Fast Approximate Bayesian Gaussian Process Regression

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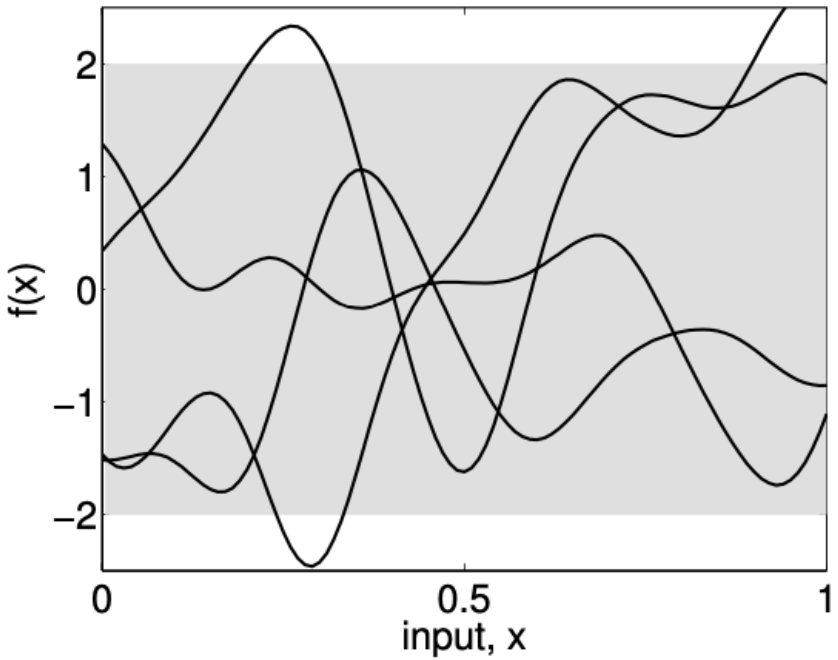
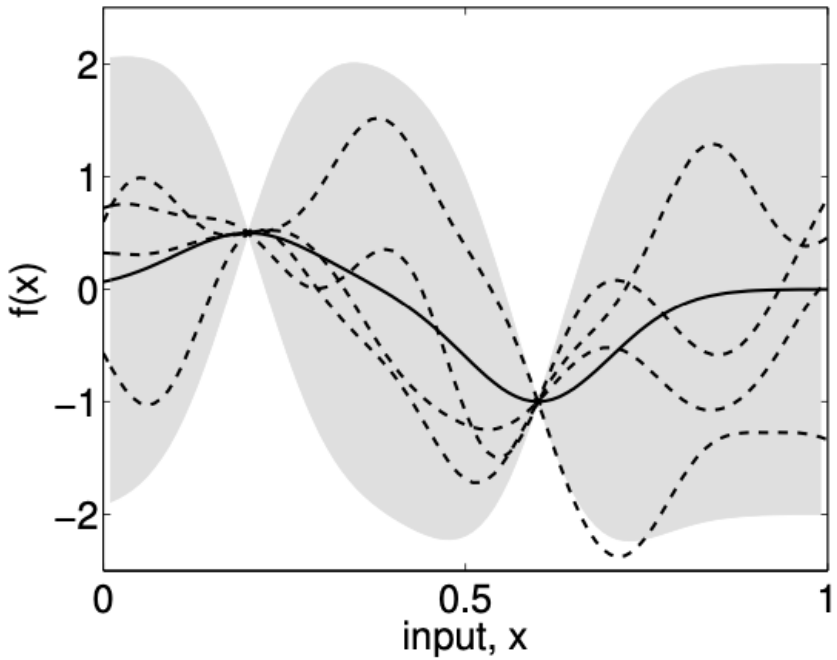
Gaussian processes (GPs)



(a), prior

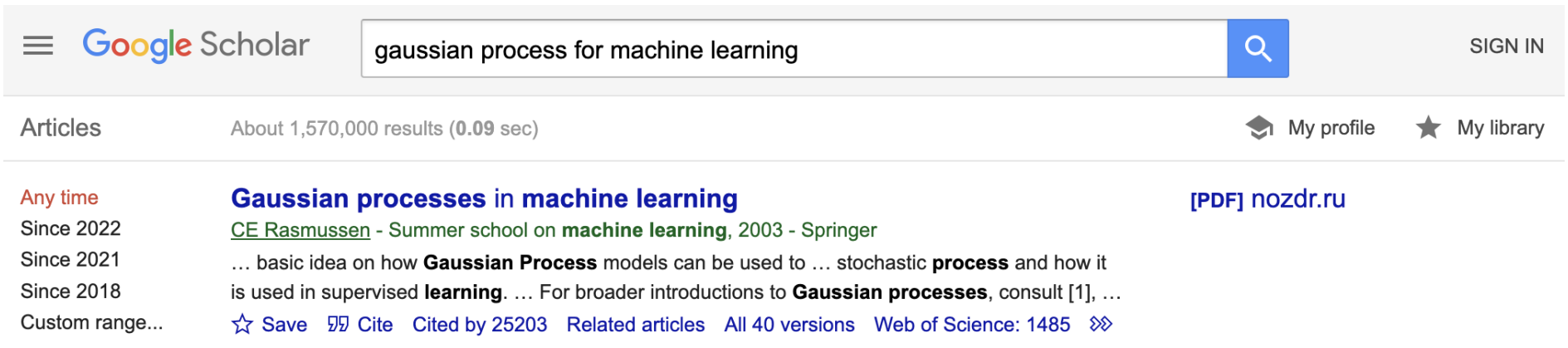


(b), posterior

Source: Gaussian Processes for Machine Learning by Rasmussen and Williams (2005).

Gaussian processes (GPs) are useful tools

- Give a reliable estimate of their own uncertainty.
- Inherit benefits of the underlying Gaussian distribution. E.g., marginals, conditionals, and derivatives are all still Gaussian.
- Enable us to encode assumptions we may have about a data set, including periodicity, smoothness (or lack thereof), wiggliness, etc.
- Not just for regression with normally distributed error structure, can be used for regression with count data, classification, as a building block in other models, etc.



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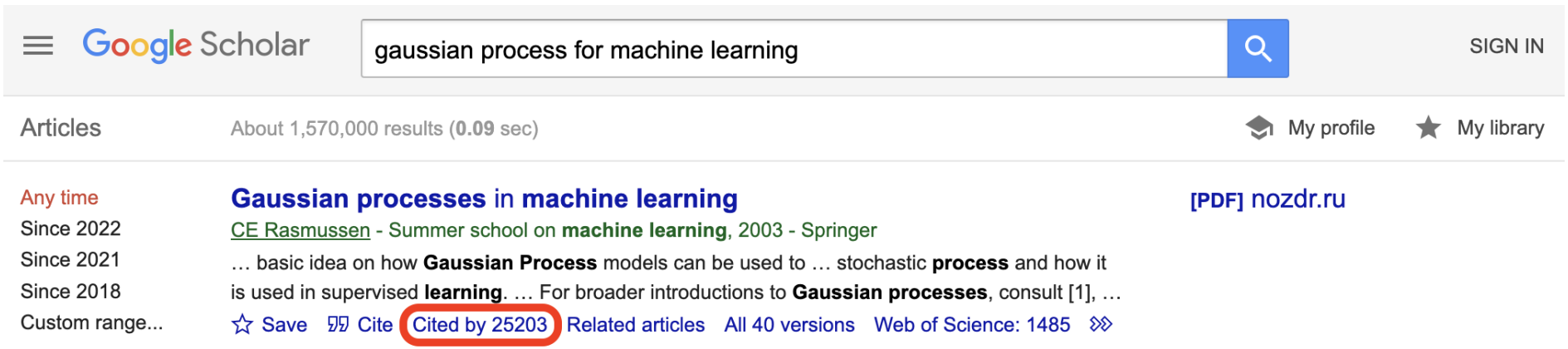


Gaussian process (GP) regression

$$y = f(x_i) + \epsilon_i, \quad \epsilon_i \sim \mathrm{N}(0, \tau^{-1})$$

Inputs $x_i \in \mathbb{R}^d, \quad i = 1, \ldots, n$

Here $f \sim GP(\mu, k)$, encodes dependence.

Covariance function/kernel k is $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ and is such that $k(x_i, x_j)$ is the covariance between $f(x_i)$ and $f(x_j)$.

