Gaussian Process Approximations in Bayesian Inverse Problems

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Master Thesis Colloquium

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Outline

1. Radial basis functions and Gaussian process regression
2. Bayesian approach to inverse problems
3. Gaussian process approximations in Bayesian inverse problems
4. Current and upcoming work

Radial basis functions and Gaussian process regression

Interpolation with radial basis functions

- $\star$ Recover $f : \Omega \to \mathbb{R}$ from values $y = f(X)$ on $X = \{x_1, ..., x_N\}$

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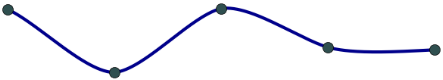

Data and RBF interpolant

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- "Works well" in reproducing kernel Hilbert space (RKHS)
- For example Matérn kernel $\varphi_\nu(z) \sim z^\nu K_\nu(z)$

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A Gaussian process (GP) is a collection of random variables, any finite number of which have a joint Gaussian distribution

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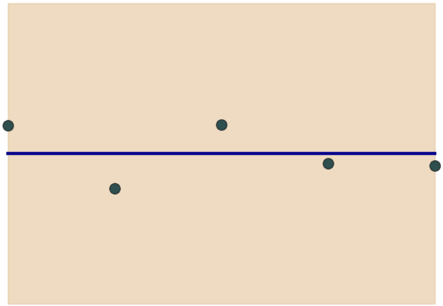

Mean and standard deviation of Gaussian process

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- $\star$ We want to reproduce f at points X_{new}

- ⋆ Condition joint distribution $(f(X), f(X_{\text{new}}))$ on hitting y

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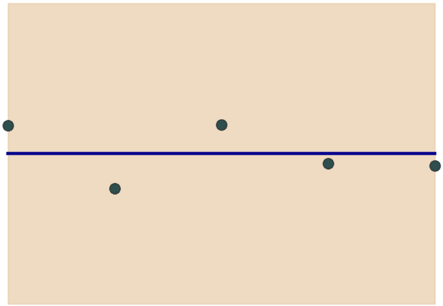

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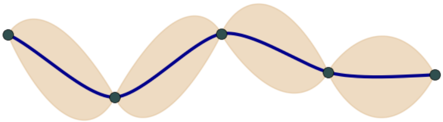
Conditioning Gaussian processes



Predictive mean and standard deviation of Gaussian process

Conditioning Gaussian processes

- ⋆ Condition joint distribution $(f(X), f(X_{\text{new}}))$ on hitting y
- ⋆ Conditioning suggests $f(X_{\text{new}}) \sim \mathcal{N}(m_{\text{new}}, K_{\text{new}})$ with predictive mean

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- The predictive mean m_{new} is the RBF interpolant!

Bayesian approach to inverse problems

Example for an inverse problem

Differential Equation on $(0,1)$

Find $a = (a_1, a_2) \in [-1,1]^2$ such that for

$$-\operatorname{div}((\sin(a_1 x) + \cos(a_2 x))\nabla u(x)) = 1, \quad u(0) = u(1) = 0$$

the measurements satisfy

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- ⋆ Operator $\mathcal{G} : \mathbb{R}^2 \to \mathbb{R}^3,\ (a_1, a_2) \mapsto (u(1/3), u(1/2), u(2/3))$
- ⋆ How can we find a from $y = \mathcal{G}(a) +$ "measurement error"

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Inverse problems

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- $\star$ Noisy measurements $y \in \mathbb{R}^n$, noise $\eta \sim \mathcal{N}(0, \sigma_\eta^2 I_n)$
- $\star$ Find input $a \in \mathcal{A}$ such that $y = \mathcal{G}(a)$ or $y = \mathcal{G}(a) + \eta$

Bayesian statistics

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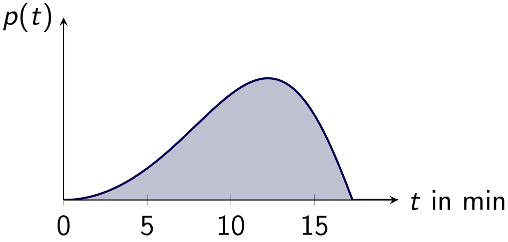

Bayesian answer to: "When will he finish?"

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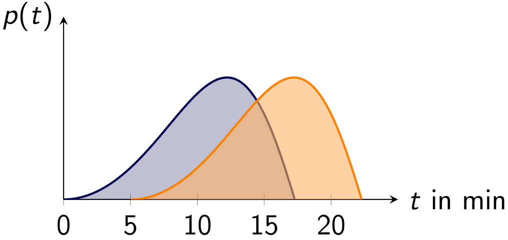

Updated answer after collecting data ("How long did 2 bullet pts. take?")

How do we find the posterior distribution?

