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Optimizing performance in Gaussian Processes

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Contents

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Symbols and Notation

Matrices are capitalized bold face letters while vectors are lowercase bold face letters.

Syntax	*Meaning*
$\triangleq$	An equality which acts as a statement
$\lvert \boldsymbol{A} \rvert$	The determinate of a matrix.
$\langle \cdot, \cdot \rangle_{\mathcal{H}}$	The inner product with respect to the Hilbert space $\mathcal{H}$, sometimes abbreviated as $\langle \cdot, \cdot \rangle$ if the Hilbert space is clear from context.
$\lVert \cdot \rVert_{\mathcal{V}}$	The norm of a vector with respect to the vector space $\mathcal{V}$, sometimes abbreviated as $\lVert \cdot \rVert$ if the vector space is clear from context.
$\boldsymbol{x}^{\mathsf{T}}, \boldsymbol{X}^{\mathsf{T}}$	The transpose operator.
$\boldsymbol{x}^{*}, \boldsymbol{X}^{*}$	The hermitian operator.
$\boldsymbol{a}. * \boldsymbol{b}$ or $\boldsymbol{A}. * \boldsymbol{B}$	Element-wise vector (matrix) multiplication, similar to Matlab.
$\propto$	Proportional to.
∇ or $\nabla_{\boldsymbol{f}}$	The partial derivative (with respect to $\boldsymbol{f}$).
∇	The Hessian.
$\sim$	Distributed according to, example $x \sim \mathcal{N}(0, 1)$
$\mathbf{0}$ or $\mathbf{0}_n$ or $\mathbf{0}_{n \times m}$	The zero vector (matrix) of appropriate length (size) or the zero vector of length n or the zero matrix with dimensions $n \times m$.
$\mathbf{1}$ or $\mathbf{1}_n$ or $\mathbf{1}_{n \times m}$	The one vector (matrix) of appropriate length (size) or the one vector of length n or the one matrix with dimensions $n \times m$.
$\mathbb{1}_{n \times m}$	The matrix with ones along the diagonal and zeros on off diagonal elements.

$\boldsymbol{A}_{(\cdot,\cdot)}$ Index slicing to extract a submatrix from the elements of $\boldsymbol{A} \in \mathbb{R}^{n \times m}$, similar to indexing slicing from the python and Matlab programming languages. Each parameter can receive a single value or a 'slice' consisting of a start and an end value separated by a semicolon. The first and second parameter describe what row and columns should be selected, respectively. A single value means that only values from the single specified row/column should be selected. A slice tells us that all rows/columns between the provided range should be selected. Additionally if now start and end values are specified in the slice then all rows/columns should be selected. For example, the slice $\boldsymbol{A}_{(1:3,j:j')}$ is the submatrix $\mathbb{R}^{3 \times (j'-j+1)}$ matrix containing the first three rows of $\boldsymbol{A}$ and columns j to j'. As another example, $\boldsymbol{A}_{(:,j)}$ is the j^{th} column of $\boldsymbol{A}$.

$\boldsymbol{A}^{\dagger}$ Denotes the unique psuedo inverse or Moore-Penore inverse of $\boldsymbol{A}$.

$\mathbb{C}$ The complex numbers.

C The classes in a classification problem.

$\mathrm{cholesky}\left(\boldsymbol{A}\right)$ A function to compute the Cholesky decomposition of the matrix $\boldsymbol{A}$, where $\boldsymbol{L}\boldsymbol{L}^{\intercal} = \boldsymbol{A}$.

$\mathrm{cov}\left(\boldsymbol{f}\right)$ Gaussian process posterior covariance.

d The number of features in the data set.

D The dimension of the feature space of the feature mapping constructed in the Random Fourier Feature method.

$\mathcal{D}$ The dataset, $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$.

$\mathrm{diag}\left(\boldsymbol{w}\right)$ Vector argument, a diagonal matrix containing the elements of vector $\boldsymbol{w}$.

$\mathrm{diag}\left(\boldsymbol{W}\right)$ Matrix argument, a vector containing the diagonal elements of the matrix $\boldsymbol{W}$.

$\mathbb{E}$ or $\mathbb{E}_{q(x)}\left[z(x)\right]$ Expectation, or expectation of $z(x)$ where $x \sim q(x)$.

$\mathcal{GP}$ Gaussian process $f \sim \mathcal{GP}\left(m(\boldsymbol{x}), k\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right)$, the function f is distributed as a Guassian process with mean function $m\left(\boldsymbol{x}\right)$ and covariance function $k\left(\boldsymbol{x}, \boldsymbol{x}'\right)$.

$k(\cdot, \cdot)$	A covariance or kernel matrix.
$\boldsymbol{K_{WW'}}$	For two data sets $\boldsymbol{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_n]^\intercal \in \mathbb{R}^{n \times d}$ and $\boldsymbol{W'} = [\boldsymbol{w}'_1, \boldsymbol{w}'_2, \ldots, \boldsymbol{w}'_m]^\intercal \in \mathbb{R}^{n' \times d}$ the matrix $\boldsymbol{K_{WW'}} \in \mathbb{R}^{n \times n'}$ has elements $(\boldsymbol{K_{WW'}})_{i,j} = k\left(\boldsymbol{w}_i, \boldsymbol{w}'_j\right)$.
lin-solve $(\boldsymbol{A}, \boldsymbol{B})$	A function used to solve $\boldsymbol{X} = \boldsymbol{A}^{-1}\boldsymbol{B}$ in the linear system $\boldsymbol{AX} = \boldsymbol{B}$.
$\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ or $\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$	(the variable $\boldsymbol{x}$ has a) Multivariate Gaussian distribution with mean vector $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$.
n and n_*	The number of training (and tests) cases.
N	The dimenion of the feature space.
$\mathbb{N}$	The natural numbers, $\mathbb{N} = \{1, 2, 3, \ldots\}$.
$\mathcal{O}(\cdot)$	Big-O notation. If a function $f \in \mathcal{O}(g)$ then the absolute value of $f(x)$ is at most a positive multiple of $g(x)$ for all sufficiently large values of x.
$y \mid x$ and $p(x \mid y)$	A conditonal random variable y given x and its probability density.
$\boldsymbol{Q}, \boldsymbol{V}$	Typically used to denote a matrix with orthonormal structure.
$\mathbb{R}$	The real numbers.
$\operatorname{tr}(\boldsymbol{A})$	The trace of a matrix.
$\mathbb{V}$ or $\mathbb{V}_{q(x)}[z(x)]$	Variance, the variance of $z(x)$ when $x \sim q(x)$.
$\mathcal{X}$	Input space.
$\boldsymbol{X}$	The $n \times d$ matrix of training inputs.
$\boldsymbol{X}_*$	The $n_* \times d$ matrix of test inputs.
$\boldsymbol{x}_i$	The i^{th} training input.
$\mathbb{Z}$	The integers, $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$.

Introduction

Time series prediction (and related regressional tasks) is a subject of high interest across many disciplines of science and mathematics. The history of time series can be traced back to the birth of science in ancient Greece where Aristotle devised a systematic approach to weather forecasting in 350 BC in his famous treatise *Meteorologica*. This method was later used to help predict when certain meteorological induced events, such as the flooding of the Nile river [HHF73]. Statistical modelling for time series prediction would not come until the 20th century where development of AutoRegressive Moving Average (ARMA) models which where first mentioned by Yule [Yul27] in 1927 and later popularized by Box and Jenkins in their book *Time Series Analysis* published in 1970 [Box08].

Given a data set of n observations $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$, where each input $x_i \in \mathbb{R}_{>0}$ is a time value and $y_i \in \mathbb{R}$ is a output or experimental observation that acts a function of time, the goal of time series prediction is to try and best predict a value $y_\star$ at a novel time $x_\star$. With computing power becoming ever more advanced and affordable, many have taken to Machine Learning (ML) to develop sophisticated models to address the problem of creating accurate yet computationally inexpensive time series predictors. Broadly speaking, ML is any class of heuristic algorithm that attempts to refine and develope some model to perform a "simple" task by learning through user provided input. ML is founded on the idea that any form of task learning is done through sensory input taken from the surrounding environment. More formally speaking, ML attempts to generate a function $f : X \to Y$, for some input set X and observation or output set Y, were the outputs given by f closely aligns to actual observations. It is tacitly assumed that the phenomena we are studying follows laws which admit mathematical formulation and that experimental results can be reproduced to some degree of accuracy. Typically, experiments will never produce exact values of the underpinning law, g. Instead experimental observations, y_i, will include a small amount of random error so that $y_i = g(x_i) + \varepsilon_i$ where $\varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}\left(0, \sigma^2\right)$.

A ML model will attempt to make accurate predictions using some simplified formulation of the world. The distribution corresponding to the probability of a prediction within the context of the "state of the world" is referred to as the *likelihood*. The uncertainty within the likelihood stems from the predictive limits of the model. These limitation usually arise as a consequence of selecting a model which is either too simple or complex. The "state of the world" is sometimes internally captured by the model as a set of mutable parameters $\boldsymbol{\theta}$. The process of taking observations and using them to form predictions is called *inference* which, in some sense, is synonymous with learning [VdW19].

ML can be applied to time series prediction in a fairly straight forward manner by simply teaching a ML algorithm the time series data set, $\mathcal{D}$, to hopefully produce a function f that serves as a good approximant for event prediction.

In this thesis we shall focus on a particular class of ML algorithms called Baysian models which, unsurprisingly, makes use of Bayesian statistics to drive inference. In Baysian models a *prior* distribution is used to quantify the uncertainty of the current state of the model before any observations are made. The model can then be updated once data is observed by using the likelihood to give a *posterior* distribution which represents the reduced uncertainty after "teaching" the model new observations. Methods of teaching a model how to change its behavior using a new set of observations often involves the use of a *loss function* L. The loss function is used as an aid in deciding what action, a, should be taken in to best minimize uncertainty. The best action, roughly speaking, can be evaluated as

$$a_{\text{opt}} = \arg\min_{a} \int L\left(y_\star, a\right) p\left(y_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y}\right) \, dy_\star.$$

Interestingly, the best action does not rely so much on the model's internalized parameters but rather on the predictive distribution $p\left(y_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y}\right)$ [VdW19]. This key insight has spawned a class of ML algorithms that focuses on infering the function f directly by computing $p\left(f \mid \mathcal{D}\right)$ instead of finding optimal internal parameters using $p\left(\boldsymbol{\theta} \mid \mathcal{D}\right)$ [Mur12]. Models that perform inference in this manner are called *non-parameteric* models. Within the *non-parameteric* model paradigm, the predictive distribution can be represented as

$$p\left(y_\star \mid x_\star, \boldsymbol{X}, \boldsymbol{y}\right) = \int p\left(y_\star \mid f, x_\star\right) p\left(f \mid \boldsymbol{X}, \boldsymbol{y}\right) \, df$$

and once new data is observed the posterior can be updated using Baye's rule

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}, \qquad p\left(\boldsymbol{f}, f_\star \mid \boldsymbol{y}\right) = \frac{p\left(\boldsymbol{y} \mid \boldsymbol{f}\right) p\left(\boldsymbol{f}, f_\star\right)}{p\left(\boldsymbol{y}\right)}$$

[Ras06]. This thesis will focus on a particular non-parameteric Bayesian ML model called Gaussian processes (GPs). The over arching idea of GPs is to assign a prior probability to every possible function mapping from X to Y. While this does not appear to be computationally tractable due to the seemingly uncountable infinite number of mappings that would require checking, it turns out, these computations can infact be carried out given we are only seeking predictions at a finite number of points using a finite number of observations. GPs occupy a special place within the realm of ML since they account for uncertainty in a principled way, are relatively simple to implement and are highly modular allowing them to easily be incorporated into a larger systems. It is no surprise then that while other kernel methods (such as kernelized k^{th} nearest neighbors and ridge regression) are still overshadowed by their neural network cousins, GPs have made a quiet comeback in the ML community [Cao18].

The following example highlights a particular GP success story: a team of researchers led by Andries Potgieter at QAAFI (UQ) are currently investigating new digital approaches to accurately derive crop phenology stages (i.e. mid green, peak, flowering, grain filling and harvest) measured at field scale across large regions. Such methods can be used to better inform farmers and industry on the optimised time to plant various crops to minimize crop loss from environmental stresses such as frost and fungal disease. This involves analysing crop growth from previous seasons (i.e. 2018-2021) to forecast when certain phenological stages will take place in the current harvest. Outputs form this tool will allow producers to accurately map the temporal and spatial extend of phenology at a field and farm levels across different regions and seasons. This problem is readily converted into a time series problem. Originally, Potgieter's team surveyed a number of different parameteric models to carry out forecasting. However, the parameteric models we serverely limited in their ability to inform when key phenological stages would take place. After seeing the success of applying GPs to other remote sensing tasks [SD22] the team investigated the use of GPs in their own research to find that they could produce much higher resolution predictions from which they could infer a far richer phenological timeline [Pot13]. A comparision of using GPs over other parameteric models is shown in Figure 1. Potgieter's team found that the only draw back to using GPs was the lengthy run time required to create predictions and fears that

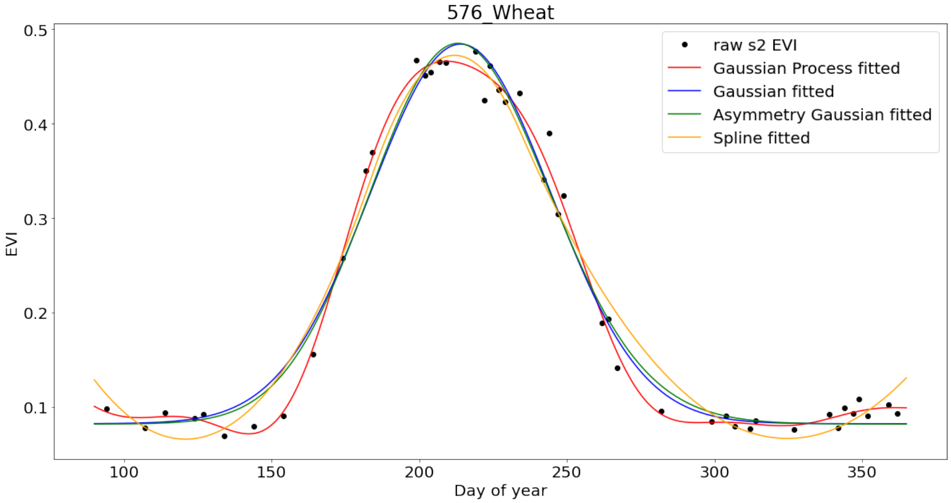


Figure 1. Potgieter's team found that GPs where superior in terms of predicting a phenological timeline for a number of common seasonal crops over other parameteric models.

collecting new data each season will only exacerbate the issue. This is a common problem shared by anyone wanting to use GPs. Due to their unwieldy $\mathcal{O}\left(n^3\right)$ runtime, where n is the number of observations, GPs become impractical to apply on datasets with $n > 10^5$ samples. As such, the goal of this thesis is to explore various avenues one can take to replace some of the more intense calculations of GPs with computationally more efficient approximations without overly sacrificing accuracy.

Chapter 1 will give a more mathematical treatment of GPs starting from the ground through a review of some fundamental material from functional analysis also the theory behind the motivation of GPs before finally concluding with concrete algorithms for GP regression and classification. Chapters 2 and **??** will cover techniques for approximating a large matrix used with GPs that provides information on how similar each observation is to one other. Chapter **??** then gives alternative methods for solving linear systems, an essential component required for the GP algorithm to work.

1. Gaussian Processes

The aim of this chapter is to explore the theory behind GPs. First, some essential theory from functional analysis on kernels and reproducing kernel Hilbert spaces will be reviewed which are not only used in GPs but are found in a vast array of machine learning models, aptly named kernel machines. Afterward, we shall go through the underlying statistics that drive GP prediction and use it to form algorithms for both regression and classification tasks. Note that most of the theory presented here is only for real-values data sets although most the time complex-valued generalizations do exist.

1.1. **Kernels.** Often in machine learning we are often met with the challenge of how to best represent data instances as fixed size feature vectors $\boldsymbol{x}_i \in X$. For certain objects it might not be obvious at all how to represent the data as a fixed length vector. Good examples of variable length data include textual documents and genomic data. For these data types we can define a method of measuring similarity between objects which requires them to first be converted to a fixed length feature vector first [Mur12]. To do this we begin by mapping the feature vectors into a Hilbert space H which enriches the vector space with an inner product $\langle\cdot,\cdot\rangle_H : H \times H \to \mathbb{R}$ and a norm $\|\cdot\|_H : H \to \mathbb{R}$. Input data is transformed into feature space vectors via a non-linear feature mapping $\Phi : X \to H$. The benefit of using feature maps in this way is that a non-linear descision boundary can be constructed using linear models. In some instances a similarity measure can be computed directly using a function $k : X \times X \to \mathbb{R}$, instead of needing to construct a Φ and then computing the inner product of the transformed instances. Functions that act directly on our data instances are known as kernel functions and using them to avoid computation associated with the underlying feature space is known as the kernel trick [Ste08]. These ideas are stated more formally in definition 1.

