



THE UNIVERSITY OF QUEENSLAND
A U S T R A L I A

OPTIMIZING PERFORMANCE
IN GAUSSIAN PROCESSES

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INTRODUCTION

The problem of time series prediction (and related regression tasks) have been a long standing subject of high interest in many disciplines of science and mathematics. The problem itself is fairly straight forward, 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 value that acts as a function of time, the question then is how do we go about predicting a value y_* for the modeled phenomena at time x_* ? With computing power becoming ever more affordable and advanced, many have taken to Machine Learning (ML) to develop sophisticated models to address the problem of developing accurate time series predictors. ML, broadly speaking, is any class of heuristic algorithm that attempts to refine and develop functionality by learning through some form of input. The idea of 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, in ML we are trying to develop a function $f : X \rightarrow Y$ for some input set X and observation set Y where the outputs of f closely align to actual observations. A model will attempt to make accurate prediction using some simplified formulation of the world required for the task. 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 limitations usually arise as a consequence of selecting a model too simple or complex for the task. The "state of the world" is sometimes internally captured by the model as a set of mutable parameters θ . The process of taking observations and using them to form predictions is called *inference* which, in some sense, is synonymous with learning.

ML can be applied to the problem of time series prediction in a fairly straight forward manner, by simply teaching a ML algorithm \mathcal{M} 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 Bayesian ML models which, unsurprisingly, makes use of Bayesian statistics to drive inference.

In Bayesian models a *prior* distribution is used to represent 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 update the state of the model to give a *posterior* distribution which represents the reduced uncertainty after "teaching" the model with these new observations. Methods of "teaching" a model how to behave using a new set of observations sometimes involves the use of a *loss function* L which is used to aid us in deciding what action a should be taken in changing the state of the model to best minimize uncertainty. The best action, roughly speaking, can be evaluated as

$$a_* = \arg \min_a \int L(y_*, a) p(y_* | x_*, \mathbf{X}, \mathbf{y}) dy_*.$$

Interestingly, the best action does not rely so much on the model internalized parameters or the structure of the model itself but more so the predictive distribution $p(y_* | x_*, \mathbf{X}, \mathbf{y})$. This key insight has spawned a class of ML algorithms that focus on inferring the function f directly by computing $p(f | \mathcal{D})$ instead of finding optimal internal parameters using $p(\theta | \mathcal{D})$. Models that perform inference in this manner are called *non-parameteric* models. Within the *non-parameteric* model paradigm, the predictive distribution can be expressed as

$$p(y_* | x_*, \mathbf{X}, \mathbf{y}) = \int p(y_* | f, x_*) p(f | \mathbf{X}, \mathbf{y}) df$$

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

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{marginal likelihood}}, \quad p(\mathbf{f}, f_{\star} | \mathbf{y}) = \frac{p(\mathbf{y} | \mathbf{f}) p(\mathbf{f}, f_{\star})}{p(\mathbf{y})}.$$

This thesis will focus on a particular non-parametric Bayesian ML model called Gaussian processes (GP). The over arching idea of GPs is to define a prior to every possible function mapping from X to Y . On the surface, this does not seem computationally tractable as we would seemingly need to check through an uncountable infinite number of mappings. It turns out, computation can be completed 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, relatively simple to implement and are highly modular allowing them to easily be incorporated into a larger systems. It is no surprise that while other kernel methods are still overshadowed by their neural network cousins, GPs have made a quiet comeback in the ML community.

To highlight a particular GP success story, a team of agriculturalists lead by Andries Potgieter are currently investigating how ML can be used to inform farmers on the best time to plant various crops to minimize crop loss from environmental stresses; such as frost and plant diseases. This involves analysing crop growth from previous seasons to forecast when certain phenological stages in the crops development of the current yield. This problem is readily converted into a time series problem. Originally, Andries' team surveyed a number of different parameteric models to provide this forecasting. However, the parameteric models we serverely limited in their ability to inform when key phenological stages would take place. They then moved onto using GPs which they found could produce much higher resolution predictions from which they could infer a far richer phenological timeline. A comparision of using GPs over other parameteric models is shown in Figure 1. Andries' team found that the only draw back to using GPs was

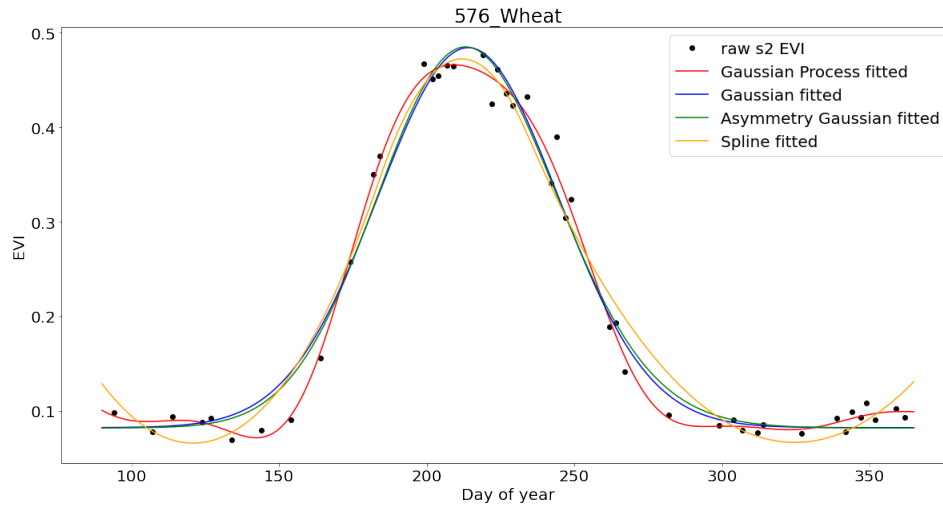


FIGURE 1. Andries' team found that GPs where superior in terms of predicting a phenological timeline for a number of common seasonal crops over other parameteric models.

the lengthy run time required to create predictions and fears that as more data is collected each season this would only exacerbate the issue. This is a common problem shared by anyone wanting to use GPs. Due to their unwieldy $\mathcal{O}(n^3)$ runtime, where n is the number of observations, GPs become impractical

to apply on datasets with $n > 10^5$. The goal of this thesis is to explore various avenues one can take to replace some of the more intense calculations with computational more efficient approximations without sacrificing a great deal of precision.

