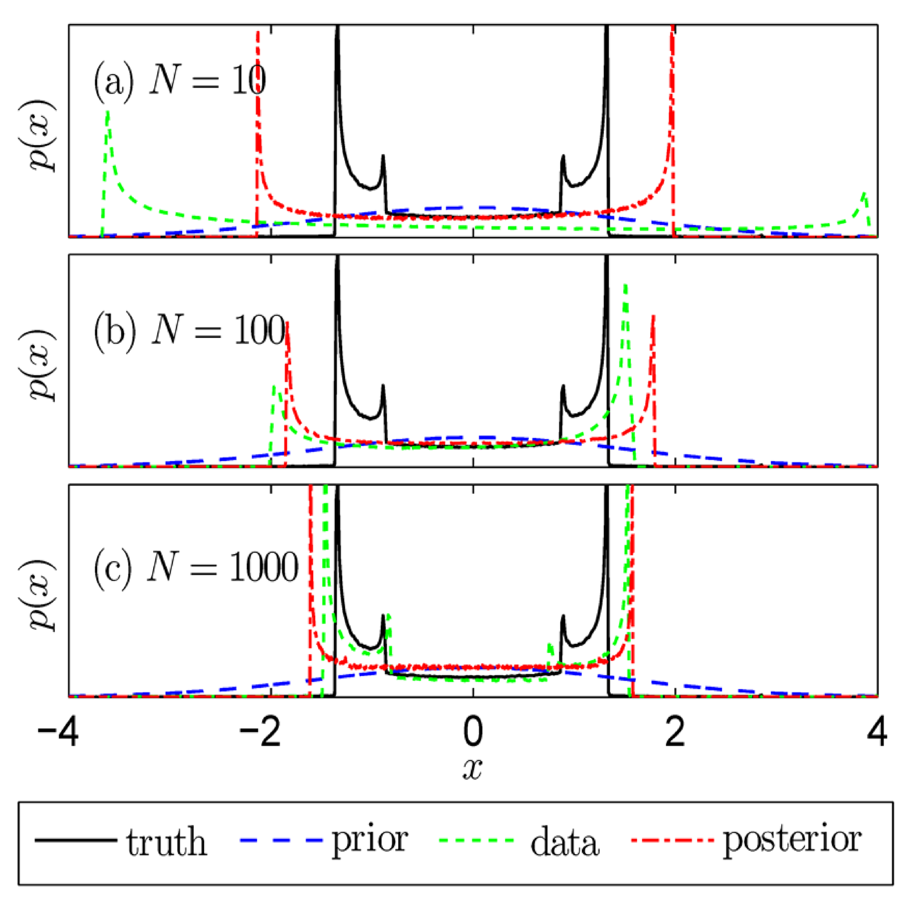

Figure 1: *pdfs for linear Bayesian update (LBU)*

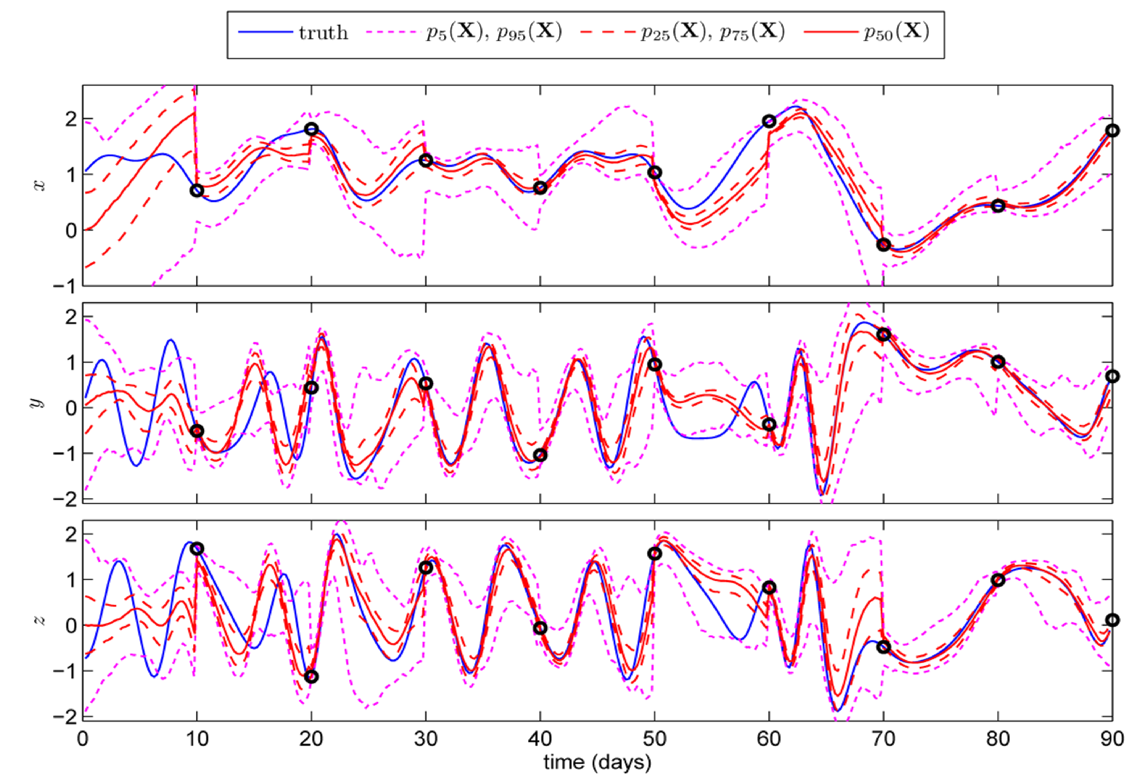

Figure 2: *Time evolution of Lorenz-84 state and uncertainty with LBU*

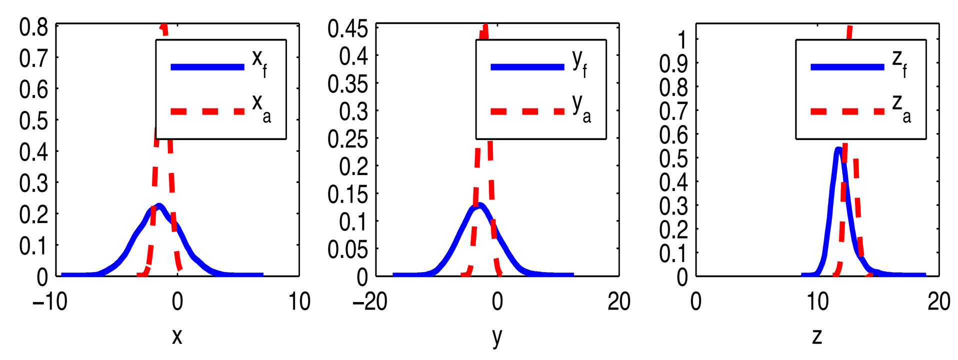

Figure 3: *Linear measurement $(x(t), y(t), z(t))$ at $t = 10$ in Lorenz-84: prior and posterior after one update*

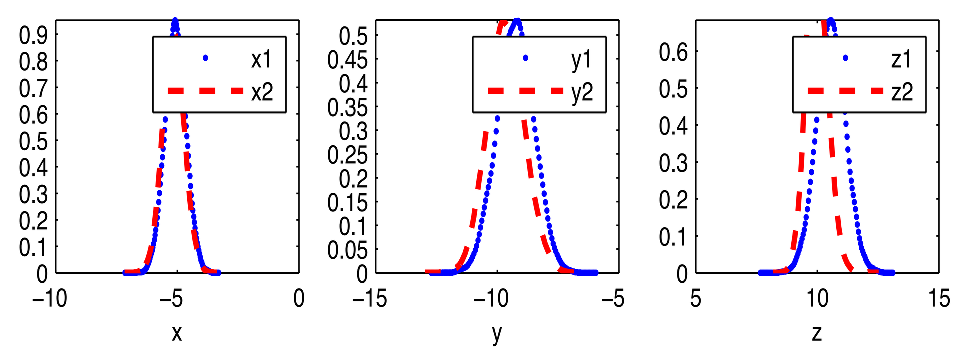

Figure 4: *Quadratic measurement $(x(t)^2, y(t)^2, z(t)^2)$ at $t = 10$ in Lorenz-84:: Comparison posterior for LBU and NLBU after one update*

Future plans

1. Compute a posteriory via MCMC and compare with results of (non-)linear BU
2. Compare linear, quadratic, cubic Bayesian updates (convergence)
3. Compute KLD between linear, non-linear and MCMC.

Conclusion

1. (non-) Linear Bayesian updates of PCE coefficients are offered. The Kalman filter is a particular case of the linear update.
2. The method is sampling free (no need for MCMC simulations).
3. To use this method (a priori) PCE coefficients of the uncertain coefficient $q(\omega)$ and of observations $Y(u(\omega))$ (or solution u) are needed.

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