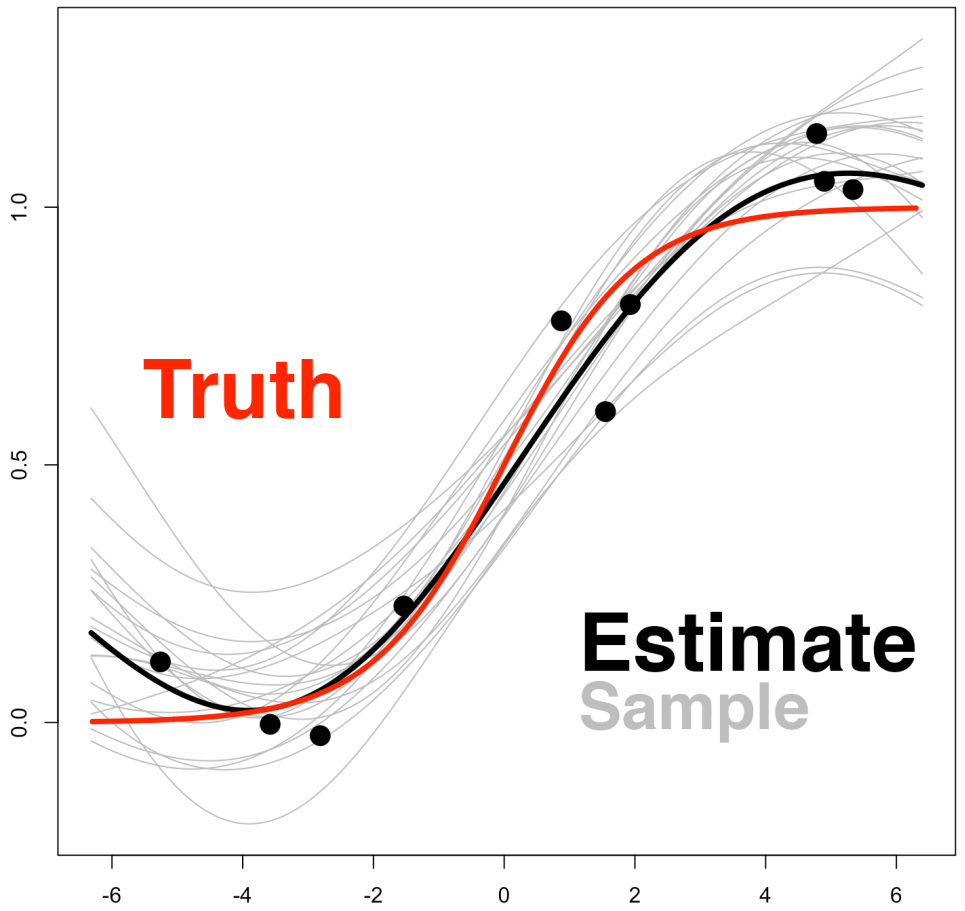
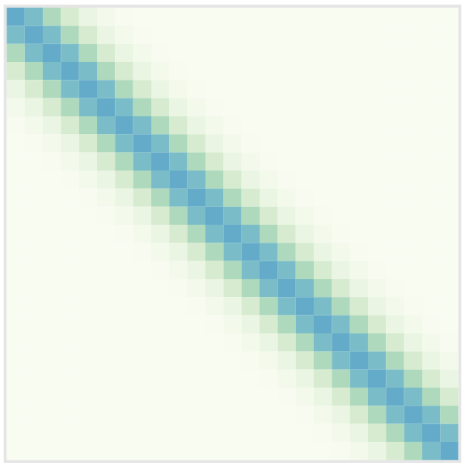


Figure: Samples from GP regression based on some observed data (black points).

Different covariance kernels

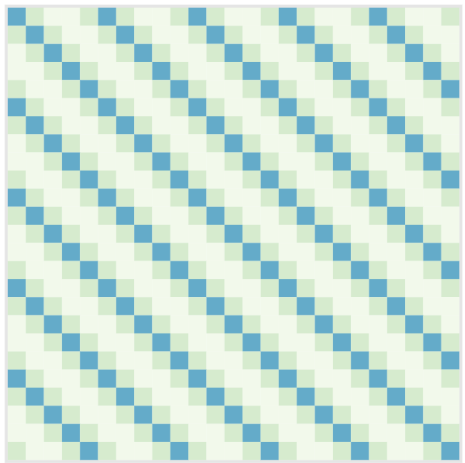
RBF KERNEL

$$\sigma^2 \exp\left(-\frac{||t-t'||^2}{2l^2}\right)$$



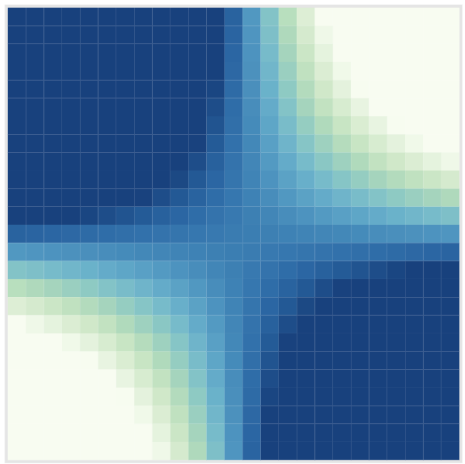
PERIODIC

$$\sigma^2 \exp\left(-\frac{2\sin^2(\pi|t-t'|/p)}{l^2}\right)$$



LINEAR

$$\sigma_b^2 + \sigma^2(t-c)(t'-c)$$



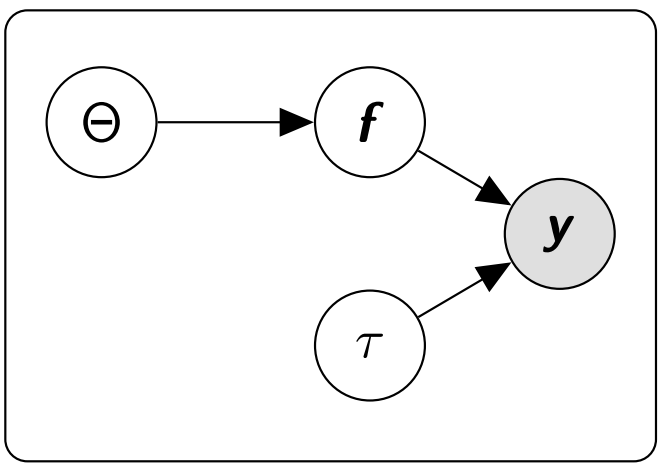
Source: `https://distill.pub/2019/visual-exploration-gaussian-processes/`.

Bayesian Gaussian process regression

- Rather than fixing the precision τ or kernel hyperparameters Θ, assign prior distributions $\pi(\cdot)$ for them.

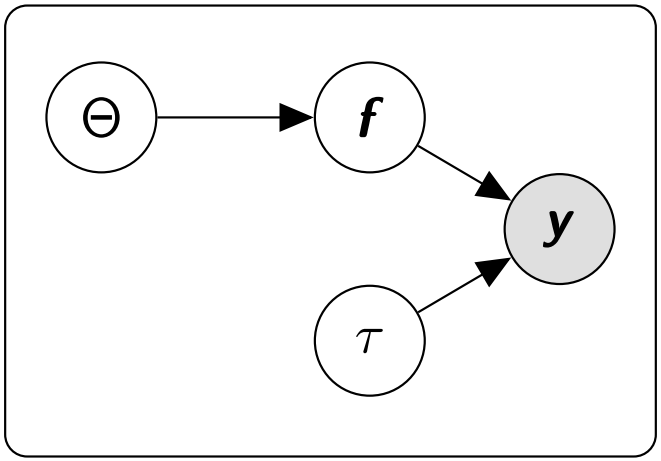
- The posterior distribution is:
  $\pi(\boldsymbol{f}, \Theta, \tau | \boldsymbol{y}) \propto \pi(\boldsymbol{y}|...)\ \pi(\boldsymbol{f}|\Theta)\ \pi(\Theta)\ \pi(\tau)$

- Can represent the model as a directed acyclic graph (DAG).

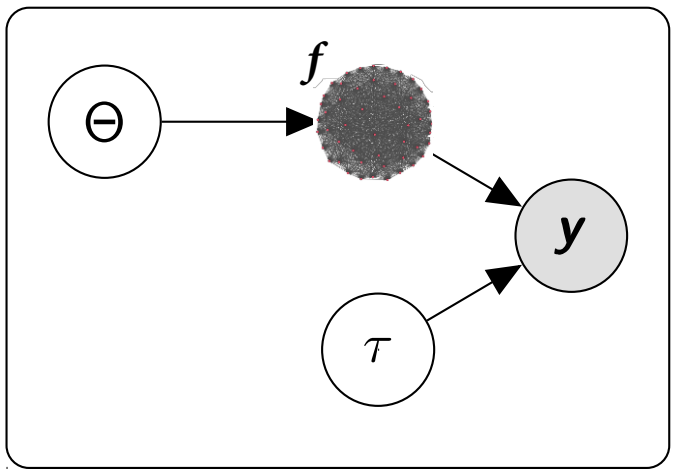


Why GP regression is expensive (DAG view)

Bayesian GP regression shown as a DAG:



But $\boldsymbol{f}$ is actually quite complex...



Why GP regression is expensive (equation view)

In equation view, the log-likelihood function is:

$$\ell_n(\Theta, \tau) = -\frac{n}{2} \log(2\pi) - \log\big[\det(K + \tau^{-1} I_n)\big] - \frac{1}{2} \boldsymbol{y}^T (K + \tau^{-1} I_n)^{-1} \boldsymbol{y},$$

and the GP function posterior is $\boldsymbol{f} | \boldsymbol{y}, X, \Theta, \tau \sim \mathrm{N}(\mu_f, \Sigma_f)$, where calculating the posterior mean μ_f and covariance Σ_f requires linear solves and matrix-matrix products.