Chapter 1 will give a more mathematical treatment of GPs starting from the ground up by first giving a review of some essential material from functional analysis and then motivating the theory behind GPs before finally ending with a concrete algorithm for GP regression and classification. In chapter FIX and 2 we shall look at techniques for approximating a large matrix that essentially provides information on how similar each observation is from one other. Chapter 3 then gives alternative methods for solving linear systems which is an essential component required for GP algorithm to work.

1. GAUSSIAN PROCESSES

The aim of this chapter is to review some essential mathematical machinery required for us to understand the core concepts of Gaussian Processes.

1.1. Kernels. Often in machine learning we are often met with the problem of how to best represent data instances as fixed size feature vectors $\mathbf{x}_i \in X$. For certain objects it might not be obvious at all on how to represent the data as a fixed length vector. Good examples of variable length data include textual documents and genomic data. For these types of data we can instead define a method of measuring similarity between object which does require them to be converted to a fixed length feature vector first [Mur12]. To do this we can begin by mapping the feature vectors into a Hilbert space H which provides us with an inner product $\langle \cdot, \cdot \rangle_H : H \times H \rightarrow \mathbb{R}$ and a norm $\| \cdot \|_H : H \rightarrow \mathbb{R}$. Input data is transformed into feature space vectors via a non-linear feature mapping $\Phi : X \rightarrow H$. The benefit of using a feature mapping in this way is that we can construct non-linear decision boundaries using linear models. In some instances a similarity measure can be computed directly using a function $k : X \times X$, instead of needing to construct a Φ and then computing the inner product of the transformed instances. We call such functions that act directly on our data instances kernel functions and using a kernel function 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 $k : X \times X \rightarrow \mathbb{R}$ is called a kernel on X if there exists a Hilbert space and a map $\Phi : X \rightarrow H$ such that for all $\mathbf{x}, \mathbf{x}' \in X$ we have $k(\mathbf{x}, \mathbf{x}') = \langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle_H$. 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 of little surprise then that neither the feature map nor the feature space are uniquely determined by the kernel. As a quick example from Ingo Steinwart and Andreas Christmann book *Support Vector Machines* [Ste08], let $X = \mathbb{R}$ and $k(x, x') = x \cdot x'$ where $x, x' \in X$. We can see that k is a kernel using the feature map $\Phi(x) \triangleq x$ and $H = \mathbb{R}$. However another suitable feature map for this particular kernel is $\Phi'(x) \triangleq (x/\sqrt{2}, x/\sqrt{2})$ 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 there 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. First, we shall need the following definition.

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

$$(1) \quad \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j k(\mathbf{x}_j, \mathbf{x}_i) \geq 0.$$

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

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

Definition 4 (Gram Matrix). For fixed $\mathbf{x}_1, \dots, \mathbf{x}_n \in X$ the matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ where $\mathbf{K}_{i,j} \triangleq k(\mathbf{x}_j, \mathbf{x}_i)$ 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 function is positive (semi) definite. If k is a real valued kernel corresponding to the feature map Φ , then k is symmetric by virtue of the fact that the inner product of a real Hilbert space is symmetric. Moreover k is positive definite since for $\alpha_1, \dots, \alpha_n \in \mathbb{R}$ and $\mathbf{x}_1, \dots, \mathbf{x}_n \in X$ we have

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

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 $k : K \times K \rightarrow \mathbb{R}$ is a kernel if and only if it is symmetric 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. We shall 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 $k : X \times X \rightarrow \mathbb{R}$ is called a reproducing kernel if we have $k(\cdot, \mathbf{x}) \in H$ for all $\mathbf{x} \in X$ and the reproducing property

$$f(\mathbf{x}) = \langle f, k(\cdot, \mathbf{x}) \rangle$$

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

- (2) The space H is called a reproducing kernel Hilbert space over X if for all $\mathbf{x} \in X$ the Dirac functional $\delta_{\mathbf{x}} : H \rightarrow \mathbb{R}$ defined by $\delta_{\mathbf{x}}(f) \triangleq f(\mathbf{x})$, $f \in H$ 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 $\|f_n - f\| \rightarrow 0$ we have $|\delta_{\mathbf{x}}(f_n) - \delta_{\mathbf{x}}(f)| = |f_n(\mathbf{x}) - f(\mathbf{x})| \rightarrow 0$. Note that because the evaluation function is both linear and continuous then it is also bounded in the sense that there is an $c \in \mathbb{R}$, $c > 0$ such that for every $f \in H$

and a fixed $\mathbf{x} \in X$ we have $|\delta_{\mathbf{x}}(f)| \leq c \|f\|_H$ [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 $\Phi : X \rightarrow H$ is given by*

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

for some $\mathbf{x} \in X$. 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

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

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

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

□

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 $k : X \times X \rightarrow \mathbb{R}$ defined by $k(\mathbf{x}', \mathbf{x}) = \langle \delta_{\mathbf{x}}, \delta_{\mathbf{x}'} \rangle_H$, $\mathbf{x}, \mathbf{x}' \in X$ 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 giving a one-to-one correspondence between kernels and RKHS. This is known as the Moore-Aronszajn theorem seen in theorem 9.

Theorem 9 (Moore-Aronszajn). *Suppose k is a symmetric 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. We shall now focus on a specific class of kernel that shall be used extensively in upcoming theory and experimentation.

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

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

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

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

[Ste08].

The Gaussian RBF kernel makes for a very simple an 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 $z, z' \in \mathbb{R}^d$ grows the corresponding measurement of similarity decays exponentially. A visual representation of this decay is shown in figure ??.

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]. Nonetheless, Gaussian RBF kernelis remains the one of the most widely used kernels in literature.