Definition 1 (Kernel)**.** *Let X be a non-empty set. Then a function $k : X \times X \to \mathbb{R}$ is called a kernel on X if there exists a Hilbert space and a map $\Phi : X \to H$ such that for all $\boldsymbol{x}, \boldsymbol{x}' \in X$ we have $k(\boldsymbol{x}, \boldsymbol{x}') = \langle \Phi(\boldsymbol{x}), \Phi(\boldsymbol{x}')\rangle_H$. We call the Φ the feature map and H the feature space of k.*

It is worth noting that almost no conditions are placed on the set X, allowing it to accommodate virtually any form of data. It is not surprising then that neither the feature map nor the feature space are uniquely determined by the kernel. As shown by the example from Steinwart and Christmann [Ste08], when $X = \mathbb{R}$ and $k(x, x') = x \cdot x'$ where $x, x' \in X$, we can see that k is a kernel using the feature map $\Phi(x) = x$ and $H = \mathbb{R}$. However, another suitable feature map for this particular kernel is $\Phi'(x) = \left(x/\sqrt{2}, x/\sqrt{2}\right)$ with a corresponding feature space of $H = \mathbb{R}^2$ since

$$\langle \Phi'(x), \Phi'(x')\rangle_{\mathbb{R}^2} = \frac{x'}{\sqrt{2}} \cdot \frac{x}{\sqrt{2}} + \frac{x'}{\sqrt{2}} \cdot \frac{x}{\sqrt{2}} = x \cdot x'$$

for $x, x' \in X$. While their might be numerous functions that provide some notion of similarity between data entries, these functions might not be valid kernels. Instead of needing to construct a feature map and feature space to verify that a chosen function is a valid kernel using definition 1, we can make use of a much simpler set of criteria. Before embarking on this train of thought, we need to define the following.

Definition 2 (Positive Definite and Positive Semidefinite)**.** *A function $k : K \times K \to \mathbb{R}$ is positive semidefinite if for all $n \in \mathbb{N}$ and $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$ and all $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in X$ we have*

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k\left(\boldsymbol{x}_j, \boldsymbol{x}_i\right) \geq 0. \tag{1}$$

Furthermore, k is said to be positive definite if for mutually distinct $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in X$ equality 1 only holds for $\alpha_1 = \ldots = \alpha_n = 0$ [Ste08].

Definition 3 (Symmetric)**.** *A function $k : K \times K \to \mathbb{R}$ is called symmetric if $k\left(\boldsymbol{x}, \boldsymbol{x}'\right) = k\left(\boldsymbol{x}', \boldsymbol{x}\right)$ for any inputs $\boldsymbol{x}', \boldsymbol{x} \in X$* [Ste08].

Definition 4 (Gram Matrix)**.** *For fixed $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in X$ the matrix $\boldsymbol{K} \in \mathbb{R}^{n \times n}$ where $\boldsymbol{K}_{i,j} \triangleq k\left(\boldsymbol{x}_j, \boldsymbol{x}_i\right)$ is the Gram matrix* [Ste08].

Note that checking if a function is positive (semi) definite is equivalent to checking that any Gram matrix produced by a function is positive (semi) definite. If k is a real valued kernel corresponding to the feature map Φ, then k is symmertic by virtue of the fact that the inner product of a real Hilbert space is symmetric. Moreover k is positive definite since for $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$ and $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in X$ we have

$$\begin{aligned}
&\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k\left(\boldsymbol{x}_j, \boldsymbol{x}_i\right) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \langle \Phi\left(\boldsymbol{x}_i\right), \Phi\left(\boldsymbol{x}_j\right) \rangle_H \\
&= \left\| \sum_{i}^{n} \alpha_i \Phi\left(\boldsymbol{x}_i\right) \right\|_H^2 \\
&\geq 0.
\end{aligned}$$

The following theorems tell us that it is not only necessary for a kernel to be positive semi definite but it is also a sufficient condition.

Theorem 5. *A function $k : K \times K \to \mathbb{R}$ is a kernel if and only if it is symmertic and positive semidefinite* [Ste08].

1.2. Reproducing Kernel Hilbert Spaces.

We shall now shift our attention towards reproducing kernel Hilbert spaces (RKHS) and describe their relation to kernels, and see that in some sense, the RKHS of a kernel k is the smallest feature space for a kernel. The formal definition of a RKHS is stated in definition 6.

Definition 6 (RKHS)**.** *Let $X \neq \emptyset$ and H be a real Hilbert space over X*

(1) *A function $k : X \times X \to \mathbb{R}$ is called a reproducing kernel if we have $k\left(\cdot, \boldsymbol{x}\right) \in H$ for all $\boldsymbol{x} \in X$ and the reproducing property*

$$f(\boldsymbol{x}) = \langle f, k\left(\cdot, \boldsymbol{x}\right) \rangle$$

holds for all $f \in H$ and $x \in X$.

(2) *The space H is called a reproducing kernel Hilbert space over X if for all $\boldsymbol{x} \in X$ the Dirac functional $\delta_{\boldsymbol{x}} : H \to \mathbb{R}$ defined by $\delta_{\boldsymbol{x}}(f) \triangleq f(x),\ f \in H$ is continuous.*

[Ste08]

An important property of the RKHS is that the convergence in the norm implies pointwise convergence. Specifically, in a RKHS for any sequence of functions $\{f_n\} \subset H$ where $\|f_n - f\| \to 0$ we have $|\delta_{\boldsymbol{x}}(f_n) - \delta_{\boldsymbol{x}}(f)| = |f_n(x) - f(x)| \to 0$. Note that because the evaluation function is both linear and continuous, then it is also bounded in the sense that there is a $c \in \mathbb{R},\ c > 0$ such that for every $f \in H$ and a fixed $\boldsymbol{x} \in X$ we have $|\delta_{\boldsymbol{x}}(f)| \leq c \|f\|_H$ [Ber96]. This property of uniform convergence implying pointwise convergence is important since it tells us that if functions $f, g \in H$ are close in norm then their evaluation at any point is also similar. The following lemma ties together the definition of an RKHS, reproducing kernel and a kernel.

Lemma 7. *Let H be a Hilbert function space over X that has a reproducing kernel k. Then H is a RKHS and H is also a feature space of k where the feature map $\Phi : X \to H$ is given by*

$$\Phi(\boldsymbol{x}) = k(\cdot, \boldsymbol{x})$$

for some $\boldsymbol{x} \in X$. We call Φ the canonical feature map.

Proof. Since the reproducing property tells us that any Dirac functional can be represented by the reproducing kernel this means

$$|\delta_{\boldsymbol{x}}(f)| = |f(\boldsymbol{x})| = |\langle f, k(\cdot, \boldsymbol{x})\rangle| \leq \|k(\cdot, \boldsymbol{x})\|_H \cdot \|f\|_H$$

for all $\boldsymbol{x} \in X,\ f \in H$. This shows continuity of $\delta_{\boldsymbol{x}}$ for $\boldsymbol{x} \in X$. In order to show that Φ is a feature map, fix an $\boldsymbol{x}' \in X$ and set $f = k(\cdot, \boldsymbol{x}')$. Then for $\boldsymbol{x} \in X$, the reproducing property yields

$$\langle \Phi(\boldsymbol{x}'), \Phi(\boldsymbol{x})\rangle_H = \langle k\left(\cdot, \boldsymbol{x}'\right), k(\cdot, \boldsymbol{x})\rangle_H = \langle f, k(\cdot, \boldsymbol{x})\rangle_H = f(\boldsymbol{x}) = k\left(\boldsymbol{x}', \boldsymbol{x}\right).$$

□

This tells us that every Hilbert space with a reproducing kernel is a RKHS. We can also show the converse, that is, every RKHS has a unique reproducing kernel seen in theorem 8.

Theorem 8. *Let H be a RKHS over X. Then $k : X \times X \to \mathbb{R}$ defined by $k(\boldsymbol{x}', \boldsymbol{x}) = \langle \delta_{\boldsymbol{x}}, \delta_{\boldsymbol{x}'}\rangle_H,\ \boldsymbol{x}, \boldsymbol{x}' \in X$ is the only reproducing kernel of H* [Ste08].

Theorem 8 shows that a RKHS is uniquely determined by its kernel. In fact the other direction can also be shown to afford a one-to-one correspondence between kernels and RKHS. This is known as the Moore-Aronszajn theorem presented in thorem 9.

Theorem 9 (Moore-Aronszajn)**.** *Suppose k is a symmertic positive definite kernel on a set X. Then there is a unique Hilbert space of functions for which k is the reproducing kernel* [Ber03].

The elements of a RKHS will often inherit the analytical properties of its corresponding kernel. This means that kernels provide a mechanism for generating spaces of functions with useful analytical properties.

1.3. **Gaussian Radial Basis Kernel.** Although there are many kernels to use at our disposal, we turn our attention to a specific class of kernel that shall be used extensively in the upcoming theory and experimentation.

Definition 10 (Gaussian Radial Basis Kernel)**.** *For $d \in \mathbb{N}$, $\sigma \in \mathbb{R}_{>0}$ and $\boldsymbol{z}, \boldsymbol{z}' \in \mathbb{R}^d$ we define*

$$k_\sigma\left(\boldsymbol{z}, \boldsymbol{z}'\right) \triangleq \exp\left(-\sigma^{-2}\sum_{j=1}^{d}\left(z_j - {z'}_j\right)^2\right).$$

Then k_σ is a real valued kernel called the Gaussian Radial Basis Kernel (RBF) kernel with bandwidth σ. Moreover k_σ can be computed as

$$\exp\left(\frac{-\left\|\boldsymbol{z} - \boldsymbol{z}'\right\|_2^2}{\sigma^2}\right)$$

[Ste08].

The Gaussian RBF kernel makes for a very simple and intuitive measurement of similarity between its inputs. One geometric interpretation of the Gaussian RBF kernel is that as the radius of the smallest d-sphere containing $\boldsymbol{z}, \boldsymbol{z}' \in \mathbb{R}^d$ grows the corresponding measurement of similarity decays exponentially. A visual representation of this decay is shown in Figure 2.

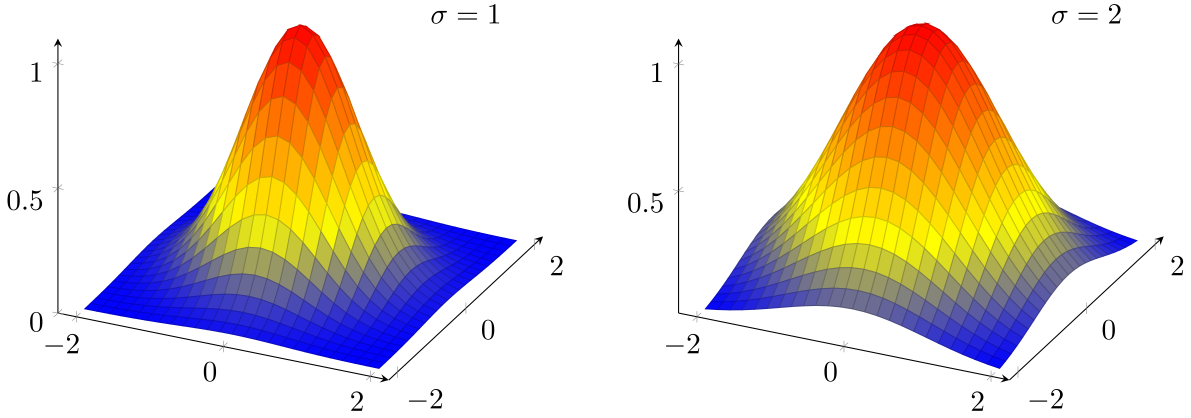


FIGURE 2. A graph of the Gaussian RBF from definition 10 for $d = 2$. Evidently, a larger value of σ slows the rate of decay increasing the similarity between the same pair of samples.

This kernel is infinitely differentiable meaning it has mean square derivatives of all orders and is therefore very smooth. In fact, some argue that such strong smoothness makes it unrealistic for modelling natural phenomena [Ras06, Ste99]. Nontheless, Gaussian RBF kernels remain the one of the most widely used in literature.

1.4. **Kernel Machines.**

1.4.1. *Introduction to Support Vector Machines for Binary Classification.* In this section, we will be investigating at two different machine learning models that make use of kernels to perform classification and regression. The first class of kernel machines to be evaluated are support vector machines (SVM). SVMs where originally designed for binary classification and as such only a model for binary classification is presented, although extensions exist that allow regression and multi-class classification.

For the binary classification problem we are tasked with labelling new samples with either one of two classes, -1 or 1. We shall assume our input space consists of vectors from $\mathbb{R}^d$ and that we provided with a labelled training set $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\}$. One simple method to classify samples is by creating an affine linear hyperplane satisfying

$$\begin{aligned} &\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b > 0, \quad y_i = +1 \\ &\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b < 0, \quad y_i = -1 \end{aligned} \tag{2}$$

for some $\boldsymbol{w} \in \mathbb{R}^d$ and $b \in \mathbb{R}$ where $\|\boldsymbol{w}\|_2 = 1$ [Ste08]. Moreover we would like $\boldsymbol{w}$ and b to maximise the margin, that is the maximal distance between the separating hyperplane and the points in D. The specific $\boldsymbol{w}$ and b obtained through the training set is denoted $\boldsymbol{w}_D$ and b_D and the resulting descision function is defined as

$$f_D(\boldsymbol{x}) \triangleq \operatorname{sign}(\langle \boldsymbol{w}_D, \boldsymbol{x} \rangle + b_D).$$

There are, however, a number of shortcomings to this model. The most obvious is that our training data may not be linearly separable in $\mathbb{R}^d$ meaning no such $\boldsymbol{w}_D$ and b_D exist. Moreover, when noise is introduced to the data set this model will prioritize finding a hyperplane that perfectly separates the two classes, making no compromises in misclassifying points, and consequently subjecting it to overfitting. SVMs where introduced by Boser *et al.* [Bos92] to address the first issue of separability. Their approach was to lift the input vector into a more malleable Hilbert space H_0 using a feature map. The inputs are then classified within the new space. Unfortunately this method does nothing to address the second issue of over fitting and, if anything, actually worsens it. Cortes and Vapnik [Cor95] attempted to address this second issue by introducing slack variables to equation 2 so that now we need to satisfy $y_i(\langle \boldsymbol{w}, \Phi(\boldsymbol{x}_i) \rangle + b) \geq 1 - \xi_i$ for some $\xi_i \in \mathbb{R}_{>0}$. These constraints can be re-written as

$$\xi_i \geq 1 - y_i(\langle \boldsymbol{w}, \Phi(\boldsymbol{x}_i) \rangle + b)$$

and combining this with our slack constraints (that is $\xi_i \geq 0$) yields

$$\xi_i \geq \max\{0, 1 - y_i(\langle \boldsymbol{w}, \Phi(\boldsymbol{x}_i) \rangle + b)\} = L_{\text{hinge}}(y_i, \langle \boldsymbol{w}, \Phi(\boldsymbol{x}_i) \rangle + b)$$

where L_{hinge} is the hinge loss defined as

$$L_{\text{hinge}}(y, \eta) \triangleq \max\{0, 1 - y\eta\}.$$

This optimization problem can be re-written is the form

$$\min_{(\boldsymbol{w}, b) \in H_0 \times \mathbb{R}} \lambda \|\boldsymbol{w}\|_{H_0} + \frac{1}{n} \sum_{i=1}^{n} L_{\text{hinge}}(y_i, f_{(\boldsymbol{w}, b)})$$

where $f_{(\boldsymbol{w}, b)} : X \to \mathbb{R}$ is defined as

$$f_{(\boldsymbol{w}, b)} \triangleq \langle \boldsymbol{w}, \Phi(x_i) \rangle + b$$

[Ste08]. Unfortunately, this new embedding requires us to solve for optimal parameters in a very high, or even infinite, dimension vector space. To get around this, the Lagrange approach is typically used to solve the corresponding dual problem. When the hinge loss is used the dual problem becomes

$$\max_{\alpha\in[0,C]^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j \langle \Phi(\boldsymbol{x}_i), \Phi(\boldsymbol{x}_j)\rangle$$

$$\text{subject to} \quad \sum_{i=1}^{n} y_i \alpha_i = 0 \tag{3}$$

Notice that in the dual problem, we find that inner products are only taken with vectors that have the feature map applied to them allowing us to employ the kernel trick described in section 1.1 so that equation 3 becomes

$$\max_{\alpha\in[0,C]^n} \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j k(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

$$\text{subject to} \quad \sum_{i=1}^{n} y_i \alpha_i = 0.$$

1.4.2. *Introduction to Gaussian Processes for Regression.* The next machine learning model of interest that uses kernels are gaussian processes. To motivate this model, consider the time series data in Figure 3 (A).