Sampling from the GP prior requires

$$\text{Cholesky}(K) \cdot \boldsymbol{z} \text{ or } K^{\frac{1}{2}} \boldsymbol{z}, \quad \boldsymbol{z} \sim N(0_n, I_n),$$

and sampling from the posterior requires

$$\mu_f + \text{Cholesky}(\Sigma_f) \cdot \boldsymbol{z} \text{ or } \mu_f + \Sigma_f^{\frac{1}{2}} \boldsymbol{z}, \quad \boldsymbol{z} \sim N(0_n, I_n).$$

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Scalable GP regression

- Fast sparse Gaussian process methods: The informative vector machine (Herbrich, Lawrence, and Seeger, 2003)
- A unifying view of sparse approximate Gaussian process regression (Quinonero-Candela and Rasmussen, 2005)
- Gaussian predictive process models for large spatial data sets (Banerjee et al. 2008)
- Bayesian treed Gaussian process models with an application to computer modeling (Gramacy and Lee, 2008)
- Variational learning of inducing variables in sparse Gaussian processes (Titsias, 2009)
- On fixed-domain asymptotics and covariance tapering in Gaussian random field models (Wang and Loh 2011)
- A full scale approximation of covariance functions for large spatial data sets (Sang and Huang 2012)
- Twenty years of mixture of experts (Yuksel, Wilson, and Gader, 2012)
- Efficient Gaussian process regression for large datasets (Banerjee, Dunson, and Tokdar 2012)
- Covariance tapering for prediction of large spatial data sets in transformed random fields (Hirano and Yajima, 2013)
- Massively Parallel Approximate Gaussian Process Regression (Gramacy, Niemi, and Weiss, 2014)
- Distributed variational inference in sparse Gaussian process regression and latent variable models (Gal et al., 2014)
- Gaussian process models with parallelization and GPU acceleration (Dai et al., 2014)
- Distributed Gaussian processes (Deisenroth and Ng, 2015)
- Local Gaussian Process Approximation for Large Computer Experiments (Gramacy and Apley, 2015)
- Fast Direct Methods for Gaussian Processes (Ambikasaran et al., 2015)
- Kernel interpolation for scalable structured Gaussian processes (KISS-GP) (Wilson and Nickisch, 2015)
- Multi-level restricted maximum likelihood covariance estimation and kriging for large non-gridded spatial datasets (Castrillon-Candás, Genton, and Yokota, 2016)
- Hierarchical nearest-neighbor Gaussian process models for large geostatistical datasets (Datta et al. 2016)
- Nonseparable dynamic nearest neighbor Gaussian process models for large spatio-temporal data with an application to particulate matter analysis (Datta et al., 2016)
- Multi-resolution approximations of Gaussian processes for large spatial datasets (Katzfuss and Gong, 2018)
- Generalized robust Bayesian committee machine for large-scale Gaussian process regression (Liu et al., 2018)
- Nested Kriging predictions for datasets with a large number of observations (Rulliere et al., 2018)
- Efficient algorithms for Bayesian Nearest Neighbor Gaussian Processes (Finley et al. 2019)
- Likelihood Approximation With Hierarchical Matrices For Large Spatial Datasets (Litvinenko et al., 2019)
- On random subsampling of Gaussian process regression: A graphon-based analysis (Hayashi, Imaizumi, and Yoshida, 2019)
- And many, many, many more not listed here (see review papers such as "When Gaussian process meets big data: A review of scalable GPs")

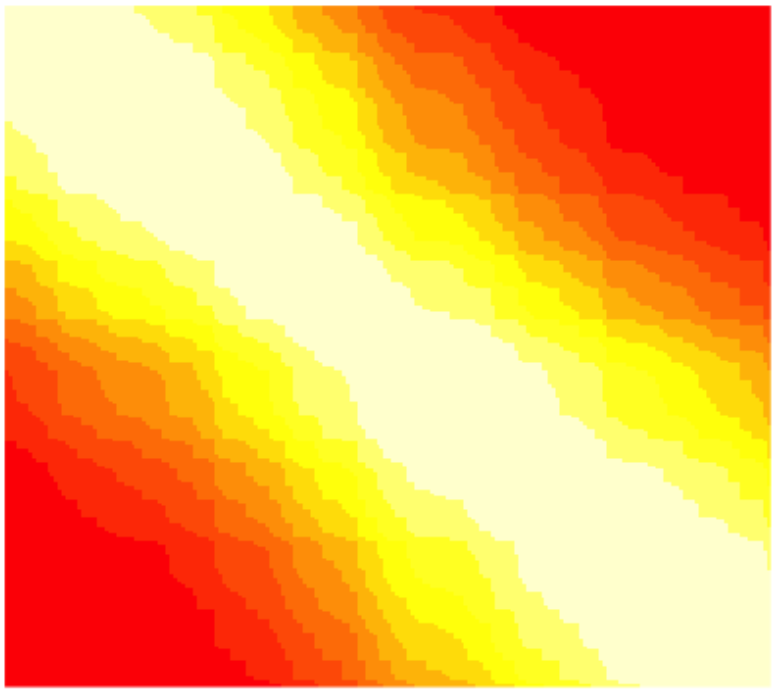
Where our approach fits in

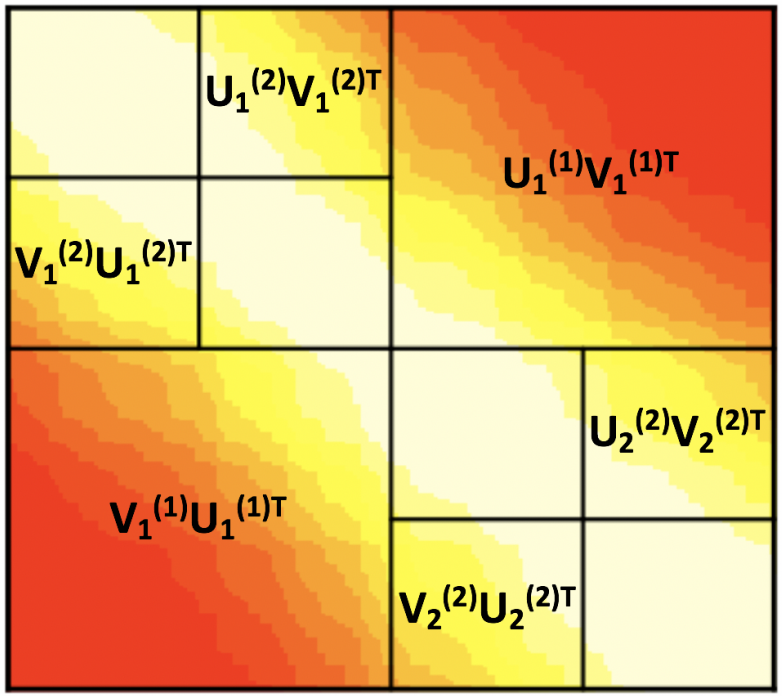
The philosophy: Rather than changing the model, approximate the covariance matrix in a way that allows you to speed up the operations necessary for fully Bayesian inference.

What we develop: A novel sampling algorithm for posterior draws of $f|y$ with a provable bound on the divergence between the true and approximate posterior, novel use of $\mathcal{H}$-matrices in the Bayesian context, and a tensor product formulation for higher-dimensional input spaces. Published in JRSS-B in 2022: See `https://doi.org/10.1111/rssb.12494`.

Where we're going: Explore alternative ways of approximating K (or k). Develop and release modular **R** code that can be incorporated into existing samplers in place of exact GPs.

Example: Approximating K using an $\mathcal{H}$-matrix





Using an approximation based on the Hierarchical Off-Diagonal Low Rank (HODLR) decomposition, a type of hierarchical matrix, you can calculate the Cholesky, perform solves, and get determinants at $\mathcal{O}(n \log n)$ cost.

$\mathcal{H}$-matrices and GPs

Prior to our work, $\mathcal{H}$-matrices had not yet been extended to fully Bayesian GP regression models. Here's why.

Say you want to sample from n-dimensional $\mathrm{N}(\mathbf{0}, C)$.

1. Get Cholesky factorization $C = LL^T$.
2. Sample n univariate standard normal random variables; call these samples $\boldsymbol{z}$, so $\boldsymbol{z} \sim \mathrm{N}(\mathbf{0}, I_n)$.
3. Then $L\boldsymbol{z}$ has the desired distribution.

The GP posterior doesn't fit neatly in this format:

$$\begin{aligned} \boldsymbol{f}|\boldsymbol{y}, X, \Theta, \tau &\sim \mathrm{N}(\mu_f, \Sigma_f), \\ \Sigma_f &= K - K(K + \tau^{-1}\mathbf{I}_n)^{-1}K \\ &= (K^{-1} + \tau\mathbf{I}_n)^{-1} \\ &= K(\tau K + \mathbf{I}_n)^{-1} \end{aligned}$$

Sampling algorithm

Algorithm 1: Recall τ is the noise precision. Let ϵ denote the tolerated difference max norm. Sampling proceeds as follows:

1. If $\tau < 1$, set $\epsilon^* = \tau\epsilon$, else set $\epsilon^* = \epsilon$.
2. Create $\mathcal{H}$ matrix decomposition of K with tolerance ϵ^*/τ and $\tau K + I$ with tolerance ϵ^*, $\tilde{K}$ and $\tilde{M}$ respectively (assembly, cost $\mathcal{O}(n \log^2 n)$).
3. Get W s.t. $\tilde{K} = WW^T$ (symmetric factorization, cost $\mathcal{O}(n \log^2 n)$).
4. Sample $\boldsymbol{a}, \boldsymbol{b} \sim \mathrm{N}(0, I_n)$.
5. Let $Z = \sqrt{\tau}\tilde{K}a + Wb$ (matrix vector products, cost $\mathcal{O}(n \log n)$).
6. Let $Z^* = \tilde{M}^{-1}Z$ (solve, cost $\mathcal{O}(n \log n)$).
7. Let $R = \tau\tilde{K}\tilde{M}^{-1}\boldsymbol{y}$ (solve then mat-vec product, cost $\mathcal{O}(n \log n)$).
8. Finally, let $Z^{**} = R + Z^*$, which is the approximated sample from $p(\boldsymbol{f}|\boldsymbol{y}, X, \Theta)$ (vector addition, cost $\mathcal{O}(n)$).

