Fast Gaussian Process Regression with Derivative Information

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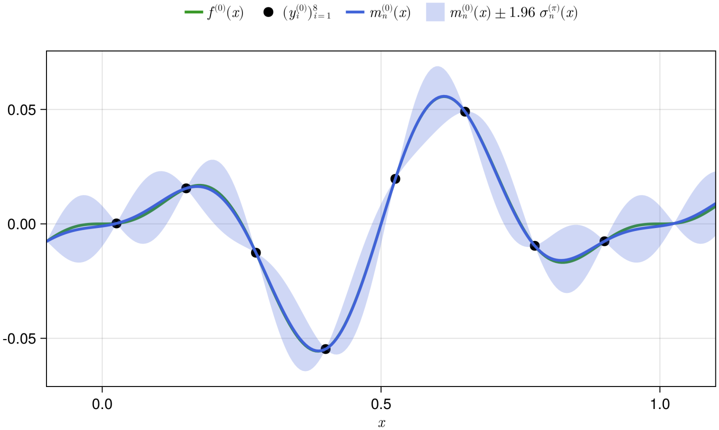
Why Gaussian Process Regression (GPR)?

- Encode simulation knowledge into model via kernel e.g. smoothness or periodicity
- Provides a distribution over simulations i.e. quantifies uncertainty in predictions



Motivation

Practitioners require fast and accurate surrogate models for real time decision making

Challenge: A GPR model costs $\mathcal{O}(n^3)$ to fit

- Applications often require GPR for $n > 10,000$ nodes which is very costly

Solution: Matching nodes and kernel reduces costs to $\mathcal{O}(n \log n)$

⋆ Require control over design of experiments

Observation: Derivative information can enhance GPR

- Derivatives available for free e.g. simulation is the numerical solution of a PDE
- Derivatives may be available at a nominal cost e.g. via automatic differentiation
- Derivatives may be the primary information source e.g. GPR for solving non-linear PDEs [Chen et al., 2021]

New Challenge: With m derivative orders, can we improve the $\mathcal{O}(n^3 m^3)$ fitting cost?
New Solution: Exploit additional structure to reduce cost to $\mathcal{O}(m^2 n \log n + m^3 n)$

Outline and Related Work

1. **GPR**: follows book on GP for Machine Learning [Rasmussen et al., 2006]
2. **Fast GPR**: follows fast Bayesian cubature of Hickernell and Jagadeeswaran
   - Flavor #1: lattice sequence designs [Jagadeeswaran and Hickernell, 2019]
   - Flavor #2: digital sequence designs [Jagadeeswaran and Hickernell, 2022]
   - Unifying thesis of Jagadeeswaran Rathinavel [Rathinavel, 2019]
   - Adjacent work in a RKHS with lattice sequences [Kaarnioja et al., 2022]
   - Application to surrogate for PDE with random coefficients [Sorokin et al., 2023]
3. **GPR with derivative information**: incorporated gradients in [Solak et al., 2002]
4. **Fast GPR with derivative information**: Our novel contribution!

Gaussian Process Regression

- Given *simulation* $f : [0,1]^s \to \mathbb{R}$
- Assume simulation an instance of a *Gaussian process*, $f \sim GP(0, K)$
  - Assume prior mean is zero (not necessary but simplifies presentation)
  - *Prior covariance kernel* $K : [0,1]^s \times [0,1]^s \to \mathbb{R}$ is symmetric positive definite

$$K(\boldsymbol{x}, \boldsymbol{x}') = \mathrm{Cov}[f(\boldsymbol{x}), f(\boldsymbol{x}')]$$

- *Sampling sequence* $\mathsf{X} = (\boldsymbol{x}_i)_{i=1}^n \in [0,1]^{n \times s}$
- *Observations* $\boldsymbol{y} = (y_i)_{i=1}^n = (f(\boldsymbol{x}_i) + \varepsilon_i)_{i=1}^n \in \mathbb{R}^{n \times 1}$ with *noise* $\varepsilon_1, \dots, \varepsilon_n \overset{\mathrm{IID}}{\sim} \mathcal{N}(0, \zeta)$
- *kernel (Gram) matrix* $\mathsf{K} = (K(\boldsymbol{x}_i, \boldsymbol{x}_j))_{i,j=1}^n \in \mathbb{R}^{n \times n}$
- *kernel vector* $\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x}) = (K(\boldsymbol{x}, \boldsymbol{x}_i))_{i=1}^n \in \mathbb{R}^{n \times 1}$

