Scalable Gaussian Process Regression with Gauss-Legendre Features

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Talk Outline

1. Gaussian Processes: From Linear to Functional Model
2. Gauss-Legendre Features
3. Parameter Computation
4. Spectral Equivalence
5. Efficient Compuations
6. Experiments

Linear Regression in Bayesian Modeling

Given: $\mathcal{D} = \{(\mathbf{x}_i, y_i) \,|i = 1, \ldots, n\} \subset \mathbb{R}^d \times \mathbb{R}$.
Let $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n]^\mathsf{T}$.

Bayesian linear regression model:

$$f(\mathbf{x}) = \mathbf{x}^\mathsf{T}\mathbf{w}, \quad y = f(\mathbf{x}) + \varepsilon, \quad \varepsilon \overset{i.i.d}{\sim} \mathcal{N}(0, \sigma_n^2)\,.$$

- We specify a **prior** over the parameters: $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$.
- Gives rise to the **likelihood**: $p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \mathcal{N}\left(\mathbf{X}\mathbf{w}, \sigma_n^2\mathbf{I}\right)$.

Bayesian Modeling

Bayesian analysis is based on Bayes rule:

$$\underbrace{p\left(\mathbf{w}|\mathbf{y},\mathbf{X}\right)}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y}|\mathbf{X},\mathbf{w})}^{\text{likelihood}}\,\overbrace{p(\mathbf{w})}^{\text{prior}}}{\underbrace{p\left(\mathbf{y}|\mathbf{X}\right)}_{\text{marginal likelihood}}}$$

where the **marginal-likelihood** is:

$$p\left(\mathbf{y}|\mathbf{X}\right) = \int p\left(\mathbf{y}|\mathbf{X},\mathbf{w}\right) p\left(\mathbf{w}\right) d\mathbf{w}\,.$$

Thus, the **posterior** can be derived:

$$p\left(\mathbf{w}|\mathbf{y},\mathbf{X}\right) \propto \mathcal{N}\left(\sigma_n^{-2}\left(\sigma_n^{-2}\mathbf{X}^\mathsf{T}\mathbf{X} + \mathbf{\Sigma}^{-1}\right)^{-1}\mathbf{X}^\mathsf{T}\mathbf{y},\left(\sigma_n^{-2}\mathbf{X}^\mathsf{T}\mathbf{X} + \mathbf{\Sigma}^{-1}\right)^{-1}\right)\,.$$

Feature Maps in Function-space View

Replace $\mathbf{x}$ with $\phi(\mathbf{x})$, and write $f(\mathbf{x}) = \phi(\mathbf{x})^\mathsf{T}\mathbf{w}$ with a prior $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$. Then:

$$\mathbb{E}[f(\mathbf{x})] = \phi(\mathbf{x})^\mathsf{T}\mathbb{E}[\mathbf{w}] = 0$$

$$\mathbb{E}\left[f(\mathbf{x})f(\mathbf{x}')\right] = \phi(\mathbf{x})^\mathsf{T}\mathbb{E}\left[\mathbf{w}\mathbf{w}^\mathsf{T}\right]\phi(\mathbf{x}') = \phi(\mathbf{x})^\mathsf{T}\boldsymbol{\Sigma}\phi(\mathbf{x}')$$

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defining the feature map $\psi(\mathbf{x}) = \mathbf{\Sigma}^{1/2}\phi(\mathbf{x}')$ yields $k(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x})^\mathsf{T}\psi(\mathbf{x}) \Rightarrow$ the ***kernel trick***.

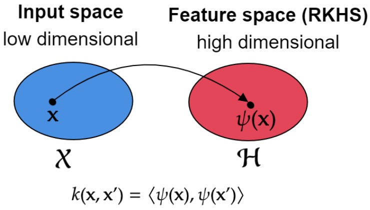
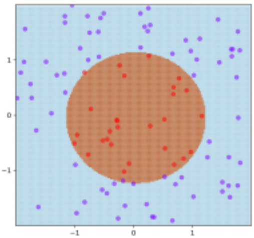


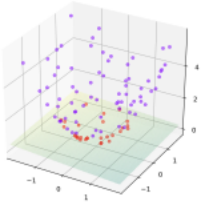
Figure: Reproducing Kernel Hilbert Space.

Feature Maps in Function-space View

For example: consider data $\mathbf{x} \in \mathbb{R}^2$.

