Fast Gaussian Process Regression with Derivative Information using Lattice and Digital Sequences

PhD Comprehensive Exam

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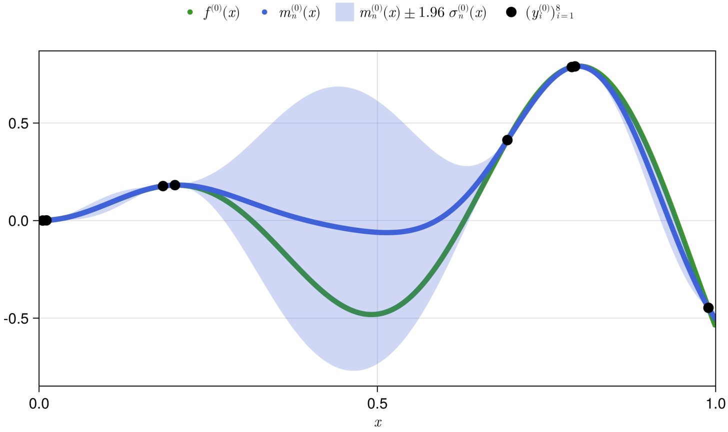
Why Gaussian Process Regression?

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



Motivation

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 (DoE)

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 derivatives, can we improve the $\mathcal{O}(n^3 m^3)$ fitting cost?

- e.g. for $f : [0,1]^s \to \mathbb{R}$ with access to f and ∇f has $m = 1 + s$

New Solution: Exploit additional structure to reduce cost to $\mathcal{O}(m^2 n \log n + m^3 n)$

Outline

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 of PDE with random coefficients [Sorokin et al., 2023a]
3. **GPR with derivative information**: incorporated gradients in [Solak et al., 2002]
4. **Fast GPR with derivative information**: our novel contribution!

My Related Work Not Mentioned in this Talk

- Articles for MCQMC conference proceedings
  - Quasi-Monte Carlo (QMC) Software [Choi et al., 2022]
  - Challenges in developing great QMC software [Choi et al., 2023]
  - QMC for vector functions of integrals [Sorokin and Rathinavel, 2023]
- Metalearning priors for Bayesian optimization with GPs [Sorokin et al., 2023b]
- Adaptive probability of failure estimation with GPs [Sorokin and Rao, 2023]
- Galactic chemical evolution modeling [Gjergo et al., 2023]

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 semi-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 Variance: $\sigma_n^2(\boldsymbol{x}) = K(\boldsymbol{x},\boldsymbol{x}) - \boldsymbol{k}_{\mathsf{X}}^\intercal(\boldsymbol{x})(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x})$

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

$$\text{Posterior Covariance: } \sigma_n^2(\boldsymbol{x}) = K(\boldsymbol{x},\boldsymbol{x}) - \boldsymbol{k}_{\mathsf{X}}^\intercal(\boldsymbol{x})(\mathsf{K}+\zeta\mathsf{I})^{-1}\boldsymbol{k}_{\mathsf{X}}(\boldsymbol{x})$$

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]

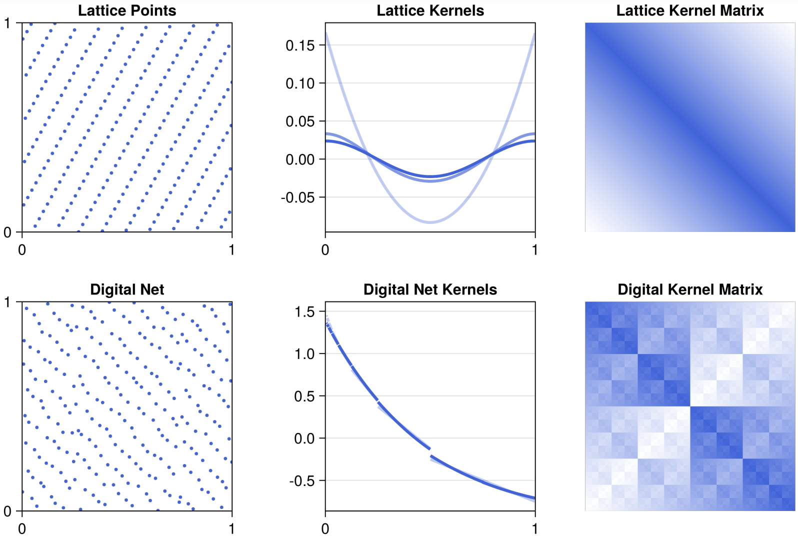
- K circulant with lattice sequence X and shift invariant kernel