1.4. Kernel Machines.

1.4.1. *Introduction to Support Vector Machines for Binary Classification.* In this section, we shall look at two different machine learning models that make use of kernels to perform classification and regression. The first kernel machine we shall look at are support vector machines (SVM). SVMs where originally designed for binary classification and as such we shall only present a model for binary classification, 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 $D = \{(x_1, y_1), (x_1, y_1), \dots, (x_n, y_n)\}$. One simple method to classify samples is by creating an affine linear hyperplane satisfying

$$(2) \quad \begin{aligned} \langle w, x_i \rangle + b &> 0, & y_i &= +1 \\ \langle w, x_i \rangle + b &< 0, & y_i &= -1 \end{aligned}$$

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

$$f_D(x) \triangleq \text{sign}(\langle w_D, x \rangle + b_D).$$

There are, however, a number of short comings to this model. The most obvious is that our training data may not be linearly separable in \mathbb{R}^d meaning no such 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 therefore leaving it subject 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 we instead need to satisfy $y_i (\langle \mathbf{w}, \Phi(\mathbf{x}_i) \rangle + b) \geq 1 - \xi_i$ for some $\xi_i \in \mathbb{R}_{>0}$. These constraints can be re-written as

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

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

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

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 in the form

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

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

$$f_{(\mathbf{w}, b)} \triangleq \langle \mathbf{w}, \Phi(\mathbf{x}_i) \rangle + b.$$

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, often the Lagrange approach is used to solve the corresponding dual problem. When the hinge loss is used the dual problem becomes

$$\begin{aligned} & \max_{\alpha \in [0, C]^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y_i y_j \alpha_i \alpha_j \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle \\ (3) \quad & \text{subject to} \quad \sum_{i=1}^n y_i \alpha_i = 0 \end{aligned}$$

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 if the corresponding kernel trick described in section 1.1 is known for the feature map used so that 3 becomes

$$\begin{aligned} & \max_{\alpha \in [0, C]^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y_i y_j \alpha_i \alpha_j k(\mathbf{x}_i, \mathbf{x}_j) \\ & \text{subject to} \quad \sum_{i=1}^n y_i \alpha_i = 0. \end{aligned}$$

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 2 (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^* . This is a classic problem of time series prediction. What seems like a good prediction for the missing value at time x^* ? Perhaps something close to the red diamond seen in figure 2 (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 as the founding ideas behind

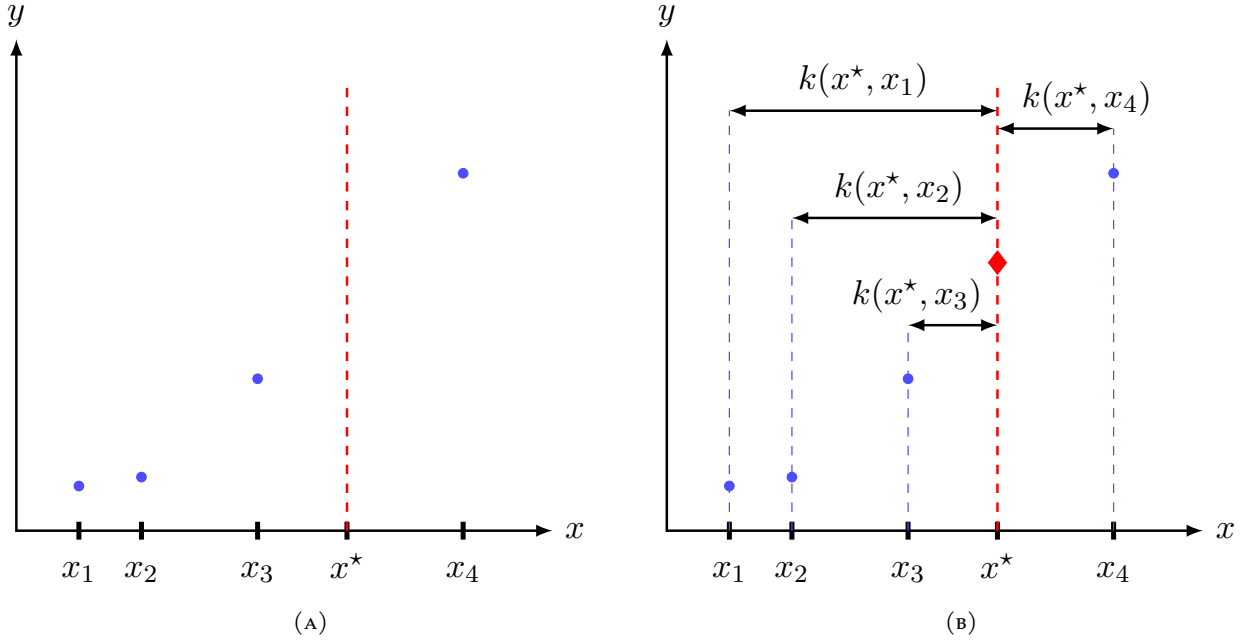


FIGURE 2. Panel (A) shows depicts the classical problem of time series prediction, guessing a value for x^* given values for surrounding times. Panel (B) shows a suitable choice for the value at time x^* with the reasoning that closely surrounding values should have greater influence over inference.

GPs, that is, training inputs that are more similar value we would like to make predictions for should have a greater influence over the prediction.

Similar to 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 motivating GP regression although we will see later on that GPs can be extended to perform binary classification and even multi-class classification. To begin, consider the following linear regression model

$$(4) \quad f(\mathbf{x}) \triangleq \langle \mathbf{w}, \mathbf{x} \rangle$$

where we are again assuming that \mathbf{x} belongs to \mathbb{R}^d and that $\mathbf{w} \in \mathbb{R}^d$ is a weight vector. Notice the striking resemblances to the linear classifier used to motivate SVMs, 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 $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ to a noisy version of f

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

where $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_n^2)$. 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

$$(5) \quad p(y | \mathbf{X}, \mathbf{w}) = \prod_{i=1}^n p(y_i | \mathbf{x}_i, \mathbf{w})$$

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

where $\mathbf{y} = [y_1, y_2, \dots, y_n]^\top \in \mathbb{R}^n$ and $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]^\top \in \mathbb{R}^{n \times d}$. 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

$$\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \Sigma_p)$$

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

$$p(\mathbf{w} \mid \mathbf{y}, \mathbf{X}) \propto p(\mathbf{y} \mid \mathbf{w}, \mathbf{X}) p(\mathbf{w}).$$

Equation 5 gives us a probability for $p(\mathbf{y} \mid \mathbf{w}, \mathbf{X})$ and since $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \Sigma_p)$ then

$$p(\mathbf{w}) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp\left(-\frac{1}{2} \mathbf{w}^\top \Sigma_p^{-1} \mathbf{w}\right)$$

[Kro14]. This means, up to proportionality

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

where $\bar{\mathbf{w}} \triangleq \sigma_n^{-2} (\sigma_n^{-2} \mathbf{X}^\top \mathbf{X} + \Sigma_p^{-1})^{-1} \mathbf{X}^\top \mathbf{y}$. Notice that this again is a multivariate Gaussian distribution with mean $\bar{\mathbf{w}}$ and covariance \mathbf{A}^{-1} where $\mathbf{A} \triangleq \sigma_n^{-2} \mathbf{X}^\top \mathbf{X} + \Sigma_p^{-1}$ so that

$$p(\mathbf{w} \mid \mathbf{X}, \mathbf{y}) \sim \mathcal{N}(\mathbf{w}, \mathbf{A}^{-1})$$

