Hierarchical matrix approximation of large covariance matrices

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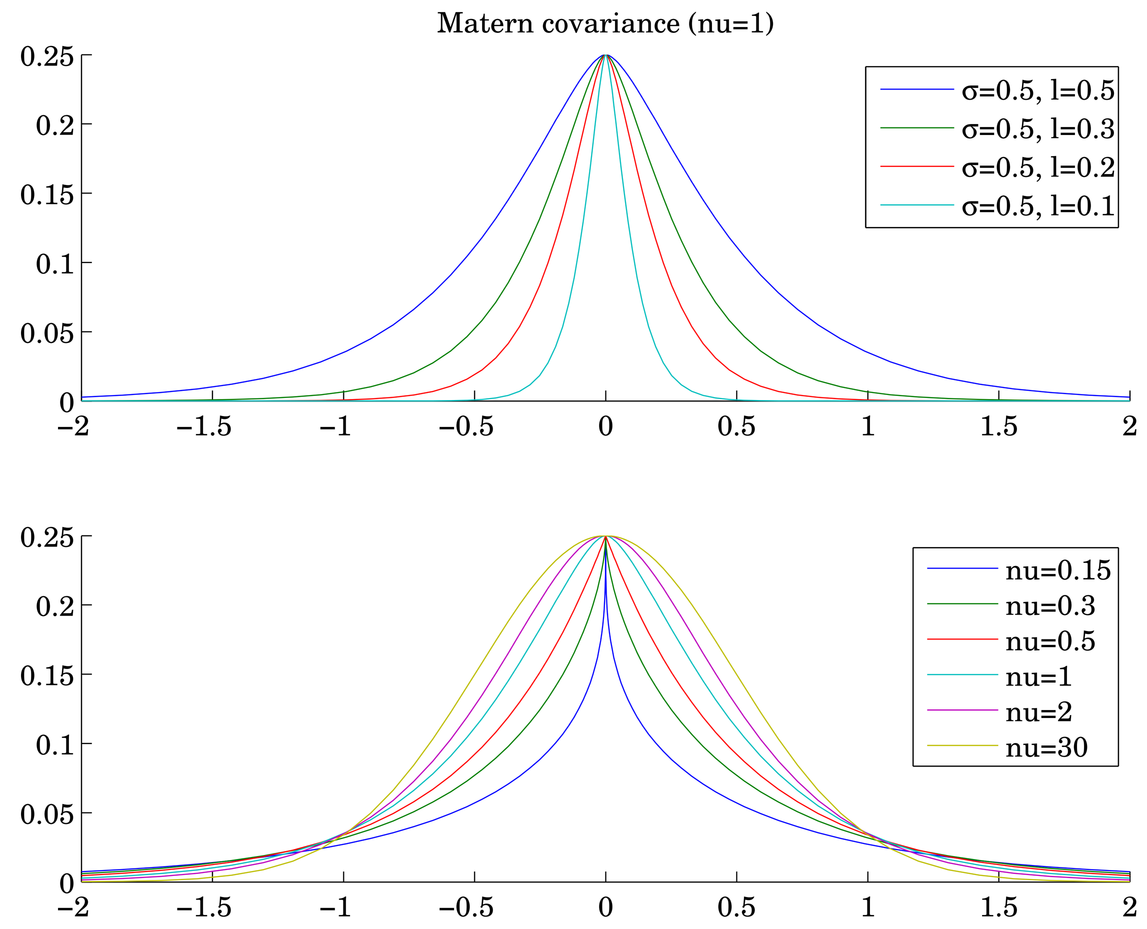
Maximum likelihood covariance estimation

We approximate large non-structured Matérn covariance matrices of size $n\times n$ in the $\mathcal{H}$-matrix format with a log-linear computational cost and storage $\mathcal{O}(kn\log n)$, where rank $k \ll n$ is a small integer. Applications are: spatial statistics, machine learning and image analysis, kriging and optimal design.