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

- 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
- Details on kernel forms available ▸ here


Lattice Points
Lattice Kernels
Lattice Kernel Matrix
Digital Net
Digital Net Kernels
Digital Kernel Matrix
0.15
0.10
0.05
0.00
-0.05
1.5
1.0
0.5
0.0
-0.5
0
1

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 $\mathbf{1}/\sqrt{n}$

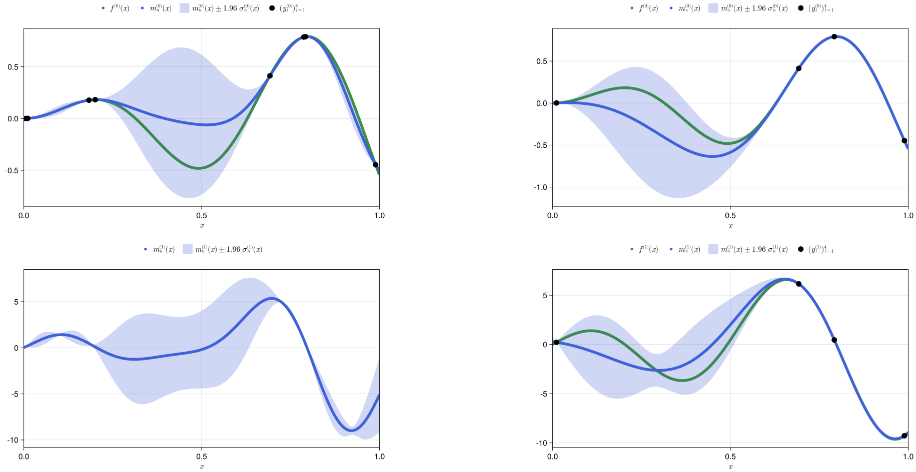
Solve $(\mathsf{K}+\zeta\mathsf{I})\boldsymbol{a}=\boldsymbol{b}$ for $\boldsymbol{a}$ at cost $\mathcal{O}(n\log n)$ with

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

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

Gaussian Kernel with IID Uniform Points

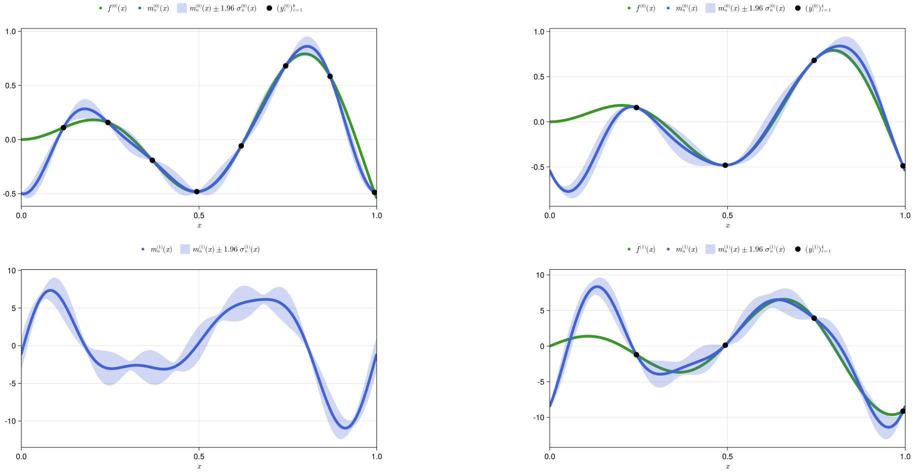
GP#1 Left | GP#2 Right



Top: f. **Bottom:** $\mathrm{d}f$. **Left:** f at 8 points. **Right:** f and $\mathrm{d}f$ at same 4 points.