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3. Get W s.t. $\tilde{\nu}$ … $(n \log^2 n)$).
4. Sample $\boldsymbol{a}$, …
5. Let $Z = \sqrt{\tau}$… products, cost $\mathcal{O}(n \log n)$).
6. Let $Z^* = \tilde{M}^{-1}$… $\mathcal{O}(n \log n)$).
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TL;DR

Approximation fidelity

Theorem

Let $\boldsymbol{p} \sim N(\mu_f, \Sigma_f)$ *where* $\mu_f = \tau \Sigma_f \boldsymbol{y}$ *and* Σ_f *is an* $n \times n$ *positive definite matrix, with* $\Sigma_f = K(\tau K + I)^{-1}$ *for* K *the* $n \times n$ *realization of some symmetric covariance kernel,* $\boldsymbol{y}$ *is a length-n vector, and* τ *is a constant. Define* $M = (\tau K + I)$ *such that* $\Sigma_f = KM^{-1}$. *Then there exists matrices* $\tilde{K}, \tilde{M} \in \mathcal{H}$ *with* $||K - \tilde{K}||_{\max} \leq \varepsilon$ *and* $||M - \tilde{M}||_{\max} \leq \varepsilon$ *such that for* $\tilde{\Sigma}_f = \tilde{K}\tilde{M}^{-1}$, $\tilde{\mu}_f = \tau \tilde{\Sigma}_f \boldsymbol{y}$, *and* $\boldsymbol{q} \sim N(\tilde{\mu}_f, \tilde{\Sigma}_f)$

$$\mathcal{D}_{KL}(\mathcal{P}||\mathcal{Q}) = E_{\mathcal{P}}\left[log\left(\frac{\mathcal{P}}{\mathcal{Q}}\right)\right] \leq c_1 n^2 \varepsilon + c_2 n^{5/2} \varepsilon + c_3 n^3 \varepsilon^2, \qquad (1)$$

with $\lim_{\varepsilon \to 0} \mathcal{D}_{KL}(\mathcal{P}||\mathcal{Q}) = 0$, *where the density functions of* $\boldsymbol{p}$ *and* $\boldsymbol{q}$ *are denoted by* $\mathcal{P}$ *and* $\mathcal{Q}$, *respectively. The constants* c_1, c_2, *and* c_3 *are dependent on the conditioning of* K *and* M.

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$$\mathcal{D}_{KL}(\mathcal{P}||\mathcal{Q}) \leq \varepsilon + c_2 n^{5/2}\varepsilon + c_3 n^3 \varepsilon^2, \qquad (1)$$

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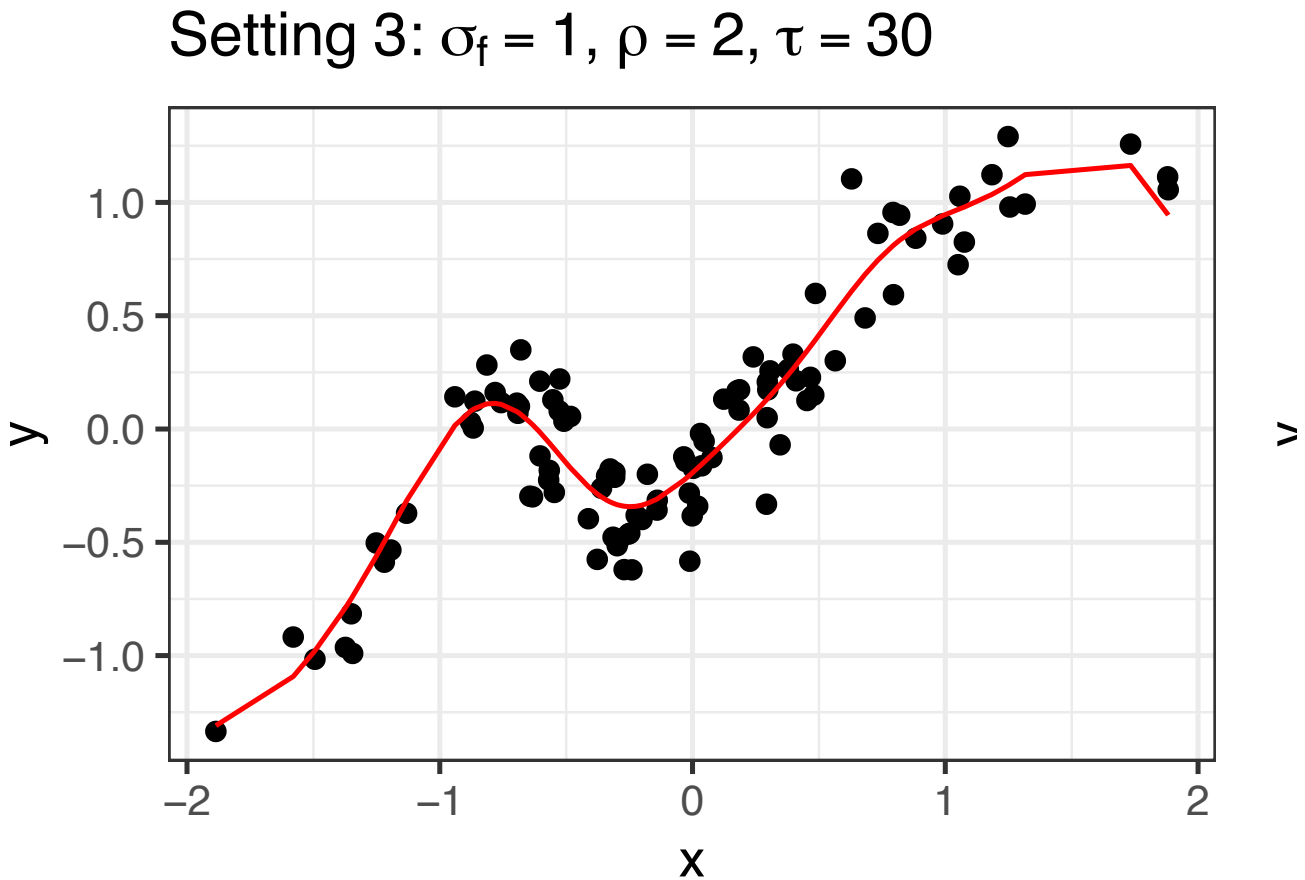
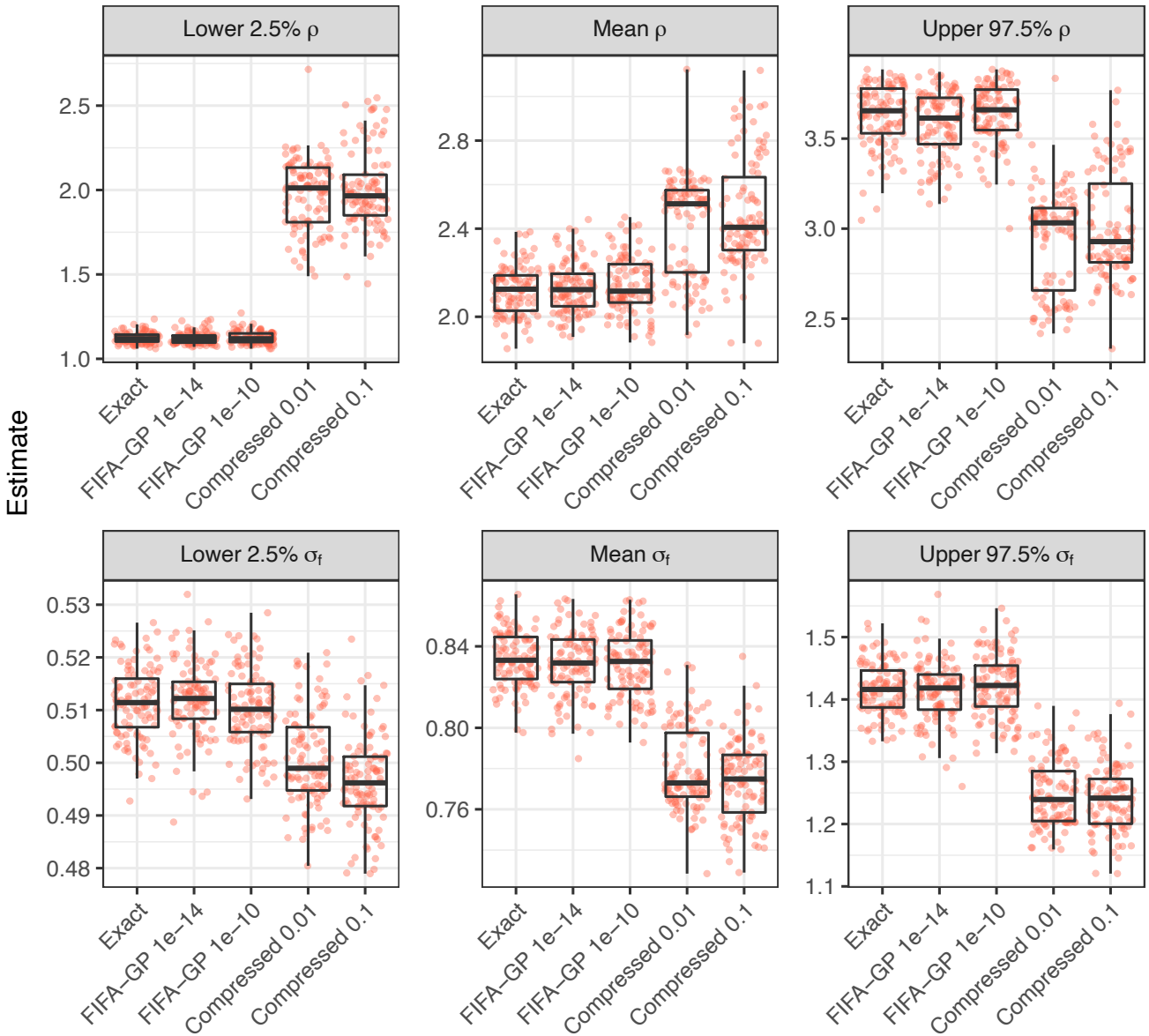
TL;DR