Matérn covariance function is defined as

$$C(r) := C_\theta(r) = \frac{2\sigma^2}{\Gamma(\nu)}\left(\frac{r}{2l}\right)^\nu K_\nu\left(\frac{r}{l}\right),\ \theta = (\sigma^2, \nu, l).$$



Shape of Matérn covariance functions.

Suppose we observe $\boldsymbol{z} = (z_1, ..., z_n)^T \sim \mathcal{N}(0, C(\theta^*))$ for some fixed $\theta = \theta^*$ (truth to be identified). To estimate uncertain parameter θ we maximize the log-likelihood

$$-2\ell(\theta) = N\log 2\pi + \log\det\{C(\theta)\} + \boldsymbol{z}^T C(\theta)^{-1}\boldsymbol{z},$$

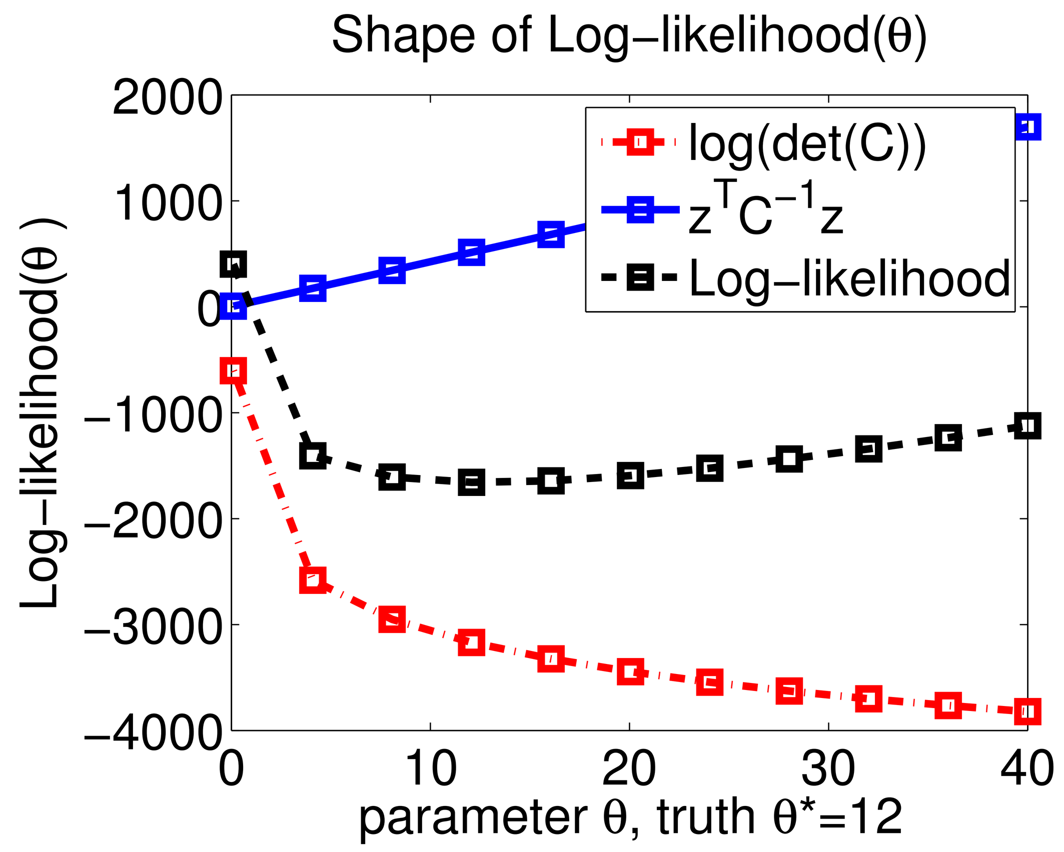
where $C = LL^T$, $\boldsymbol{z} = L(\theta^*)\cdot y$, $y \sim \mathcal{N}(0, I)$- normal distributed. On each iteration i of a maximization algorithm we have a new matrix $C(\theta_i)$. Approximate the likelihood $\ell(\theta)$ by $\tilde{\ell}(\theta, k)$, where k is the $\mathcal{H}$-matrix rank used for approximation of the covariance matrix $C(\theta) \approx C^{\mathcal{H}}(\theta, k)$.