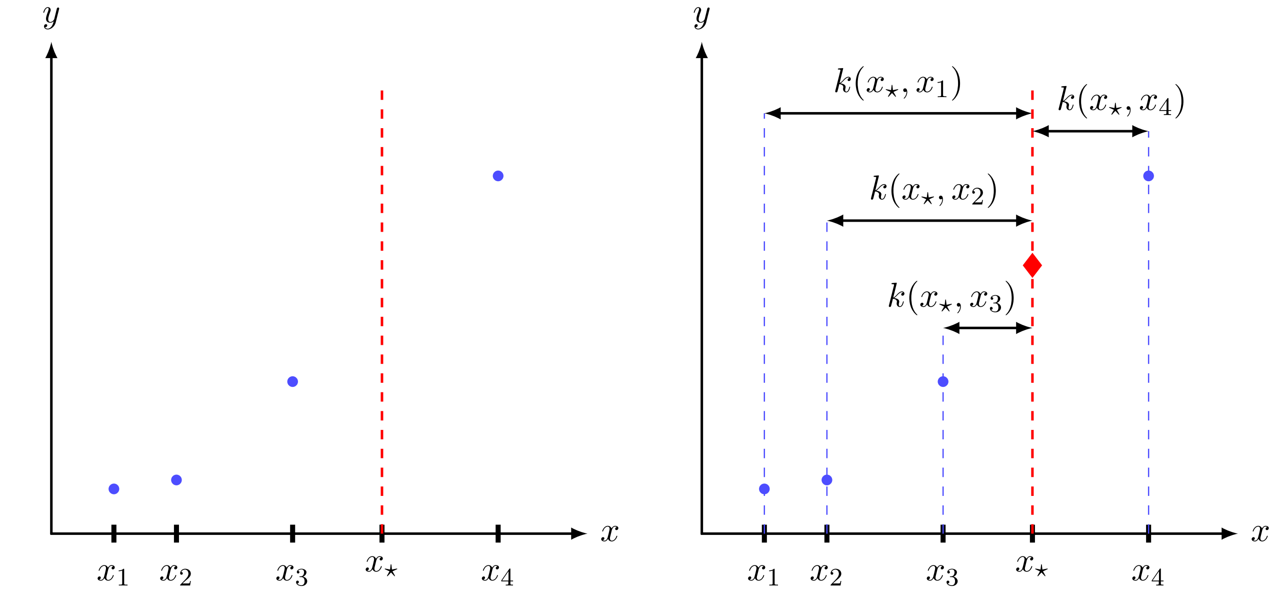
In this diagram there is a number of observed values $D = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)\}$ (blue labels) as well as a missing observation at time $x_\star$. This is a classic problem of time series prediction, that is what is a good prediction for the missing value at time $x_\star$? Perhaps something close to the red diamond seen in Figure 3 (B)? Why does this red diamond seem like a good choice? Because for known data for which the measurement of similarity is small, we expect the corresponding outputs should also be similar since most natural phenomena are continuous by nature. This reasoning is used to underpin GPs, that is, training inputs that are more similar to the input value should have greater influence over the prediction.

Like SVMs, we can motivate the mathematical model of a GP through a linear model. Since GPs are designed for regression tasks, we shall only focus on GP regression although we will see later that GPs can be extended to perform binary classification and even multi-class classification. To begin, consider the following linear regression model

$$f(\boldsymbol{x}) \triangleq \langle \boldsymbol{w}, \boldsymbol{x}\rangle \tag{4}$$

where we again assuming that $\boldsymbol{x}$ belongs to $\mathbb{R}^d$ and that $\boldsymbol{w} \in \mathbb{R}^d$ is a weight vector. Notice the striking resemblances to the linear classifier used in our derivation for the SVM model, although this time we are using the value computed by the inner product directly to infer instead of fitting it over a sign function to force it into a binary class. Suppose we have independently sampled observations $D = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$ to a noisy version of f

$$y_i = f(\boldsymbol{x}_i) + \varepsilon_i$$



(A)

(B)

FIGURE 3. Panel (A) shows depicts the classical problem of time series prediction, guessing a value for $x_\star$ given values for surrounding times. Panel (B) shows a suitable choice for the value at time $x_\star$ with the reasoning that closely surrounding values should have greater influence over inference. Example taken from the 2013 Machine Learning course CPSC 540 instructed by Nando de Freitas [NdF13].

where $\varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}\left(0, \sigma_n^2\right)$. Together the assumption of noise and the base linear model give rise to a likelihood, or more specifically, a probability density over the observations given the inputs and weight parameters. Due to the assumption of independence in our observations

$$
\begin{aligned}
p\left(y \mid \boldsymbol{X}, \boldsymbol{w}\right) &= \prod_{i=1}^{n} p\left(y_i \mid \boldsymbol{x}_i, \boldsymbol{w}\right) \\
&= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_n} \exp\left(-\frac{\left(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i\rangle\right)^2}{2\sigma_n^2}\right) \\
&= \frac{1}{\left(2\pi\sigma_n^2\right)^{\frac{n}{2}}} \exp\left(-\frac{1}{2\sigma_n^2}\left(\sum_{i=1}^{n}\left(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i\rangle\right)^2\right)\right) \\
&= \frac{1}{\left(2\pi\sigma_n^2\right)^{\frac{n}{2}}} \exp\left(-\frac{1}{2\sigma_n^2}\left\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\right\|_2^2\right) \\
&= \mathcal{N}\left(\boldsymbol{X}\boldsymbol{w}, \sigma_n^2\, \mathbb{1}_{n\times n}\right)
\end{aligned}
\tag{5}
$$

where $\boldsymbol{y} = [y_1, y_2, \ldots, y_n]^\intercal \in \mathbb{R}^n$ and $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]^\intercal \in \mathbb{R}^{n\times d}$ [Ras06, page 9]. Within the Bayesian paradigm, a prior is required to represent our beliefs about the parameters in the absence of any information. Typically, the following prior is used for the weight vector

$$
\boldsymbol{w} \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{\Sigma}_p\right)
$$

where $\boldsymbol{\Sigma}_p$ is an appropriate covariance matrix. Ideally, we would like to know the posterior pdf $p\left(\boldsymbol{w} \mid \boldsymbol{y}, \boldsymbol{X}\right)$ which refines our choices of $\boldsymbol{w}$ by taking into account our observations. The posterior can be computed using Bayes rule

$$p\left(\boldsymbol{w} \mid \boldsymbol{y}, \boldsymbol{X}\right) \propto p\left(\boldsymbol{y} \mid \boldsymbol{w}, \boldsymbol{X}\right) p\left(\boldsymbol{w}\right).$$

Equation 5 gives us a probability for $p\left(\boldsymbol{y} \mid \boldsymbol{w}, \boldsymbol{X}\right)$ and since $\boldsymbol{w} \sim \mathcal{N}\left(\boldsymbol{0}, \boldsymbol{\Sigma}_p\right)$ then

$$p\left(\boldsymbol{w}\right) = \frac{1}{\sqrt{\left(2\pi\right)^d \left|\boldsymbol{\Sigma}\right|}} \exp\left(-\frac{1}{2}\boldsymbol{w}^\intercal \boldsymbol{\Sigma}_p^{-1} \boldsymbol{w}\right)$$

[Kro14]. This means, up to proportionality

$$\begin{aligned} p\left(\boldsymbol{w} \mid \boldsymbol{y}, \boldsymbol{X}\right) &\propto \exp\left(-\frac{1}{2\sigma_n^2}\left(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\right)^\intercal \left(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\right)\right) \exp\left(-\frac{1}{2}\boldsymbol{w}^\intercal \boldsymbol{\Sigma}_p^{-1} \boldsymbol{w}\right) \\ &\propto \exp\left(-\frac{1}{2}\left(\boldsymbol{w} - \bar{\boldsymbol{w}}\right)^\intercal \left(\frac{1}{\sigma_n^2}\boldsymbol{X}^\intercal \boldsymbol{X} + \boldsymbol{\Sigma}_p^{-1}\right)\left(\boldsymbol{w} - \bar{\boldsymbol{w}}\right)\right) \end{aligned}$$

where $\bar{\boldsymbol{w}} \triangleq \sigma_n^{-2}\left(\sigma_n^{-2}\boldsymbol{X}^\intercal \boldsymbol{X} + \boldsymbol{\Sigma}_p^{-1}\right)^{-1} \boldsymbol{X}^\intercal \boldsymbol{y}$. Notice that this again is a multivariate Gaussian distribution with mean $\bar{\boldsymbol{w}}$ and covariance $\boldsymbol{A}^{-1}$ where $\boldsymbol{A} \triangleq \sigma_n^{-2}\boldsymbol{X}^\intercal \boldsymbol{X} + \boldsymbol{\Sigma}_p^{-1}$ so that

$$p\left(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}\right) \sim \mathcal{N}\left(\boldsymbol{w}, \boldsymbol{A}^{-1}\right).$$

To make a prediction of our target function for an input, $\boldsymbol{x}_\star$, outside our observed values we can take the average over all possible parameter values weighted by the posterior to predict $f_\star \triangleq f\left(\boldsymbol{x}_\star\right)$ which yields

$$p\left(f_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y}\right) = \int_{\mathbb{R}^d} p\left(f_\star \mid \boldsymbol{x}_\star, \boldsymbol{w}\right) p\left(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}\right)\, d\boldsymbol{w} = \mathcal{N}\left(\boldsymbol{x}_\star{}^\intercal \bar{\boldsymbol{w}}, \boldsymbol{x}_\star{}^\intercal \boldsymbol{A}^{-1} \boldsymbol{x}_\star\right).$$

This gives another Gaussian distribution whose means is the mean of the posterior distribution of the weight vectors multiplied by the input vector, and whose covariance in the quadratic form of the covariance of the weight vectors again with the input vectors. This makes sense since it tells us that the uncertainty of the model grows quadratically with the magnitude of the input.

We can now employ the kernel trick in the exact same manner in the derivation of the SVM model, that is, by using a feature mapping Φ to lift the inputs of our linear regression model from equation 4 into a higher dimension and more workable Hilbert space so that our model now becomes

$$f\left(\boldsymbol{x}\right) \triangleq \langle \boldsymbol{w}, \Phi\left(\boldsymbol{x}\right)\rangle.$$

The derivation for the new model is identical with the only difference being that $\boldsymbol{x}_\star$ is replaced with $\Phi\left(\boldsymbol{x}_\star\right)$ and $\boldsymbol{X}$ is replaced with $\Phi\left(\boldsymbol{X}\right) \triangleq \left[\Phi\left(\boldsymbol{x}_1\right), \Phi\left(\boldsymbol{x}_2\right), \ldots, \Phi\left(\boldsymbol{x}_n\right)\right]^\intercal \in \mathbb{R}^{n \times N}$ where N is the dimension of the feature space. The new predictive distribution can be expressed as

$$f_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y} \sim \mathcal{N}\left(\frac{1}{\sigma_n^2}\Phi\left(\boldsymbol{x}_\star\right)^\intercal \boldsymbol{A}^{-1} \Phi\left(\boldsymbol{X}\right)^\intercal \boldsymbol{y}, \Phi\left(\boldsymbol{x}_\star\right)^\intercal \boldsymbol{A}^{-1} \Phi\left(\boldsymbol{x}_\star\right)\right) \tag{6}$$

where $\boldsymbol{A}$ is now $\boldsymbol{A} \triangleq \frac{1}{\sigma_n^2}\Phi\left(\boldsymbol{X}\right)^\intercal \Phi\left(\boldsymbol{X}\right) + \boldsymbol{\Sigma}_p^{-1} \in \mathbb{R}^{N \times N}$. From this, it becomes evident that the inverse of $\boldsymbol{A}$ is required to compute both the mean and the covariance. This is not favourable since this would require knowledge of the feature space into which the feature map sends inputs. Moreover, computing $\boldsymbol{A}^{-1}$ may become impractical in the dimension of the feature space is incredibly large. Remember, the whole point of the kernel trick is to avoid any computation that involves direct knowledge of H but rather to use a kernel k to bypass these obstacles and indirectly produce inner products of the data applied to the feature map. With this in mind, let us try and find different expressions for the mean and the covariance of equation 6 that will enable us to apply the kernel trick. Before starting, we need to find a suitable expression for the mean. First define the notation

$$\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'} \triangleq \Phi\left(\boldsymbol{W}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{W}'\right)^{\intercal} \in \mathbb{R}^{n \times n'}$$

where $\boldsymbol{W} \in \mathbb{R}^{n \times d}$ and $\boldsymbol{W}' \in \mathbb{R}^{n' \times d}$ are two data matrices. Consider the following

$$\begin{aligned}
&\boldsymbol{A}\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal} \\
&= \left(\sigma_n^{-2}\Phi\left(\boldsymbol{X}\right)^{\intercal}\Phi\left(\boldsymbol{X}\right) + \boldsymbol{\Sigma}_p^{-1}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal} \\
&= \sigma_n^{-2}\ \Phi\left(\boldsymbol{X}\right)^{\intercal}\Phi\left(\boldsymbol{X}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal} + \Phi\left(\boldsymbol{X}\right)^{\intercal} \\
&= \sigma_n^{-2}\ \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\Phi\left(\boldsymbol{X}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal} + \sigma_n^2 \mathbb{1}_{n \times n}\right) \\
&= \sigma_n^{-2}\ \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right)
\end{aligned}$$

meaning

$$\begin{aligned}
\sigma_n^{-2}\ \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right) &= \boldsymbol{A}\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal} \\
\sigma_n^{-2}\ \boldsymbol{A}^{-1}\Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right) &= \boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal} \\
\sigma_n^{-2}\ \boldsymbol{A}^{-1}\Phi\left(\boldsymbol{X}\right)^{\intercal} &= \boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right)^{-1}
\end{aligned}$$

so that the current mean of

$$\frac{1}{\sigma_n^2}\Phi\left(\boldsymbol{x}_\star\right)^{\intercal}\boldsymbol{A}^{-1}\Phi\left(\boldsymbol{X}\right)^{\intercal}\boldsymbol{y}$$

in equation 6 can be replaced with

$$\Phi\left(\boldsymbol{x}_\star\right)^{\intercal}\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right)^{-1}\boldsymbol{y}.$$

To find a more suitable expression for the covariance matrix, we will need the assistance of the matrix inversion lemma stated without proof in lemma 11.

Lemma 11 (Matrix Inversion Lemma)**.** *For $\boldsymbol{Z} \in \mathbb{K}^{n \times m}$, $\boldsymbol{W} \in \mathbb{K}^{m \times m}$ and $\boldsymbol{U}, \boldsymbol{V} \in \mathbb{K}^{n \times m}$ then*

$$\left(\boldsymbol{Z} + \boldsymbol{U}\boldsymbol{W}\boldsymbol{V}^{\intercal}\right)^{-1} = \boldsymbol{Z}^{-1} - \boldsymbol{Z}^{-1}\boldsymbol{U}\left(\boldsymbol{W}^{-1} + \boldsymbol{V}^{\intercal}\boldsymbol{Z}^{-1}\boldsymbol{U}\right)^{-1}\boldsymbol{V}^{\intercal}\boldsymbol{Z}^{-1}$$

assuming the relevant inverses exist [Pre92, page 75].