Theorem (Bayes, simplified)

Let $\mathcal{G} \in C(\mathcal{A}; \mathbb{R}^n)$ *and* $\mu_0(\mathcal{A}) = 1$. *Then* $\mu^y \ll \mu_0$ *with density*

$$\frac{\mathrm{d}\mu^y}{\mathrm{d}\mu_0}(a) \propto \exp\left(-\frac{1}{2\sigma_\eta^2}\|y - \mathcal{G}(a)\|^2\right)$$

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- ⋆ Maximum-a-posteriori estimator (mode)

Gaussian process approximations in Bayesian inverse problems

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- **Good setting for approximations!**

Approximations in Bayesian inverse problems

- Replace $\mathcal{G}$ by its GP/RBF approximation

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- New approximation results (Stuart, Teckentrup (2018))

Theoretical preliminaries

Assumptions

1. $\mathcal{G} \in H^{\nu+m/2}(\mathcal{A}; \mathbb{R}^n)$ for some $\nu > 0$ (recall $\mathcal{A} \subseteq \mathbb{R}^m$)
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Hellinger distance:

$$d_{\mathrm{Hell}}(\mu_1, \mu_2) = \left(\frac{1}{2} \int_{\mathcal{A}} \left(\sqrt{\frac{\mathrm{d}\mu_1}{\mathrm{d}\mu_0}} - \sqrt{\frac{\mathrm{d}\mu_2}{\mathrm{d}\mu_0}} \right)^2 \, \mathrm{d}\mu_0 \right)^{1/2}$$

Main results

Theorem (Stuart, Teckentrup (2018))

Under the previous assumptions, there exists C_2 independent of X and N such that

$$d_{Hell}(\mu^y, \mu^y_{app}) \leq C_2 \|\mathcal{G} - m^{\mathcal{G}}\|_{L^2_{\mu_0}(\mathcal{A},\mathbb{R}^n)}$$

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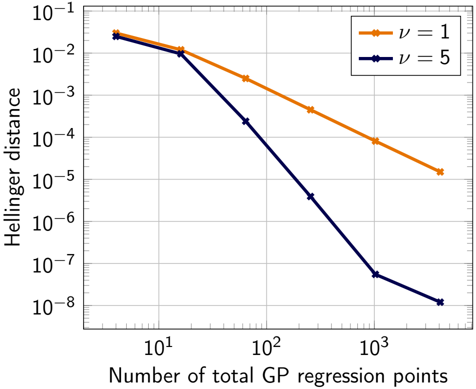
- ⋆ ...use the full process instead of only the mean, e.g. sample a random approximation from $\mathrm{GP}(m^{\mathcal{G}}(\cdot), K^{\mathcal{G}}(\cdot, \cdot))$
- ⋆ ...do all of this with $\Phi(a) = \frac{1}{2\sigma_\eta^2}\|y - \mathcal{G}(a)\|^2$ instead of $\mathcal{G}$

Hellinger distance for problem with $m = 2$ inputs



Different regularities of GP approximation on uniform tensor grid

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1. RBF-interpolants and predictive means are the same
2. Error estimates from RBF-interpolation come from the regularity of the kernel
3. Forward maps from Bayesian inverse problems are expensive to evaluate
4. They are easy to approximate with radial basis functions

Current and upcoming work

Currently: “Tidying up” some theory (for myself)

- Some approximation errors seem neglected
  - Forward model is only approximately available (FEM for PDE)
  - Numerical error in $\cong$ “noise” in evaluations
- Which error has which influence...
  - ... on the conditional mean?
  - ... on the hellinger distance?
- Some quantities seem arbitrary
  - Why the Matérn kernel–which parameters?
  - **Which pointset for GP approximation?**

Soon: Optimising the choice of GP locations

- Pick design points intelligently
- *Bayesian optimisation*
- Non-adaptively: *experimental design*
- Adaptively: *sequential design*
- Make computations a little bit more efficient
- ...while trying not to blow up the runtime with unnecessary optimisations
- More about this next time

Further readings on radial basis functions

RBF interpolation:
Scattered Data Approximation
H. Wendland, Cambridge University Press, 2004

Relationship between GP regression and RBF interpolation:
Interpolation of spatial data–a stochastic or a deterministic problem?
M. Scheuerer, R. Schaback, M. Schlather, European Journal of Applied Mathematics, 2013

Further readings on Bayesian inverse problems

Bayesian approach to inverse problems:
The Bayesian approach to inverse problems
M. Dashti, A. M. Stuart, Handbook of Uncertainty Quantification, Springer, 2017

GP approximations in Bayesian inverse problems:
Posterior consistency for Gaussian process approximations of Bayesian posterior distributions
A. M. Stuart, A.L. Teckentrup, Mathematics of Computation, 2018

Thanks!