Lattice Points with Matching Kernel

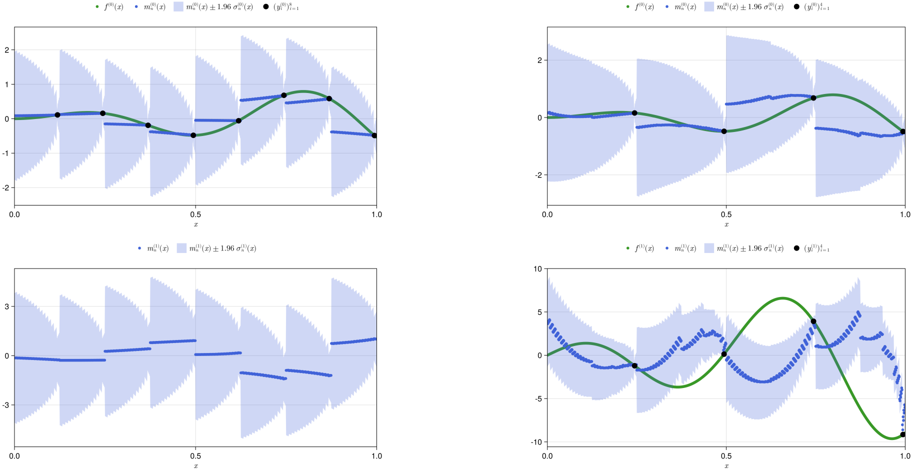
GP#1 Left | GP#2 Right



Top: f. **Bottom:** $\mathrm{d}f$. **Left:** f at 8 points. **Right:** f and $\mathrm{d}f$ at same 4 points.

Digital Net with Matching Kernel

GP#1 Left | GP#2 Right



Top: f. **Bottom:** $\mathrm{d}^+ f$. **Left:** f at 8 points. **Right:** f and $\mathrm{d}^+ f$ at same 4 points.

Linear functional of a Gaussian process is still a Gaussian process

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

(Right derivative for digitally shift invariant kernels)

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

With m derivative multi-indices $\boldsymbol{\beta}_1,\dots,\boldsymbol{\beta}_m \in \mathbb{N}_0^s$ 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

New! 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

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

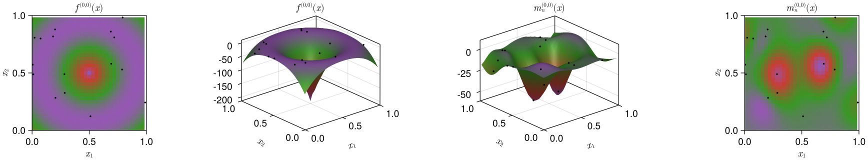
where

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

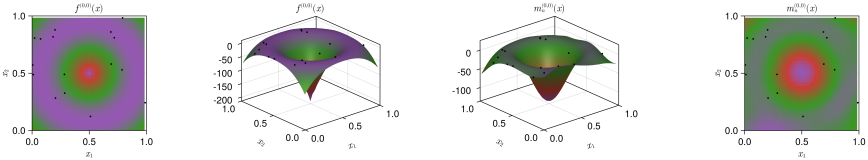
Both $L(\boldsymbol{\theta}|\boldsymbol{y})$ and $\partial_{\theta_j} L(\boldsymbol{\theta}|\boldsymbol{y})$ can still be computed in $\mathcal{O}(m^2 n\log n + m^3 n)$

Analytic Donut[1] in UMBridge [Seelinger et al., 2023]

