Optimizing Gaussian Processes

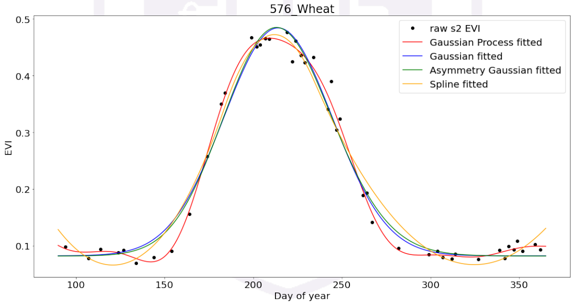
Honours Research Project

Michael Ciccotosto-Camp - 44302913

THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

Problem Setting and Motivation

- The idea of studying time series prediction came from a research group from the Gatton campus, lead by Andries Potgieter, analysing crop growth from previous seasons to forecast when certain phenological stages will take place in the current harvest.



Introduction to Gaussian Processes

- A Gaussian Process (GP) is a collection of random variables with index set I, such that every finite subset of random variables has a joint Gaussian distribution and are completely characterized by a mean function $m : X \to \mathbb{R}$ and a kernel $k : X \times X \to \mathbb{R}$ (in this context, think of the kernel as a function that provides some notion of similarity between points).

$$\begin{aligned} m(\boldsymbol{x}) &= \mathbb{E}\left[f(\boldsymbol{x})\right] \\ k(\boldsymbol{x}, \boldsymbol{x}') &= \mathbb{E}\left[(f(\boldsymbol{x}) - m(\boldsymbol{x}))(f(\boldsymbol{x}') - m(\boldsymbol{x}'))\right]. \end{aligned}$$

Predictions

- Using the assumption that our data can be modelled as a Gaussian process, we can write out the new distribution of the observed noisy values along the points at which we wish to test the underlying function as

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_\star \end{bmatrix} \sim \mathbb{N}\left(\mathbf{0}, \quad \begin{bmatrix} \boldsymbol{K}_{\boldsymbol{XX}} + \sigma_n^2 \mathbb{I}_{n\times n} & \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal \\ \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} & \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star} \end{bmatrix}\right).$$

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- The mean and covariance can then be computed as

$$\overline{\boldsymbol{f}_\star} = \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \left[\boldsymbol{K}_{\boldsymbol{XX}} + \sigma_n^2 \mathbb{I}_{n \times n}\right]^{-1} \boldsymbol{y}$$
$$\operatorname{cov}(\boldsymbol{f}_\star) = \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star} - \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \left[\boldsymbol{K}_{\boldsymbol{XX}} + \sigma_n^2 \mathbb{I}_{n \times n}\right]^{-1} \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal.$$

Unoptimized GPR

Algorithm 1: Unoptimized GPR

input : Observations $\boldsymbol{X}, \boldsymbol{y}$ and a test input $\boldsymbol{x}_\star$.
output: A prediction $\overline{f_\star}$ with its corresponding variance $\mathbb{V}[f_\star]$.

```
1 $\boldsymbol{L} = \text{cholesky}\left(\boldsymbol{K_{XX}} + \sigma_n^2 \mathbb{I}_{n\times n}\right)$
2 $\alpha = \text{lin-solve}\left(\boldsymbol{L}^\intercal, \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{y}\right)\right)$
3 $\overline{f_\star} = \boldsymbol{K_{X_\star X}} \alpha$
4 $\boldsymbol{v} = \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{K_{X_\star X}}\right)$
5 $\mathbb{V}[f_\star] = \boldsymbol{K_{X_\star X_\star}} - \boldsymbol{v}^\intercal \boldsymbol{v}$
6 **return** $\overline{f_\star}, \mathbb{V}[f_\star]$
```

Problems with Unoptimized GPR

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Algorithm 2: Unoptimized GPR
input  : Observations $\boldsymbol{X}, \boldsymbol{y}$ and a prediction inputs $\boldsymbol{X}_{\star}$.
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```

- Lines 1,2 and 4 can be incredibly slow as computing $\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}$ doing a Cholesky decomposition and performing linear solves scale poorly as the number of inputs, n, grows.