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

$$p(f^* \mid \mathbf{x}^*, \mathbf{X}, \mathbf{y}) = \int_{\mathbb{R}^d} p(f^* \mid \mathbf{x}^*, \mathbf{w}) p(\mathbf{w} \mid \mathbf{X}, \mathbf{y}) d\mathbf{w} = \mathcal{N}(\mathbf{x}^{*\top} \bar{\mathbf{w}}, \mathbf{x}^{*\top} \mathbf{A}^{-1} \mathbf{x}^*).$$

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 use 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.

$$f(\mathbf{x}) \triangleq \langle \mathbf{w}, \Phi(\mathbf{x}) \rangle.$$

The derivation for the new model is identical with the only difference being that \mathbf{x}^* is replaced with $\Phi(\mathbf{x}^*)$ and \mathbf{X} is replaced with $\Phi(\mathbf{X}) \triangleq [\Phi(\mathbf{x}_1), \Phi(\mathbf{x}_2), \dots, \Phi(\mathbf{x}_n)]^\top \in \mathbb{R}^{n \times N}$ where N is the dimension of the Hilbert space. The new predictive distribution becomes

$$(6) \quad f^* | \mathbf{x}^*, \mathbf{X}, \mathbf{y} \sim \mathcal{N} \left(\frac{1}{\sigma_n^2} \Phi(\mathbf{x}^*)^\top \mathbf{A}^{-1} \Phi(\mathbf{X})^\top \mathbf{y}, \Phi(\mathbf{x}^*)^\top \mathbf{A}^{-1} \Phi(\mathbf{x}^*) \right)$$

where \mathbf{A} is now $\mathbf{A} \triangleq \frac{1}{\sigma_n^2} \Phi(\mathbf{X})^\top \Phi(\mathbf{X}) + \Sigma_p^{-1} \in \mathbb{R}^{N \times N}$. From this, it becomes evident that the inverse of \mathbf{A} is required to compute both the mean and the covariance. This is not favourable since this would require knowledge of the Hilbert space into which the feature map send inputs. Moreover, computing \mathbf{A}^{-1} may become impractical in the dimension of the Hilbert space is incredibly large. Remember, the whole point of the kernel trick is to avoid any computation that involves direct knowledge of H and to instead 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 the will enable us to apply the kernel trick. To start we can find a suitable expression for the mean. First define the notation

$$\mathbf{K}_{\mathbf{W}\mathbf{W}'} \triangleq \Phi(\mathbf{W}) \Sigma_p \Phi(\mathbf{W}')^\top \in \mathbb{R}^{n \times n'}$$

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

$$\begin{aligned} & \mathbf{A} \Sigma_p \Phi(\mathbf{X})^\top \\ &= (\sigma_n^{-2} \Phi(\mathbf{X})^\top \Phi(\mathbf{X}) + \Sigma_p^{-1}) \Sigma_p \Phi(\mathbf{X})^\top \\ &= \sigma_n^{-2} \Phi(\mathbf{X})^\top \Phi(\mathbf{X}) \Sigma_p \Phi(\mathbf{X})^\top + \Phi(\mathbf{X})^\top \\ &= \sigma_n^{-2} \Phi(\mathbf{X})^\top (\Phi(\mathbf{X}) \Sigma_p \Phi(\mathbf{X})^\top + \sigma_n^2 \mathbb{1}_{n \times n}) \\ &= \sigma_n^{-2} \Phi(\mathbf{X})^\top (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}) \end{aligned}$$

meaning

$$\begin{aligned} \sigma_n^{-2} \Phi(\mathbf{X})^\top (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}) &= \mathbf{A} \Sigma_p \Phi(\mathbf{X})^\top \\ \sigma_n^{-2} \mathbf{A}^{-1} \Phi(\mathbf{X})^\top (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}) &= \Sigma_p \Phi(\mathbf{X})^\top \\ \sigma_n^{-2} \mathbf{A}^{-1} \Phi(\mathbf{X})^\top &= \Sigma_p \Phi(\mathbf{X})^\top (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})^{-1} \end{aligned}$$

so that the current mean of

$$\frac{1}{\sigma_n^2} \Phi(\mathbf{x}^*)^\top \mathbf{A}^{-1} \Phi(\mathbf{X})^\top \mathbf{y}$$

in equation 6 can be replaced with

$$\Phi(\mathbf{x}^*)^\top \Sigma_p \Phi(\mathbf{X})^\top (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})^{-1} \mathbf{y}.$$

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 $\mathbf{Z} \in \mathbb{K}^{n \times m}$, $\mathbf{W} \in \mathbb{K}^{m \times m}$ and $\mathbf{U}, \mathbf{V} \in \mathbb{K}^{n \times m}$ then

$$(\mathbf{Z} + \mathbf{U}\mathbf{W}\mathbf{V}^\top)^{-1} = \mathbf{Z}^{-1} - \mathbf{Z}^{-1}\mathbf{U}(\mathbf{W}^{-1} + \mathbf{V}^\top\mathbf{Z}^{-1}\mathbf{U})^{-1}\mathbf{V}^\top\mathbf{Z}^{-1}$$

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

Consider

$$(7) \quad \mathbf{A} = \Sigma_p^{-1} + \Phi(\mathbf{X})^\top (\sigma_n^{-2} \mathbb{1}_{n \times n}) \Phi(\mathbf{X})$$

then setting $\mathbf{Z}^{-1} = \Sigma_p$, $\mathbf{W}^{-1} = \sigma_n^2 \mathbb{1}_{n \times n}$ and $\mathbf{V} = \mathbf{U} = \Phi(\mathbf{X})$ then equation 7 becomes

$$\Sigma_p - \Sigma_p \Phi(\mathbf{X})^\top (\sigma_n^2 \mathbb{1}_{n \times n} + \Phi(\mathbf{X}) \Sigma_p \Phi(\mathbf{X})^\top)^{-1} \Phi(\mathbf{X}) \Sigma_p$$

via the matrix inversion lemma. Thus equation 6 can be equivalently formulated as

$$(8) \quad f^* | \mathbf{x}^*, \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\Phi(\mathbf{x}^*)^\top \Sigma_p \Phi(\mathbf{X})^\top (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})^{-1} \mathbf{y}, \\ \Phi(\mathbf{x}^*)^\top \Sigma_p \Phi(\mathbf{x}^*) - \Phi(\mathbf{x}^*)^\top \Sigma_p \Phi(\mathbf{X})^\top (\sigma_n^2 \mathbb{1}_{n \times n} + \Phi(\mathbf{X}) \Sigma_p \Phi(\mathbf{X})^\top)^{-1} \Phi(\mathbf{X}) \Sigma_p \Phi(\mathbf{x}^*))$$