Posterior Mean: $m_n(\boldsymbol{x}) = \boldsymbol{k}_{\mathsf{X}}^\intercal(\boldsymbol{x})(\mathsf{K} + \zeta \mathsf{I})^{-1}\boldsymbol{y}$

Posterior Covariance: $K_n(\boldsymbol{x}, \boldsymbol{x}') = K(\boldsymbol{x}, \boldsymbol{x}') - \boldsymbol{k}_{\mathsf{X}}^\intercal(\boldsymbol{x})(\mathsf{K} + \zeta \mathsf{I})^{-1}\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x}')$

$$\text{Posterior Mean: } m_n(\boldsymbol{x}) = \boldsymbol{k}_{\mathsf{X}}^{\mathsf{T}}(\boldsymbol{x})(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{y}$$

$$\text{Posterior Covariance: } K_n(\boldsymbol{x},\boldsymbol{x}') = K(\boldsymbol{x},\boldsymbol{x}') - \boldsymbol{k}_{\mathsf{X}}^{\mathsf{T}}(\boldsymbol{x})(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x}')$$

Key is to solve systems of the form

$$(\mathsf{K}+\zeta\mathsf{I})\boldsymbol{a} = \boldsymbol{b}$$

for $\boldsymbol{a} \in \mathbb{C}^n$ where $\boldsymbol{b} \in \mathbb{R}^n$

- $(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{y}$ precomputed during fitting, typically costs $\mathcal{O}(n^3)$
- $(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x}')$ computed when evaluating uncertainty, typically costs $\mathcal{O}(n^2)$ after precomputing factorization of $\mathsf{K}+\zeta\mathsf{I}$

Fast Gaussian Process Regression

What? Induce structure in $\mathsf{K}+\zeta\mathsf{I}$ so solving $(\mathsf{K}+\zeta\mathsf{I})\boldsymbol{a}=\boldsymbol{b}$ for $\boldsymbol{a}$ costs $\mathcal{O}(n\log n)$
How? Match quasi-random sequences with structured kernels [Rathinavel, 2019]

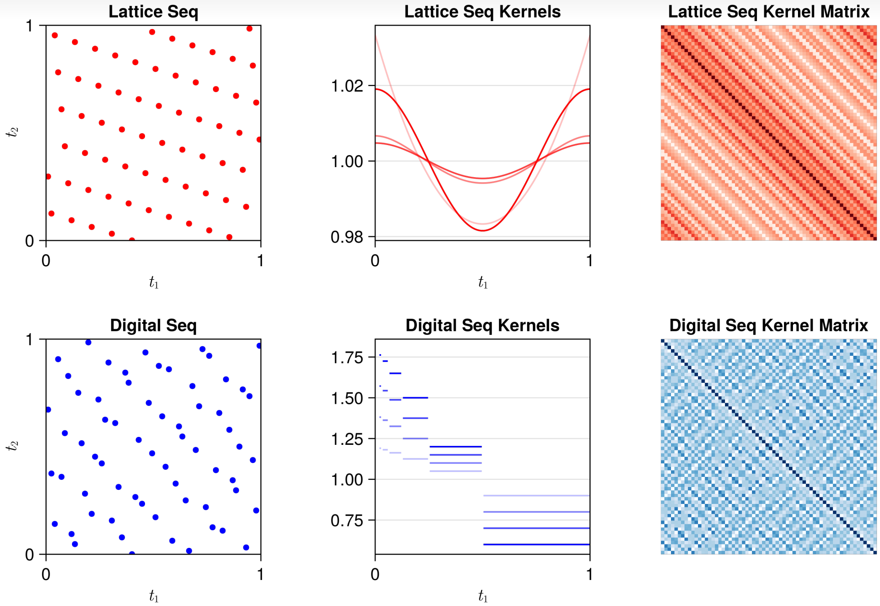
- K circulant with lattice sequence X and shift invariant kernel

$$K(\boldsymbol{x},\boldsymbol{x}')=K((\boldsymbol{x}-\boldsymbol{x}')\mod 1)$$

- K block-Toeplitz with digital sequence X and digitally shift invariant kernel

$$K(\boldsymbol{x},\boldsymbol{x}')=K(\boldsymbol{x}\ominus\boldsymbol{x}')$$

where $\ominus$ is XOR (exclusive or) of base 2 digits


Lattice Seq
Lattice Seq Kernels
Lattice Seq Kernel Matrix
Digital Seq
Digital Seq Kernels
Digital Seq Kernel Matrix
t_1
t_2
0
1
1.02
1.00
0.98
1.75
1.50
1.25
1.00
0.75