IID Points, Gaussian Kernel: No Gradient Information

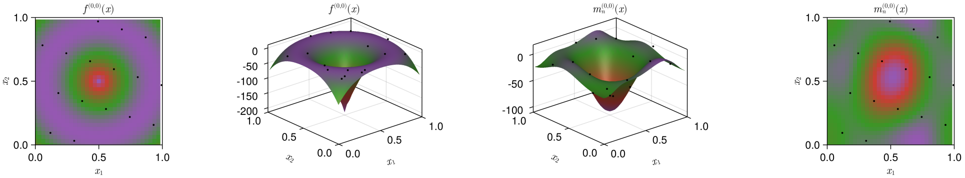


IID Points with Gaussian Kernel: With Gradient Information

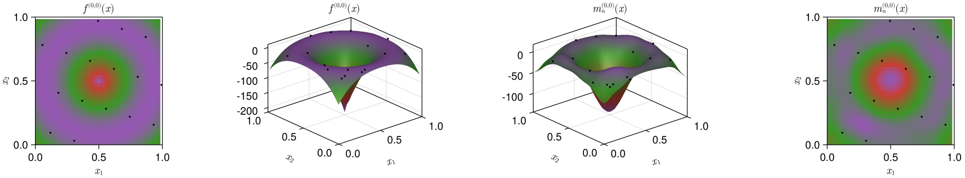


[1] https://um-bridge-benchmarks.readthedocs.io/en/docs/inverse-benchmarks/analytic-donut.html

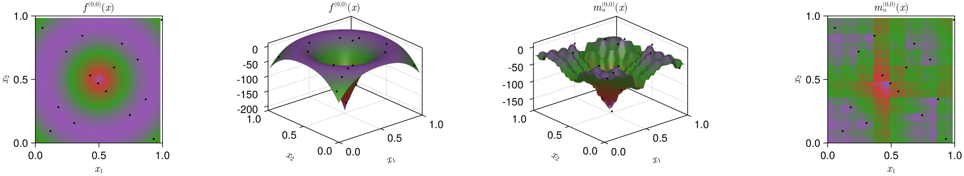
Lattice Points, Matching Kernel: No Gradient Information



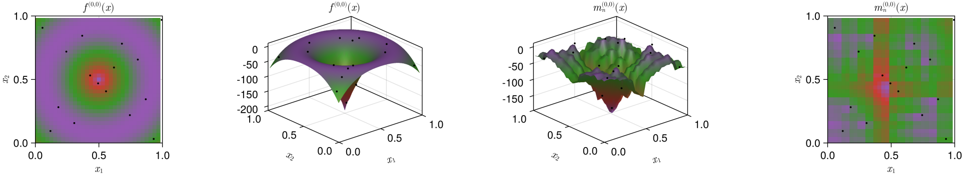
Lattice Points, Matching Kernel: With Gradient Information



Digital Net, Matching Kernel: No Gradient Information



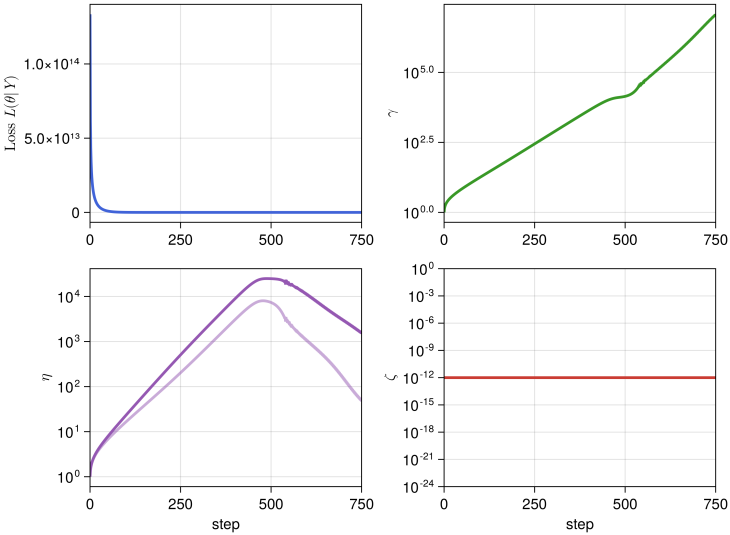
Digital Net, Matching Kernel: With Right Gradient Information