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

$$(9) \quad f^* | \mathbf{x}^*, \mathbf{X}, \mathbf{y} \sim \mathcal{N}(\mathbf{K}_{\mathbf{x}^*\mathbf{X}} (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})^{-1} \mathbf{y}, \mathbf{K}_{\mathbf{x}^*\mathbf{x}^*} - \mathbf{K}_{\mathbf{x}^*\mathbf{X}} (\sigma_n^2 \mathbb{1}_{n \times n} + \mathbf{K}_{\mathbf{X}\mathbf{X}})^{-1} \mathbf{K}_{\mathbf{X}\mathbf{x}^*})$$

. To get a better idea of the connection to kernels, since Σ_p is a symmetric positive semi definite matrix, it defines an inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_{\Sigma_p} = \mathbf{y}^* \Sigma_p \mathbf{x}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{K}^N$$

[Wan][page 34] so that

$$(10) \quad (\mathbf{K}_{\mathbf{W}\mathbf{W}'})_{ij} = \langle \Phi(\mathbf{w}_i), \Phi(\mathbf{w}_j) \rangle_{\Sigma_p} = k(\mathbf{w}_i, \mathbf{w}_j)$$

where k is the kernel with feature map Φ and inner product $\langle \cdot, \cdot \rangle_{\Sigma_p}$. In fact when $\mathbf{W} = \mathbf{W}'$ 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 using observed values.

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 $p(f | D)$ instead of a vector of parameteric values $p(\theta | D)$. 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 we choose a suitable f by 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 evaluate 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 characterised by a mean function $m(\mathbf{x})$ and a kernel, which in the context of GPs is sometimes called a covariance function, $k(\mathbf{x}, \mathbf{x}')$ on a real process as

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

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 function 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 $m(\mathbf{x}) = 0$. A function $f(\mathbf{x})$ sampled from a GP with mean $m(\mathbf{x})$ and covariance $k(\mathbf{x}, \mathbf{x}')$ is written as

$$f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$$

Since a GP is a collection of random variables it must satisfy the consistency requirement, that is, an observation of a set of variables should not the distribution of any small sub set of the observed values. More specifically if

$$(\mathbf{y}_1, \mathbf{y}_2) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

then

$$\begin{aligned} \mathbf{y}_1 &\sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{1,1}) \\ \mathbf{y}_2 &\sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_{2,2}) \end{aligned}$$

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

$$(\mathbf{K}_{\mathbf{W}\mathbf{W}'})_{i,j} \triangleq k(\mathbf{w}_i, \mathbf{w}'_j)$$

where $\mathbf{K}_{\mathbf{W}\mathbf{W}'} \in \mathbb{R}^{n \times n'}$. The covariance function completely characterized by its kernel. Unless otherwise stated, the kernel or covariance function used in examples and experimentation in the Gaussian RBF kernel, definition 10. To understand this better, as a small exercise we can select a number of inputs $\mathbf{X}^* = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n^*}]^\top \in \mathbb{R}^{n^* \times d}$ of compute the corresponding covariance matrix using the Gaussian RBF kernel. Gaussian vectors can then be sampled using a joint Gaussian distribution using the covariance matrix from the distribution

$$\mathbf{f}^* \sim \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathbf{X}^* \mathbf{X}^*})$$

graph its values as a function of its inputs.

Figure 3 (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 3 (A) represents twice the standard deviation about the mean.

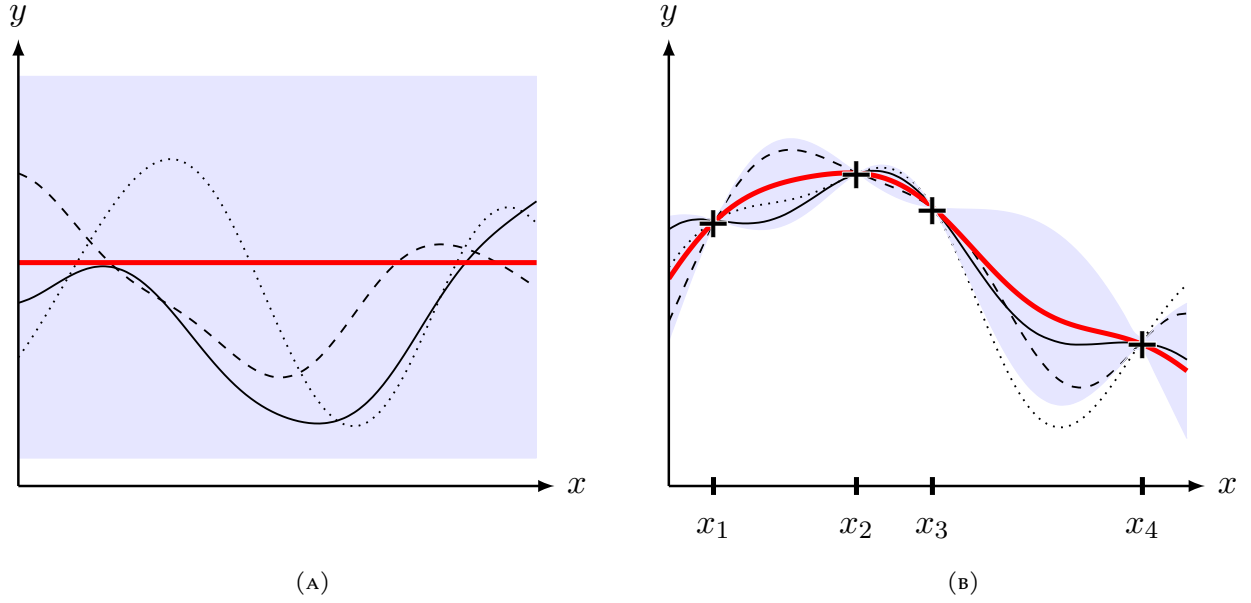


FIGURE 3. Panel (A) shows three function drawn from the prior distribution. Panel (B) shows three function drawn from the prior distribution after four observations have been made. In both panels the mean function is drawn in red, sampled functions in black and twice the standard deviation shaded in light blue.