Consider

$$\boldsymbol{A} = \boldsymbol{\Sigma}_p^{-1} + \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\sigma_n^{-2}\mathbb{1}_{n \times n}\right)\Phi\left(\boldsymbol{X}\right) \tag{7}$$

then applying the matrix inversion lemma by setting $\boldsymbol{Z}^{-1} = \boldsymbol{\Sigma}_p, \boldsymbol{W}^{-1} = \sigma_n^2 \mathbb{1}_{n \times n}$ and $\boldsymbol{V} = \boldsymbol{U} = \Phi\left(\boldsymbol{X}\right)$ equation 7 then becomes

$$\boldsymbol{\Sigma}_p - \boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\sigma_n^2 \mathbb{1}_{n \times n} + \Phi\left(\boldsymbol{X}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\right)^{-1}\Phi\left(\boldsymbol{X}\right)\boldsymbol{\Sigma}_p.$$

Thus equation 6 can be equivalently formulated as

$$\begin{aligned}
f_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y} \sim \mathcal{N}(&\Phi\left(\boldsymbol{x}_\star\right)^{\intercal}\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right)^{-1}\boldsymbol{y}, \\
&\Phi\left(\boldsymbol{x}_\star\right)^{\intercal}\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{x}_\star\right) - \Phi\left(\boldsymbol{x}_\star\right)^{\intercal}\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\left(\sigma_n^2 \mathbb{1}_{n \times n} + \Phi\left(\boldsymbol{X}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{X}\right)^{\intercal}\right)^{-1}\Phi\left(\boldsymbol{X}\right)\boldsymbol{\Sigma}_p \Phi\left(\boldsymbol{x}_\star\right)).
\end{aligned} \tag{8}$$

The astute reader may have noticed the very suggestive notation of labelling matrices of the form $\Phi\left(\boldsymbol{W}\right)\boldsymbol{\Sigma}_p\Phi\left(\boldsymbol{W}'\right)^\intercal$ as $\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'}$ as though it may have some sort of connection to a kernel. To make this even more obvious, notice that each occurance of the feature map in both expressions for the mean and covariance in equation 8 can be replaced with a $\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'}$ for some appropriate choice of $\boldsymbol{W}$ and $\boldsymbol{W}'$ giving a more notationally cleaner expression

$$f_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y} \sim \mathcal{N}(\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2\mathbb{1}_{n\times n}\right)^{-1}\boldsymbol{y}, k(\boldsymbol{x}_\star,\boldsymbol{x}_\star) - \boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\left(\sigma_n^2\mathbb{1}_{n\times n} + \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}\right)^{-1}\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}^\intercal). \tag{9}$$

To get a better idea of the connection to kernels, since $\boldsymbol{\Sigma}_p$ is a symmetric positive semi definite matrix, it defines an inner product

$$\langle \boldsymbol{x}, \boldsymbol{y}\rangle_{\boldsymbol{\Sigma}_p} = \boldsymbol{y}^*\boldsymbol{\Sigma}_p\boldsymbol{x}, \quad \boldsymbol{x},\boldsymbol{y} \in \mathbb{K}^N$$

[Wan, page 34] so that

$$\left(\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'}\right)_{ij} = \langle \Phi\left(\boldsymbol{w}_i\right), \Phi\left(\boldsymbol{w}_j\right)\rangle_{\boldsymbol{\Sigma}_p} = k\left(\boldsymbol{w}_i, \boldsymbol{w}_j\right) \tag{10}$$

where k is the kernel with feature map Φ and inner product $\langle\cdot,\cdot\rangle_{\boldsymbol{\Sigma}_p}$. In fact when $\boldsymbol{W} = \boldsymbol{W}'$ equation 10 is exactly the Gram matrix with said kernel. Thus GPs are another great example of models that take advantage of the kernel trick. We shall see in the coming chapters on how exactly we can compute predictions at novel points.

1.5. **Gaussian Processes for Regression.** We saw in section 1.4 that, unlike most other machine learning models, GPs infer over a distribution of functions $p\left(f \mid \mathcal{D}\right)$ instead of a vector of parameteric values $p\left(\boldsymbol{\theta} \mid \mathcal{D}\right)$. Naively, one may attempt to find a suitable f by fixing a class of functions $\mathcal{F}$ and then search over this class to find a function that best represents the data. However, this may not work well if there is not enough richness in $\mathcal{F}$ to represent the data. Instead, a suitable f is selected by first assigning a prior probability to every possible function using the training data and then to select the function with the highest probability. To keep this computation tractable we only evalute our predicted function at a finite number of points. The prediction itself is found by taking the mean over all functions with respect to the posterior conditioned on the observed data which is assumed to be jointly Gaussian with the input value. This gives rise to Gaussian Process more formally stated in definition 12.

Definition 12 (Gaussian Process)**.** *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* [Ras06, Mur12].

A GP is completely characterized by a mean function $m(\boldsymbol{x})$ and a kernel, which in the context of GPs is sometimes called a covariance function, $k(\boldsymbol{x}, \boldsymbol{x'})$ on a real process as

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

GPs define a prior over all possible functions which can be used to create a posterior once enough data has been observed. The prior is used to represent the functions we expect to see before any observations are made. Although defining a prior over all possible functions may seem computationally intractable, we actually only need to define a distribution over a finite number of points. Before any observations are made, we typically assume that the mean function is the constant zero function, that is $m\left(\boldsymbol{x}\right) = 0$. A function $f(\boldsymbol{x})$ sampled from a GP with mean $m(\boldsymbol{x})$ and covariance $k(\boldsymbol{x}, \boldsymbol{x'})$ is written as

$$f(\boldsymbol{x}) \sim \mathcal{GP}\left(m(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x'})\right)$$

Since a GP is a collection of random variables it must satisfy the consistency requirement, that is, observing some of the values should not change the distribution of any small subset of unobserved values. More specifically if

$$(\boldsymbol{y_1}, \boldsymbol{y_2}) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

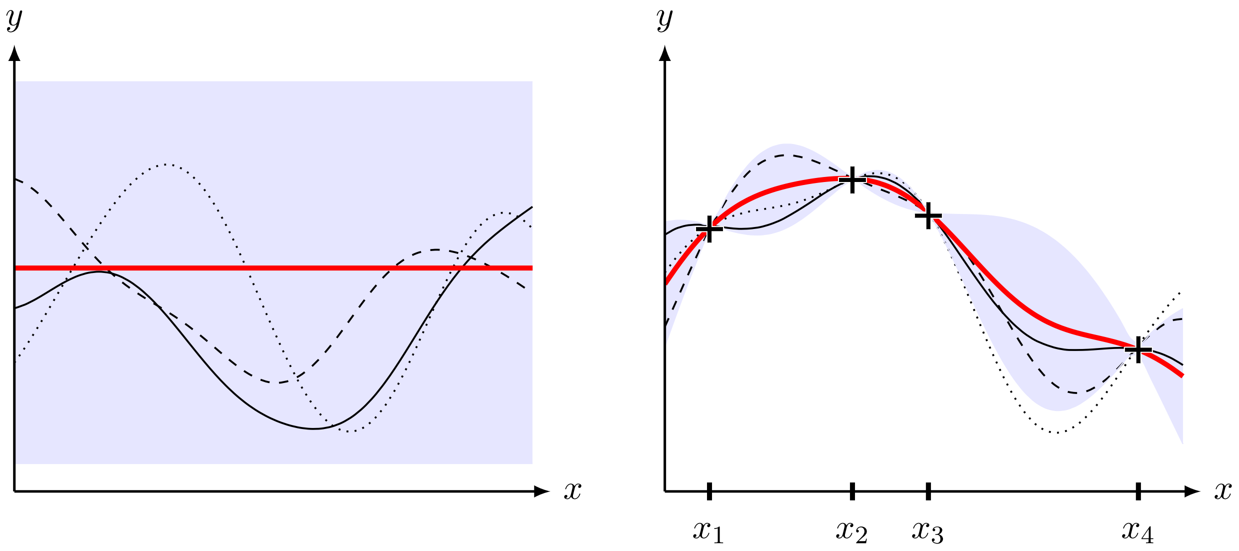
then

$$\boldsymbol{y_1} \sim \mathcal{N}(\boldsymbol{\mu_1}, \boldsymbol{\Sigma_{1,1}})$$
$$\boldsymbol{y_2} \sim \mathcal{N}(\boldsymbol{\mu_2}, \boldsymbol{\Sigma_{2,2}})$$

where $\boldsymbol{\Sigma_{1,1}}$ and $\boldsymbol{\Sigma_{2,2}}$ are the relevant sub matrices. Again, we shall us the notation that for set of data $\boldsymbol{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_n]^\intercal \in \mathbb{R}^{n \times d}$ and $\boldsymbol{W'} = [\boldsymbol{w}'_1, \boldsymbol{w}'_2, \ldots, \boldsymbol{w}'_m]^\intercal \in \mathbb{R}^{n' \times d}$ we use the notation

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

where $\boldsymbol{K_{WW'}} \in \mathbb{R}^{n \times n'}$. The covariance function completely characterized by its kernel. Unless otherwise stated, the kernel or covariance function used in examples and experimentation is the Gaussian RBF kernel, definition 10.



(A)

(B)

FIGURE 4. Panel (A) shows three function drawn from the prior distribution. Panel (B) shows three function drawn from the prior distribution after four observations have been made. In both panels the mean function is drawn in red, sampled functions in black and twice the standard deviation shaded in light blue.

Figure 4 (A) shows three samples drawn from the prior before any observations are made. GPs also allow us to compute the pointwise variance which can provide some measure of variability for predicted values. The blue shaded area of Figure 4 (A) represents twice the standard deviation about the mean.

1.5.1. *Noise-free observations.* Typically when using GP we would like to incorporate data from observations, or training data, into our predictions on unobserved values. Let us suppose there is some obsevered data $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{f}_i) \mid i \in \{1, 2, \ldots, n\}\}$ which is (unrealistically) noise-free that we would like to model as a GP. In other words, for any sample in our dataset we can be certain that the observed value is the true value of the underlying function we wish to model. Then for the observed data

$$\boldsymbol{f} \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}\right).$$

We would then like to make a prediction for unobserved values say $\boldsymbol{X}_\star = [\boldsymbol{x}_{1\star}, \boldsymbol{x}_{2\star}, \ldots, \boldsymbol{x}_{n\star}]$ with value $f_\star$ as has a distribution of

$$\boldsymbol{f}_\star \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{K}_{\boldsymbol{X}_\star\boldsymbol{X}_\star}\right).$$

Here $\boldsymbol{f}$ and $\boldsymbol{f}_\star$ are independent but we would like to give them some sort of correlation. We can do this by having them originate from the same joint distribution. According to the prior, we can write the joint distribution of the training points $\boldsymbol{f}$ and the test points $\boldsymbol{f}_\star$ as

$$\begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{f}_\star \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} & \boldsymbol{K}^\intercal_{\boldsymbol{X}_\star\boldsymbol{X}} \\ \boldsymbol{K}_{\boldsymbol{X}_\star\boldsymbol{X}} & \boldsymbol{K}_{\boldsymbol{X}_\star\boldsymbol{X}_\star} \end{bmatrix}\right).$$

While the above does give us some information that $\boldsymbol{f}_\star$ is related to the observed data and the test inputs, it does not provide any method to evalute $\boldsymbol{f}_\star$. To do this we shall need the assistance of the following theorem.

Theorem 13. (*Marginals and conditionals of an MVN* [Mur12]) *Suppose* $\boldsymbol{x} = (\boldsymbol{x}_1, \boldsymbol{x}_2)$ *is jointly Gaussian with parameters*

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{1,1} & \boldsymbol{\Sigma}_{1,2} \\ \boldsymbol{\Sigma}_{2,1} & \boldsymbol{\Sigma}_{2,2} \end{bmatrix}$$

then the posterior conditional is given by

$$\begin{aligned} \boldsymbol{x}_2 \mid \boldsymbol{x}_1 &\sim \mathcal{N}\left(\boldsymbol{x}_2 \mid \boldsymbol{\mu}_{2|1}, \boldsymbol{\Sigma}_{2|1}\right) \\ \boldsymbol{\mu}_{2|1} &= \boldsymbol{\mu}_2 + \boldsymbol{\Sigma}_{2,1}\boldsymbol{\Sigma}_{1,1}^{-1}\left(\boldsymbol{x}_1 - \boldsymbol{\mu}_1\right) \\ \boldsymbol{\Sigma}_{2|1} &= \boldsymbol{\Sigma}_{2,2} - \boldsymbol{\Sigma}_{2,1}\boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\Sigma}_{1,2}. \end{aligned}$$

Thus, once data has been observed, finding a mean and covariance for $\boldsymbol{f}_\star$ involves a direct application of theorem 13 which gives

$$\boldsymbol{f}_\star \mid \boldsymbol{K}^\intercal_{\boldsymbol{X}_\star\boldsymbol{X}}, \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}, \boldsymbol{f} \sim \mathcal{N}\left(\boldsymbol{\mu}_\star, \boldsymbol{\Sigma}_\star\right)$$

where

$$\begin{aligned} \boldsymbol{\mu}_\star &= \mathbf{0} + \boldsymbol{K}_{\boldsymbol{X}_\star\boldsymbol{X}}\boldsymbol{K}^{-1}_{\boldsymbol{X}\boldsymbol{X}}\left(\boldsymbol{f} - \mathbf{0}\right) \\ &= \boldsymbol{K}_{\boldsymbol{X}_\star\boldsymbol{X}}\boldsymbol{K}^{-1}_{\boldsymbol{X}\boldsymbol{X}}\boldsymbol{f} \end{aligned}$$

and

$$\boldsymbol{\Sigma}_\star = \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star} - \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1} \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}$$

meaning we can write a distribution for $\boldsymbol{f}_\star$ as

$$\boldsymbol{f}_\star \mid \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal, \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}, \boldsymbol{f} \sim \mathcal{N}\left(\boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1} \boldsymbol{f}, \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star} - \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1} \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal\right). \tag{11}$$

Function values from the unobserved inputs $\boldsymbol{X}_\star$, that is $\boldsymbol{f}_\star$, can be estimated using the joint posterior distribution by evaulting the mean of 11. Figure 4 (B) shows these computations given a data set $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)\}$. Notice that the variance tightens around the observed values since (assuming no noise in our data is present) we now know for certain this is how our target function should behave at x_1, x_2, x_3 and x_4. Clearly, specifying the properties of the prior is important since it fixes the properties of the functions considered during inference.

1.5.2. *Prediction with Noisy observations.* When attempting to model our value function we usually do not have access to the value function itself but a noisy version thereof, $y = f(\boldsymbol{x}) + \varepsilon$ where $\varepsilon \sim \mathcal{N}(0, \sigma_n^2)$ meaning the prior on the noisy values becomes

$$\operatorname{cov}(\boldsymbol{y}) = \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \boldsymbol{I}.$$

The reason why noise is only added along the diagonal follows from the assumption of independence of noise in our data. 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

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_\star \end{bmatrix} \sim \mathcal{N}\left(\boldsymbol{0}, \begin{bmatrix} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n\times n} & \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal \\ \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} & \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star} \end{bmatrix}\right).$$

Using a similar we arrive at a similar condition distribution of $\boldsymbol{f}_\star \mid \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal, \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}, \boldsymbol{f}$ we arrive at one of the most fundamental equations for GP regression tasks

$$\boldsymbol{f}_\star \mid \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal, \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}, \boldsymbol{y} \sim \mathcal{N}\left(\overline{\boldsymbol{f}_\star}, \operatorname{cov}(\boldsymbol{f}_\star)\right) \tag{12}$$

where

$$\overline{\boldsymbol{f}_\star} \triangleq \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \left[\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n\times n}\right]^{-1} \boldsymbol{y} \tag{13}$$

$$\operatorname{cov}(\boldsymbol{f}_\star) = \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star} - \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \left[\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n\times n}\right]^{-1} \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal \tag{14}$$

Remarkably, this gives us the the exact same posterior distribution ascertained from the weight space derivation in equation 9. Notice that the prediction of the mean in equation 13 is a linear combination of the observations, somtimes referred to as a *linear predictor*. Another way of looking at the prediction is seeing it as a linear combination of n kernel evaluations centered at the input $\boldsymbol{x}_\star$

$$\boldsymbol{f}_\star = \sum_{i=1}^{n} \alpha_i k\left(\boldsymbol{x}_i, \boldsymbol{x}_\star\right)$$

where $\boldsymbol{\alpha} = \left[\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n\times n}\right]^{-1} \boldsymbol{y}$. Intuitively, this expression can be understood by realising that, despite defining the GP using a joint Gaussian distribution over the observations, when making predictions GPs only care about the $(n+1)$-dimension distribution defined by the n observations and the single test point. When the GP is marginalized by taking the relevant submatrix block of the covariance matrix, this conditioning gives us our desired 1-dimensional prediction.

Also notice that the covariance does not depend on observations but scales quadratically to the norm of the testing inputs. This is a key feature of GPs. The variance is comprised of the difference between the prior covariance, $\boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}_\star}$, and positive term $\boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}} \left[\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right]^{-1} \boldsymbol{K}_{\boldsymbol{X}_\star \boldsymbol{X}}^\intercal$ which represents knowledge given by the observations about the underlying function.