Nystrom Approximation

- The Nystrom method we seek a matrix $\boldsymbol{Q} \in \mathbb{R}^{n \times k}$ that satisfies $\|\boldsymbol{A} - \boldsymbol{Q}\boldsymbol{Q}^{*}\boldsymbol{A}\|_F \leq \varepsilon$, where $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is positive semi definite matrix, to form the rank$-k$ approximation

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Random Fourier Feature Approximation

- The RFF technique hinges on Bochners theorem which characterises positive definite functions (namely kernels) and states that any positive definite functions can be represented as

$$k\left(\boldsymbol{x}-\boldsymbol{y}\right)=k\left(\boldsymbol{x}-\boldsymbol{y}\right)=\int_{\mathbb{C}^d}\exp\left(i\langle\boldsymbol{\omega},\boldsymbol{x}-\boldsymbol{y}\rangle\right)\mu_k\left(d\boldsymbol{\omega}\right)$$

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- This integral can then be approximated via the following Monte Carlo estimate

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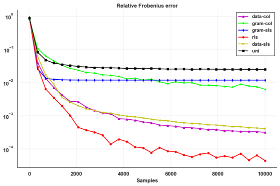
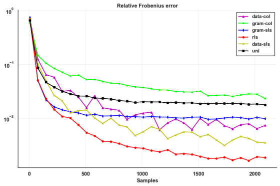
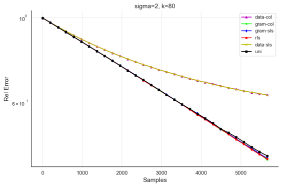


(a) 3D-Spatial network

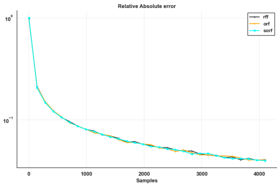


(b) Abalone



(c) Temperature

Figure: Comparison of Nystrom methods for various datasets.



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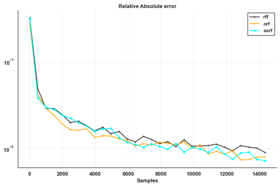

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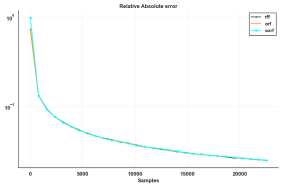

(c) Wine

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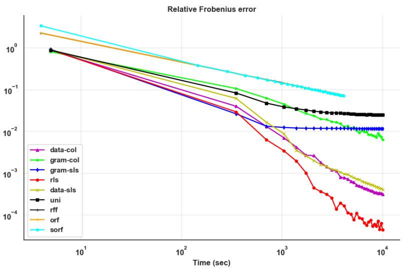
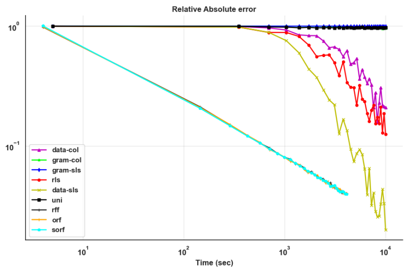


(a) Relative error



(b) Absolute error

Figure: Comparison between Nystrom and RFF approximations for the 3D-Spatial network data.

Moving Forward

- We saw that the Nystrom technique is better at producing approximations of the Gram matrix, $\boldsymbol{K_{XX}}$, with smaller *relative Frobenius errors* while the RFF technique is better at producing approximations with smaller *relative absolute errors*. Which is better for GP prediction?
- Recall, the other bottle neck in the GPR algorithm was the Cholesky decomposition. We can employ faster linear system solvers, namely the *Conjugate Gradient* (CG) and *Minimum Residual* (MINRES) method.