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 observed data $D = \{(\mathbf{x}_i, \mathbf{f}_i) \mid i \in \{1, 2, \dots, n\}\}$ 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

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

We would then like to make a prediction for unobserved values say $\mathbf{X}^* = [\mathbf{x}_1^*, \mathbf{x}_2^*, \dots, \mathbf{x}_{n_*}^*]$ with value \mathbf{f}_* as has a distribution of

$$\mathbf{f}_* \sim \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathbf{X}^*\mathbf{X}^*}).$$

where $\mathbf{K}_{\mathbf{X}^*\mathbf{X}^*} = k(\mathbf{X}^*, \mathbf{X}^*) \in \mathbb{R}^{n_* \times n_*}$. Here \mathbf{f} and \mathbf{f}_* 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 \mathbf{f} and the test points \mathbf{f}_* as

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K}_{\mathbf{X}\mathbf{X}} & \mathbf{K}_{\mathbf{X}\mathbf{X}^*} \\ \mathbf{K}_{\mathbf{X}^*\mathbf{X}}^\top & \mathbf{K}_{\mathbf{X}^*\mathbf{X}^*} \end{bmatrix}\right)$$

where $\mathbf{K}_{\mathbf{X}\mathbf{X}^*} = k(\mathbf{X}, \mathbf{X}^*) \in \mathbb{R}^{n \times n_*}$.

While the above does give us some information on \mathbf{f}_* is related to the observed data and the test inputs, it does not provide any method to evaluate \mathbf{f}_* . To do this we shall need the assistance of the following lemma

Theorem 13. (Marginals and conditionals of an MVN [Mur12]) Suppose $\mathbf{x} = (x_1, x_2)$ is jointly Gaussian with parameters

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_{1,1} & \Sigma_{1,2} \\ \Sigma_{2,1} & \Sigma_{2,2} \end{bmatrix}$$

then the posterior conditional is given by

$$\begin{aligned} x_2 \mid x_1 &\sim \mathcal{N}(x_2 \mid \mu_{2|1}, \Sigma_{2|1}) \\ \mu_{2|1} &= \mu_2 + \Sigma_{2,1} \Sigma_{1,1}^{-1} (x_1 - \mu_1) \\ \Sigma_{2|1} &= \Sigma_{2,2} - \Sigma_{2,1} \Sigma_{1,1}^{-1} \Sigma_{1,2} \end{aligned}$$

Thus finding a mean and covariance for \mathbf{f}_\star requires a direct application of Theorem 13 which gives

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

where

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

and

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

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

$$(11) \quad \mathbf{f}_\star \mid \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}, \mathbf{K}_{\mathbf{X}\mathbf{X}}, \mathbf{f} \sim \mathcal{N}(\mathbf{K}_{\mathbf{X}\mathbf{X}^\star}^\top \mathbf{K}_{\mathbf{X}\mathbf{X}}^{-1} \mathbf{f}, \mathbf{K}_{\mathbf{X}^\star\mathbf{X}^\star} - \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}^\top \mathbf{K}_{\mathbf{X}\mathbf{X}}^{-1} \mathbf{K}_{\mathbf{X}\mathbf{X}^\star})$$

Function values from the unobserved inputs \mathbf{X}^\star , that is \mathbf{f}_\star , can be estimated using the joint posterior distribution by evaluating the mean of 11. Figure 3 (B) shows these computations given a data set $D = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)\}$. Notice that the variance tightens around the observed values since (assuming no noise in our data is present) we know for certain this is how our target function should behave at x_1, x_2, x_3 and x_4 . 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, $y = f(\mathbf{x}) + \varepsilon$ where $\varepsilon \sim \mathcal{N}(0, \sigma_n^2)$ meaning the prior on the noisy values becomes

$$\text{cov}(\mathbf{y}) = \mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbf{I}$$

The reason why noise is only added along the diagonal follows from the assumption of independence 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

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

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

$$(12) \quad \mathbf{f}_\star \mid \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}, \mathbf{K}_{\mathbf{X}\mathbf{X}}, \mathbf{y} \sim \mathcal{N}(\bar{\mathbf{f}}_\star, \text{cov}(\mathbf{f}_\star))$$

where

$$(13) \quad \bar{\mathbf{f}}_\star \triangleq \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}^\top [\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}]^{-1} \mathbf{y}$$

$$(14) \quad \text{cov}(\mathbf{f}_\star) = \mathbf{K}_{\mathbf{X}^\star \mathbf{X}^\star} - \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}^\top [\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}]^{-1} \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}$$

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, sometimes 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 \mathbf{x}^\star

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

where $\alpha = [\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}]^{-1} \mathbf{y}$. Intuitively, this expression can be understood by realising that despite defining the GP defining a joint Gaussian distribution over the observations when making predictions GPs only require the $(n + 1)$ -dimension distribution defined by the n observations and the single test point. Marginalising by taking the relevant submatrix block of the covariance matrix yields 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, $\mathbf{K}_{\mathbf{X}^\star \mathbf{X}^\star}$, and positive term $\mathbf{K}_{\mathbf{X}\mathbf{X}^\star}^\top [\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}]^{-1} \mathbf{K}_{\mathbf{X}\mathbf{X}^\star}$ 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 \mathbf{X}, \mathbf{y} and a test input \mathbf{x}^\star .

output: A prediction $\bar{\mathbf{f}}_\star$ with its corresponding variance $\mathbb{V}[\mathbf{f}_\star]$.

$\mathbf{L} = \text{cholesky}(\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})$

$\alpha = \text{lin-solve}(\mathbf{L}^\top, \text{lin-solve}(\mathbf{L}, \mathbf{y}))$

$\bar{\mathbf{f}}_\star = \mathbf{K}_{\mathbf{x}^\star \mathbf{X}} \alpha$

$\mathbf{v} = \text{lin-solve}(\mathbf{L}, \mathbf{K}_{\mathbf{x}^\star \mathbf{X}})$