Feature map	Kernel
$\psi(\mathbf{x}) = (x_1, x_2, x_1^2 + x_2^2)$	$k(\mathbf{x}, \mathbf{x}') = \mathbf{x} \cdot \mathbf{x}' + \lVert\mathbf{x}\rVert_2^2 \lVert\mathbf{x}'\rVert_2^2$





Some Popular Kernels

- **Polynomial:** $k(\mathbf{x}, \mathbf{x}') = (\gamma \mathbf{x}^\mathsf{T} \mathbf{x}' + c)^q$.
- **Exponential:** $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|_2}{\sigma}\right)$.
- **Gaussian:** $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|_2^2}{2\sigma^2}\right)$.
- **Matérn:** $k(\mathbf{x}, \mathbf{x}') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{\ell}\|\mathbf{x}-\mathbf{x}'\|_2\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}}{\ell}\|\mathbf{x}-\mathbf{x}'\|_2\right)$.
- **Periodic kernel:** $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{2\sin^2(\pi\|\mathbf{x}-\mathbf{x}'\|_2/p)}{\sigma^2}\right)$.

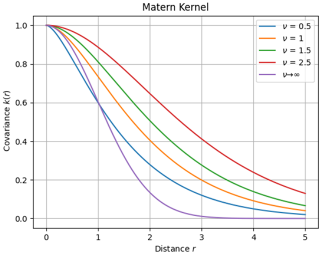


Figure: Matérn kernel.

Gaussian Processes

Definition

A *Gaussian Process* (GP) is a finite collection of random variables, which have a joint Gaussian distribution.

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Assume that $f(\mathbf{x}) \sim \mathcal{GP}\left(\mu\left(\mathbf{x}\right), k(\mathbf{x}, \mathbf{x}')\right)$, where:

- The mean is $\mu(\mathbf{x}) := \mathbb{E}\left[f(\mathbf{x})\right]$ (usually $= \mathbf{0}$).
- The covariance is:
  $k(\mathbf{x}, \mathbf{x}') := \mathbb{E}\left[\left(f(\mathbf{x}) - \mu(\mathbf{x})\right)\left(f(\mathbf{x}') - \mu(\mathbf{x}')\right)\right]$.

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For any $\mathbf{x}_1, \ldots, \mathbf{x}_m \in \mathbb{R}^d$, the vector $\mathbf{f} = \left[f(\mathbf{x}_1), \ldots, f(\mathbf{x}_m)\right]^\mathsf{T}$ is Gaussian random vector with covariance matrix $\mathbf{K}(\mathbf{X}, \mathbf{X})$ defined by $\mathbf{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$.

Gaussian Processes Regression

- The prior is Gaussian $\mathbf{f}|\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \mathbf{K})$.
- The log marginal-likelihood can be obtained:

$$\log p(\mathbf{y}|\mathbf{X}) = -\frac{1}{2}\mathbf{y}^{\mathsf{T}} \left(\mathbf{K} + \sigma_n^2 \mathbf{I}\right)^{-1} \mathbf{y} - \frac{1}{2} \log |\mathbf{K} + \sigma_n^2 \mathbf{I}| - \frac{n}{2} \log 2\pi$$

- The predictive mean and variance are

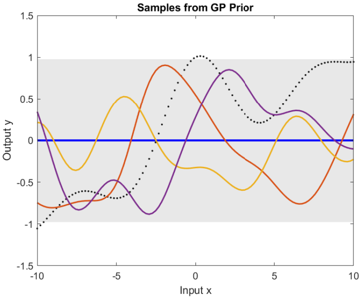
$$\mathbf{f}^{\star}(\mathbf{x}) = \mathbf{K}(\mathbf{x}, \mathbf{X}) \left(\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma_n^2 \mathbf{I}_n\right)^{-1} \mathbf{y}$$

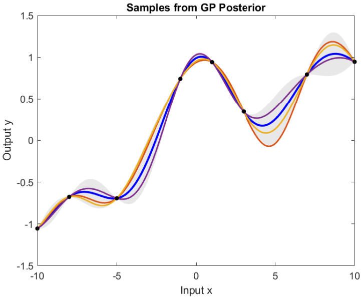
$$\mathbf{f}^{\star}_{\mathsf{var}}(\mathbf{x}) = \mathbf{K}(\mathbf{x}, \mathbf{x}) - \mathbf{K}(\mathbf{x}, \mathbf{X}) \left(\mathbf{K}(\mathbf{X}, \mathbf{X}) + \sigma_n^2 \mathbf{I}_n\right)^{-1} \mathbf{K}(\mathbf{x}, \mathbf{X})^{*}.$$

$O(n^3)$ is expensive!