Maximize $\tilde{\ell}(\theta, k)$ and find the parameter $\hat{\theta}(k)$, where this maximum is achieved. Here $C(\theta)^{-1}\boldsymbol{z}(\theta^*)$ is computed in two steps

$$1) L(\theta)x(\theta) = \boldsymbol{z}(\theta^*) \quad\text{and}\quad 2) L(\theta)^T r(\theta) = x(\theta).$$

$$\log\det\{C\} = \log\det\{\prod_{i=1}^n \lambda_i^2\} = 2\sum_{i=1}^n \log\lambda_i,$$

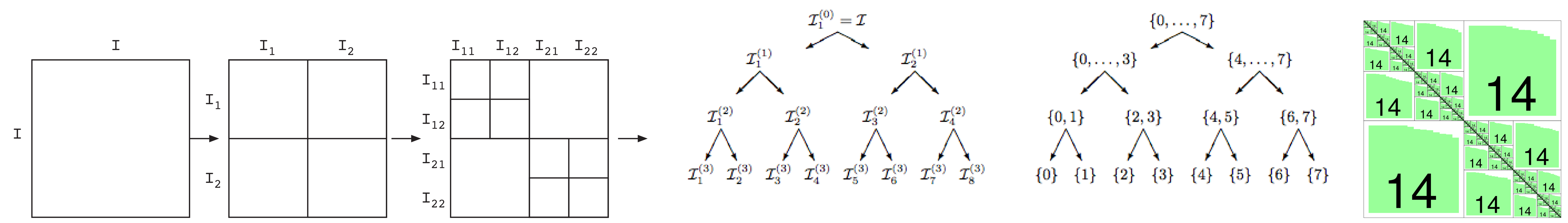
where λ_i are diagonal elements of $\mathcal{H}$-Cholesky factor L.



Minimum of negative log-likelihood (black) is at $\theta = (\cdot,\cdot,l) \approx 12$ (σ^2 and ν are fixed).

Hierarchical matrices

Advantages to approximate C by $C^{\mathcal{H}}$: $\mathcal{H}$-approximation is cheap, storage and MV $\mathcal{O}(kn\log n)$, LU and M^{-1} $\mathcal{O}(k^2 n\log^2 n)$, efficient parallel implementations exist.



$\mathcal{H}$-matrix approximations of exponential covariance $C \approx C^{\mathcal{H}} \in \mathbb{R}^{n\times n}$, $n = 32^2$, cov. lengths in x and in y directions are 0.15 and 0.2, domain $[0,1]^2$. Dense (red/dark) blocks $\in \mathbb{R}^{32\times 32}$, max. rank $k = 14$.

Numerical examples

n	rank k for $C^{\mathcal{H}}$	size, MB C	size, MB $C^{\mathcal{H}}$	t, sec. C	t, sec. $C^{\mathcal{H}}$	ε	$\max_{i=1..10} \lvert\lambda_i - \tilde{\lambda}_i\rvert$, i	ε_2
$4.0\cdot 10^3$	10	48	3	0.8	0.08	$7\cdot 10^{-3}$	$7.0\cdot 10^{-2}$, 9	$2.0\cdot 10^{-4}$
$1.05\cdot 10^4$	18	439	19	7.0	0.4	$7\cdot 10^{-4}$	$5.5\cdot 10^{-2}$, 2	$1.0\cdot 10^{-4}$
$2.1\cdot 10^4$	25	2054	64	45.0	1.4	$1\cdot 10^{-5}$	$5.0\cdot 10^{-2}$, 9	$4.4\cdot 10^{-6}$

$\mathcal{H}$-matrix approximation of exp. cov. function, cov. lengths in x, y, z directions are 0.1, 0.5 and 0.1. Column 6. Accuracy of 10 largest eigenvalues. $\varepsilon_2 := \frac{\lvert\|C\|_2 - \|\tilde{C}\|_2\rvert}{\|C\|_2}$, $\varepsilon := \frac{\|(C-\tilde{C})v\|_2}{\|C\|_2\|v\|_2}$, v - random vector.

