Optimizing Gaussian Processes

Honours Research Project

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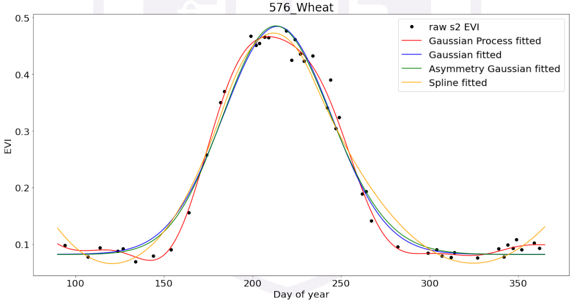
Problem Setting and Motivation

- The idea of studying time series prediction came from a research group from the Gatton campus, lead by Dr 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

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

(using the notation $\left(\boldsymbol{K}_{\boldsymbol{WW}'}\right)_{i,j} \triangleq k\left(\boldsymbol{w}_i, \boldsymbol{w}_j'\right)$)

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(using the notation $\left(\boldsymbol{K}_{\boldsymbol{WW'}}\right)_{i,j} \triangleq k\left(\boldsymbol{w}_i, \boldsymbol{w}'_j\right)$)

- The mean and covariance can then be computed as

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

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 $\mathbb{V}\left[f_\star\right]$.

$\boldsymbol{L} = \text{cholesky}\left(\boldsymbol{K}_{\boldsymbol{XX}} + \sigma_n^2 \mathbb{I}_{n\times n}\right)$

$\alpha = \text{lin-solve}\left(\boldsymbol{L}^\intercal, \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{y}\right)\right)$

$\overline{y_\star} = \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{X}} \alpha$

$\boldsymbol{v} = \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{X}}\right)$

$\mathbb{V}\left[f_\star\right] = \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{x}_\star} - \boldsymbol{v}^\intercal \boldsymbol{v}$

return $\overline{f_\star}, \mathbb{V}\left[f_\star\right]$

Problems with Unoptimized GPR

Algorithm 2: Unoptimized GPR

input : Observations $\boldsymbol{X}, \boldsymbol{y}$ and a prediction inputs $\boldsymbol{x}_\star$.
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3 $\overline{f_\star} = \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{X}} \alpha$
4 $\boldsymbol{v} = \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{X}}\right)$
5 $\mathbb{V}[f_\star] = \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{x}_\star} - \boldsymbol{v}^\intercal \boldsymbol{v}$
6 **return** $\overline{f_\star}, \mathbb{V}[f_\star]$

- Lines 1,2 and 4 can be incredibly slow as computing $\boldsymbol{K}_{\boldsymbol{XX}}$ 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

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

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&= \langle \varphi(\boldsymbol{x}), \varphi(\boldsymbol{y}) \rangle_{\mathbb{C}^D}
\end{aligned}$$

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- CG: $\|\boldsymbol{x} - \boldsymbol{x}^{\star}\|_{\boldsymbol{A}}$ is minimized.
- MINRES: $\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|_2$ is minimized.