Gaussian Processes Regression

Sampled functions from prior and posterior:





- Furher reading about GPs for machine learning [1].

[1] Christopher KI Williams and Carl Edward Rasmussen. *Gaussian processes for machine learning*, volume 2. MIT Press Cambridge, MA, 2006.

Maximum Likelihood

Typically, the kernel $k_{\boldsymbol{\theta}}$ depends on a *hyperparameters* vector $\boldsymbol{\theta}$, determined by:

$$\boldsymbol{\theta}^{\star} = \arg\max_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}), \quad \mathcal{L}(\boldsymbol{\theta}) = \log p\left(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}\right) .$$

- Global maximum is not guaranteed (local search).
- Optimization of $\mathcal{L}(\boldsymbol{\theta})$ is **expensive**.

Feature Maps

Denote $\boldsymbol{\theta} = [\boldsymbol{\theta}_0, \sigma_f^2, \sigma_n^2]$. Our method builds feature maps for kernel families $\{k_{\boldsymbol{\theta}}\}_{\boldsymbol{\theta}\in\Theta}$ that can be written as:

$$k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \int_{\mathbb{R}^d} \varphi(\mathbf{x}, \boldsymbol{\eta})\varphi(\mathbf{x}', \boldsymbol{\eta})^* p(\boldsymbol{\eta}; \boldsymbol{\theta}_0) d\boldsymbol{\eta} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'}$$

where for every $\boldsymbol{\theta}_0$, $p(\cdot; \boldsymbol{\theta}_0)$ is an even on $\mathbb{R}^d$, and

$$\varphi(\mathbf{x}, \boldsymbol{\eta}) = \varphi(\mathbf{x}, -\boldsymbol{\eta})^* \, \forall \boldsymbol{\eta} \in \mathbb{R}^d \, .$$

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Important case:

A shift-invariant kernel $k(\mathbf{x}, \mathbf{x}') = k_0(\mathbf{x} - \mathbf{x}')$ can be written as **(Bochner's theorem)**

$$k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \int_{\mathbb{R}^d} e^{-i(\mathbf{x}-\mathbf{x}')^\mathsf{T}\boldsymbol{\eta}} p(\boldsymbol{\eta}; \boldsymbol{\theta}_0) d\boldsymbol{\eta} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'} \, .$$

Random Fourier Features Method

For **shift-invariant kernels**:

$$\begin{aligned} k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}') &= \sigma_f^2 \int_{\mathbb{R}^d} e^{-i(\mathbf{x}-\mathbf{x}')^\top \boldsymbol{\eta}} p(\boldsymbol{\eta}; \boldsymbol{\theta}_0) d\boldsymbol{\eta} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'} \\ &\approx \frac{\sigma_f^2}{s} \sum_{j=1}^{s} e^{-i(\mathbf{x}-\mathbf{x}')^\top \boldsymbol{\eta}_j} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'} \\ &=: \tilde{k}_{\boldsymbol{\theta}}^{(\mathsf{RFF})}(\mathbf{x}, \mathbf{x}') \,. \end{aligned}$$

RFF [2] is based on **Monte-Carlo** sampling, where $\boldsymbol{\eta}_1, \ldots, \boldsymbol{\eta}_s$ are sampled from $p(\boldsymbol{\eta}; \boldsymbol{\theta}_0)$.

[2] Rahimi and Recht, *Random features for large-scale kernel machines*, NeurIPS (2008).

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- We have $k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \mathbb{E}_{\boldsymbol{\eta}_1, \ldots \boldsymbol{\eta}_s} \left[\varphi(\mathbf{x}, \cdot)^* \varphi(\mathbf{x}', \cdot)\right]$ where $\varphi(\mathbf{x}, \boldsymbol{\eta}) = \sqrt{\frac{\sigma_f^2}{s}} \left(e^{-2\pi i \boldsymbol{\eta}_1^\mathsf{T}\mathbf{x}}, \ldots, e^{-2\pi i \boldsymbol{\eta}_s^\mathsf{T}\mathbf{x}}\right)^* \,.$