$\mathbb{V}[\mathbf{f}_\star] = \mathbf{K}_{\mathbf{x}^\star \mathbf{x}^\star} - \mathbf{v}^\top \mathbf{v}$

return $\bar{\mathbf{f}}_\star, \mathbb{V}[\mathbf{f}_\star]$

A cholesky decomposition is typically used since \mathbf{L} can be used twice to assist in solving both the linear systems in the mean and covariance. Unfortunately, a cholesky decomposition incurs a runtime of $\mathcal{O}(n^3)$ 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 classifications model, the Gaussian processes classifier (GPC) seeks an estimate for the joint probability $p(y, \mathbf{x})$ where $\mathbf{x} \in \mathbb{R}^d$ 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 $p(y) p(\mathbf{x} | y)$ or $p(\mathbf{x}) p(y | \mathbf{x})$ giving rise to the *generative* and *discriminative* approaches respectively [Ras06, page 34]. The generative approach models the prior probabilities of each class, $p(\mathcal{C}_i)$, as well as the class conditional probabilities for each input $p(\mathbf{x} | \mathcal{C}_i)$ and computes the posterior as

$$p(y | \mathbf{x}) = \frac{p(y) p(\mathbf{x} | y)}{\sum_{i=1}^C p(\mathcal{C}_i) p(\mathbf{x} | \mathcal{C}_i)}.$$

On the other hand, the discriminative method focuses on modelling $p(y | \mathbf{x})$ directly. With both these paradigms at our disposal, which one should we prefer 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 want, that is $p(y | \mathbf{x})$. Also the density estimation of $p(\mathbf{x} | \mathcal{C}_i)$ 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 may mean we are trying to solve a harder problem than what we need to. 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 simplest 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 \mathbf{x} to a class of either -1 or $+1$. For a linear model likelihood can be formulated as

$$(15) \quad p(y = +1 | \mathbf{x}, \mathbf{w}) = \sigma(\langle \mathbf{x}, \mathbf{w} \rangle)$$

given a weight vector \mathbf{w} and where $\sigma(z)$ 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

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

will take the role of the sigmoid function in equation 15, graphed in Figure 4. 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

$$p(y | \mathbf{x}, \mathbf{w}) = \sigma(\langle \mathbf{x}, \mathbf{w} \rangle)^y (1 - \sigma(\langle \mathbf{x}, \mathbf{w} \rangle))^{1-y}$$

which for symmetric likelihood functions can be written more concisely as

$$p(y_i | \mathbf{x}_i, \mathbf{w}) = \sigma(y_i f_i)$$

where

$$(17) \quad f_i \triangleq f(\mathbf{x}_i) = \langle \mathbf{x}_i, \mathbf{w} \rangle.$$

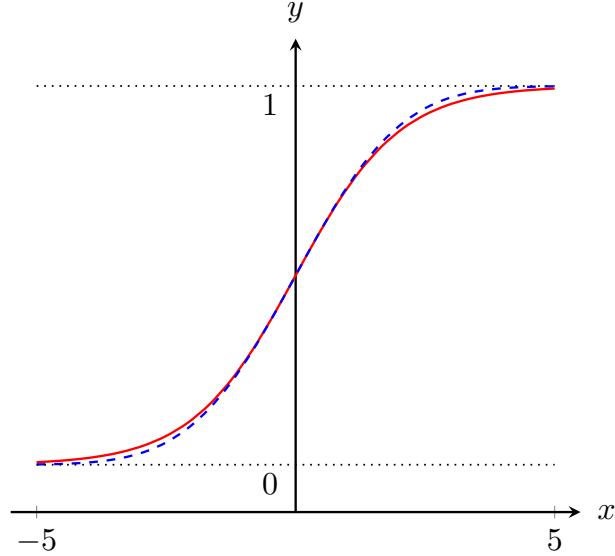


FIGURE 4. The logistic function from equation 16 (solid red) juxtaposed with a close approximation, the scaled probit function (dashed blue).

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

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

where logit is commonly referred to as the logit transformation. For a given dataset $\mathcal{D} = (\mathbf{X}, \mathbf{y})$ where $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]^\top \in \mathbb{R}^{n \times d}$ and $\mathbf{y} = [y_1, y_2, \dots, y_n]^\top \in \{-1, +1\}^n$ we assume each observation is independently generated conditioned over $f(\mathbf{x})$. Similar to GPR, a Gaussian prior is used for the weights so that $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \sigma_p)$ giving an un-normalised log posterior of

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

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. However, when using the logistic function it is easy enough to show that the log likelihood is concave as a function of \mathbf{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].

The idea behind Gaussian process classification for binary classes is that a Gaussian process regression model is placed over a latent function $f(\mathbf{x})$ with the output being "squashed" through a sigmoid function to obtain a prior on

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

This construction is illustrated in Figure 5 and provides a natural extension to the linear logistic regression model.

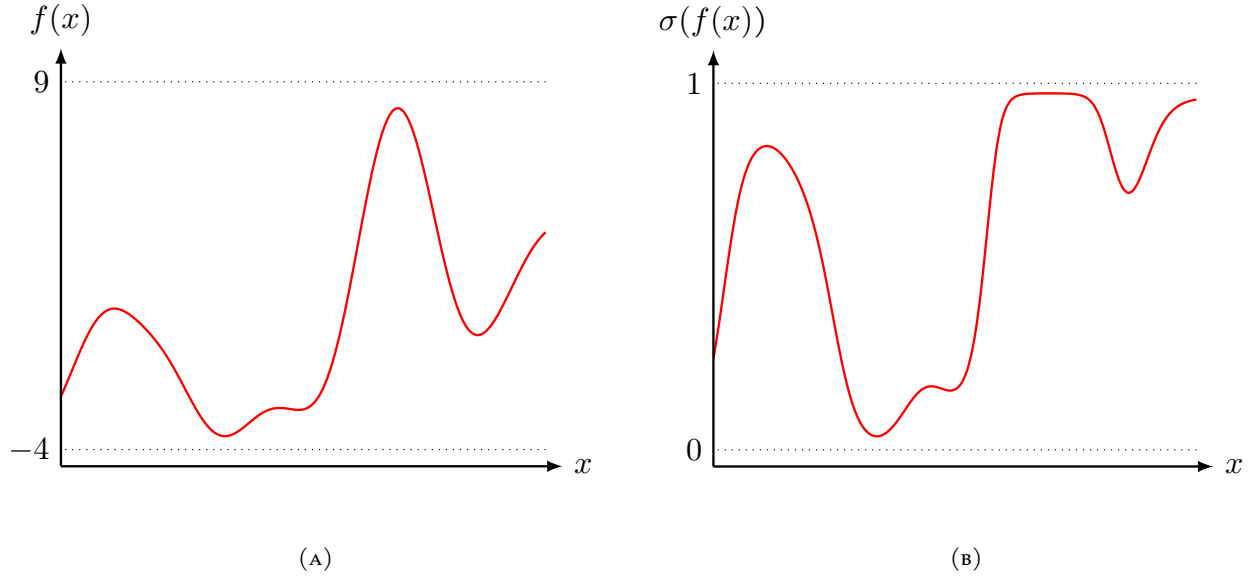


FIGURE 5. The latent function f , panel (A), is transformed using a sigmoid function, panel (B), to provide a probabilistic interpretation of x belonging to the class +1.