Small n simulation, 1D input (example data set)

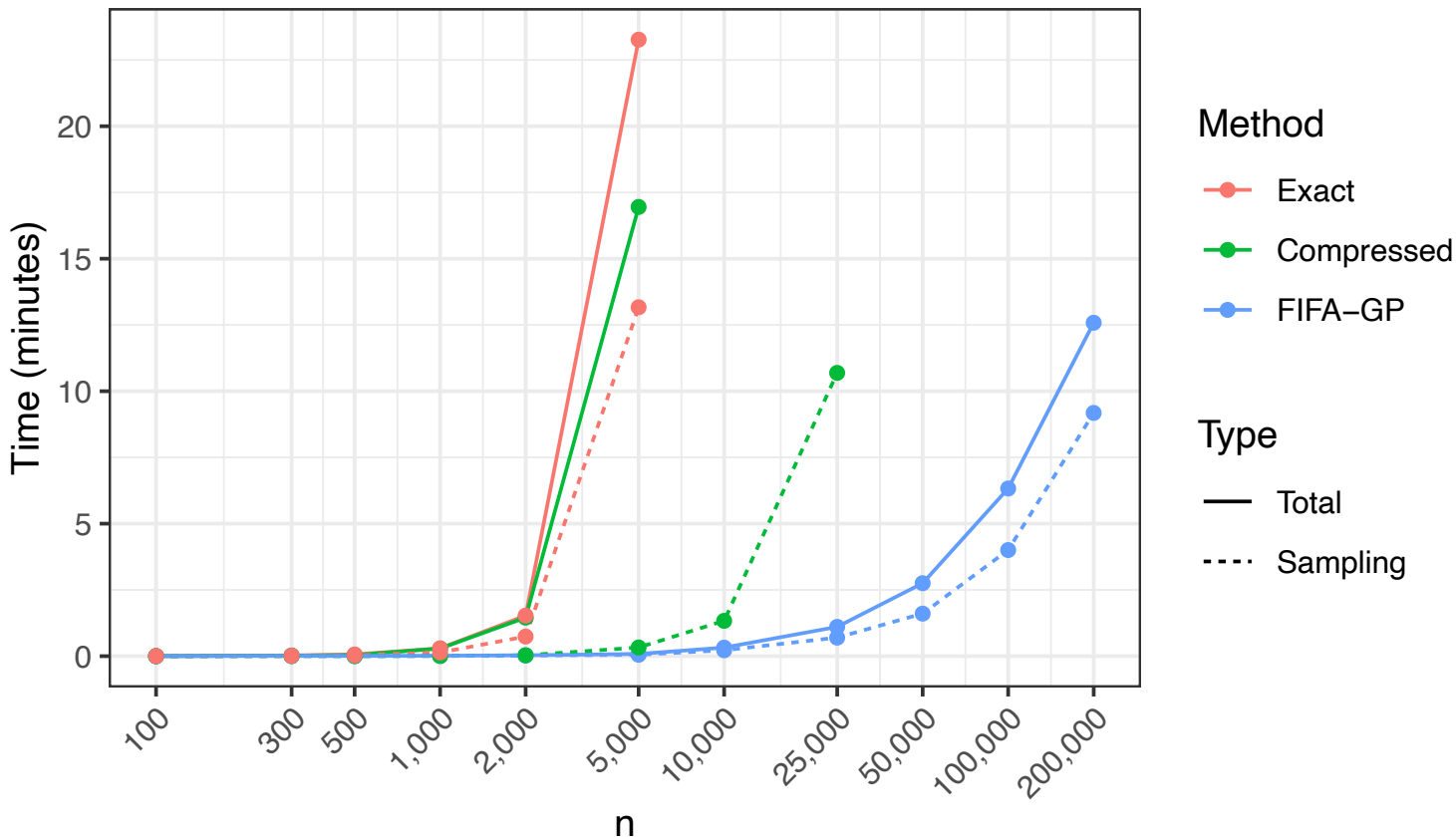


Small n simulation, 1D input (example results, more in paper)



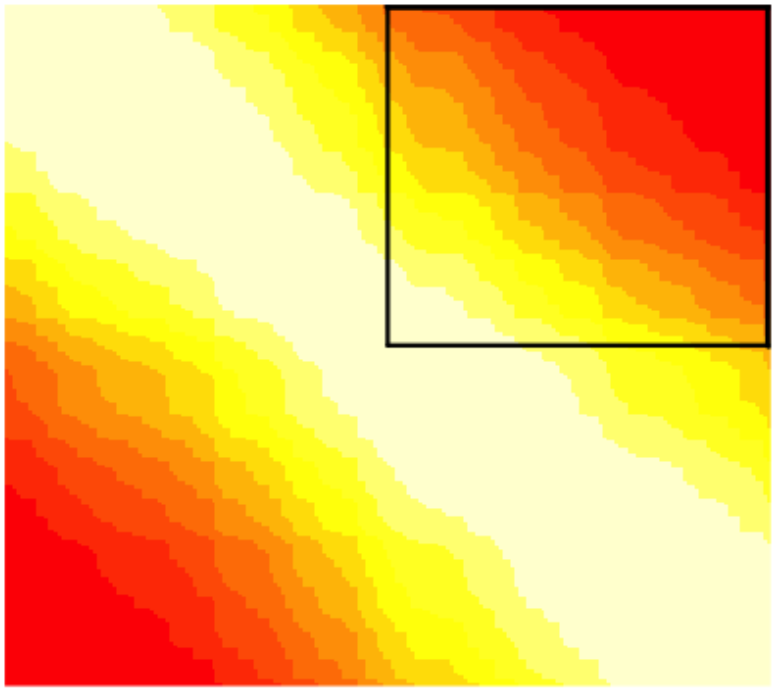
Large n simulation, 1D input (timing for 100 samples)

Observations have mean $f(x) = \sin 2x + \frac{1}{8}e^x$ and precision $\tau = 2$.

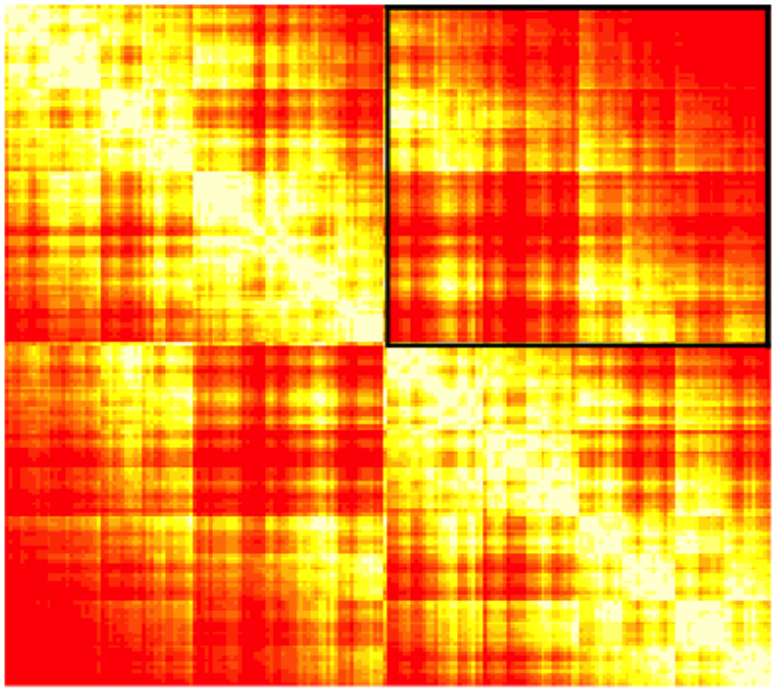


MSE and MSPE for FIFA-GP are similar to the exact GP and compressed GP, and superior to the NNGP.

Dimension of input space



1D input requires rank $r = 8$ matrix to approximate to tolerance 10^{-12}.



2D input requires rank $r = 56$ matrix to approximate to tolerance 10^{-12}.