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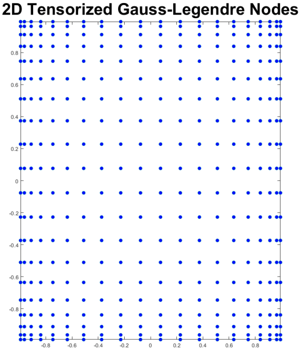
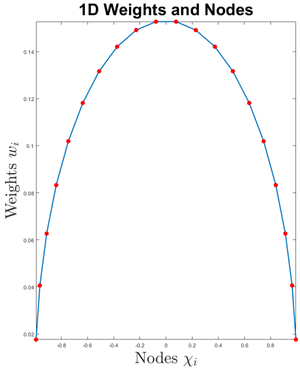
Reminder: Gauss-Legendre Quadrature

- Approximate (exactness holds for all $p \in \mathbb{P}_{2s-1}$)

$$\int_\Omega f(\boldsymbol{\eta}) p(\boldsymbol{\eta}) d\boldsymbol{\eta} \approx \sum_{j \in \{1,\ldots,s\}^d} w_j f(\boldsymbol{\eta}_j) \, .$$

- Gauss-Legendre rule (uniform pdf):
  η_j are the roots of L_s and $w_j = \frac{2}{(1-\eta_j^2)(L_s'(\eta_j))^2}$.





Gauss-Legendre Features: Integral Error

($\boldsymbol{\theta}$ is fixed).

The goal: set $\mathbf{U}$ and $\mathbf{s}$ s.t. for every dataset $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{X}$

$$(1-\Delta)\mathbf{K} \preceq \tilde{\mathbf{K}} \preceq (1+\Delta)\mathbf{K}\,.$$

$$\Updownarrow$$

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$$\left| \int_{\mathbb{R}^d} f(\boldsymbol{\eta}) p(\boldsymbol{\eta}; \boldsymbol{\theta}_0) d\boldsymbol{\eta} - \sum_{j=1}^{s} w_j(\boldsymbol{\theta}) f(\boldsymbol{\eta}_j) p(\boldsymbol{\eta}_j; \boldsymbol{\theta}_0) \right| \leq \frac{\Delta}{\sigma_f^2}$$

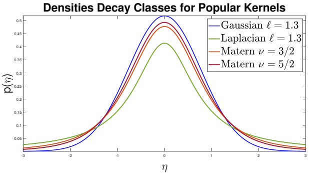
where

$$f(\boldsymbol{\eta}) = \sigma_f^2 \mathbf{z}(\boldsymbol{\eta}) \mathbf{z}(\boldsymbol{\eta})^*, \quad \mathbf{z}(\boldsymbol{\eta}) := [\varphi(\mathbf{x}_1, \boldsymbol{\eta}), \ldots, \varphi(\mathbf{x}_n, \boldsymbol{\eta})]^\mathsf{T}\ .$$

Gauss-Legendre Features for Gaussian Process Regression

1. Truncate the integral

$$\approx \int_{\Pi_{k=1}^{d}[-U_k,U_k]} f(\boldsymbol{\eta})p(\boldsymbol{\eta};\boldsymbol{\theta}_0)d\boldsymbol{\eta}$$



Faster density decay $\Leftrightarrow$ smaller $\mathbf{U}$.

2. Approximate via Gauss-Legendre quadrature

$$\approx \sum_{j=1}^{s} w_j(\boldsymbol{\theta}) f(\boldsymbol{\eta}_j) p(\boldsymbol{\eta}_j;\boldsymbol{\theta})$$

Faster Chebyshev's coefficients decay $\Leftrightarrow$ smaller s.

- Decay of Chebyshev's coefficients for analytic functions.
- For most kernels: $s = \prod_{k=1}^{d} s_k = O((\ln n)^d)$.

Truncating The Integral

We assume that p has a decay property. Consider a few decay classes of $p(\boldsymbol{\eta};\boldsymbol{\theta}_0)$ for well known kernels:

$$\begin{aligned}
\mathcal{P}_{C,\mathbf{L}} &= \left\{ p(\boldsymbol{\eta}) \le C \cdot \Pi_{k=1}^{d} \frac{1}{1+L_k^2\eta_k^2} \right\} \\
\mathcal{P}_{C,\mathbf{L}}^{(r)} &= \left\{ p(\boldsymbol{\eta}) \le C \cdot \left(1+\|\mathbf{L}\boldsymbol{\eta}\|_2^2\right)^{-r} \right\} \\
\mathcal{E}_{C,\mathbf{L}}^{(2)} &= \left\{ p(\boldsymbol{\eta}) \le C \cdot e^{-\|\mathbf{L}\boldsymbol{\eta}\|_2^2} \right\}
\end{aligned}$$

where $\mathbf{L} = \mathbf{diag}\left(L_1,\ldots,L_d\right) \ge 0$.
For each class, we set $\mathbf{U}$ s.t. the first integral error bound holds.