For circulant or block-Toeplitz K we have

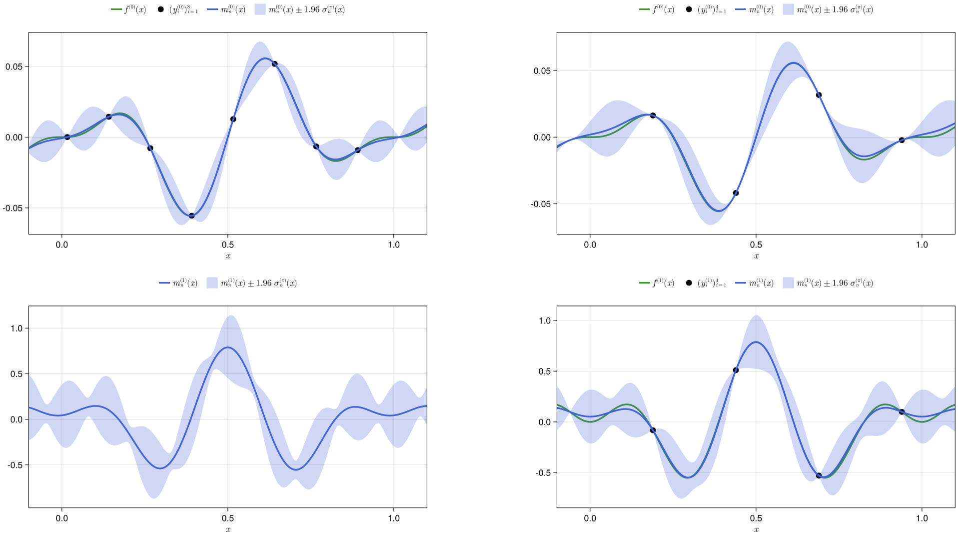
- $\mathsf{K} + \zeta \mathsf{I}$ inherits same structure as K
- Eigendecomposition $\mathsf{K} = \mathsf{V} \Lambda \mathsf{V}^\dagger$ with $\mathsf{V}^{-1} = \mathsf{V}^\dagger =$ Hermitian of V
- $\mathcal{F}(\boldsymbol{a}) := \mathsf{V}^\dagger \boldsymbol{a}$ and $\mathcal{F}^{-1}(\boldsymbol{b}) := \mathsf{V} \boldsymbol{b}$ can be computed in $\mathcal{O}(n \log n)$
  - Circulant K means $\mathcal{F}(\boldsymbol{a})$ is the fast Fourier transform of $\boldsymbol{a}$
  - Block-Toeplitz K means $\mathcal{F}(\boldsymbol{a})$ is the fast Walsh-Hadamard transform of $\boldsymbol{a}$
- First column of V is $\mathbf{1}/\sqrt{n}$

Solve $(\mathsf{K} + \zeta \mathsf{I}) \boldsymbol{a} = \boldsymbol{b}$ for $\boldsymbol{a}$ at cost $\mathcal{O}(n \log n)$ with

$$\boldsymbol{a} = \mathcal{F}^{-1} \left(\frac{\mathcal{F}(\boldsymbol{b})}{\boldsymbol{\lambda} + \zeta} \right)$$

where $\boldsymbol{\lambda} = \operatorname{diag}(\Lambda) = \sqrt{n} \mathcal{F}(\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x}_1))$ and the division is done elementwise

Derivative Informed Gaussian Process Regression



Linear functional of a Gaussian process is still a Gaussian process

$$f^{(\boldsymbol{\beta})}(\boldsymbol{x}) := \frac{\partial^{|\boldsymbol{\beta}|}}{\partial \boldsymbol{x}^{\boldsymbol{\beta}}} f(\boldsymbol{x}) := \frac{\partial^{|\boldsymbol{\beta}|}}{\partial x_1^{\beta_1} \cdots \partial x_s^{\beta_s}} f(\boldsymbol{x})$$

$$\mathrm{Cov}[f^{(\boldsymbol{\beta})}(\boldsymbol{x}), f^{(\boldsymbol{\beta}')}(\boldsymbol{x}')] = \frac{\partial^{|\boldsymbol{\beta}|}}{\partial \boldsymbol{x}^{\boldsymbol{\beta}}} \frac{\partial^{|\boldsymbol{\beta}'|}}{\partial \boldsymbol{x}^{\boldsymbol{\beta}'}} \mathrm{Cov}[f(\boldsymbol{x}), f(\boldsymbol{x}')] =: K^{(\boldsymbol{\beta},\boldsymbol{\beta}')}(\boldsymbol{x},\boldsymbol{x}')$$