The curse of dimensionality

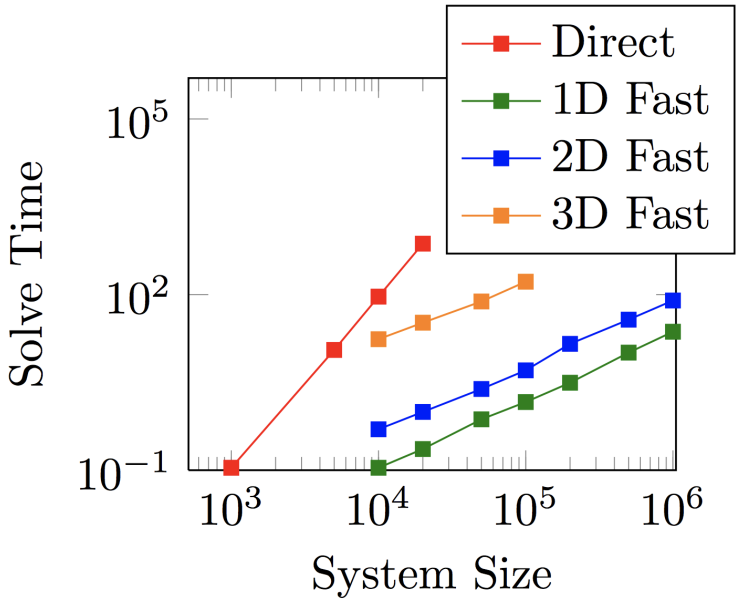


TABLE II

TIMINGS FOR GAUSSIAN COVARIANCE FUNCTIONS IN ONE, TWO, AND THREE DIMENSIONS. THE MATRIX ENTRIES ARE GIVEN AS $C_{ij} = 2\delta_{ij} + \exp\left(-||r_i - r_j||^2\right)$, WHERE r_i ARE RANDOM UNIFORMLY DISTRIBUTED POINTS IN THE INTERVAL $[-3, 3]^d$ $(d = 1, 2, 3)$.

	One-dimensional data					Two-dimensional data					Three-dimensional data				
n	Assembly	Factor	Solve	Det.	Error	Assembly	Factor	Solve	Det.	Error	Assembly	Factor	Solve	Det.	Error
$10,000$	0.12	0.11	0.008	0.01	10^{-13}	0.56	0.50	0.018	0.03	10^{-13}	15.4	17.3	0.113	0.91	10^{-12}
$20,000$	0.15	0.23	0.016	0.03	10^{-13}	1.16	0.99	0.028	0.05	10^{-13}	30.9	33.1	0.224	1.06	10^{-12}
$50,000$	0.47	0.71	0.036	0.12	10^{-12}	2.74	2.44	0.067	0.12	10^{-13}	75.5	76.3	0.434	1.68	10^{-11}
$100,000$	1.24	1.46	0.052	0.24	10^{-12}	5.43	5.08	0.165	0.23	10^{-12}	149	166	0.923	3.11	10^{-11}
$200,000$	2.14	3.12	0.121	0.39	10^{-13}	12.4	14.4	0.485	0.44	10^{-12}					
$500,000$	6.13	10.2	0.388	0.56	10^{-12}	31.7	37.3	1.33	1.17	10^{-12}					
$1,000,000$	14.1	23.2	0.834	1.52	10^{-12}	70.8	79.2	3.15	2.24	10^{-12}					

From "Fast Direct Methods for Gaussian Processes" by Ambikasaran et al. (2015).

Extending to higher dimensional inputs

- Our original solution was to model the d-dimensional surface as a tensor product of 1-dimensional GPs:

$$y_i = f_1(x_{1,i}) \otimes f_2(x_{2,i}) \otimes \ldots \otimes f_d(x_{d,i}) + e_i,$$
$$e_i \sim \mathrm{N}(0, \tau^{-1}), \quad f_h(\cdot) \sim GP(m_h(\cdot), k_h(\cdot,\cdot)),$$
$$i = 1, \ldots, n, \quad h = 1, \ldots, d.$$

- This approach can work well for some problems; see JRSS-B paper for a proof and details on simulated and non-synthetic performance.

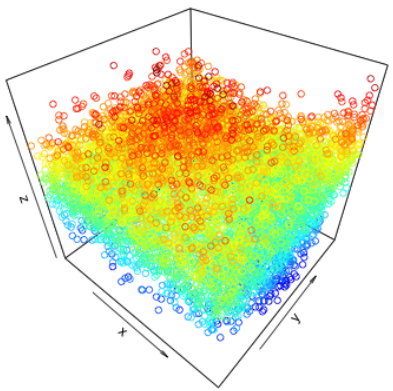
- But if we don't want to fiddle with tensor products, we could utilize a non-HODLR $\mathcal{H}$-matrix class that scales better with d (e.g. `H2Lib`, `HLIBCov`, or `SMASH`), or rethink the best stage at which to perform the approximation (i.e., perhaps approximate the kernel k rather than the realization of that kernel K).

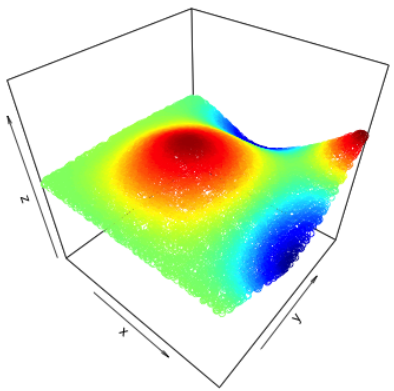
Tensor product simulation (data/surfaces)

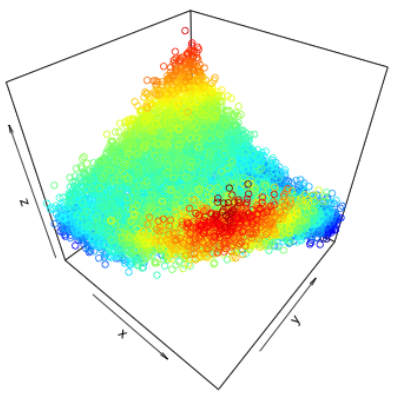
Simulate data from:

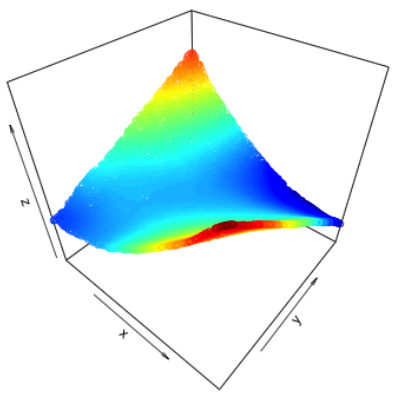
(Top) $g_1(x_1, x_2) = \sin(x_1)\sin(x_2)\sqrt{x_1 x_2}$