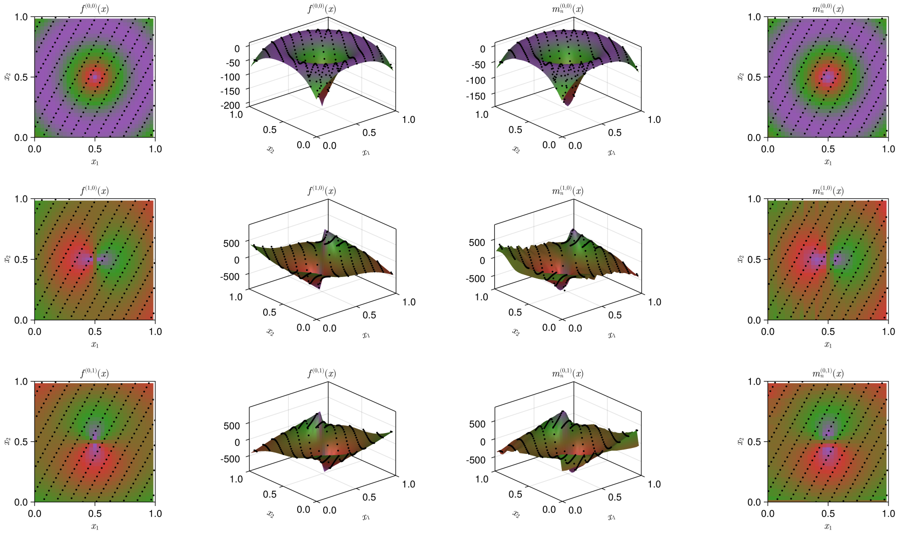
Full Lattice GP with Gradients for Donut Example

```julia
import FastGaussianProcesses; import QMCGenerators; import UMBridge

# docker run -it -p 4243:4243 linusseelinger/benchmark-analytic-donut
model = UMBridge.HTTPModel("posterior", "http://localhost:4243")
β = [0 0; 1 0; 0 1] # observe f^{(0,0)}, f^{(1,0)}, f^{(0,1)}

function f(x::Vector{Float64})
    z = [6*x[1]-3, 6*x[2]-3] # both componenets between -3 and 3
    [    UMBridge.evaluate(model,[z],Dict())[1][1], # f^{(0,0)}
        (UMBridge.gradient(model,0,0,[z],[1]) .* [6, 6])...] # f^{(1,0)}, f^{(0,1)}
end

seq = QMCGenerators.RandomShift(QMCGenerators.LatticeSeqB2(2),1,7) # s=2, seed=7
gp = FastGaussianProcesses.FastGaussianProcess(f,seq,2^8;β=β,optim_steps=750) # n=2^10
FastGaussianProcesses.plot_gp_optimization(gp,figpath=joinpath(@__DIR__,"optim.png"))
FastGaussianProcesses.plot_gp_2s(gp;f=f,β=β,figpath=joinpath(@__DIR__,"gp.png"))
```

Kernel Parameter Optimization

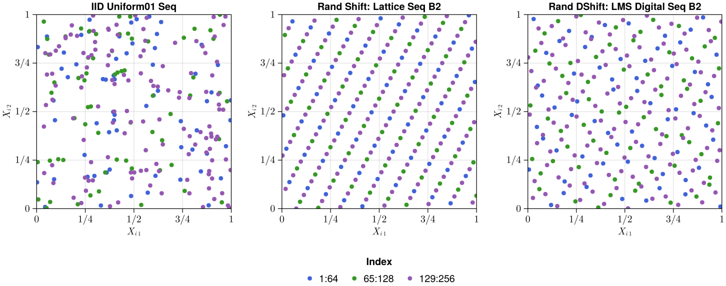


Gaussian Process and Gradient Visualization



Theoretical Next Steps

Efficient updates and error quantification when adding new points



Fast GP with mix of lattice / digital net and unstructured points

- Unstructured points on boundary of $[0,1]^s$
- Unstructured refinement sampling after initial structured sampling