Algorithm 1 shows one possible implementation for computing the mean and covariance of a single test input.

```
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 $\mathbb{V}\left[f_\star\right]$.
  $\boldsymbol{L} = \text{cholesky}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \sigma_n^2 \mathbb{1}_{n \times n}\right)$
  $\boldsymbol{\alpha} = \text{lin-solve}\left(\boldsymbol{L}^\intercal, \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{y}\right)\right)$
  $\overline{f_\star} = \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{X}} \boldsymbol{\alpha}$
  $\boldsymbol{v} = \text{lin-solve}\left(\boldsymbol{L}, \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{X}}\right)$
  $\mathbb{V}\left[f_\star\right] = \boldsymbol{K}_{\boldsymbol{x}_\star \boldsymbol{x}_\star} - \boldsymbol{v}^\intercal \boldsymbol{v}$
  return $\overline{f_\star}, \mathbb{V}\left[f_\star\right]$
```

A Cholesky decomposition is typically used since $\boldsymbol{L}$ can be used twice to assist in solving both the linear systems in the mean and covariance. Unfortunately, a Cholesky decomposition incurres a runtime of $\mathcal{O}\left(n^3\right)$ where n is the number of samples making it impractical for large data sets. In the later chapters we shall consider other methods for solving these linear systems.

1.6. **Gaussian Processes for Classification.** As with most classification models, the Gaussian processes classifier (GPC) seeks an estimate for the joint probability $p\left(y, \boldsymbol{x}\right)$ where $\boldsymbol{x} \in \mathbb{R}^d$ is an input, as in the regression case, but y is now a class taking on a discrete and finite number of values $\{\mathcal{C}_i\}_{i=1}^C$. Using Baye's theorem the joint probability density can be decomposed into either $p\left(y\right) p\left(\boldsymbol{x} \mid y\right)$ or $p\left(\boldsymbol{x}\right) p\left(\boldsymbol{y} \mid \boldsymbol{x}\right)$ giving rise to the *generative* and *discriminative* approaches respectively [Ras06, page 34]. The generative approach models the prior probabilities of each class, $p\left(\mathcal{C}_i\right)$, as well as the class conditional probabilities for each input $p\left(\boldsymbol{x} \mid \mathcal{C}_i\right)$ and computes the posterior as

$$p\left(y \mid \boldsymbol{x}\right) = \frac{p\left(y\right) p\left(\boldsymbol{x} \mid y\right)}{\sum_{i=1}^C p\left(\mathcal{C}_i\right) p\left(\boldsymbol{x} \mid \mathcal{C}_i\right)}.$$

On the other hand, the discriminative method focuses on modelling $p\left(y \mid \boldsymbol{x}\right)$ directly. With both these paradigms at our disposal, which one would be preferred for our GPC? While there are strengths and weaknesses associated with both models, the discriminative approach is usually chosen as it has a rather attractive property of directly modeling what we require, that is $p\left(y \mid \boldsymbol{x}\right)$. Aditionally, the density estimation of $p\left(\boldsymbol{x} \mid \mathcal{C}_i\right)$ using in the generative model presents a number of difficulties, especially for larger values of d. If we are only focused on classifying inputs, the generative approach could mean trying to solve a harder problem than what is necessary. For this reason we focus on GPCs that adopt the discriminative approach.

1.6.1. *Linear Models for Classification.* We can start by reviewing linear models for the simplist form of classification, that is binary classification. Adopting the notation from SVM (see section 1.4.1) literature, the binary classification problem involves assigning an input $\boldsymbol{x}$ to a class of either -1 or $+1$. For a linear model likelihood can be formulated as

$$p\left(y=+1 \mid \boldsymbol{x}, \boldsymbol{w}\right)=\sigma\left(\langle\boldsymbol{x}, \boldsymbol{w}\rangle\right) \tag{15}$$

given a weight vector $\boldsymbol{w}$ and where $\sigma(\boldsymbol{z})$ is chosen to be any sigmoid function, see definition 14.

Definition 14 (Sigmoid Function)**.** *A sigmoid function is a monotonically increasing function mapping from* $\mathbb{R}$ *to* $[0,1]$ [Ras06, page 35].

In this text, the commonly used logistic function

$$\sigma(z)=\frac{1}{1+\exp(-z)} \tag{16}$$

will take the role of the sigmoid function in equation 15, graphed in Figure 5. This type of model is aptly named the logistic regression. Unlike GPR, the likelihood is no longer a Gaussian distribution. Instead it follows the Bernoulli distribution

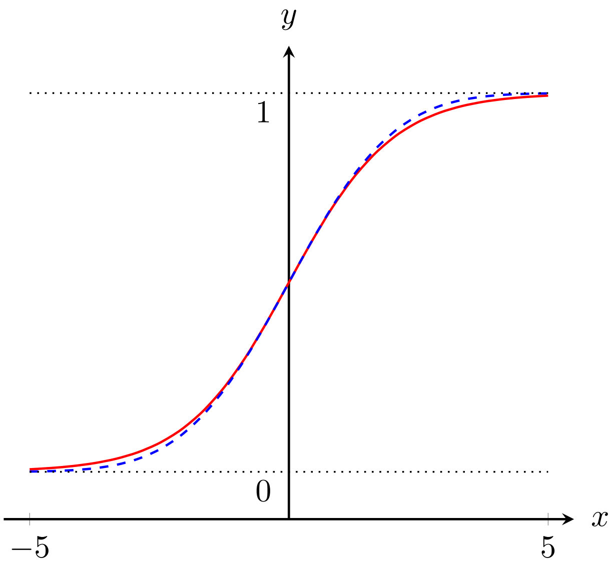


FIGURE 5. The logistic function from equation 16 (solid red) juxtaposed with a close approximation, the scaled probit function (dashed blue).

$$p\left(y \mid \boldsymbol{x}, \boldsymbol{w}\right)=\sigma\left(\langle\boldsymbol{x}, \boldsymbol{w}\rangle\right)^{y}\left(1-\sigma\left(\langle\boldsymbol{x}, \boldsymbol{w}\rangle\right)\right)^{\frac{1-y}{2}}$$

which for symmeteric likelihood functions can be written more concisely as

$$p\left(y_i \mid \boldsymbol{x}_i, \boldsymbol{w}\right)=\sigma\left(y_i f_i\right)$$

where

$$f_i \triangleq f\left(\boldsymbol{x}_i\right)=\langle\boldsymbol{x}, \boldsymbol{w}\rangle. \tag{17}$$

Thus, the logistic regression model can be written as the log ratio of the likelihoods of the input belonging to either class, that is

$$\mathrm{logit}\left(\boldsymbol{x}\right) \triangleq \langle \boldsymbol{x}, \boldsymbol{w} \rangle = \log\left(\frac{p\left(y=+1\right)}{p\left(y=-1\right)}\right)$$

where logit is commonly referred to as the logit transformation [Ras06, page 37]. For a given dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$ we assume each observation is independently generated conditioned over $f\left(\boldsymbol{x}\right)$. Similar to GPR, a Gaussian prior is used for the weights so that $\boldsymbol{w} \sim \mathcal{N}\left(\boldsymbol{0}, \sigma_p\right)$ giving an un-normalised log posterior of

$$\log p\left(\boldsymbol{w} \mid \boldsymbol{X}, \boldsymbol{y}\right) \propto -\frac{1}{2}\boldsymbol{w}^{\intercal}\Sigma_p^{-1}\boldsymbol{w} + \sum_{i=1}^{n} \log \sigma\left(y_i f_i\right).$$

However, unlike GPR an analytic form for the mean and variance for the posterior is not available due to the non-Gaussian nature of the likelihood, although, when using the logistic function it is easy enough to show that the log likelihood is concave as a function of $\boldsymbol{w}$ for a fixed dataset. This means a number of numerical optimization techniques, such as Newton's method or the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm [Fle00] can be used to solve these values.

The idea behind Gaussian process classification for binary classes is that a Gaussian process prior is placed over a latent function $f\left(\boldsymbol{x}\right)$ where the output is then "squashed" through a sigmoid function to obtain a prior on

$$\pi\left(\boldsymbol{x}\right) \triangleq p\left(y=+1 \mid \boldsymbol{x}\right) = \sigma\left(f\left(\boldsymbol{x}\right)\right).$$

This construction is illustrated in Figure 6 and provides a natural extension to the linear logistic regression model.

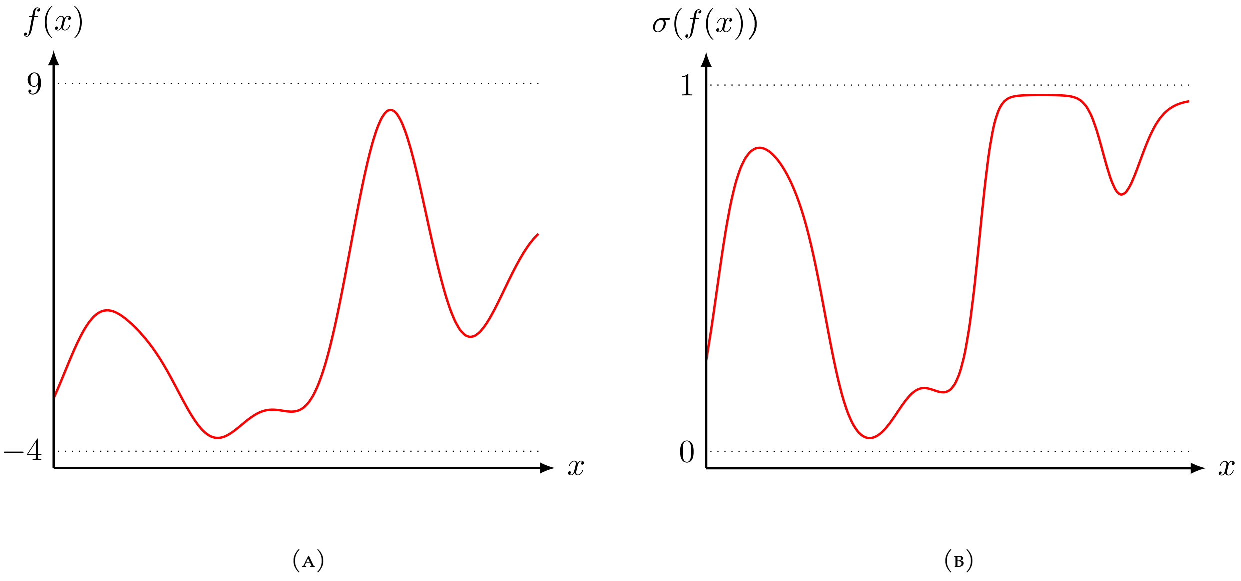


FIGURE 6. The latent function f, panel (A), is transformed using a sigmoid function, panel (B), to provide a probabilistic interpretation of x belonging to the class $+1$.

Specifically, the linear model from equation 17 is replaced with a GPR model and the Gaussian prior on the weights with a GPR weight prior with

$$p\left(\begin{bmatrix}\boldsymbol{f}\\ f_\star\end{bmatrix}\right)=\mathcal{N}\left(\mathbf{0},\begin{bmatrix}\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} & \boldsymbol{K}_{\boldsymbol{x}^\star\boldsymbol{X}}^\intercal\\ \boldsymbol{K}_{\boldsymbol{x}^\star\boldsymbol{X}} & k\left(\boldsymbol{x}_\star,\boldsymbol{x}_\star\right)\end{bmatrix}\right)$$

where $f_\star = f(\boldsymbol{x}_\star)$ and $\boldsymbol{f} = f\left(\boldsymbol{X}\right)$. For classification tasks, we assume that each observation has received the correct label which is why no noise is added to the covariance matrix.

Note that values of f are also never observed within the phenomena we are modelling, nor are we particularly interested in them. The function f serves the role of a *nuisance function* and acts solely as a convenience tool within our formulations. The ultimate goal is to make predictions for π, not f, and the goal of the coming sections will be to eventually integrate out f.

Subsequently, predictions for $\pi_\star = \pi\left(\boldsymbol{x}_\star\right)$ are made by average over all possible latent functions weighted by the posterior giving the prediction

$$\overline{\pi_\star} \triangleq p\left(y_\star = +1 \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{x}_\star\right) = \int \sigma\left(f_\star\right) p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{x}_\star\right)\, df_\star \tag{18}$$

While this is a sound model, computing predictions is not so straight forward since the integral in 18 is not analytically tractable for the same reason as the linear binary classifier. Later on we will see how we can make use of our numerical toolbox to derive a good approximation for $\overline{\pi_\star}$.

1.6.2. *Lapace Approximation for Posterior.* We saw that the integral in 18 could not be used to make predictions for $\overline{\pi_\star}$ analytically. In this section we shall address how the distribution for the latent process, $p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{x}_\star\right)$, can be numerically approximated to provide a numerically tractable succedaneum. Using Baye's theorem

$$\begin{aligned}
p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{x}_\star\right) &= \int p\left(f_\star, \boldsymbol{f} \mid \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{x}_\star\right)\, d\boldsymbol{f}\\
&= \frac{1}{p\left(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{x}_\star\right)} \int p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}\right) p\left(\boldsymbol{f} \mid \boldsymbol{X}\right) p\left(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}\right)\, d\boldsymbol{f}\\
&= \int p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}\right) p\left(\boldsymbol{f} \mid \boldsymbol{X}, \boldsymbol{y}\right)\, d\boldsymbol{f}
\end{aligned}$$

using the fact that $p\left(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}, f_\star\right) = p\left(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}\right)$ [Bis06, Ras06]. The conditional distribution $p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}\right)$ can be derived as

$$p\left(f_\star \mid \boldsymbol{X}, \boldsymbol{x}_\star, \boldsymbol{f}\right) = \mathcal{N}\left(f_\star \mid \boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1} \boldsymbol{y}, k\left(\boldsymbol{x}_\star, \boldsymbol{x}_\star\right) - \boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1} \boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}^\intercal\right)$$

through the use of equation 13 and 14. Unfortunately

$$p\left(\boldsymbol{f} \mid \boldsymbol{X}, \boldsymbol{y}\right) = \frac{p\left(\boldsymbol{y} \mid \boldsymbol{f}\right) p\left(\boldsymbol{f} \mid \boldsymbol{X}\right)}{p\left(\boldsymbol{y} \mid \boldsymbol{X}\right)}$$

does not follow a Gaussian distribution. Instead we can use a Lapace approximation to estimate $p\left(\boldsymbol{f} \mid \boldsymbol{X}, \boldsymbol{y}\right)$ as a Gaussian distribution. Breifly, the Lapace approximation works by assuming the distribution at hand, $p\left(\boldsymbol{z}\right)$, can be modelled as

$$p\left(\boldsymbol{z}\right) = \frac{1}{c} q\left(\boldsymbol{z}\right)$$

where $q(\boldsymbol{z})$ is multivariate Gaussian and c is some normalization constant [Bis06, page 214]. To do this, first the centre of $q(\boldsymbol{z})$ is placed at the mode of $p(\boldsymbol{z})$. The mode of $p(\boldsymbol{z})$ is

$$\boldsymbol{z}_0 = \arg\min_{\boldsymbol{z}} p(\boldsymbol{z})$$

which can be computed by solving

$$\nabla p(\boldsymbol{z}_0) = \mathbf{0}. \tag{19}$$

To ensure the covariance of the synthesized multivariate Gaussian behaves similar to the original distribution we can make use of an important property of the Gaussian distribution which is its logarithm being is a quadratic function of its inputs. Taking the Taylor series expansion of $\ln q(\boldsymbol{z})$ centered at $\boldsymbol{z}_0$ yields

$$\ln q(\boldsymbol{z}) \simeq \ln q(\boldsymbol{z}_0) - \frac{1}{2}(\boldsymbol{z}-\boldsymbol{z}_0)^\intercal \boldsymbol{A}(\boldsymbol{z}-\boldsymbol{z}_0)$$

where

$$\boldsymbol{A} = -\nabla\nabla \ln q(\boldsymbol{z})|_{\boldsymbol{z}=\boldsymbol{z}_0}.$$

Expotentiating both sides gives

$$\begin{aligned} q(\boldsymbol{z}) &\simeq q(\boldsymbol{z}_0)\exp\left(-\frac{1}{2}(\boldsymbol{z}-\boldsymbol{z}_0)^\intercal \boldsymbol{A}(\boldsymbol{z}-\boldsymbol{z}_0)\right) \\ &\propto \mathcal{N}\left(\boldsymbol{z} \mid \boldsymbol{z}_0, \boldsymbol{A}^{-1}\right). \end{aligned} \tag{20}$$