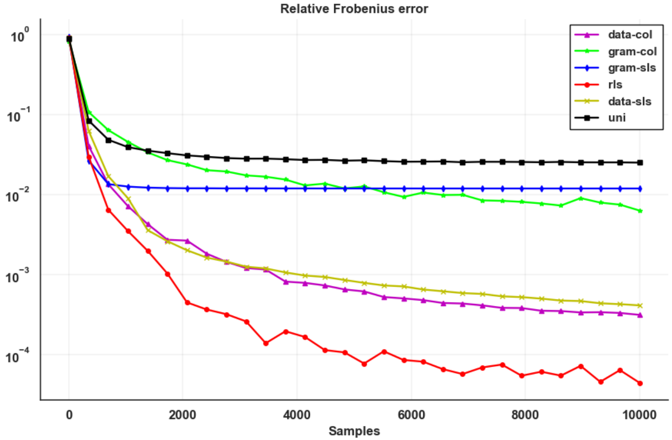


Figure: 3D-Spatial Network dataset using Nystrom

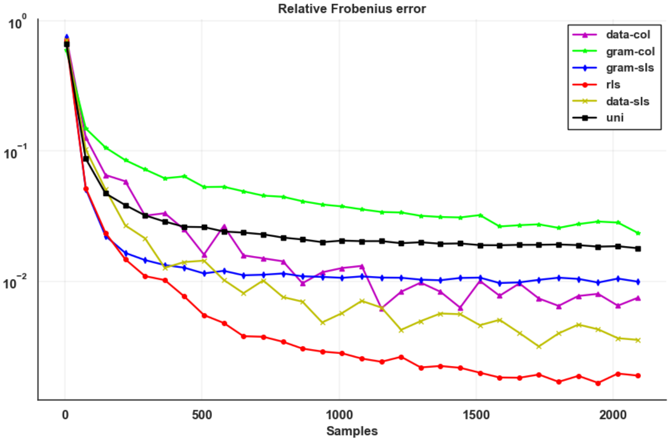


Figure: Abalone dataset using Nystrom

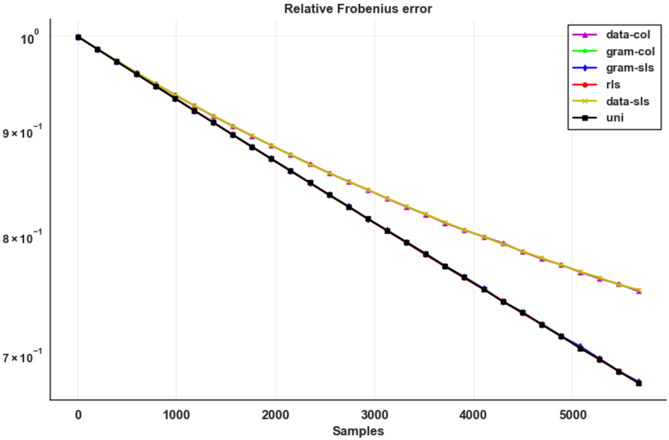


Figure: Temperature dataset using Nystrom

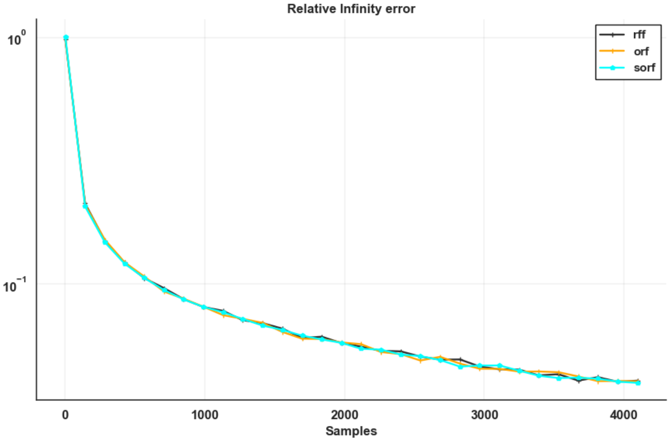
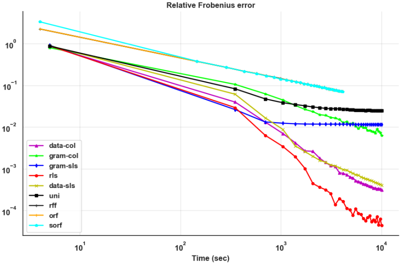
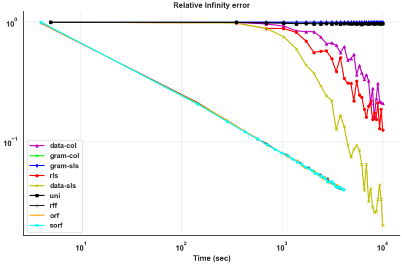


Figure: 3D-Spatial Network dataset using RFF



(a) Frobenius error



(b) Infinity error

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

- How do Nystrom and RFF methods compare in terms of prediction?

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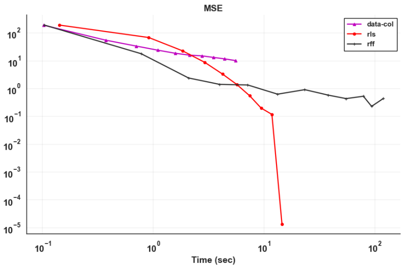
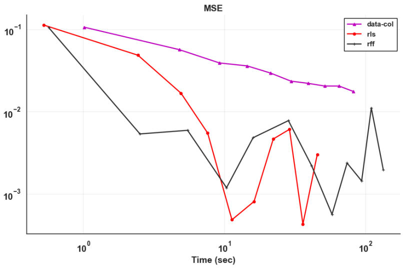


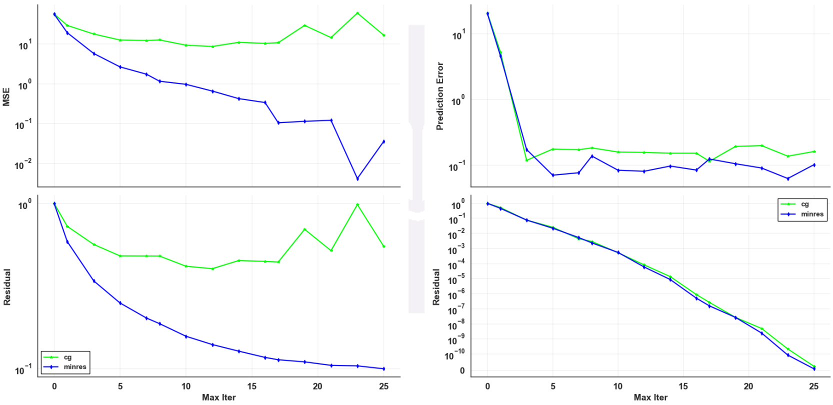
(a) Stock Market dataset



(b) Temperature dataset

Figure: Comparison between Nystrom and RFF approximations in GP prediction.

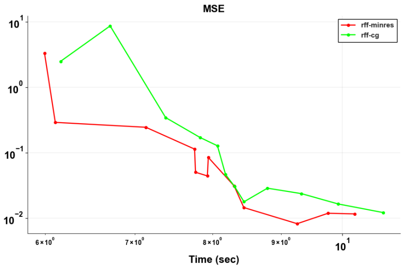
- How do MINRES and CG methods compare in terms of prediction?



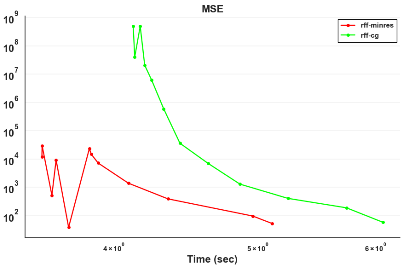
(a) Abalone dataset (b) Quadratic dataset

Figure: Comparison between MINRES and CG in GP prediction.

- Using approximation techniques together.



(a) Stock Market dataset



(b) Abalone dataset

Figure: Comparison between CG and MINRES when paried with RFF.

Moving Forward

- Write these results up.
- Apply our findings to our initial remote sensing task.
- Look at multi-output Gaussian Processes for remote sensing.