Gaussian Processes and Uncertainty Quantification

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Outline

1. Gaussian Process Regression
2. Uncertainty Quantification and Inverse Problems
3. Emulators for Inverse Problems
4. Numerical Linear Algebra with Covariances

Gaussian Process Regression

Gaussian Processes

Definition (Gaussian process)

A Gaussian process $Z \sim \mathrm{GP}$ is a random field, for which any finite number of evaluations has multivariate Gaussian distribution.

- Generalisation of multivariate Gaussian distribution
- Uniquely defined by mean function $m = m(\cdot)$ and covariance function $k = k(\cdot, \cdot)$
- Write: $Z \sim \mathrm{GP}(m, k)$

Gaussian Processes

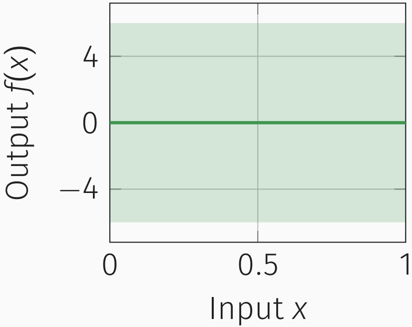


Figure 1: Gaussian process (prior distribution) with constant mean.

Gaussian Process Regression

- Goal: recover a function $f : \mathcal{X} \to \mathbb{R}$ from evaluations $f(\mathcal{X}_N) = (f(x_1), \dots, f(x_N))$ at $\mathcal{X}_N$
- Condition law of GP on attaining measurements
- Result: $\hat{Z} \sim \mathrm{GP}(m_f, k_f)$ with $m_f(x) = \sum_{i=1}^N c_i k(x, x_i)$
- Here, $k(\mathcal{X}_N, \mathcal{X}_N)c = f(\mathcal{X}_N)$.

Gaussian Process Regression

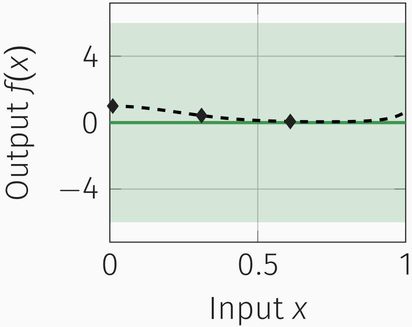


Figure 2: Gaussian process prior distribution with constant mean (green), true function (black; dashed), observations.

Gaussian Process Regression

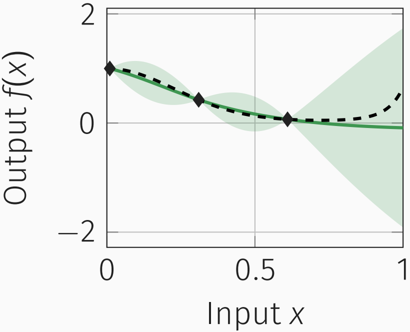


Figure 3: Gaussian process posterior distribution (green), true function (black; dashed), observations.

Error estimates

- Use Matérn kernel $k_\nu(x, y) = \varphi_\nu(\|x - y\|)$, $\varphi_\nu(s) \sim s^\nu K_\nu(s)$
- Repr. kernel Hilbert space $\mathcal{H}_k \cong H^{\nu+d/2}(\mathcal{X})$, $d = \dim(\mathcal{X})$
- Approximation order: $\|f - m_f\|_{L^2} \lesssim h^{\nu+d/2}$
- h is fill distance of $\mathcal{X}_N$

F. J. Narcowich and J. D. Ward and H. Wendland
Sobolev error estimates and a Bernstein inequality for scattered data interpolation via radial basis functions.
Constr. Approx., 24, pp. 175–186, 2006

Uncertainty Quantification and Inverse Problems

Uncertainty Quantification

- Goal: reduce uncertainty arising in computations (uncertain modelling, uncertain algorithms, ...)
- Inverse problem
- Given $\mathcal{G} : A \to Y$ and (noisy) measurements $y \in Y$, find $a \in A$ from

$$y = \mathcal{G}(a) + \eta, \quad \eta \sim \mathcal{N}(0, \sigma^2), \quad \sigma > 0$$

Inverse Problems: Differential Equation

Find $a \in [-1, 1]$ such that for

$$-\operatorname{div}(e^{1+0.5\sin(ax)}\nabla u(x)) = 1, \quad u(0) = u(1) = 0$$

the measurements satisfy

$$u(1/3) = 1.1241, \quad u(1/2) = 1.34235, \quad u(2/3) = 1.87.$$

Bayesian Approach

- Knowledge is probability distribution
- Statistical estimators using that distribution

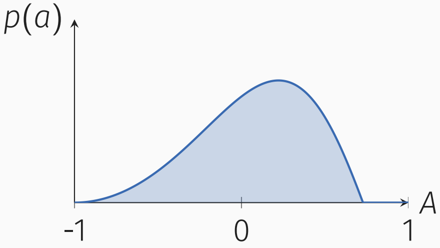


Figure 4: Bayesian answer to: “Which input parameter?”