Practical Next Steps

Available software

- `QMCGenerators.jl`[2]: Quasi-random sequence generators with randomizations
- `FastGaussianProcesses.jl`[3]: Fast GPR with derivatives (in development)
- `QMCPy`[4] [Choi et al., 2022]: Quasi-Monte Carlo Software
  - Quasi-random sequence generators with randomizations
  - Fast GPR cubature [Rathinavel, 2019]

SCGSR program with Pieterjan Robbe at Sandia National Laboratory?

- Operator learning for PDE solver with high dimensional output (no derivatives)
- Small number of input parameters, numerical solver outputs PDE solution function
- Extend software to support HPC systems via CPU / GPU

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

Long Term Next Steps

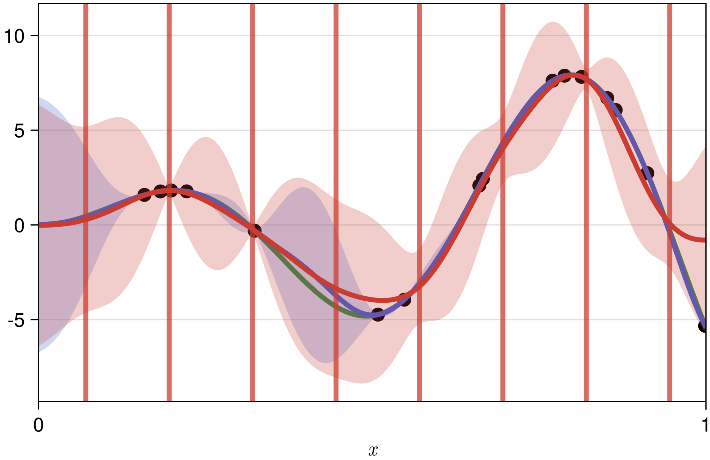
Fast(er) GPR without DoE via inducing points [Snelson and Ghahramani, 2005]

- Typical cost of GPR with p unstructured data points is $\mathcal{O}(p^3)$
- Induce onto n unstructured points at cost $\mathcal{O}(p^2n+pn^3)$
- Induce onto n lattice / digital net points at cost $\mathcal{O}(p^2n+n^3+pn\log n)$
- Induce onto mix of lattice / digital net and unstructured samples?
- Induce derivative observations?

Application to learning nonlinear PDEs with GPs [Chen et al., 2021]

- No simulation. Instead, optimize derivative outputs to fit PDE
- Lattice / digital net points in $(0,1)^s$ with unstructured sampling of BCs

Inducing Points Sketch



Green: function. **Blue**: Standard GP. **Red**: GP with Vertical Line Inducing Points.

References I

Yifan Chen, Bamdad Hosseini, Houman Owhadi, and Andrew M. Stuart. Solving and learning nonlinear pdes with gaussian processes. *Journal of Computational Physics*, 447:110668, 2021. ISSN 0021-9991. doi: https://doi.org/10.1016/j.jcp.2021.110668. URL https://www.sciencedirect.com/science/article/pii/S0021999121005635.

Sou-Cheng T. Choi, Fred J. Hickernell, Rathinavel Jagadeeswaran, Michael J. McCourt, and Aleksei G. Sorokin. Quasi-monte carlo software. In Alexander Keller, editor, *Monte Carlo and Quasi-Monte Carlo Methods*, pages 23–47, Cham, 2022. Springer International Publishing. ISBN 978-3-030-98319-2.