With m derivative orders $\boldsymbol{\beta}_1,\dots,\boldsymbol{\beta}_m$ the kernel (Gram) matrix becomes

$$\mathsf{K} = \begin{pmatrix} \mathsf{K}^{(\boldsymbol{\beta}_1,\boldsymbol{\beta}_1)} & \dots & \mathsf{K}^{(\boldsymbol{\beta}_1,\boldsymbol{\beta}_m)} \\ \vdots & \ddots & \vdots \\ \mathsf{K}^{(\boldsymbol{\beta}_m,\boldsymbol{\beta}_1)} & \dots & \mathsf{K}^{(\boldsymbol{\beta}_m,\boldsymbol{\beta}_m)} \end{pmatrix} \in \mathbb{R}^{nm \times nm}, \quad \mathsf{K}^{(\boldsymbol{\beta}_k,\boldsymbol{\beta}_l)} = \left(K^{(\boldsymbol{\beta}_k,\boldsymbol{\beta}_l)}(\boldsymbol{x}_i,\boldsymbol{x}_j)\right)_{i,j=1}^{n}$$

so solving $(\mathsf{K}+\zeta\mathsf{I})\boldsymbol{a} = \boldsymbol{b}$ for $\boldsymbol{a} \in \mathbb{C}^{mn}$ where $\boldsymbol{b} \in \mathbb{R}^{mn}$ costs $\mathcal{O}(m^3 n^3)$ in general

Fast Gaussian Process Regression with Derivative Information

$\mathsf{K}^{(\boldsymbol{\beta}_k,\boldsymbol{\beta}_l)}$ retains structure of $\mathsf{K}^{(\mathbf{0},\mathbf{0})}$ e.g. circulant or block Toeplitz

$$\begin{pmatrix} \mathsf{K}^{(\boldsymbol{\beta}_1,\boldsymbol{\beta}_1)} & \dots & \mathsf{K}^{(\boldsymbol{\beta}_1,\boldsymbol{\beta}_m)} \\ \vdots & \ddots & \vdots \\ \mathsf{K}^{(\boldsymbol{\beta}_m,\boldsymbol{\beta}_1)} & \dots & \mathsf{K}^{(\boldsymbol{\beta}_m,\boldsymbol{\beta}_m)} \end{pmatrix} = \begin{pmatrix} \mathsf{V} & & \\ & \ddots & \\ & & \mathsf{V} \end{pmatrix} \underbrace{\begin{pmatrix} \Lambda^{(\boldsymbol{\beta}_1,\boldsymbol{\beta}_1)} & \dots & \Lambda^{(\boldsymbol{\beta}_1,\boldsymbol{\beta}_m)} \\ \vdots & \ddots & \vdots \\ \Lambda^{(\boldsymbol{\beta}_m,\boldsymbol{\beta}_1)} & \dots & \Lambda^{(\boldsymbol{\beta}_m,\boldsymbol{\beta}_m)} \end{pmatrix}}_{\Lambda \in \mathbb{R}^{nm \times nm}} \begin{pmatrix} \mathsf{V}^\dagger & & \\ & \ddots & \\ & & \mathsf{V}^\dagger \end{pmatrix}$$

Let $\otimes$ be the Kronecker product so

$$\mathsf{K} + \zeta \mathsf{I} = (\mathsf{I} \otimes \mathsf{V})(\Lambda + \zeta \mathsf{I})(\mathsf{I} \otimes \mathsf{V}^\dagger)$$

$$\mathsf{K} + \zeta \mathsf{I} = (\mathsf{I} \otimes \mathsf{V})(\Lambda + \zeta \mathsf{I})(\mathsf{I} \otimes \mathsf{V}^\dagger)$$

Since Λ is a diagonal block (striped) matrix, there is some permutation matrix P with

$$\mathsf{P}^\intercal(\Lambda + \zeta \mathsf{I})\mathsf{P} = \Upsilon + \zeta \mathsf{I}$$

where

$$\Upsilon = \begin{pmatrix} \Upsilon_1 & & \\ & \ddots & \\ & & \Upsilon_n \end{pmatrix}$$

is block diagonal with $\Upsilon_{i,kl} = \lambda_i^{(\boldsymbol{\beta}_k, \boldsymbol{\beta}_l)}$. Then

$$\mathsf{K} + \zeta \mathsf{I} = (\mathsf{I} \otimes \mathsf{V})\mathsf{P}(\Upsilon + \zeta \mathsf{I})\mathsf{P}^\intercal(\mathsf{I} \otimes \mathsf{V}^\dagger)$$