Mathematically

- Prior distribution μ_0 on A
- Posterior distribution μ^y on A via Radon–Nikodym derivative

$$\frac{\mathrm{d}\mu^y}{\mathrm{d}\mu_0}(a) \propto e^{-\Phi(a)}, \qquad \Phi(a) = \|y - \mathcal{G}(a)\|_2^2/(2\sigma^2)$$

- Estimators: mean of μ^y, mode of μ^y, … EXPENSIVE

A. M. Stuart
Inverse problems: A Bayesian perspective.
Acta Numerica, 2010

Emulators for Inverse Problems

Statistical Estimators

- Quadrature for conditional mean estimator:

$$\hat{x}_{\mathrm{CM}} = \int_A s \, \mathrm{d}\mu^y(s) \approx \sum_{m=1}^{M} \omega_m \xi_m \frac{\mathrm{d}\mu^y}{\mu_0}(\xi_m)$$

- ***Challenge:*** evaluations of R.–N. derivative need evaluation of $\mathcal{G}$ which tends to be expensive
- Solution: use an approximation of $\mathcal{G}$
- Gaussian process: $m_{\mathcal{G}} \approx \mathcal{G}$

Approximate probability distributions

- “New” posterior distribution via Radon–Nikodym derivative:

$$\frac{\mathrm{d}\mu_N^y}{\mathrm{d}\mu_0}(a) \propto \exp\left(-\frac{\|y - m_{\mathcal{G}}(a)\|_2^2}{2\sigma^2}\right)$$

- Hope: $\mu_N^y \approx \mu^y$ as long as $m_{\mathcal{G}} \approx \mathcal{G}$

Posterior consistency

Theorem (Stuart & Teckentrup (2018); simplified)

Assuming $\mathcal{X}$ *compact and* $\mathcal{G} \in H^s(\mathcal{X})$, $s > \dim(\mathcal{X})/2$,

$$d_{Hell}(\mu^y, \mu_N^y) \leq C_2 \|\mathcal{G} - m^{\mathcal{G}}\|_{L^2}$$

A. M. Stuart and A. L. Teckentrup
Posterior consistency for Gaussian process approximations of Bayesian posterior distributions.
Mathematics of Computation, 2018

Convergence rates

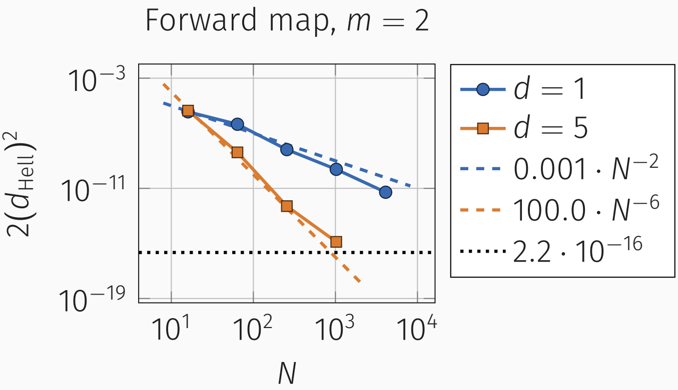


Figure 5: Approximation of Hellinger distance and expected convergence rates for a model problem, $s \in \{1, 5\}$ unknown inputs.

What we could have covered as well...

- Approximation of $\Phi(a) = \|y - \mathcal{G}(a)\|_2^2/(2\sigma^2)$ instead of $\mathcal{G}$
  $\rightarrow$ Same rates
- Use sample paths of $\mathrm{GP}(m_f, k_f)$ instead of m_f to approximate $\mathcal{G}$ or Φ
  $\rightarrow$ slightly lower rates (h^{ν} instead of $h^{\nu+m/2}$)

A. M. Stuart and A. L. Teckentrup
Posterior consistency for Gaussian process approximations of Bayesian posterior distributions.
Mathematics of Computation, 2018

Likelihood Functions

- Denote the likelihood function $\ell(a) := e^{-\Phi}(a)$
- Approximation of likelihood function gives same results!
- Let $m_\ell \approx \ell$ be a GP approx.