Sou-Cheng T. Choi, Yuhan Ding, Fred J. Hickernell, Jagadeeswaran Rathinavel, and Aleksei G. Sorokin. Challenges in developing great quasi-monte carlo software, 2023.

Josef Dick. Walsh spaces containing smooth functions and quasi–monte carlo rules of arbitrary high order. *SIAM Journal on Numerical Analysis*, 46(3):1519–1553, 2008.

References II

Josef Dick. The decay of the walsh coefficients of smooth functions. *Bulletin of the Australian Mathematical Society*, 80(3):430–453, 2009.

Josef Dick and Friedrich Pillichshammer. Multivariate integration in weighted hilbert spaces based on walsh functions and weighted sobolev spaces. *Journal of Complexity*, 21(2):149–195, 2005.

Eda Gjergo, Aleksei G. Sorokin, Anthony Ruth, Emanuele Spitoni, Francesca Matteucci, Xilong Fan, Jinning Liang, Marco Limongi, Yuta Yamazaki, Motohiko Kusakabe, and Toshitaka Kajino. Galcem. i. an open-source detailed isotopic chemical evolution code, feb 2023. URL https://dx.doi.org/10.3847/1538-4365/aca7c7.

R. Jagadeeswaran and Fred J. Hickernell. Fast automatic bayesian cubature using lattice sampling. *Statistics and Computing*, 29(6):1215–1229, Sep 2019. ISSN 1573-1375. doi: 10.1007/s11222-019-09895-9. URL http://dx.doi.org/10.1007/s11222-019-09895-9.

References III

Rathinavel Jagadeeswaran and Fred J Hickernell. Fast automatic bayesian cubature using sobol sampling. In *Advances in Modeling and Simulation: Festschrift for Pierre L'Ecuyer*, pages 301–318. Springer, 2022.

Vesa Kaarnioja, Yoshihito Kazashi, Frances Y Kuo, Fabio Nobile, and Ian H Sloan. Fast approximation by periodic kernel-based lattice-point interpolation with application in uncertainty quantification. *Numerische Mathematik*, 150(1):33–77, 2022.

Motonobu Kanagawa, Philipp Hennig, Dino Sejdinovic, and Bharath K Sriperumbudur. Gaussian processes and kernel methods: A review on connections and equivalences. *arXiv preprint arXiv:1807.02582*, 2018.

Carl Edward Rasmussen, Christopher KI Williams, et al. *Gaussian processes for machine learning*, volume 1. Springer, 2006.

Jagadeeswaran Rathinavel. *Fast automatic Bayesian cubature using matching kernels and designs*. Illinois Institute of Technology, 2019.

References IV

Linus Seelinger, Vivian Cheng-Seelinger, Andrew Davis, Matthew Parno, and Anne Reinarz. Um-bridge: Uncertainty quantification and modeling bridge. *Journal of Open Source Software*, 8(83):4748, 2023.

Edward Snelson and Zoubin Ghahramani. Sparse gaussian processes using pseudo-inputs. *Advances in neural information processing systems*, 18, 2005.

Ercan Solak, Roderick Murray-Smith, WE Leithead, D Leith, and Carl Rasmussen. Derivative observations in gaussian process models of dynamic systems. *Advances in neural information processing systems*, 15, 2002.

Aleksei G. Sorokin and Vishwas Rao. Credible intervals for probability of failure with gaussian processes, 2023.

Aleksei G. Sorokin and Jagadeeswaran Rathinavel. On bounding and approximating functions of multiple expectations using quasi-monte carlo, 2023.

References V

Aleksei G. Sorokin, Aleksandra Pachalieva, Daniel O'Malley, James M. Hyman, Fred J. Hickernell, and Nicolas W. Hengartner. Computationally efficient and error aware surrogate construction for numerical solutions of subsurface flow through porous media, 2023a.