Returning to our original problem of estimating $p(\boldsymbol{f} \mid \boldsymbol{X}, \boldsymbol{y}) \propto p(\boldsymbol{y} \mid \boldsymbol{f})\, p(\boldsymbol{f} \mid \boldsymbol{X})$ as a Gaussian distribution, the prior $p(\boldsymbol{f} \mid \boldsymbol{X})$ follows a Gaussian distribution with zero mean and covariance $\boldsymbol{K}_{\boldsymbol{XX}}$ and the distribution of $p(\boldsymbol{y} \mid \boldsymbol{f})$ (assuming independence of samples) can be written as

$$p(\boldsymbol{y} \mid \boldsymbol{f}) = \prod_{i=1}^{n} \sigma(y_i f_i).$$

To find a Laplace approximation for $p(\boldsymbol{f} \mid \boldsymbol{X}, \boldsymbol{y})$ we only need to consider an unnormalized posterior when maximizing with respect to $\boldsymbol{f}$ since $p(\boldsymbol{y} \mid \boldsymbol{f})$ does not depend on $\boldsymbol{f}$. Thus, the log of the unnormalized posterior is

$$\begin{aligned} \Psi(\boldsymbol{f}) &\triangleq \ln p(\boldsymbol{y} \mid \boldsymbol{f}) + \ln p(\boldsymbol{f} \mid \boldsymbol{X}) \\ &= -\sum_{i=1}^{n} \ln(1+\exp(y_i f_i)) - \frac{1}{2}\boldsymbol{f}^\intercal \boldsymbol{K}_{\boldsymbol{XX}}^{-1}\boldsymbol{f} - \frac{1}{2}\ln|\boldsymbol{K}_{\boldsymbol{XX}}| - \frac{n}{2}\ln 2\pi. \end{aligned}$$

The gradient and Hessian of the unnormalized posterior then becomes

$$\begin{aligned} \nabla\Psi(\boldsymbol{f}) &= \nabla \ln p(\boldsymbol{y} \mid \boldsymbol{f}) - \boldsymbol{K}_{\boldsymbol{XX}}^{-1}\boldsymbol{f} = (\boldsymbol{t}-\boldsymbol{\pi}) - \boldsymbol{K}_{\boldsymbol{XX}}^{-1}\boldsymbol{f} \\ \nabla\nabla\Psi(\boldsymbol{f}) &= \nabla\nabla \ln p(\boldsymbol{y} \mid \boldsymbol{f}) - \boldsymbol{K}_{\boldsymbol{XX}}^{-1} = -\boldsymbol{W} - \boldsymbol{K}_{\boldsymbol{XX}}^{-1} \end{aligned}$$

where $\pi_i = p(y_i = +1 \mid f_i) = \sigma(f_i)$, $\boldsymbol{t} = (\boldsymbol{y}+\mathbf{1})/2 \in \mathbb{R}^n$ and $\boldsymbol{W} \triangleq -\nabla\nabla \ln p(\boldsymbol{y} \mid \boldsymbol{f})$ is a diagonal matrix (since the distribution of y_i only depends on f_i and not $f_{j\neq i}$) with entries $\boldsymbol{W}_{ii} = \sigma(y_i f_i)$ [Bis06, Ras06]. From equation 19, the mode of $\hat{\boldsymbol{f}}$ of $\boldsymbol{\Psi}$ can be computed as

$$\begin{aligned} \nabla\Psi\left(\hat{\boldsymbol{f}}\right) &= \mathbf{0} = (\boldsymbol{t}-\boldsymbol{\pi}) - \boldsymbol{K}_{\boldsymbol{XX}}^{-1}\hat{\boldsymbol{f}} \\ \iff \hat{\boldsymbol{f}} &= \boldsymbol{K}_{\boldsymbol{XX}}(\boldsymbol{t}-\boldsymbol{\pi}). \end{aligned} \tag{21}$$

Since $\boldsymbol{t}-\boldsymbol{\pi}$ is a non-linear function, a non-linear optimization technique method is required to solve $\hat{\boldsymbol{f}}$ in 21. Since the Hessian of $\Psi(\boldsymbol{f})$ is available, Newton's method is typically employed as fast iterative method to approximate $\hat{\boldsymbol{f}}$ where $\hat{\boldsymbol{f}}$ is updated as

$$\hat{\boldsymbol{f}}^{\text{ new}} = \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}\left(\mathbb{1}_{n\times n}+\boldsymbol{W}\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}\right)^{-1}\left(\boldsymbol{W}\hat{\boldsymbol{f}}^{\text{ old}}+\nabla\ln\left(\boldsymbol{y}\mid\hat{\boldsymbol{f}}^{\text{ old}}\right)\right).$$

Once a suitable mode is found, using equation 20, the Lapacian approximation for $p(\boldsymbol{f}\mid\boldsymbol{X},\boldsymbol{y})$ becomes

$$p(\boldsymbol{f}\mid\boldsymbol{X},\boldsymbol{y})\simeq q(\boldsymbol{f}\mid\boldsymbol{X},\boldsymbol{y})=\mathcal{N}\left(\hat{\boldsymbol{f}},\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1}+\boldsymbol{W}\right)^{-1}\right). \tag{22}$$

1.6.3. *Predictions.* With the Lapace approximation for $p(\boldsymbol{f}\mid\boldsymbol{X},\boldsymbol{y})$ (equation 22) and an exact probability distribution for $p(f_\star\mid\boldsymbol{X},\boldsymbol{x}_\star,\boldsymbol{f})$, a mean for the latent process, $p(f_\star\mid\boldsymbol{X},\boldsymbol{y},\boldsymbol{x}_\star)$, can now be computed by invoking 13 to give

$$\begin{aligned}\mu_{f_\star}=\mathbb{E}\left[f_\star\mid\boldsymbol{X},\boldsymbol{y},\boldsymbol{x}_\star\right]&=\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}^{-1}\hat{\boldsymbol{f}}\\&=\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\nabla\ln\left(\boldsymbol{y}\mid\hat{\boldsymbol{f}}\right)\\&=\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\left(\boldsymbol{t}-\boldsymbol{\pi}\right).\end{aligned} \tag{23}$$

Similarly, the variance can be computed using equation 14 to give

$$\sigma_{f_\star}^2=\mathbb{V}\left[f_\star\mid\boldsymbol{X},\boldsymbol{y},\boldsymbol{x}_\star\right]=k\left(\boldsymbol{x}_\star,\boldsymbol{x}_\star\right)-\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}+\boldsymbol{W}^{-1}\right)^{-1}\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}^{\intercal}. \tag{24}$$

Using equation 18, predictions can now be made as

$$\overline{\pi_\star}\simeq\int\sigma\left(f_\star\right)q\left(f_\star\mid\boldsymbol{X},\boldsymbol{y},\boldsymbol{x}_\star\right)\,df_\star \tag{25}$$

where $q(f_\star\mid\boldsymbol{X},\boldsymbol{y},\boldsymbol{x}_\star)$ is a multivariate Gaussian distribution with mean and variance given by equations 23 and 24 respectively. Notice that the prediction given in 25 is a convolution of a Gaussian and logistic function which unfortunately cannot be evaluated analytically. However, Spiegelhalter and Lauritzen [Spi90] show that a good approximation can be found by replacing the sigmoid function with the probit function $\Phi(\lambda a)$ which is simply the cumulative distribution function (CDF) of the standard Gaussian distribution. To get the best approximation using the probit function, the constant factor λ is adjusted to equate their slopes at the origin. The value of λ that gives this equality is $\lambda=\sqrt{\pi/8}$. The similarity between the sigmoid function and probit function rescaled by a factor of $\sqrt{\pi/8}$ is illustrated in Figure 5. The reason for replacing the sigmoid function with a probit function is that the convolution of a Gaussian distribution and probit function can be analytically evaluated as

$$\int\Phi(\lambda a)\mathcal{N}\left(a\mid\mu,\sigma^2\right)\,da=\Phi\left(\frac{\mu}{\left(\lambda^{-2}+\sigma^2\right)^{\frac{1}{2}}}\right). \tag{26}$$

Again apply the approximation $\sigma(a)\simeq\Phi(\lambda a)$ to left hand side of 26 gives the following estimate for the convolution of a Gaussian and sigmoid function

$$\int\sigma(a)\mathcal{N}\left(a\mid\mu,\sigma^2\right)\,da\simeq\sigma\left(\frac{\mu}{\left(1+\pi\sigma^2/8\right)^{\frac{1}{2}}}\right) \tag{27}$$

[Bis06, page 219]. The integral used to approximate $\overline{\pi_\star}$ in 25 can now be estimated using 27 to give

$$\overline{\pi_\star} = \sigma\left(\frac{\mu_{f_\star}}{\left(1+\pi\sigma_{f_\star}^2/8\right)^{\frac{1}{2}}}\right).$$

This theory justifies Algorithm 2 which creates predictions based on the GPC method.

```
Algorithm 2: Unoptimized GPC
  input  : Observations $\boldsymbol{X}, \boldsymbol{y}$ and a test input $\boldsymbol{x}^\star$.
  output: A prediction $\overline{f_\star}$ with its corresponding variance $\mathbb{V}\left[f_\star\right]$.
  $\boldsymbol{t} = \left(\boldsymbol{y} + \boldsymbol{1}\right)/2$
  $\boldsymbol{f} = \boldsymbol{0}$
  repeat
      $\boldsymbol{W} = \mathrm{diag}\left(\sigma\left(\boldsymbol{y}.^{*}\boldsymbol{f}\right)\right)$
      $\boldsymbol{\alpha} = \text{lin-solve}\left(\mathbb{1}_{n\times n} + \boldsymbol{W}\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}, \boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}}\right)$
      $\boldsymbol{f} = \boldsymbol{\alpha}\left(\boldsymbol{t} - \sigma(\boldsymbol{f}) + \boldsymbol{W}\boldsymbol{f}\right)$
  until convergence
  $\mu_{f_\star} = \boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\left(\boldsymbol{t} - \sigma(\boldsymbol{f})\right)$
  $\sigma_{f_\star}^2 = k\left(\boldsymbol{x}_\star, \boldsymbol{x}_\star\right) - \boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}\left(\boldsymbol{K}_{\boldsymbol{X}\boldsymbol{X}} + \boldsymbol{W}^{-1}\right)^{-1}\boldsymbol{K}_{\boldsymbol{x}_\star\boldsymbol{X}}^{\intercal}$
  $\overline{\pi_\star} = \sigma\left(\mu_{f_\star}/\left(1+\pi\sigma_{f_\star}^2/8\right)^{\frac{1}{2}}\right)$
  return $\overline{\pi_\star}, \mu_{f_\star}, \sigma_{f_\star}^2$
```

2. The Nystrom Method

In chapter 1 we saw that GP regression and classification relied on a Gram matrix (see definition 4) to produce predictions. Unfortunately, from a computational perspective, constructing the Gram matrix for a data set $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$ brings about a nasty bottle neck on account of the $\mathcal{O}\left(n^2\right)$ kernel evaluations. Even before the rise of ML, a lot of research devoted to creating numerical methods that quickly construct a low rank approximation of large matrices, $\boldsymbol{A}$, which ordinarily are a computational burden to build exactly. These methods are based on the idea of capturing the columns space of the matrix that best describes the the action of $\boldsymbol{A}$ as an operator. Mahoney provides an enlightened summary as to why the column space is of paramount importance in these approximation techniques

> *"To understand why sampling columns (or rows) from a matrix is of interest,recall that matrices are "about" their columns and rows that is, linear combinations are taken with respect to them; one all but understands a given matrix if one understands its column space, row space, and null spaces; and understanding the subspace structure of a matrix sheds a great deal of light on the linear transformation that the matrix represents."*
> [MWM11, page 13]

Moreover, this class of algorithms lend very nice forms when $\boldsymbol{A}$ possess positive definite structure, which is exactly the case for Gram matrices.

2.1. The Nystrom Method.

Attempting to compute an entire kernel matrix can be a computational headache prompting an investigation of estimative alternatives. The approximation techniques studied in this chapter have been spurred on by the John-Lindenstrauss lemma stated in lemma 15.

Lemma 15 (John-Lindenstrauss)**.** *Given $0 < \varepsilon < 0$, any set of n points, X, in a high dimensional Euclidean space can be embedded into a $\ell-$dimensional Euclidean space where $\ell = \mathcal{O}\left(\ln(n)\right)$ via some linear map $\boldsymbol{\Omega} \in \mathbb{R}^{n\times\ell}$ which satisfies*

$$(1-\varepsilon)\left\|\boldsymbol{u}-\boldsymbol{v}\right\|^2 \leq \left\|\boldsymbol{\Omega u}-\boldsymbol{\Omega v}\right\|^2 \leq \varepsilon\left\|\boldsymbol{u}-\boldsymbol{v}\right\|^2$$

for any $\boldsymbol{u}, \boldsymbol{v} \in X$ [MWM11, page 15].

The John-Lindenstrauss lemma tells us that $\boldsymbol{QQ}^*\boldsymbol{A}$ will serve as a good approximation to some matrix $\boldsymbol{A} \in \mathbb{R}^{n\times m}$ where $\boldsymbol{QQ}^*$, in some sense, projects onto a rank-k subspace of $\boldsymbol{A}$'s column space. This is because if $\boldsymbol{QQ}^*$ closesly matches the behavior of $\boldsymbol{\Omega}$ from the lemma then the pair-wise distances between points before and after applying $\boldsymbol{QQ}^*$ should remain fairly similar. To state this a little more explicitly, for a matrix $\boldsymbol{A}$ and a positive error tolerance ε we seek a matrix $\boldsymbol{Q} \in \mathbb{R}^{n\times k_\varepsilon}$ with orthonormal columns such that

$$\left\|\boldsymbol{A}-\boldsymbol{QQ}^*\boldsymbol{A}\right\|_F \leq \varepsilon$$

which can be expressed in a more short hand notation as

$$\boldsymbol{A} \simeq \boldsymbol{QQ}^*\boldsymbol{A}. \tag{28}$$

This is commonly called the *fixed precision approximation problem*. To simplify algorithmic development, a value of k is specified in advance (instead of ε, thus removing k's dependence on ε) which is instead given the name *fixed rank problem*. Within the fixed rank problem framework, when $\boldsymbol{A}$ is hermitian, the matrix $\boldsymbol{QQ}^*$ acts as a good projection for both the columns and row space of $\boldsymbol{A}$ so that we have both $\boldsymbol{A} \simeq \boldsymbol{QQ}^*\boldsymbol{A}$ and $\boldsymbol{A} \simeq \boldsymbol{AQQ}^*$ meaning

$$\boldsymbol{A} \simeq \boldsymbol{QQ}^* (\boldsymbol{A}) \simeq \boldsymbol{QQ}^*\boldsymbol{AQQ}^*. \tag{29}$$

Furthermore, if $\boldsymbol{A}$ is positive semi-definite we can improve the quality of our approximation of our approximation at almost no additional cost [Hal11, page 32]. Using the approximation from 29

$$\begin{aligned} \boldsymbol{A} &\simeq \boldsymbol{Q}\left(\boldsymbol{Q}^*\boldsymbol{AQ}\right)\boldsymbol{Q}^* \\ &= \boldsymbol{Q}\left(\boldsymbol{Q}^*\boldsymbol{AQ}\right)\left(\boldsymbol{Q}^*\boldsymbol{AQ}\right)^\dagger\left(\boldsymbol{Q}^*\boldsymbol{AQ}\right)\boldsymbol{Q}^* \\ &\simeq \left(\boldsymbol{AQ}\right)\left(\boldsymbol{Q}^*\boldsymbol{AQ}\right)^\dagger\left(\boldsymbol{Q}^*\boldsymbol{A}\right). \end{aligned} \tag{30}$$

This is known as the Nystrom method. Since any Gram matrix is positive semi-definite, we can always applied the Nystrom method to find an approximation to it. A general Nystrom framework is presented in Algorithm 3.

```
Algorithm 3: General Nystrom Framework
  input : A positive semi-definite matrix $\boldsymbol{A} \in \mathbb{R}^{n\times m}$, a matrix $\boldsymbol{Q} \in n \times k$ that
          satisfies 28.
  output: A rank $k$ approximation $\overline{\boldsymbol{A}} \simeq \boldsymbol{A}$.
  $\boldsymbol{C} = \boldsymbol{AQ}$
  $\boldsymbol{W} = \boldsymbol{Q}^*\boldsymbol{C}$
  return $\boldsymbol{CW}^\dagger\boldsymbol{C}^*$
```

However, Algorithm 3 assumes that $\boldsymbol{Q}$ has already been computed. Naturally, the next question is then how to efficiently construct a suitable matrix $\boldsymbol{Q}$ that satisfies equation 28? We can do this through a very popular column sampling technique ubiquitous in numerical linear algebra literature. This technique has been driven by theorem 16.

Theorem 16. *Every $\boldsymbol{A} \in \mathbb{R}^{n\times m}$ matrix contains a $k-$column submatrix $\boldsymbol{C}$ for which*

$$\left\|\boldsymbol{A} - \boldsymbol{CC}^\dagger\boldsymbol{A}\right\|_F \leq \sqrt{1 + k(n-k)} \cdot \|\boldsymbol{A} - \boldsymbol{A}_k\|$$

where $\boldsymbol{A}_k$ is the best rank$-k$ approximation of $\boldsymbol{A}$ [Hal11, page 11].