(Bottom) $g_2(x_1, x_2) = x^2 - 2xy + 3y + 2$

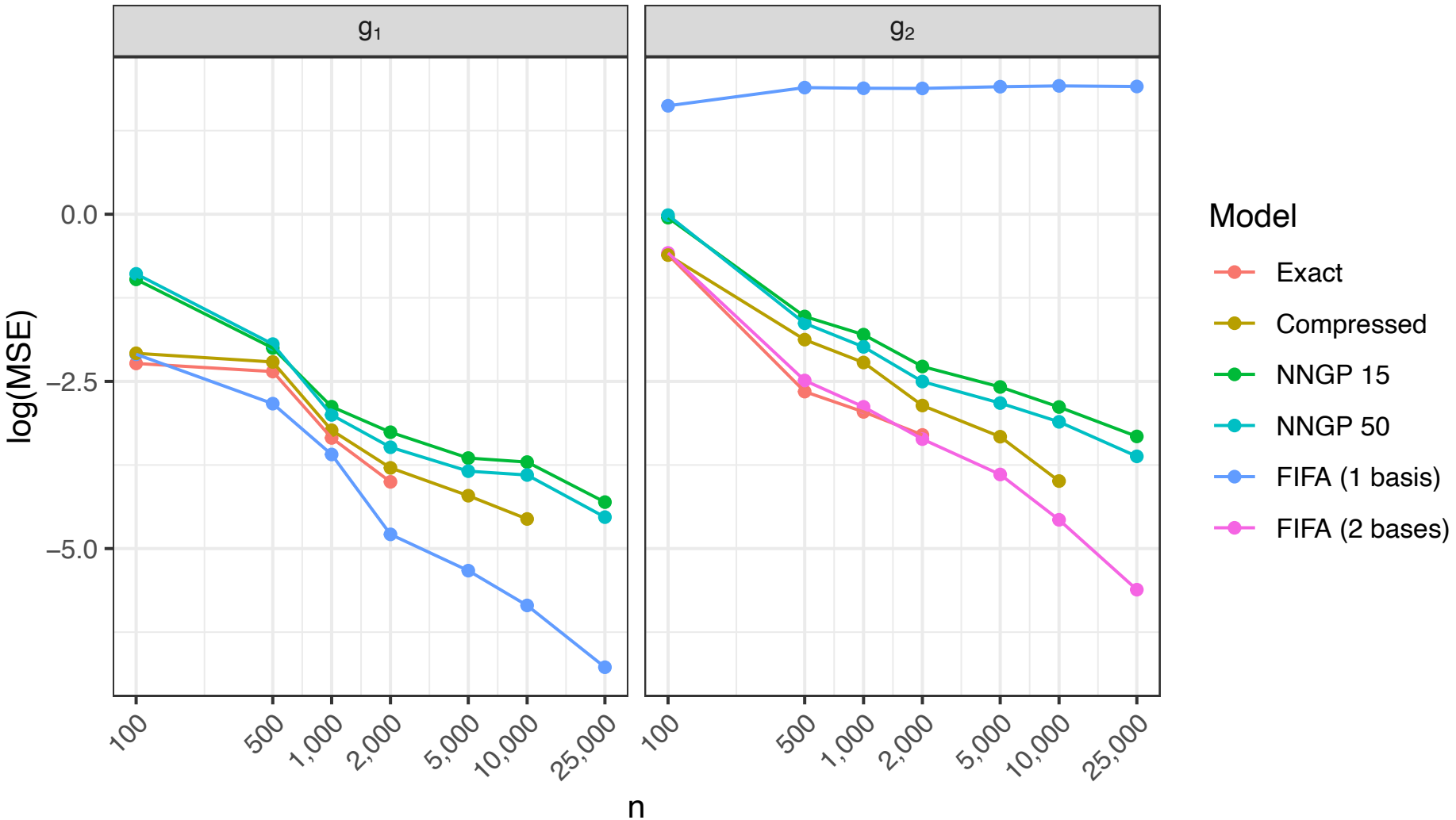




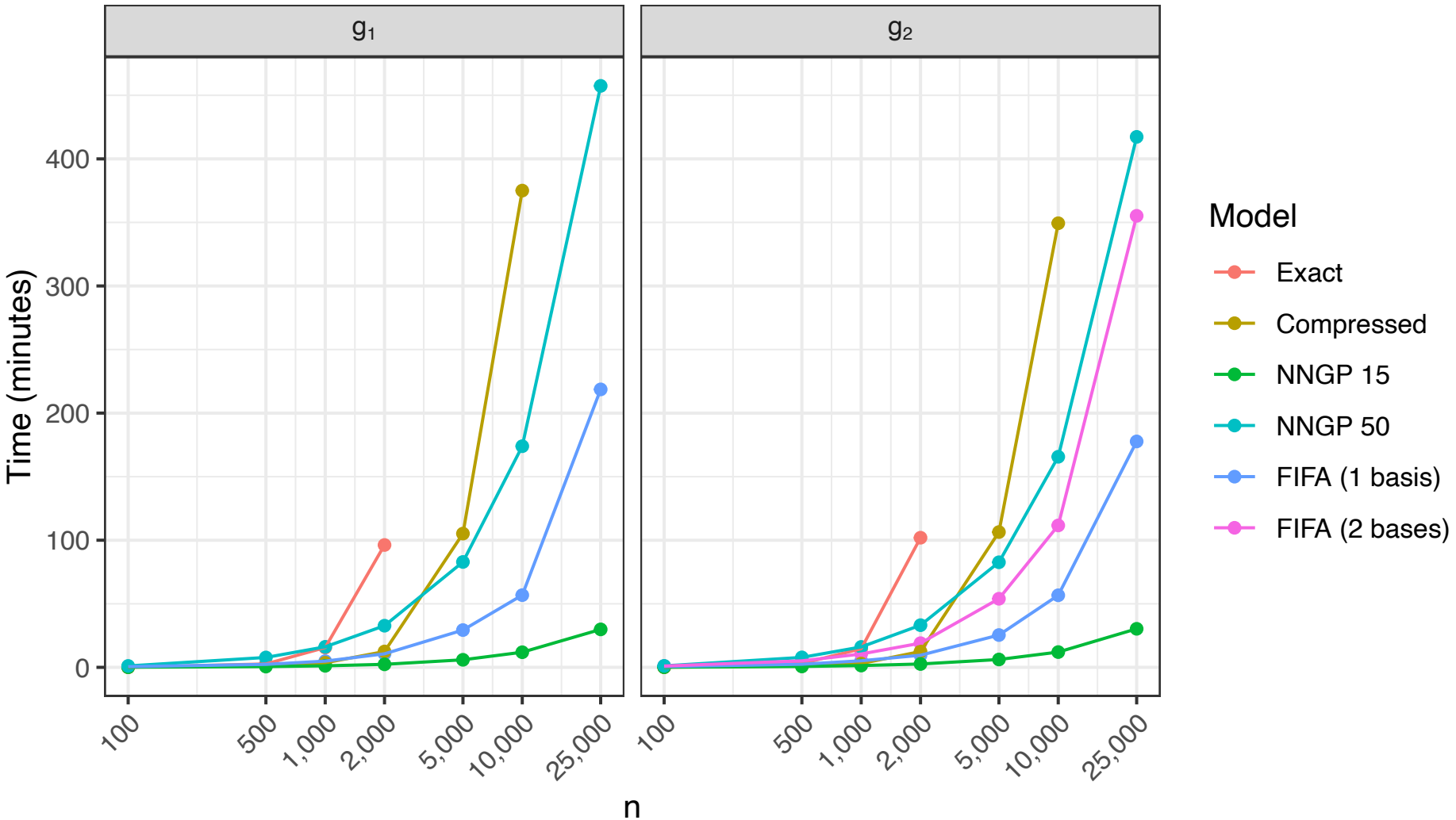




Tensor product simulation (MSE)



Tensor product simulation (timing for 7,000 iterations)



Illustrative real data examples

Atmospheric CO2 at Mauna Loa, HI:

- 358,253 observations, data at hourly level from 1974 to present.
- FIFA-GP **outperforms** the NNGP in MSPE for **75%** of hold-out years and consistently takes 1/3 the computation time (around 30 minutes for 7,000 samples).

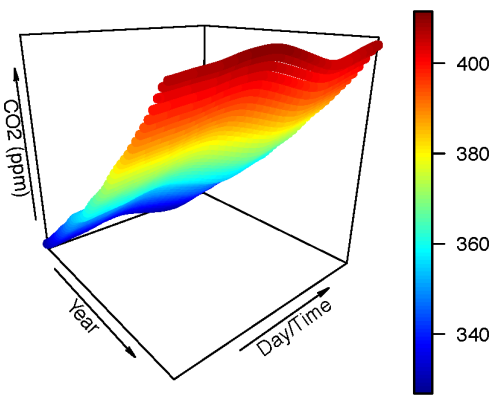


Figure: Model predicted atmospheric CO2 surface.

Particulate matter ($PM_{2.5}$) in USA:

- 4,977,391 observations, daily data for contiguous US since 1999.
- FIFA-GP yielded an **18% improvement** relative to the NNGP for hold-out predictive performance, and completed 7,000 samples in about **an hour**.

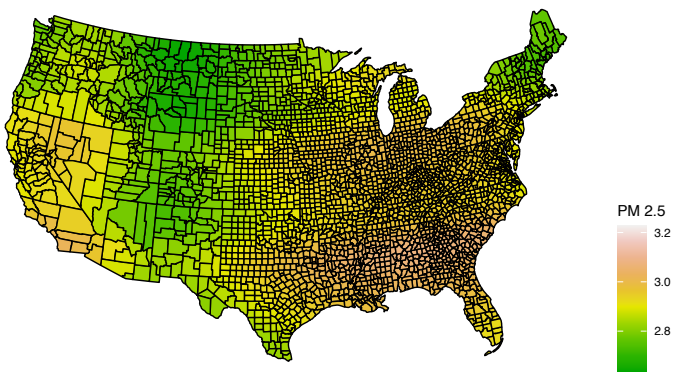
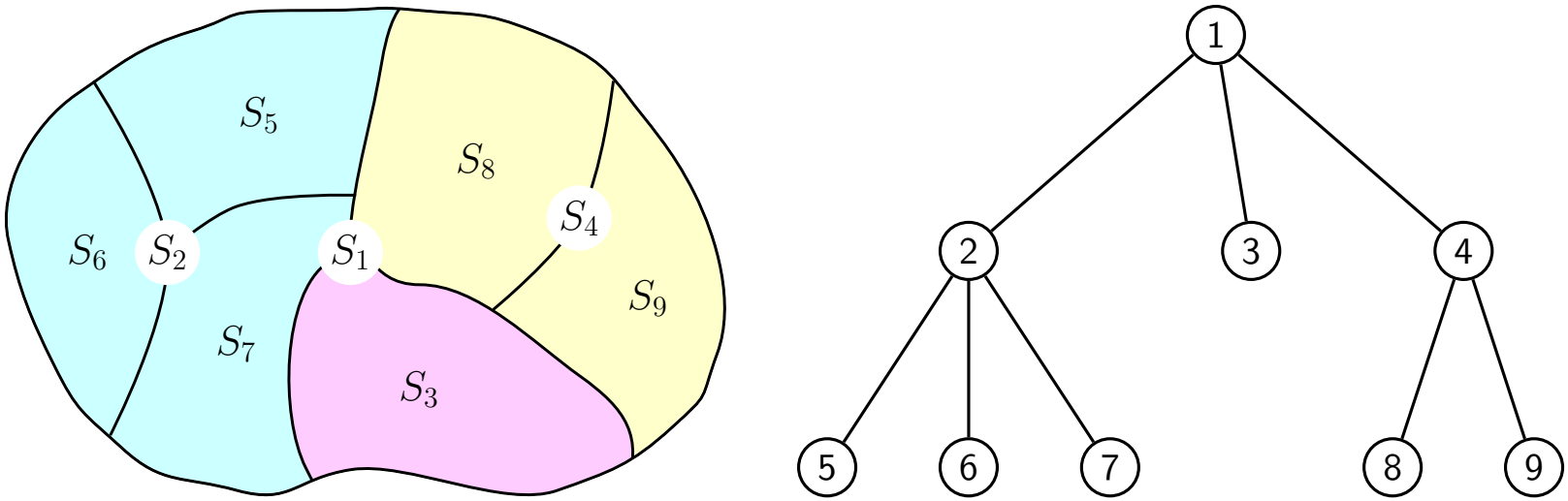


Figure: Model predicted 2019 $PM_{2.5}$ surface.