Truncating The Integral

$k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}')$	$p(\boldsymbol{\eta}; \boldsymbol{\theta}_0)$	Decay Class
Non-isotropic Laplacian $\exp(-\lVert \mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}') \rVert_1)$	$\pi^{-d} \prod_{k=1}^{d} \frac{\ell_k}{1 + \ell_k^2 \eta_k^2}$ $L_k = \ell_k$	$\mathcal{P}_{C,\mathbf{L}}$ $C = \pi^{-d} \prod_{k=1}^{d} \ell_k$
Matèrn $\frac{2^{1-\nu}}{\Gamma(\nu)} (\sqrt{2\nu} \lVert \mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}') \rVert_2)^{\nu} \cdot K_{\nu}(\sqrt{2\nu} \lVert \mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}') \rVert_2)$	$\frac{\Gamma(\nu + d/2)}{\pi^{d/2} \Gamma(\nu)(2\nu)^{d/2}} \prod_{k=1}^{d} \ell_k \cdot \left(1 + \lVert \mathbf{L}\boldsymbol{\eta} \rVert_2^2\right)^{-(\nu + d/2)}$ $L_k = \ell_k / \sqrt{2\nu}$	$\mathcal{P}_{C,\mathbf{L}}^{(r)}$ $r = \nu + d/2$ $C = \frac{\Gamma(\nu + d/2)}{\Gamma(\nu)(2\pi\nu)^{d/2}} \prod_{k=1}^{d} \ell_k$
Non-isotropic Gaussian $\exp(-\lVert \mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}') \rVert_2^2 / 2)$	$(2\pi)^{-d/2} \prod_{k=1}^{d} \ell_k \exp(-\lVert \mathbf{L}\boldsymbol{\eta} \rVert_2^2 / 2)$ $L_k = \ell_k$	$\mathcal{E}_{C,\mathbf{L}}^{(2)}$ $C = (2\pi)^{-d/2} \prod_{k=1}^{d} \ell_k$

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1. For $\mathcal{P}_{C,\mathbf{L}}$: $U_k^{(\min)} = O(\cot(n^{-2/d}))$.
2. For $\mathcal{P}_{C,\mathbf{L}}^{(r)}$ and $r > d/2$: $U_k^{(\min)} = O(n^{2/(r-1)})$ for $d = 2$, and $O(n^{2/(2r-d)})$ otherwise.
3. For $\mathcal{E}_{C,\mathbf{L}}^{(2)}$: $U_k^{(\min)} = O(\sqrt{\ln n})$.

Spectrally Equivalent Kernel Approximations

- Scaling up GPR by $k_{\boldsymbol{\theta}} \approx \tilde{k}_{\boldsymbol{\theta}}$. How well $\tilde{k}$ approximates k?
- It depends on how much $\mathcal{N}(\boldsymbol{\mu}, \tilde{\mathbf{K}}(\mathbf{X}, \mathbf{X}))$ is different from $\mathcal{N}(\boldsymbol{\mu}, \mathbf{K}(\mathbf{X}, \mathbf{X}))$.

Definition

We say $\tilde{\mathbf{K}}$ is *spectrally equivalent* to $\mathbf{K}$ if

$$(1 - n^{-1})\mathbf{K} \preceq \tilde{\mathbf{K}} \preceq (1 + n^{-1})\mathbf{K}\,.$$

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Lemma:

If $\tilde{\mathbf{K}}$ is *spectrally equivalent* to $\mathbf{K}$, then

$$D_{\mathbf{KL}}\left(\mathcal{N}(\boldsymbol{\mu}, \mathbf{K}), \mathcal{N}(\boldsymbol{\mu}, \tilde{\mathbf{K}})\right) \leq 1 - O(n^{-1})\,.$$

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- Use $(2n)^{-1}$ as the truncation error and as the quadrature error ($\Delta = n^{-1}$).