Before we delve further into this column sampling Nystrom method, we must first cover the random matrix multiplication algorithm which serves as a backbone for this technique. Therefore, let $\boldsymbol{A} \in \mathbb{R}^{n\times m}$ be a target matrix we would like to approximate and suppose that $\boldsymbol{A}$ can be represented as the sum of 'simpler' (for example, sparse or low-rank) matrices, $\boldsymbol{A}_i$, so that

$$\boldsymbol{A} = \sum_{i=1}^{I} \boldsymbol{A}_i. \tag{31}$$

The basic idea is to consider a Monte-Carlo approximation of equation 31 that randomly selects $\boldsymbol{A}_i$ according to the distribution $\{p_i\}_{i=1}^I$ to give an estimate

$$\boldsymbol{A} \simeq \frac{1}{c}\sum_{t=1}^{c} p_{t_i}^{-1}\boldsymbol{A}_{t_i} \tag{32}$$

where c is the number of samples and each summand is rescaled by a factor of $p_{t_i}^{-1}$ to ensure our estimate is unbiased [PGMaJT21, pages 24-27]. The random matrix multiplication algorithm works by attempting to find a Monte-Carlo estimate for $\boldsymbol{AB}$, where $\boldsymbol{A} \in \mathbb{R}^{n \times I}$ and $\boldsymbol{B} \in \mathbb{R}^{I \times m}$. Recall that any matrix multiplication can be written in its outter product form

$$\boldsymbol{AB} = \sum_{i=1}^{I} \boldsymbol{A}_{(:,i)} \boldsymbol{B}_{(i,:)}$$

[FR20, Dri06]. A straight forward way to approximate this using the Monte-Carlo estimate is to simply set each $\boldsymbol{A}_i$ in 31 to the corresponding rank-1 outter product summand $\boldsymbol{A}_{(:,i)}\boldsymbol{B}_{(i,:)}$. This justifies the random matrix multiplication algorithm seen in Algorithm 4 [PDaMWM17, page 16].

```
Algorithm 4: Random Matrix Multiplication
input : $\boldsymbol{A} \in \mathbb{R}^{n\times I}$ and $\boldsymbol{B} \in \mathbb{R}^{I\times m}$, the number of samples $1 \leq c \leq I$ and a
        probability distribution over $I$, $\{p_i\}_{i=1}^{I}$ .
output: Matricies $\boldsymbol{C} \in \mathbb{R}^{n\times c}$ and $\boldsymbol{R} \in \mathbb{R}^{c\times m}$ such that $\boldsymbol{CR} \simeq \boldsymbol{AB}$.

for $t = 1, \dots, c$ do
    Pick $i_t \in \{1, \dots, I\}$ with $\mathbb{P}[i_t = k] = p_k$, independently and with replacement.
    $\boldsymbol{C}_{(:,t)} = \frac{1}{\sqrt{cp_{i_t}}} \boldsymbol{A}_{(:,i_t)}$
    $\boldsymbol{R}_{(:,t)} = \frac{1}{\sqrt{cp_{i_t}}} \boldsymbol{B}_{(i_t,:)}$
end
return $\boldsymbol{CR} = \sum_{t=1}^{c} \frac{1}{cp_{i_t}} \boldsymbol{A}_{(:,i_t)} \boldsymbol{B}_{(i_t,:)}$
```

This algorithm makes this idea a little more precise, taking in the two matrices to multiply together as well as a probability distribution over I to provide an estimate for $\boldsymbol{AB}$ of the form

$$\boldsymbol{AB} \simeq \sum_{t=1}^{c} \frac{1}{cp_{i_t}} \boldsymbol{A}_{(:,i_t)} \boldsymbol{B}_{(i_t,:)}.$$

Equivalently, the above can be restated as the product of two matrices $\boldsymbol{CR}$ formed by Algorithm 4, where $\boldsymbol{C}$ consists of c randomly selected rescaled columns of $\boldsymbol{A}$ and $\boldsymbol{R}$ is c randomly selected rescaled rows of $\boldsymbol{B}$. Notice that

$$\boldsymbol{CR} = \sum_{t=1}^{c} \boldsymbol{C}_{(:,i_t)} \boldsymbol{R}_{(i_t,:)} = \sum_{t=1}^{c} \left(\frac{1}{\sqrt{cp_{i_t}}} \boldsymbol{A}_{(:,i_t)} \right) \left(\frac{1}{\sqrt{cp_{i_t}}} \boldsymbol{B}_{(i_t,:)} \right) = \frac{1}{c} \sum_{t=1}^{c} \frac{1}{p_{i_t}} \boldsymbol{A}_{(:,i_t)} \boldsymbol{B}_{(i_t,:)}.$$

To make development easier, let us define a sampling and rescaling matrix, usually referred to as a sketching matrix, $\boldsymbol{S} \in \mathbb{R}^{n\times c}$ to be the the matrix with elements $\boldsymbol{S}_{i_t,t} = 1\sqrt{cp_{i_t}}$ if the i_t column of $\boldsymbol{A}$ is chosen during the t^{th} trial and all other entries of $\boldsymbol{S}$ are set to 0. Then we have

$$\boldsymbol{C} = \boldsymbol{AS} \quad \text{and} \quad \boldsymbol{R} = \boldsymbol{S}^{\intercal}\boldsymbol{B}$$

so that

$$\boldsymbol{CR} = \boldsymbol{ASS}^{\intercal}\boldsymbol{B} \simeq \boldsymbol{AB}. \tag{33}$$

Notice that $\boldsymbol{S}$ is generally a very sparse matrix and therefore is generally not constructed explicitly and instead the matrix products $\boldsymbol{AS}$ and $\boldsymbol{S}^\intercal \boldsymbol{B}$ are done through row and column rescaling [PDaMWM17, page 17]. Lemma 17 provides some bounds on $\boldsymbol{CR}$ as an estimate for $\boldsymbol{AB}$.

Lemma 17. *Let $\boldsymbol{C}$ and $\boldsymbol{R}$ be constructed as described in Algorithm 4, then*

$$\mathbb{E}\left[(\boldsymbol{CR})_{ij}\right] = (\boldsymbol{AB})_{ij}\,.$$

That is, $\boldsymbol{CR}$ is an unbiased estimate of $\boldsymbol{AB}$. Furthermore

$$\mathbb{V}\left[(\boldsymbol{CR})_{ij}\right] \leq \frac{1}{c}\sum_{k=1}^{n}\frac{\boldsymbol{A}_{ik}^2\boldsymbol{B}_{kj}^2}{p_k}.$$

Proof. For some fixed pair i, j for each $t = 1, \ldots, c$ define $\boldsymbol{X}_t = \left(\frac{\boldsymbol{A}_{(:,i_t)}\boldsymbol{B}_{(i_t,:)}}{cp_{i_t}}\right)_{ij} = \frac{\boldsymbol{A}_{(i,i_t)}\boldsymbol{B}_{(i_t,j)}}{cp_{i_t}}$. Thus, for any t,

$$\mathbb{E}\left[\boldsymbol{X}_t\right] = \sum_{k=1}^{n} p_k \frac{\boldsymbol{A}_{ik}\boldsymbol{B}_{kj}}{cp_k} = \frac{1}{c}\sum_{k=1}^{n}\boldsymbol{A}_{ik}\boldsymbol{B}_{kj} = \frac{1}{c}\left(\boldsymbol{AB}\right)_{ij}.$$

Since we have $(\boldsymbol{CR})_{ij} = \sum_{t=1}^{c}\boldsymbol{X}_t$, it follows that

$$\mathbb{E}\left[(\boldsymbol{CR})_{ij}\right] = \mathbb{E}\left[\sum_{t=1}^{c}\boldsymbol{X}_t\right] = \sum_{t=1}^{c}\left[\mathbb{E}\boldsymbol{X}_t\right] = (\boldsymbol{AB})_{ij}\,.$$

Hence, $\boldsymbol{CR}$ is an unbiased estimator of $\boldsymbol{AB}$, regardless of the choice of the sampling probabilities. Using the fact that $(\boldsymbol{CR})_{ij}$ is the sum of c independent random variables, we get

$$\mathbb{V}\left[(\boldsymbol{CR})_{ij}\right] = \mathbb{V}\left[\sum_{t=1}^{c}\boldsymbol{X}_t\right] = \sum_{t=1}^{c}\mathbb{V}\left[\boldsymbol{X}_t\right].$$

Using the fact $\mathbb{V}\left[\boldsymbol{X}_t\right] \leq \mathbb{E}\left[\boldsymbol{X}_t^2\right] = \sum_{k=1}^{n}\frac{\boldsymbol{A}_{ik}^2\boldsymbol{B}_{kj}^2}{c^2p_k}$, we get

$$\mathbb{V}\left[(\boldsymbol{CR})_{ij}\right] = \sum_{t=1}^{c}\mathbb{V}\left[\boldsymbol{X}_t\right] \leq c\sum_{k=1}^{n}\frac{\boldsymbol{A}_{ik}^2\boldsymbol{B}_{kj}^2}{c^2p_k} = \frac{1}{c}\frac{\boldsymbol{A}_{ik}^2\boldsymbol{B}_{kj}^2}{p_k}.$$

□

So how does this help us with the Nystrom method? Consider using the random matrix multiplication algorithm to approximate the matrix multiplication of a Gram matrix $\boldsymbol{K} \in \mathbb{R}^{n\times n}$ and $\mathbb{1}_{n\times n}$. Equation 33 gives

$$\boldsymbol{KSS}^\intercal\mathbb{1}_{n\times n} = \boldsymbol{KSS}^\intercal \simeq \boldsymbol{K}.$$

We see now that the sketching matrix produced by Algorithm 4 provides a sketching matrix $\boldsymbol{S}$ that satisfies the properties of $\boldsymbol{Q}$ from equation 28 meaning that $\boldsymbol{S}$ can be used in place of $\boldsymbol{Q}$ within the Nystrom estimate from equation 30. These ideas are used together in Algorithm 5 that uses the column sampling technique from Algorithm 4 together with the general Nystrom framework (Algorithm 3) to provide a new column sampling Nystrom method to approximate a Gram matrix for a provided dataset and probability distribution [PDaMWM05, AGaMWM13].

Algorithm 5: Nystrom Method via Column Sampling

```
input  : Data matrix $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^\intercal \in \mathbb{R}^{n \times d}$, the number of samples $1 \leq c \leq n$
         and a probability distribution over $n$, $\{p_i\}_{i=1}^{n}$ .
output: An approximation of the Gram matrix corresponding to $\boldsymbol{X}$, that is
         $\overline{\boldsymbol{K}} \simeq \boldsymbol{K}$ where $\boldsymbol{K}_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$.
Initialize $\boldsymbol{C}$ as an empty $n \times c$ matrix.
Pick $c$ columns with the probability of choosing the $k^{th}$ column $(1 \leq k \leq n)$ as
  $\mathbb{P}[k = i] = p_i$, independently and with replacement and let $I$ a list of indices of
  the sampled columns.
for $i \in I$ do
    $\boldsymbol{K}_{(:,i)} = [k(\boldsymbol{x}_1, \boldsymbol{x}_i), \ldots, k(\boldsymbol{x}_n, \boldsymbol{x}_i)]^\intercal$
    $\boldsymbol{C}_{(:,i)} = \boldsymbol{K}_{(:,i)} / \sqrt{c p_i}$
end
$\boldsymbol{W} = \boldsymbol{K}_{(I,I)} \in \mathbb{R}^{c \times c}$
Rescale each entry of $\boldsymbol{W}$, $\boldsymbol{W}_{ij}$, by $1/c\sqrt{p_i p_j}$.
Compute $\boldsymbol{W}^\dagger$
return $\boldsymbol{C}\boldsymbol{W}^\dagger\boldsymbol{C}^*$
```

As we can tell from the algorithms inputs, this requires some sort of probability distribution to select the columns. As seen in lemma 17 any probability distribution will provide an unbiased estimate. However, some probability distributions can be used to lower the variance faster than others. Naively, we could just employ uniform sampling where each column in selected with equal probability although it should be cautioned that this is seldom a good idea since uniform sampling tend to over sample landmarks from one large cluster while under sampling or even missing entire small but important clusters. As a result, the approximation for $\boldsymbol{K}$ will decline [CMaCM17, page 3]. This is demonstarted in graphic form in Figure 7.

To combat this issue, alternative probabilites density can be constructed to take into account a measure of importance in landmark selection. Indeed there has been a plethora of research that has shown the importance of using data-dependent non-uniform probability distributions to obtain proveably better error bounds within the Nystrom framework [PDaMWM05, AGaMWM13, CMaCM17, PDe11, MBCaC-MaCM15, Kum09]. A few of the more common distributions will be discussed in the coming sections.

2.2. **Column Probabilities.** Recall that the Nystrom method from Algorithm 5 is largely dependent on the random matrix multiplication algorithm (Algorithm 4) to produce a suitable sketching matrix. Moreover, improvements in the sketching matrix produced by the random matrix multiplication algorithm are reflected as smaller errors in the Nystrom approximation. Now, consider using the random matrix multiplication algorithm to approximate $\boldsymbol{A}\boldsymbol{A}^\intercal$ by setting $\boldsymbol{B} = \boldsymbol{A}$. The output is an approximation of the form

$$\boldsymbol{A}\boldsymbol{A}^\intercal \simeq \boldsymbol{C}\boldsymbol{C}^\intercal = \boldsymbol{C}\boldsymbol{R}.$$

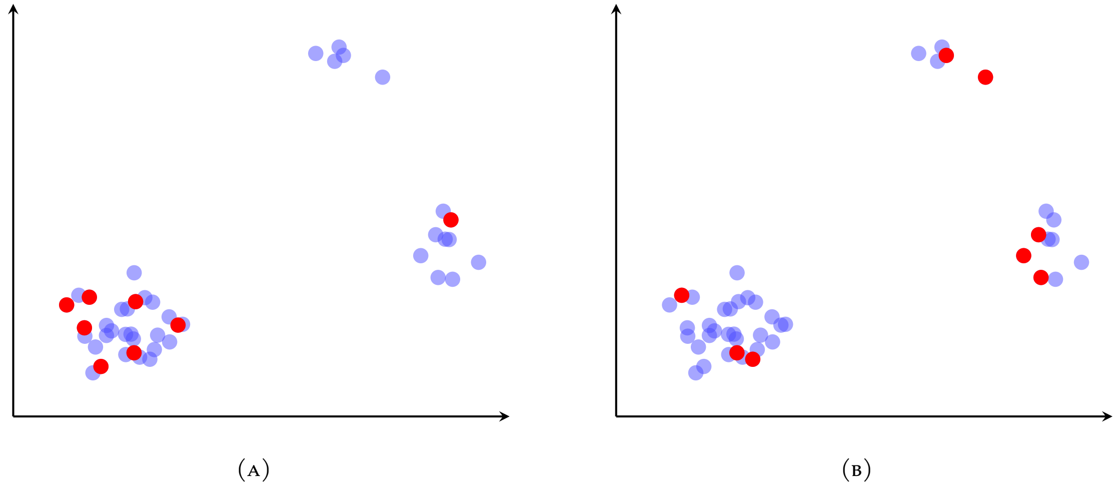


Figure 7. Employing uniform sampling in the column sampling Nystrom estimate can lead to oversampling from denser parts of the data set (Panel (A)). Instead data dependent probability densities are commonly used to better cover the relevant data (Panel (B)). Example taken from [CMaCM17, page 4].

The probability distribution

$$p_i = \frac{\left\|\boldsymbol{A}_{(:,i)}\right\|_2^2}{\|\boldsymbol{A}\|_F}.$$

aims to minimize the error between $\boldsymbol{A}\boldsymbol{A}^\intercal$ and the approximation $\boldsymbol{C}\boldsymbol{C}^\intercal$. As a result, we should expect that $\boldsymbol{C}$ becomes a better estimate for $\boldsymbol{A}\boldsymbol{S}$, implying that the sketching matrix, $\boldsymbol{S}$, is using a better sampling and landmark selection criteria. Drineas and Mahoney give a precise bound on this error presented in theorem 18 [PDaMWM05, page 2158].

Theorem 18. *Given $\boldsymbol{A} \in \mathbb{R}^{n \times I}$, $1 \leq c \leq I$ and the probability distribution $\{p_i\}_{i=1}^I$ described in equation 2.2. Construct $\boldsymbol{C}$ using algorithm 4, then*

$$\mathbb{E}\left[\left\|\boldsymbol{A}\boldsymbol{A}^\intercal - \boldsymbol{C}\boldsymbol{C}^\intercal\right\|_F\right] \leq \frac{1}{\sqrt{c}} \|\boldsymbol{A}\|_F^2$$

[PDaMWM05, page 2158].

To show theorem 18, we can actually prove something a little more general.