Approximate k instead of K

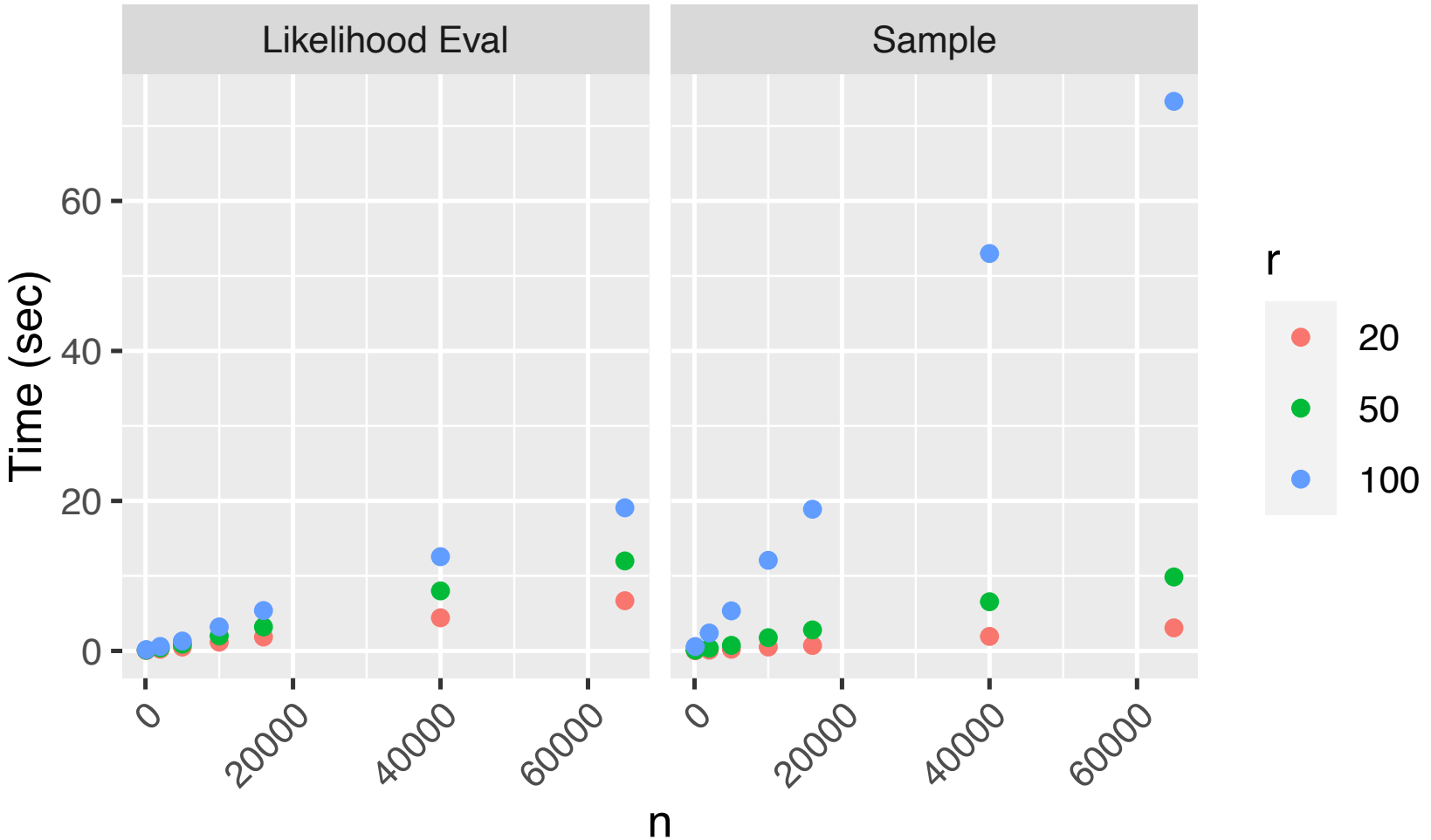
Hierarchical partitioning of domain $S =: S_1$



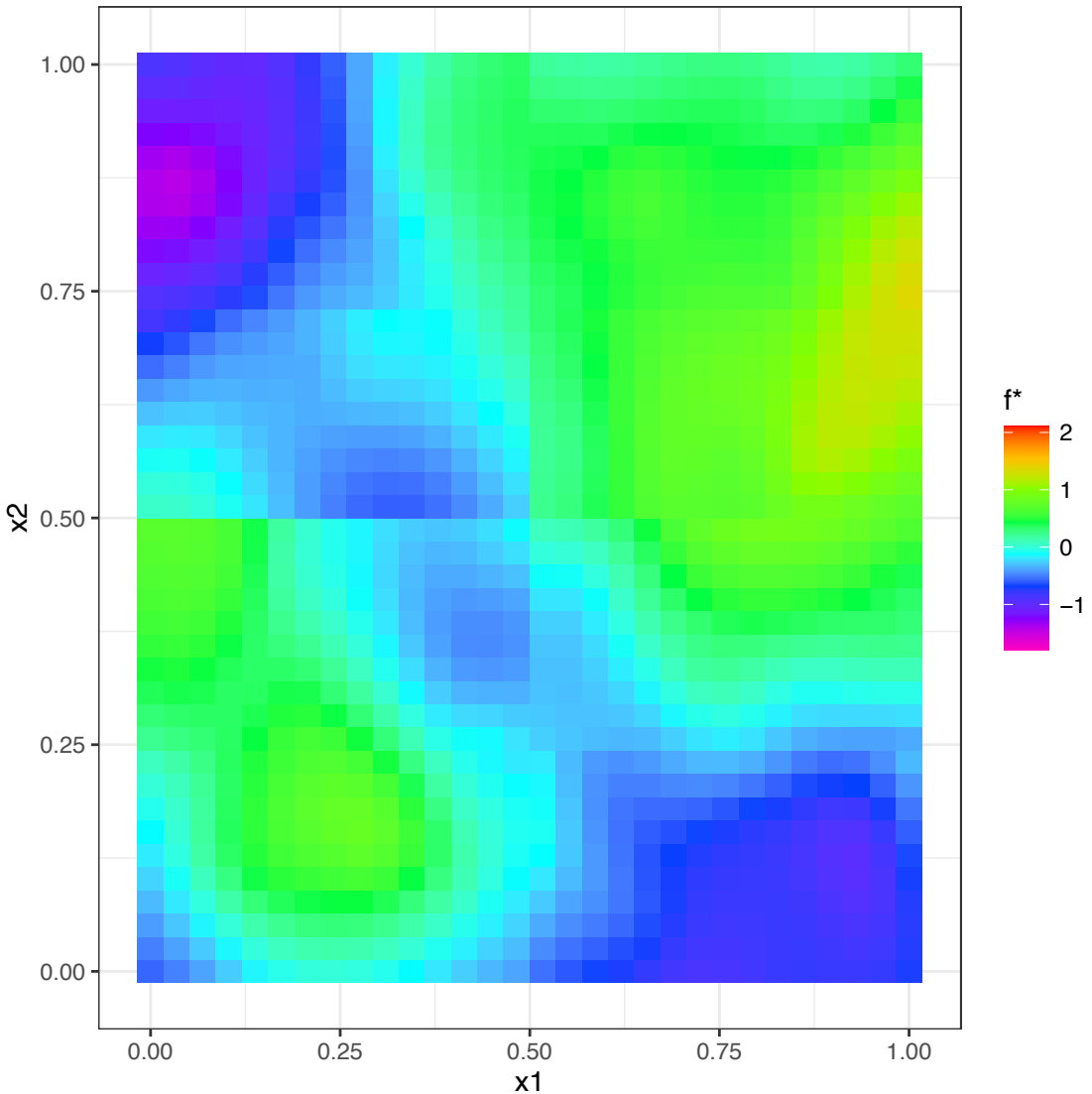
- For each nonleaf node i, find a set of landmark points $\underline{X}_i \subset S_i$
- Definition of k_{h} (informal example):
  - [Same leaf node] $\boldsymbol{x}, \boldsymbol{x}' \in S_8$: $k_{\mathsf{h}}(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}')$
  - [One level higher] $\boldsymbol{x} \in S_8$, $\boldsymbol{x}' \in S_9$:
    $k_{\mathsf{h}}(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \underline{X}_4) k(\underline{X}_4, \underline{X}_4)^{-1} k(\underline{X}_4, \boldsymbol{x}')$

Recursively Low-Rank Compressed Matrices (RLCMs) were used for kernel approximation in the frequentist GP context in "Linear-Cost Covariance Functions for Gaussian Random Fields" [Chen and Stein 2021].

Timing using different numbers of landmark points



Samples using few landmark points



Upcoming

- My co-author Matthew Wheeler along with Wesley Burr have an **R** package for fast Bayesian GP sampling using H-matrices at `https://github.com/wesleyburr/schnellerGP` (caveat: still very much in the development stage).

- Working on ideas for the potential improvements to sampling using RLCMs with few landmark points.

- If RLCM-based posterior sampling continues to seem promising, will develop an **R** package for Bayesian GP sampling leveraging RLCMs.

Questions?

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JRSS-B paper link: https://doi.org/10.1111/rssb.12494

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