Aleksei G. Sorokin, Xinran Zhu, Eric Hans Lee, and Bolong Cheng. Sigopt mulch: An intelligent system for automl of gradient boosted trees. *Knowledge-Based Systems*, page 110604, 2023b. ISSN 0950-7051. doi: https://doi.org/10.1016/j.knosys.2023.110604. URL https://www.sciencedirect.com/science/article/pii/S0950705123003544.

Weighted Tensor Product Kernels

$$K_{\boldsymbol{\alpha}}(\boldsymbol{x},\boldsymbol{y}) = \gamma \sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \eta_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \mathcal{K}_{\alpha_j}(x_j, y_j)$$

- Used in QMC literature e.g. [Kaarnioja et al., 2022]
- Optimizing kernel parameters equivalent to optimizing weights $(\eta_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1,\dots,s\}}$
- Costs $\mathcal{O}(2^s)$ to evaluate

Product Weight Kernels require $\eta_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \eta_{\{j\}}$ for $\emptyset \neq \mathfrak{u} \subseteq \{1,\dots,s\}$ and $\eta_{\emptyset} = 1$

$$K_{\boldsymbol{\alpha}}(\boldsymbol{x},\boldsymbol{y}) = \gamma \prod_{j \in \{1,\dots,s\}} \left[1 + \eta_{\{j\}} \mathcal{K}_{\alpha_j}(x_j, y_j)\right]$$

- Cost $\mathcal{O}(s)$ to evaluate

Fourier Series and Shift Invariant Kernels for Lattices

Let $\{x-y\} = (x-y) \mod 1$ and let B_i denote th i^{th} Bernoulli polynomial.

$$\mathring{K}_\alpha(x,y) = \sum_{k\in\mathbb{Z}_0} \frac{e^{2\pi \mathrm{i} k(x-y)}}{k^{2\alpha}} = \frac{(-1)^{\alpha+1}(2\pi)^{2\alpha}}{(2\alpha)!} B_{2\alpha}(\{x-y\}) = \mathring{K}_\alpha(\{x-y\})$$

is the kernel of Sobolev RKHS $\mathring{\mathcal{H}}_\alpha$ with $\alpha \in \mathbb{N}$ and

$$\langle f,g\rangle = (-1)^\alpha (2\pi)^{-2\alpha} \int_0^1 f^{(\alpha)}(x) g^{(\alpha)}(x) \mathrm{d}x.$$

[Kanagawa et al., 2018] discusses GPR and RKHS kernel interpolation connections

New! Walsh Series and Digitally Shift Invariant Kernels for Digital Nets

For $\alpha \geq 2$ the Sobolev RKHS $\mathcal{H}_\alpha$ with inner product

$$\langle f, g \rangle_\alpha = \sum_{\beta=1}^{\alpha-1} \int_0^1 f^{(\beta)}(x)\mathrm{d}x \int_0^1 g^{(\beta)}(x)\mathrm{d}x + \int_0^1 f^{(\alpha)}(x) g^{(\alpha)}(x)\mathrm{d}x$$

has kernel

$$\mathcal{K}_\alpha(x,y) = \sum_{\beta=1}^{\alpha-1} \frac{B_\beta(x)B_\beta(y)}{(\beta!)^2} + \overbrace{(-1)^{\alpha+1}\frac{B_{2\alpha}(\{x-y\})}{(2\alpha)!}}^{\mathring{\mathcal{K}}(\{x-y\})}.$$

[Dick, 2008, 2009] can be used to show $\mathcal{H}_\alpha \subset \widetilde{\mathcal{H}}_\alpha$ where $\widetilde{\mathcal{H}}_\alpha$ is an RKHS with kernel

$$\widetilde{\mathcal{K}}_\alpha(x,y) = \sum_{k \in \mathbb{N}} \frac{\mathrm{wal}_k(x \ominus y)}{b^{\mu_\alpha(k)}} = \widetilde{\mathcal{K}}_\alpha(x \ominus y).$$

Explicit forms for $b = 2, \alpha \in \{2, 3, 4\}$. For $\alpha = 1$ see [Dick and Pillichshammer, 2005].