Kullback-Leibler divergence (KLD) for miltivariate normal distributions (μ_0, C) and $(\mu_1, C^{\mathcal{H}})$ is

$$D_{KL}(\mathcal{N}_0\|\mathcal{N}_1) = 0.5\left(tr((C^{\mathcal{H}})^{-1}C) + (\mu_1-\mu_0)^T(C^{\mathcal{H}})^{-1}(\mu_1-\mu_0) - n - \log_e\left(\frac{\det C}{\det C^{\mathcal{H}}}\right)\right)$$

k	KLD $l=0.25$	KLD $l=0.75$	$\|C-C^{\mathcal{H}}\|_2$ $l=0.25$	$\|C-C^{\mathcal{H}}\|_2$ $l=0.75$	$\|C(C^{\mathcal{H}})^{-1}-I\|_2$ $l=0.25$	$\|C(C^{\mathcal{H}})^{-1}-I\|_2$ $l=0.75$
10	2.6e-3	0.2	7.7e-4	7.0e-4	6.0e-2	3.1
15	1.0e-5	9e-4	2.0e-5	1.1e-5	8.0e-4	0.02
50	3.4e-13	5e-12	2.0e-13	2.4e-13	4e-11	2.7e-9

Dependence of KLD on the approximation $\mathcal{H}$-matrix rank k, Matérn covariance with cov. length $\{0.25, 0.75\}$ in x and y directions and $\nu = 0.5$, domain $\mathcal{G} = [0,1]^2$, $\|C_{(0.25,0.75)}\|_2 = \{212, 568\}$, $n = 129^2$.

matrix, $n\times n$	n	size, GB	set up t, s.	$\mathcal{H}$-Chol. t, s.	t maximizing, s.	# iters
$\mathcal{H}$-matrix, $k=10$	66049	1	7	115	1994	13
$\mathcal{H}$-matrix, $k=20$	66049	1.7	11	370	5445	9
dense	66049	38	42	657	∞	-

Detailed computing time and number of iterations for maximization of log-likelihood $\tilde{\ell}(\theta, k)$.

Conclusion

1. We have successfully applied $\mathcal{H}$-matrix technique for the approximation of covariance matrices.
2. Parallel $\mathcal{H}$-matrix approximation is natural for huge covariance matrices.
3. Further low-rank approximation of a) Kriging, b) variance and c) geostatistical optimal design:

a) Kriging estimate $s = C_{sy}C_{yy}^{-1}y$, y - measurements, C_{sy} and C_{yy} are cross and auto-covariance matrices.
b) $\sigma = \mathrm{diag}(C_{ss|y}) = \mathrm{diag}(C_{ss} - C_{sy}C_{yy}^{-1}C_{ys})$
c) $\phi_A = n^{-1}\mathrm{trace}(C_{ss|y})$, $\phi_C = v^T\left(C_{ss} - C_{sy}C_{yy}^{-1}C_{ys}\right)v$, v a vector.

References and Acknowledgements

[1] B. N. Khoromskij, A. Litvinenko, H. G. Matthies, *Application of hierarchical matrices for computing the Karhunen-Loe?ve expan-sion*, Computing, Vol. 84, Issue 1-2, pp 49-67, 2008.

[2] Y. Sun, M. Stein, *Statistically and computationally efficient estimating equations for large spatial datasets*, JCGS,? 2015, to appear.

[3] J. Castrillon-Candas, M. Genton, and R. Yokota, *Multi-Level Restricted Maximum Likelihood Covariance Estimation and Kriging for Large Non-Gridded Spatial Datasets*, arXiv:1504.00302v1, 2015.

[4] W. Nowak, A. Litvinenko, *Kriging and spatial design accelerated by orders of magnitude: combining low-rank covariance approxi-mations with FFT-techniques*, JMathematical Geosciences, Vol. 45, N4, pp411-435, 2013.

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