Efficient Gaussian Process Regression

The approximation has a low-rank structure. Given a dataset $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{X}$, let

$$\mathbf{Z} \in \mathbb{C}^{n \times s}, \quad \mathbf{Z}_{lj} := \varphi(\mathbf{x}_l, \boldsymbol{\eta}_j),$$

and

$$\mathbf{W} : \Theta \to \mathbb{R}_+^{s \times s}, \quad \mathbf{W}(\boldsymbol{\theta}) := \mathbf{diag}\left(w_1(\boldsymbol{\theta}_0), \ldots, w_s(\boldsymbol{\theta}_0)\right) .$$

Then, the approximate kernel matrix is

$$\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{X}) = \sigma_f^2 \mathbf{Z}\mathbf{W}(\boldsymbol{\theta})\mathbf{Z}^* + \sigma_n^2 \mathbf{I}_n .$$

Efficient Gaussian Process Regression

- **Hyperparameter learning:** for each gradient iteration of:

$$\boldsymbol{\theta}^\star = \arg\max_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta})$$

we compute $O(ns + s^3 + sd)$ vs $O(n^3)$. We have:

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$$\mathcal{L}(\boldsymbol{\theta}) = -\frac{1}{2}\mathbf{y}^\mathsf{T}\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})^{-1}\mathbf{y} - \frac{1}{2}\log\det\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X}) - \frac{n}{2}\log 2\pi$$

$$\frac{\partial\mathcal{L}}{\partial\theta_i} = -\frac{1}{2}\mathbf{Tr}\left(\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})^{-1}\frac{\partial\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})}{\partial\theta_i}\right) + \frac{1}{2}\mathbf{y}^\mathsf{T}\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})^{-1}\frac{\partial\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})}{\partial\theta_i}\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})^{-1}\mathbf{y}\,.$$

where

$$\frac{\partial\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})}{\partial\sigma_f^2} = \mathbf{Z}\mathbf{W}(\boldsymbol{\theta})\mathbf{Z}^*, \quad \frac{\partial\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})}{\partial\sigma_n^2} = \mathbf{I}_n, \quad \frac{\partial\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})}{\partial\theta_i} = \sigma_f^2\mathbf{Z}\frac{\partial\mathbf{W}(\boldsymbol{\theta})}{\partial\theta_i}\mathbf{Z}^*\,.$$

Efficient Gaussian Process Regression

- **Training:** we compute

$$\mathbf{w} := \mathbf{Z}^*\boldsymbol{\alpha} = \mathbf{W}(\boldsymbol{\theta}_0)^{-1}(\sigma_f^2\mathbf{Z}^*\mathbf{Z} + \sigma_n^2\mathbf{W}(\boldsymbol{\theta}_0)^{-1})^{-1}\mathbf{Z}^*\mathbf{y}\,.$$

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- **Prediction:** Given a test set $\mathbf{x}_1^{(t)},\dots,\mathbf{x}_t^{(t)}$, let

$$\mathbf{Z}^{(t)} \in \mathbb{C}^{t\times s}, \quad \mathbf{Z}_{lj}^{(t)} := \varphi(\mathbf{x}_l^{(t)},\boldsymbol{\eta}_j)\,.$$

  We compute

$$\mathbf{y}_{\text{mean}}^{(t)} := \tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}^{(t)},\mathbf{X})\boldsymbol{\alpha} = \sigma_f^2\mathbf{Z}^{(t)}\mathbf{W}(\boldsymbol{\theta})\mathbf{w}$$
$$\mathbf{Y}_{\text{var}}^{(t)} := \tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}^{(t)},\mathbf{X}^{(t)}) - \tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}^{(t)},\mathbf{X})\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})^{-1}\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X}^{(t)})$$

  in $O(st)$ vs $O(nt)$ for mean and $O(s^3+ts^2)$ vs $O(n^3+tn^2)$ for covariance.

Efficient Gaussian Process Regression

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$$\begin{aligned}
\mathbf{y}_{\text{mean}}^{(t)} &:= \tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}^{(t)},\mathbf{X})\boldsymbol{\alpha} = \sigma_f^2\mathbf{Z}^{(t)}\mathbf{W}(\boldsymbol{\theta})\mathbf{w} \\
\mathbf{Y}_{\text{var}}^{(t)} &:= \tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}^{(t)},\mathbf{X}^{(t)}) - \tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X}^{(t)},\mathbf{X})\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X})^{-1}\tilde{\mathbf{K}}_{\boldsymbol{\theta}}(\mathbf{X},\mathbf{X}^{(t)})
\end{aligned}$$

  in $O(st)$ vs $O(nt)$ for mean and $O(s^3+ts^2)$ vs $O(n^3+tn^2)$ for covariance.