Theorem ($\rightarrow$ this thesis; simplified)

Assuming $\mathcal{X}$ compact and $\mathcal{G} \in H^s(\mathcal{X})$, $s > \dim(\mathcal{X})/2$,

$$d_{Hell}(\mu^y, \mu^y_{N,\ell}) \leq C_2 \|\ell - m_\ell\|_{L^2}$$

Essential to the proof

Lemma (→ this thesis; simplified)

There exist constants $C_1, C_2 > 0$ and $N_0 \in \mathbb{N}$ such that

$$C_1 \leq \mathbb{E}[m_{\ell,n}] \leq C_2$$

holds for all $n \geq N_0$.

Use additionally: Use $(a-b)^2 = (a^2-b^2)^2/(a+b)^2$ as well as straightforward inequalities

Convergence rates

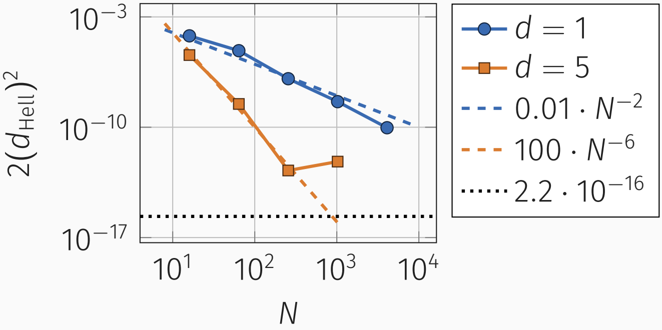


Figure 6: Approximation of Hellinger distance and expected convergence rates for a model problem, $s \in \{1, 5\}$ unknown inputs.

Furthermore

More rates:

- If using sample path–approximations, we may recover the same rate h^ν as for an approximation of $\mathcal{G}$ or Φ
- See the thesis for proofs and more simulations

Connection to Bayesian quadrature:

- Integrals of Gaussian processes are Gaussian processes
- If m_ℓ is available, $\mathbb{E}[m_\ell]$ is free

Conclusion (so far)

- Approximate posterior distributions are as good as the approximation of the forward map/potential
- The same can be shown for the likelihood function
- The rates can be observed in practice

Further work

- Slightly weaken assumptions for consistency estimates
- Emulation of vector–valued functions (in high dimension)

Numerical Linear Algebra with Covariances

Gaussian process regression

- Gaussian process regression requires solving the linear system $k(\mathcal{X}_N, \mathcal{X}_N)c = f(\mathcal{X}_N)$
- $K := k(\mathcal{X}_N, \mathcal{X}_N)$ is symmetric and positive definite
- It is also not sparse and ill–conditioned

Covariances are ill-conditioned

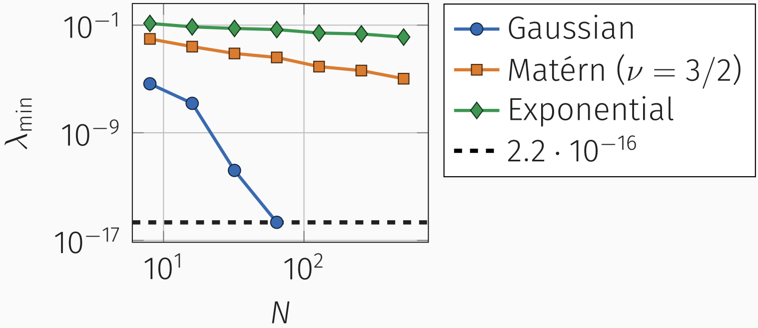
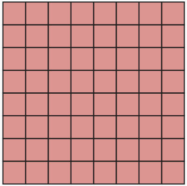


Figure 7: Smallest eigenvalue $\lambda_{\min}$ of covariance matrices constructed on Halton points in $d = 2$.