Cost of solving $(\mathsf{K}+\zeta\mathsf{I})\boldsymbol{a}=\boldsymbol{b}$ for $\boldsymbol{a}$ with structured $\mathsf{K}+\zeta\mathsf{I}$

$$\mathsf{K}+\zeta\mathsf{I}=(\mathsf{I}\otimes\mathsf{V})\mathsf{P}(\Upsilon+\zeta\mathsf{I})\mathsf{P}^\intercal(\mathsf{I}\otimes\mathsf{V}^\dagger)$$

Reduce cost from $\mathcal{O}(m^3n^3)$ to $\mathcal{O}(m^2n\log n+m^3n)$ with the following algorithm

1. Constructing Υ from eigenvalues $\boldsymbol{\lambda}^{(\boldsymbol{\beta}_k,\boldsymbol{\beta}_l)}=\mathcal{F}\left(\boldsymbol{k}_{\mathsf{X}}^{(\boldsymbol{\beta}_k,\boldsymbol{\beta}_l)}(\boldsymbol{x}_1)\right)$ costs $\mathcal{O}(m^2n\log n)$
2. $\check{\boldsymbol{b}}:=\mathsf{P}^\intercal(\mathsf{I}\otimes\mathsf{V}^\dagger)\boldsymbol{b}$ can be computed at cost $\mathcal{O}(mn\log n)$
3. $\check{\boldsymbol{a}}:=(\Upsilon+\zeta\mathsf{I})^{-1}\check{\boldsymbol{b}}$ can be computed at cost $\mathcal{O}(m^3n)$
4. $\boldsymbol{a}=(\mathsf{I}\otimes\mathsf{V})\mathsf{P}\check{\boldsymbol{a}}$ can be computed at cost $\mathcal{O}(mn\log n)$

Fast Kernel Parameter Optimization

K often depends on parameters $\boldsymbol{\theta}$ e.g. scaling factor, lengthscales, noise variance ζ
$\boldsymbol{\theta}$ which maximizes the marginal log likelihood is

$$\operatorname*{argmin}_{\boldsymbol{\theta}} L(\boldsymbol{\theta}|\boldsymbol{y}) = \operatorname*{argmin}_{\boldsymbol{\theta}} \left[\log\det(\mathsf{K}+\zeta\mathsf{I}) + \boldsymbol{y}^\intercal(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{y}\right]$$
$$= \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n}\left[\log\det(\Upsilon_i+\zeta\mathsf{I}) + \check{\boldsymbol{y}}_i^\dagger(\Upsilon_i+\zeta\mathsf{I})^{-1}\check{\boldsymbol{y}}_i\right]$$

where

$$\check{\boldsymbol{y}} := \begin{pmatrix}\check{\boldsymbol{y}}_1\\ \vdots \\ \check{\boldsymbol{y}}_n\end{pmatrix} := \mathsf{P}^\intercal(\mathsf{I}\otimes\mathsf{V}^\dagger)\boldsymbol{y}.$$

Both $L(\boldsymbol{\theta}|\boldsymbol{y})$ and $\partial_{\theta_j}L(\boldsymbol{\theta}|\boldsymbol{y})$ can still be computed in $\mathcal{O}(m^2 n\log n + m^3 n)$

Future Work

Theory

- Can we improve the $\mathcal{O}(m^2 n \log n + m^3 n)$ cost by relating $\boldsymbol{\lambda}^{(\boldsymbol{\beta},\boldsymbol{\kappa})}$ to $\boldsymbol{\lambda}^{(\boldsymbol{\beta}',\boldsymbol{\kappa}')}$?
- Link with RKHS setting
  - General GPR and RKHS kernel interpolation connections in [Kanagawa et al., 2018]
  - Optimize weights in [Kaarnioja et al., 2022] with GPR kernel parameter optimization
- Analogous developments for digital sequences

Practical Software

- `QMCGenerators.jl`[1]: Quasi-random sequence generators with randomizations
- `FastGaussianProcesses.jl`[2]: Fast GPR with derivatives (in development)
- `QMCPy`[3] [Choi et al., 2022]
  - Quasi-random sequence generators with randomizations
  - Fast GPR cubature [Rathinavel, 2019]

[1] https://github.com/alegresor/QMCGenerators.jl
[2] https://github.com/alegresor/FastGaussianProcesses.jl
[3] https://github.com/QMCSoftware/QMCSoftware

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