Woodbury matrix identity

$$\left(\sigma_f^2\mathbf{Z}\mathbf{W}(\boldsymbol{\theta}_0)\mathbf{Z}^* + \sigma_n^2\mathbf{I}_n\right)^{-1} = \sigma_n^{-2}\left(\mathbf{I}_n - \sigma_f^2\mathbf{Z}\left(\sigma_f^2\mathbf{Z}^*\mathbf{Z} + \sigma_n^2\mathbf{W}(\boldsymbol{\theta}_0)^{-1}\right)^{-1}\mathbf{Z}^*\right).$$

Main Competitive Method: RFF

- Consider a restricted class of **shift-invariant kernels** of the form:

$$k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 k_0(\mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}')) + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'}$$

  where $\mathbf{L} = \mathbf{diag}\,(L_1, \ldots, L_d) \geq 0$ (i.e., $\boldsymbol{\theta}_0$).

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  where $\mathbf{L} = \mathbf{diag}\,(L_1, \ldots, L_d) \geq 0$ (i.e., $\boldsymbol{\theta}_0$).
- The approximate kernel is

$$\tilde{k}_{\boldsymbol{\theta}}^{(\mathsf{RFF})}(\mathbf{x}, \mathbf{x}') = \frac{\sigma_f^2}{s} \sum_{j=1}^{s} e^{-i(\mathbf{x}-\mathbf{x}')^{\mathsf{T}} \boldsymbol{\eta}_j} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'}$$

  with the associated matrix

$$\tilde{\mathbf{K}}_{\boldsymbol{\theta}}^{(\mathsf{RFF})}(\mathbf{X}, \mathbf{X}) = \sigma_f^2 \mathbf{Z}(\mathbf{L}) \mathbf{Z}(\mathbf{L})^* + \sigma_n^2 \mathbf{I}_n$$

  where

$$\mathbf{Z}(\mathbf{L}) = \frac{1}{\sqrt{s}} \exp\left(-i \mathbf{X} \mathbf{L}^{-1} \boldsymbol{\Sigma}\right), \quad \boldsymbol{\Sigma} = \left[\begin{array}{ccc} \boldsymbol{\eta}_1 & \ldots & \boldsymbol{\eta}_s \end{array}\right].$$

Comparison Between The Methods

Let I be the number of gradient computations for hyperparameter learning.

Table: Computational complexities (arithmetic operations) comparison between Gauss-Legendre Features and Random Fourier Features.

	Gauss-Legendre Features	Random Fourier Features
Training	$O(ns^2)$	$O(ns^2)$
Prediction	$O(st)$	$O(st)$
Hyperparameter learning	$O(ns^2+I(ns+s^3+sd))$	$O(I(ns^2+nsd^2))$

Other Types of Kernels

Semigroup kernels are defined on $\mathbb{R}^d_+$, and can be written as

$$k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \int_{\mathbb{R}^d_+} e^{-\boldsymbol{\eta}^\mathsf{T}(\mathbf{x}+\mathbf{x}')} p(\boldsymbol{\eta}; \lambda) d\boldsymbol{\eta} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'} \,.$$

For example, the *reciprocal semigroup kernel*:

$$k_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \prod_{k=1}^{d} \frac{\lambda}{x_k + x_k' + \lambda} + \sigma_n^2 \delta_{\mathbf{x},\mathbf{x}'} \,.$$

All the methodology above can be adapted also for these types of kernels.

Hyperparameter Domain

We define a hyperparameter domain Θ for each problem, e.g.

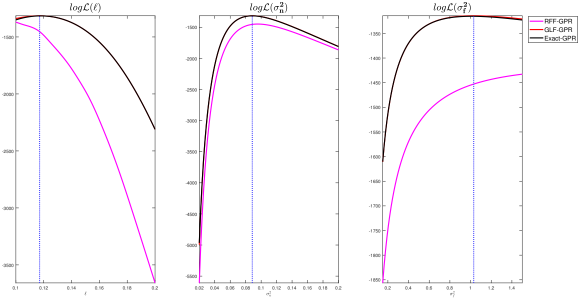
$$\Theta = \{[\ell, \sigma_n^2, \sigma_f^2] : \ell_0 \leq \ell \leq \ell_1, \sigma_{n0}^2 \leq \sigma_n^2 \leq \sigma_{n1}^2, \sigma_{f1}^2 \leq \sigma_f^2 \leq \sigma_{f0}^2\}$$

where $[\ell_0, \sigma_{f0}^2, \sigma_{n0}^2]$ is considered as the initial guess for optimization, for which we set the parameters $\mathbf{U}$ and $\mathbf{s}$.