Lemma 19. *Given $\boldsymbol{A} \in \mathbb{R}^{n \times I}$, $\boldsymbol{B} \in \mathbb{R}^{I \times m}$, $1 \leq c \leq I$ and the probability distribution $\{p_i\}_{i=1}^I$ as follows*

$$p_i = \frac{\left\|\boldsymbol{A}_{(:,i)}\right\|_2 \left\|\boldsymbol{B}_{(i,:)}\right\|_2}{\sum_{j=1}^I \left\|\boldsymbol{A}_{(:,j)}\right\|_2 \left\|\boldsymbol{B}_{(j,:)}\right\|}.$$

Construct $\boldsymbol{C}$ using algorithm 4, using the probability distribution described above, then

$$\mathbb{E}\left[\left\|\boldsymbol{A}\boldsymbol{B} - \boldsymbol{C}\boldsymbol{R}\right\|_F\right] \leq \frac{1}{\sqrt{c}} \|\boldsymbol{A}\|_F^2 \|\boldsymbol{B}\|_F^2.$$

This choice of probability distribution minimises $\mathbb{E}\left[\left\|\boldsymbol{A}\boldsymbol{B} - \boldsymbol{C}\boldsymbol{R}\right\|_F\right]$ among all possible sampling probabilites [Dri06, pages 9-12].

Proof. First note that

$$\mathbb{E}\left[\|\boldsymbol{AB}-\boldsymbol{CR}\|_F^2\right]=\sum_{k=1}^{n}\sum_{j=1}^{m}\mathbb{E}\left[(\boldsymbol{AB}-\boldsymbol{CR})_{kj}^2\right]=\sum_{k=1}^{n}\sum_{j=1}^{m}\mathbb{V}\left[(\boldsymbol{CR})_{kj}\right].$$

Thus from lemma 17, it follows that

$$\begin{aligned}&\mathbb{E}\left[\|\boldsymbol{AB}-\boldsymbol{CR}\|_F^2\right]\\ =&\frac{1}{c}\sum_{i=1}^{I}\frac{1}{p_i}\left(\sum_{k=1}^{n}\boldsymbol{A}_{ki}^2\right)\left(\sum_{j=1}^{m}\boldsymbol{B}_{ij}^2\right)-\frac{1}{c}\|\boldsymbol{AB}\|_F^2\\ =&\frac{1}{c}\sum_{i=1}^{I}\frac{1}{p_i}\left\|\boldsymbol{A}_{(:,i)}\right\|_2^2\left\|\boldsymbol{B}_{(i,:)}\right\|_2^2-\frac{1}{c}\|\boldsymbol{AB}\|_F^2.\end{aligned}$$

Substituting in a probability of

$$p_i=\frac{\left\|\boldsymbol{A}_{(:,i)}\right\|_2\left\|\boldsymbol{B}_{(i,:)}\right\|_2}{\sum_{j=1}^{I}\left\|\boldsymbol{A}_{(j,:)}\right\|_2\left\|\boldsymbol{B}_{(:,j)}\right\|}.$$

yields

$$\begin{aligned}\mathbb{E}\left[\|\boldsymbol{AB}-\boldsymbol{CR}\|_F^2\right]=&\frac{1}{c}\left(\sum_{i=1}^{I}\left\|\boldsymbol{A}_{(:,i)}\right\|_2\left\|\boldsymbol{B}_{(i,:)}\right\|_2\right)^2-\frac{1}{c}\|\boldsymbol{AB}\|_F^2\\ \le&\frac{1}{c}\|\boldsymbol{A}\|_F^2\|\boldsymbol{B}\|_F^2.\end{aligned}$$

To verify that this choice of probability distribution minimises $\mathbb{E}\left[\|\boldsymbol{AB}-\boldsymbol{CR}\|_F\right]$ define the function

$$f\left(p_1,\ldots,p_n\right)=\sum_{i=1}^{I}\frac{1}{p_i}\left\|\boldsymbol{A}_{(:,i)}\right\|_2^2\cdot\left\|\boldsymbol{B}_{(i,:)}\right\|_2^2$$

which characterises the dependence of $\mathbb{E}\left[\|\boldsymbol{AB}-\boldsymbol{CR}\|_F\right]$ on the probability distribution. To minimise f subject to $\sum_{i=1}^{I}p_i=1$, we introduce the Lagrange multiplier λ and define the function

$$g\left(p_1,\ldots,p_n\right)=f\left(p_i,\ldots,p_n\right)+\lambda\left(\sum_{i=1}^{I}p_i-1\right).$$

The minimum is then

$$0=\frac{\partial g}{\partial p_i}=-\frac{1}{p_i^2}\left\|\boldsymbol{A}_{(:,i)}\right\|_2^2\cdot\left\|\boldsymbol{B}_{(i,:)}\right\|_2^2+\lambda.$$

Thus

$$p_i=\frac{\left\|\boldsymbol{A}_{(:,i)}\right\|_2\cdot\left\|\boldsymbol{B}_{(i,:)}\right\|_2}{\sqrt{\lambda}}=\frac{\left\|\boldsymbol{A}_{(:,i)}\right\|_2\cdot\left\|\boldsymbol{B}_{(i,:)}\right\|_2}{\sum_{j=1}^{I}\left\|\boldsymbol{A}_{(j,:)}\right\|_2\left\|\boldsymbol{B}_{(:,j)}\right\|_2}$$

where the second equality comes from solving for $\sqrt{\lambda}$ in $\sum_{i=1}^{I-1}p_i=1$. These probabilities are indeed minimizing since $\frac{\partial^2 g}{\partial p_i^2}>0$ for every i such that $\left\|\boldsymbol{A}_{(:,i)}\right\|_2^2\cdot\left\|\boldsymbol{B}_{(i,:)}\right\|_2^2>0$. □

2.3. Leverage Scores.

2.3.1. *Statistical Leverage Scores.* Our next distribution originates from the least-squares problem. Breifly, in an over constrained least-squares problem, where $\boldsymbol{A} \in \mathbb{R}^{n \times m}$, $\boldsymbol{b} \in \mathbb{R}^{n}$, for $m \ll n$ there usually are not any $\boldsymbol{x} \in \mathbb{R}^{m}$ for which $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$. Instead, alternative criteria must be employed to seek a $\boldsymbol{x}$ which in some way comes "closest" to satisfying this equality. Perhaps one of the more popular criterion is to minimize the ℓ^2-norm, that is

$$\boldsymbol{x}_{opt} = \arg\min_{x} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|$$

[MWM11, page 19-21]. The optimal value for $\boldsymbol{x}$ can be solved as $\boldsymbol{x}_{opt} = \left(\boldsymbol{A}^{\intercal}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\intercal}\boldsymbol{b}$. The least-squares solution is commonly used to find the best weight vector (in this case $\boldsymbol{x}$) for a linear model, given a dataset. Fitted or predicted values are usually obtained from $\hat{\boldsymbol{b}} = \boldsymbol{H}\boldsymbol{b}$ where the projector onto the column space of $\boldsymbol{A}$

$$\boldsymbol{H} = \boldsymbol{A}\left(\boldsymbol{A}^{\intercal}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\intercal}$$

is sometimes referred to as the *hat matrix*. The element $\boldsymbol{H}_{ij}$ has the direct interpretation as the influence or statistical leverage exerted on $\hat{\boldsymbol{b}}_i$. Thus, examining the hat matrix can reveal to us columns of $\boldsymbol{A}$ which bear a significant impact on $\hat{\boldsymbol{b}}$ [Hoa78, page 17]. Relatedly, if the element $\boldsymbol{H}_{ii}$ is particularly large this is indicative of the i^{th} column of $\boldsymbol{A}$ having a strong influence over values of $\hat{\boldsymbol{b}}$, justifying the interpretation of $\boldsymbol{H}_{ii}$ as *statistical leverage scores*.

The statistical leverage scores are maximised when $\boldsymbol{A}_{(:,i)}$ is linearly independent from $\boldsymbol{A}$'s other columns and decreases when it aligns with many other columns or when the value of $\left\|\boldsymbol{A}_{(:,i)}\right\|$ is small [MBCaC-MaCM15, page 5]. To compute the statistical leverage scores, if $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\intercal}$ is the SVD of $\boldsymbol{A}$, then

$$\begin{aligned}\boldsymbol{H}_{ii} &= \left(\boldsymbol{A}\left(\boldsymbol{A}^{\intercal}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\intercal}\right)_{ii} \\ &= \left(\boldsymbol{U}\boldsymbol{\Sigma}^{2}\left(\boldsymbol{\Sigma}^{2}\right)^{-1}\boldsymbol{U}\right)_{ii} \\ &= \left\|\boldsymbol{U}_{(i,:)}\right\|_{2}^{2}.\end{aligned}$$

Note that $\boldsymbol{H}_{ii}$ may not constitute as a probability distribution, as may the other leverage scores which we will soon discuss. This is easily remedied through normalisation, in this case dividing each statistical leverage score by $\operatorname{tr}(\boldsymbol{H})$. The idea behind using statistical leverage scores as a probability distribution in the Nystrom method is that they help prioritize selection of columns that are more linearly independent from other columns so that the range of our approximate better aligns with the range of our original $\boldsymbol{A}$.

2.3.2. *Rank$-k$ Statistical Leverage Scores.* We can generalize this notion of statistical leverage scores to include lower rank approximations. Let $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\intercal}$ be the compact SVD of a $\boldsymbol{A}$ real $n \times m$ matrix. Setting $r = \min\{n, m\}$, the compact SVD can be partitioned as

$$\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2] \in \mathbb{R}^{n \times r}, \qquad \boldsymbol{\Sigma} = \begin{bmatrix}\boldsymbol{\Sigma}_1 & \\ & \boldsymbol{\Sigma}_2\end{bmatrix} \in \mathbb{R}^{r \times r}, \qquad \boldsymbol{V} = [\boldsymbol{V}_1, \boldsymbol{V}_2] \in \mathbb{R}^{m \times r}.$$

Here $\boldsymbol{U}_1$ contains the first $k \le r$ columns of $\boldsymbol{U}$, $\boldsymbol{V}_1$ the first k rows of $\boldsymbol{V}$ and $\boldsymbol{\Sigma}_1$ is a $k \times k$ matrix containing the top k singular values across its diagonal. The matrix $\boldsymbol{A}_k = \boldsymbol{U}_1\boldsymbol{\Sigma}_1\boldsymbol{V}_1$ serves as the best rank$-k$ approximation to $\boldsymbol{A}$. The statistical leverage scores relative to the best rank$-k$ approximation are again

$\boldsymbol{H}_{ii}$, but this time $\boldsymbol{H}$ is computed only using the best rank$-k$ approximation of $\boldsymbol{A}$, that is $\boldsymbol{A}_k$. These low rank scores can be evaluated as

$$\ell_i^k \triangleq \left(\boldsymbol{A}_k \left(\boldsymbol{A}_k^\intercal \boldsymbol{A}_k\right)^{-1} \boldsymbol{A}_k^\intercal\right)_{ii} = \left\|\left(\boldsymbol{U}_1\right)_{(i,:)}\right\|_2^2.$$

What makes low-rank statistical leverage scores particularly appealing is that they can be approximated quickly with a truncated SVD [AGaMWM13, pages 3-4].

2.3.3. *Ridge Leverage Scores.* The low rank leverage scores we saw in equation 2.3.2 will not always be unique and can be sensitive to perturbations [MBCaCMaCM15, page 6]. Consequently these scores can vary drastically when $\boldsymbol{A}$ is modified slightly or when we only have access to partial information on the matrix. This undermines the the possibility of computing good quality low rank approximations from statistical leverage scores. This shortcoming is addressed in the next class of leverage score, that is, ridge leverage scores. Ridge leverage scores are similar to statistical leverage scores although a ridge regression term (hence the name) is added to the hat matrix with a regularization parameter λ. The $\lambda-$ridge leverage score is defined as

$$r_i^\lambda \triangleq \left(\boldsymbol{A}\left(\boldsymbol{A}^\intercal \boldsymbol{A} + \lambda \mathbb{1}_{n\times n}\right)^{-1} \boldsymbol{A}^\intercal\right)_{ii}.$$

A regularization parameter of

$$\lambda = \frac{\|\boldsymbol{A} - \boldsymbol{A}_k\|_F^2}{k}$$

is typically used since this choice of λ will guarantee that the sum of the ridge leverage scores (keep in mind that the raw ridge leverage scores do not necessarily form a probability distribution) is bounded by $2k$, stated more formally in lemma 20.

Lemma 20. *When using a regularization parameter of* $\lambda = \frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}$ *we have* $\sum_{i=1}^n r_i^\lambda \leq 2k$ [MBCaCMaCM15, pages 6-7].

Proof. Writing r_i^λ using the SVD of $\boldsymbol{A}$ where $\lambda = \frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}$ gives

$$\begin{aligned} r_i^\lambda &= \boldsymbol{A}_{(i,:)}\left(\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{U}^\intercal + \frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}\boldsymbol{U}\boldsymbol{U}^\intercal\right)^{-1} \boldsymbol{A}_{(i,:)}^\intercal \\ &= \boldsymbol{A}_{(i,:)}\left(\boldsymbol{U}\overline{\boldsymbol{\Sigma}}^2\boldsymbol{U}^\intercal\right)^{-1} \boldsymbol{A}_{(i,:)}^\intercal \\ &= \boldsymbol{A}_{(i,:)}\left(\boldsymbol{U}\overline{\boldsymbol{\Sigma}}^{-2}\boldsymbol{U}^\intercal\right) \boldsymbol{A}_{(i,:)}^\intercal \end{aligned}$$

where $\overline{\boldsymbol{\Sigma}}_{ii}^2 = \sigma_i^2\left(\boldsymbol{A}\right) + \frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}$. Then

$$\begin{aligned} \sum_{i=1}^n r_i^\lambda &= \operatorname{tr}\left(\boldsymbol{A}^\intercal\boldsymbol{U}\overline{\boldsymbol{\Sigma}}^{-2}\boldsymbol{U}^\intercal\boldsymbol{A}\right) \\ &= \operatorname{tr}\left(\boldsymbol{V}\boldsymbol{\Sigma}\overline{\boldsymbol{\Sigma}}^{-2}\boldsymbol{\Sigma}\boldsymbol{V}^\intercal\right) \\ &= \operatorname{tr}\left(\boldsymbol{\Sigma}^2\overline{\boldsymbol{\Sigma}}^{-2}\right). \end{aligned}$$

Here we have

$$\left(\boldsymbol{\Sigma}^2\overline{\boldsymbol{\Sigma}}^{-2}\right)_{ii} = \frac{\sigma_i^2\left(\boldsymbol{A}\right)}{\sigma_i^2\left(\boldsymbol{A}\right) + \frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}}.$$

For $i \leq k$ we simply upper bound this by 1, yielding

$$\operatorname{tr}\left(\boldsymbol{\Sigma}^2\overline{\boldsymbol{\Sigma}}^{-2}\right) = k + \sum_{i=k+1}^{n} \frac{\sigma_i^2\left(\boldsymbol{A}\right)}{\sigma_i^2\left(\boldsymbol{A}\right) + \frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}} \leq k + \sum_{i=k+1}^{n} \frac{\sigma_i^2\left(\boldsymbol{A}\right)}{\frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}} = k + \frac{\sum_{i=k+1}^{n} \sigma_i^2\left(\boldsymbol{A}\right)}{\frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}} \leq k + k.$$

□

From now on (unless otherwise stated) the regularization parameter seen in 2.3.3 will always be used for ridge leverage scores where the notation

$$r_i^k \triangleq \left(\boldsymbol{A}\left(\boldsymbol{A}^\intercal\boldsymbol{A} + \left(\frac{\|\boldsymbol{A}-\boldsymbol{A}_k\|_F^2}{k}\right)\mathbb{1}_{n\times n}\right)^{-1}\boldsymbol{A}^\intercal\right)_{ii}$$

is employed to show that the best rank$-k$ matrix is utilized in the regularization parameter. Adding regularization to the hat matrix offers a smoother alternative which 'washes out' small singular directions meaning they are sampled with proportionally lower probability [MBCaCMaCM15, page 6]. Alaoui and Mahoney [Ala15] prove that ridge leverage scores provide theoretically better bounds over uniform sampling techniques when the number of sampled columns is proportional to $\operatorname{tr}\left(\boldsymbol{H}_\lambda\right) \cdot \ln\left(n\right)$ where $\boldsymbol{H}_\lambda$ is the hat matrix with added regularization, that is $\boldsymbol{H}_\lambda = \boldsymbol{A}\left(\boldsymbol{A}^\intercal\boldsymbol{A} + \lambda\mathbb{1}_{n\times n}\right)^{-1}\boldsymbol{A}^\intercal$. With the rising popularity of ridged leverage scores, a number of iterative methods have been devised (and continue to be developed) that take advantage of parallel computing to provide fast approximations [PGMaJT21, page 90].

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