Hierarchical Matrices

- Approximate blocks of K with low rank approximations
- $K \approx H_K$ tree of low rank approximations
- Storage and MVM in $O(N \log N)$



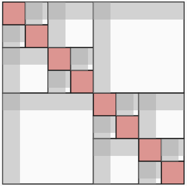


Figure 8: ***Left:*** full matrix, ***right:*** hierarchical matrix

Inverting Hierarchical Matrices

N	Relative error
400	$5.28 \cdot 10^{-8}$
800	$5.96 \cdot 10^{-7}$
1600	$5.63 \cdot 10^{-6}$
3200	$6.28 \cdot 10^{-5}$

Table 1: Relative error of solving $Kc = f$ with LU decomposition: $\mathcal{H}^2$–matrix and full matrix

MVM is more stable

N	Relative error
512	$3.9 \cdot 10^{-13}$
1024	$3.5 \cdot 10^{-13}$
2048	$6.3 \cdot 10^{-13}$
4096	$6.9 \cdot 10^{-13}$
8192	$8.3 \cdot 10^{-13}$

Table 2: Relative error of matrix–vector multiplication (MVM) using compression accuracy $\epsilon = 10^{-12}$.

Krylov Solvers & Preconditioners

- MVM is “reliable” and cheap ($O(N \log N)$)
- This motivates use of Krylov solvers: CG, GMRES, ...
- Problem: extreme ill–conditioning of covariance matrices
- Solution: Preconditioners
    - Nyström, incomplete Cholesky, ...
    - Localized Kernel spaces

Localised Kernel Spaces

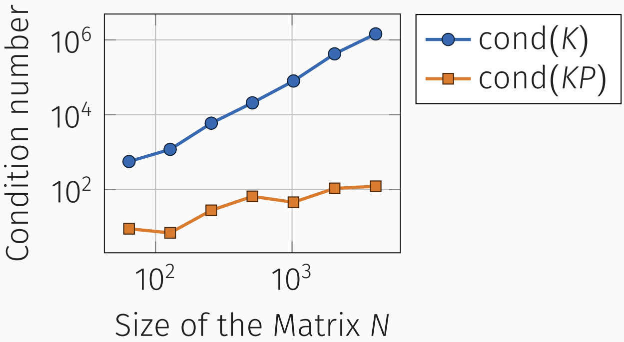


Figure 9: Condition numbers cond(K) and cond(KP) where the preconditioner is constructed with localised bases on $X = \mathbb{S}^2$.

Localised Kernel Spaces

N	n	Iter.	Runtime GMRES	RMSE of Interp.
4096	91	7	$<$ 1.0 sec	$5.2 \cdot 10^{-10}$
8192	111	11	1.0 sec	$4.8 \cdot 10^{-9}$
16384	124	12	2.0 sec	$3.9 \cdot 10^{-9}$
32768	142	8	3.0 sec	$3.3 \cdot 10^{-9}$
65536	162	13	15.0 sec	$8.4 \cdot 10^{-9}$
131072	183	8	13.0 sec	$1.4 \cdot 10^{-9}$

Table 3: GMRES with localised kernel spaces on the sphere $X = \mathbb{S}^2$; thin–plate spline kernel.

Bounded domains

N	n	Iterations	RMSE of Interp.
512	88	8	$1.3 \cdot 10^{-4}$
1024	108	13	$4.4 \cdot 10^{-5}$
2048	131	16	$1.4 \cdot 10^{-5}$
4096	156	44	$4.9 \cdot 10^{-6}$
8192	183	127	$1.2 \cdot 10^{-6}$

Table 4: GMRES with localised kernel spaces on $X = [0, 1]^2$ for the Matérn covariance.

Further work

Algorithm:

- Good *preconditioners* for covariance matrices
- Efficient assembly of hierarchical matrices

Hierarchical matrices and covariances

- Establish asymptotic smoothness of covariance functions (only done for very few)
- Error estimates w.r.t. interpolation error

Further Reading

Localised Bases for Kernel Spaces:

Localised Bases for Kernel Spaces on the Unit Sphere

E. Fuselier, T. Hangelbroek, F.J. Narcowich, J.D. Ward, G.B. Wright, SIAM Journal Numerical Analysis, 2013

ASKIT:

ASKIT: An Efficient, Parallel Library for High-Dimensional Kernel Summations

W. B. March, B. Xiao, C. D. Yu, G. Biros, SIAM Journal Scientific Computing, 2016

Further Reading

Gaussian processes, hierarchical matrices, Krylov methods:

Approximating Gaussian processes with H^2–matrices.

S. Börm, J. Garcke, ECML, 2007

Hierarchical Matrices and RBF Interpolation:

Hierarchical Matrix Approximation for Kernel-Based Scattered Data Interpolation.

A. Iske, S. Le Borne, M. Wende, SIAM Journal Scientific Computing, 2017