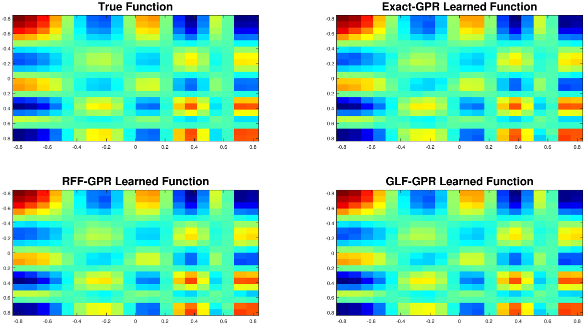
Synthetic Data

We consider $[-1,1] \times [-1,1]$ with $n = 4096$ training points and 400 test samples, generated by noisily sampling a predetermined function:

$$y_i = f^\star(\mathbf{x}_i) + \tau_i \,, \tau_i \sim \mathcal{N}(\mathbf{0}, 0.3^2\mathbf{I}_2)$$
$$f^\star(x_1, x_2) = (\sin(x_1) + \sin(10e^{x_1}))(\sin(x_2) + \sin(10e^{x_2}))\,.$$

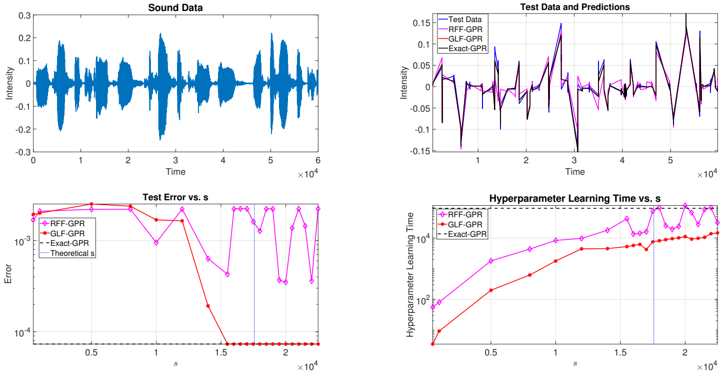


Synthetic Data



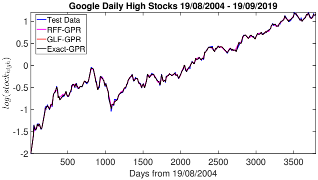
Natural Sound Modeling

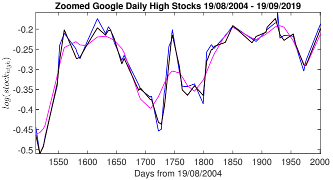
The goal is to recover contiguous missing regions in a waveform with $n = 59309$ training points. The test consists of 691 samples. The Gaussian kernel is used for learning.

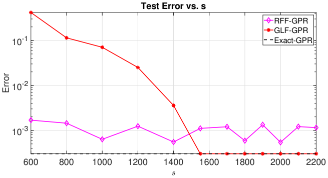


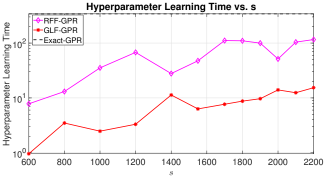
Google Daily High Stock Price

We consider a time series data of the daily high stock price of Google spanning 3797 days $19/08/2004 - 19/09/2019$. The data is $x \in \{1, \ldots, 3797\}$, $y = \log(Stock_{high})$. The test consists of 502 days. We use the Matèrn kernel with $\nu = 5/2$.



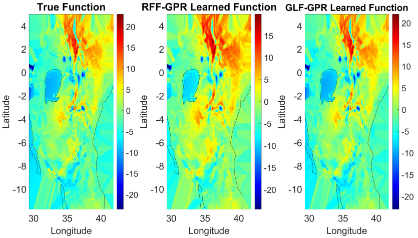


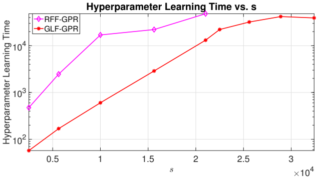




Spatial Temperature Anomaly for East Africa in 2016

We consider MOD11A2 Land Surface Temperature (LST) 8-day composite 2D data of synoptic yearly mean for 2016 in the East Africa region. Training data consists 77404 random locations $\mathbf{x} \in \{(Longitude, Latitude)\}$, $y = \{temperature\}$. The test consists of the remaining 6005 locations. We use the anisotropic Matèrn kernel with $\nu = 1$.





Thank you for your attention!

Questions?

P. Fink Shustin and Haim Avron,
Gauss-Legendre Features for Gaussian Process Regression,
Journal of Machine Learning Research (2022).