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

$$p\left(\begin{bmatrix} \mathbf{f} \\ f_{\star} \end{bmatrix}\right) = \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K}_{XX} & \mathbf{K}_{Xx_{\star}} \\ \mathbf{K}_{Xx_{\star}}^{\top} & k(x_{\star}, x_{\star}) \end{bmatrix}\right)$$

where $f_{\star} = f(x_{\star})$ and $\mathbf{f} = f(\mathbf{X})$. 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, neither are value of f ever 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. Remember the ultimate goal is to make predictions for π , not f , and that the goal of the coming sections will be to eventually integrate our f .

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

$$(18) \quad \overline{\pi}_{\star} \triangleq p(y_{\star} = +1 \mid \mathbf{X}, \mathbf{y}, x_{\star}) = \int \sigma(f_{\star}) p(f_{\star} \mid \mathbf{X}, \mathbf{y}, x_{\star}) df_{\star}$$

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 instead come up with a good approximation for $\overline{\pi}_{\star}$.

1.6.2. Laplace 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,

$p(f_\star | \mathbf{X}, \mathbf{y}, \mathbf{x}_\star)$, can be numerically approximated to provide a numerically tractable succedaneum. Using Baye's theorem

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

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

$$p(f_\star | \mathbf{X}, \mathbf{x}_\star, \mathbf{f}) = \mathcal{N}(f_\star | \mathbf{K}_{\mathbf{X}\mathbf{x}_\star}^\top \mathbf{K}_{\mathbf{X}\mathbf{X}}^{-1} \mathbf{y}, k(\mathbf{x}_\star, \mathbf{x}_\star) - \mathbf{K}_{\mathbf{X}\mathbf{x}_\star}^\top \mathbf{K}_{\mathbf{X}\mathbf{X}}^{-1} \mathbf{K}_{\mathbf{X}\mathbf{x}_\star})$$

through the use of equation 13 and 14. Unfortunately

$$p(\mathbf{f} | \mathbf{X}, \mathbf{y}) = \frac{p(\mathbf{y} | \mathbf{f}) p(\mathbf{f} | \mathbf{X})}{p(\mathbf{y} | \mathbf{X})}$$

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

$$p(\mathbf{z}) = \frac{1}{c} q(\mathbf{z})$$

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

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

which can be computed by solving

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

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 is a quadratic function of its inputs. Taking the Taylor series expansion of $\ln q(\mathbf{z})$ centered at \mathbf{z}_0 yields

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

where

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

Exponentiating both sides gives

$$\begin{aligned} f(\mathbf{z}) &\simeq f(\mathbf{z}_0) \exp\left(-\frac{1}{2} (\mathbf{z} - \mathbf{z}_0)^\top \mathbf{A} (\mathbf{z} - \mathbf{z}_0)\right) \\ (20) \quad &\propto \mathcal{N}(\mathbf{z} | \mathbf{z}_0, \mathbf{A}^{-1}). \end{aligned}$$

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

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

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

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

The gradient and Hessian of the unnormalized posterior then become

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

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

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

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

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

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

$$(22) \quad p(\mathbf{f} | \mathbf{X}, \mathbf{y}) \simeq q(\mathbf{f} | \mathbf{X}, \mathbf{y}) = \mathcal{N}(\hat{\mathbf{f}}, (\mathbf{K}_{\mathbf{X}\mathbf{X}}^{-1} + \mathbf{W})^{-1}).$$

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

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

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

$$(24) \quad \sigma_{f_\star}^2 = \mathbb{V}[f_\star | \mathbf{X}, \mathbf{y}, \mathbf{x}_\star] = k(\mathbf{x}_\star, \mathbf{x}_\star) - \mathbf{K}_{\mathbf{x}_\star \mathbf{X}} (\mathbf{K}_{\mathbf{X}\mathbf{X}} + \mathbf{W}^{-1})^{-1} \mathbf{K}_{\mathbf{x}_\star \mathbf{X}}^\top.$$

Using equation 18, predictions can now be made as

$$(25) \quad \overline{\pi}_\star \simeq \int \sigma(f_\star) q(f_\star | \mathbf{X}, \mathbf{y}, \mathbf{x}_\star) df_\star$$

where $q(f_\star | \mathbf{X}, \mathbf{y}, \mathbf{x}_\star)$ 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 4. 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

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

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

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

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

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

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

Algorithm 2: Unoptimized GPC

input : Observations \mathbf{X} , \mathbf{y} and a test input \mathbf{x}^* .

output: A prediction \overline{f}_* with its corresponding variance $\mathbb{V}[f_*]$.

$\mathbf{t} = (\mathbf{y} + \mathbf{1}) / 2$

$\mathbf{f} = \mathbf{0}$

repeat

$\mathbf{W} = \text{diag}(\sigma(\mathbf{y} \cdot^* \mathbf{f}))$

$\boldsymbol{\alpha} = \text{lin-solve}(\mathbb{1}_{n \times n} + \mathbf{W} \mathbf{K}_{\mathbf{X}\mathbf{X}}, \mathbf{K}_{\mathbf{X}\mathbf{X}})$

$\mathbf{f} = \boldsymbol{\alpha}(\mathbf{t} - \sigma(\mathbf{f}) + \mathbf{W} \mathbf{f})$

until *convergence*

$\mu_{f_*} = \mathbf{K}_{\mathbf{x}_* \mathbf{X}}(\mathbf{t} - \sigma(\mathbf{f}))$

$\sigma_{f_*}^2 = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{K}_{\mathbf{x}_* \mathbf{X}}(\mathbf{K}_{\mathbf{X}\mathbf{X}} + \mathbf{W}^{-1})^{-1} \mathbf{K}_{\mathbf{x}_* \mathbf{X}}^\top$

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

return $\overline{\pi}_*, \mu_{f_*}, \sigma_{f_*}^2$

2. RANDOM FOURIER FEATURES

As seen in section 1 GPs rely heavily on the Gram matrix (see definition 4) to create predictions based on training data $\mathcal{D} = (\mathbf{X}, \mathbf{y})$ where $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]^\top \in \mathbb{R}^{n \times d}$ and $\mathbf{y} = [y_1, y_2, \dots, y_n]^\top \in \mathbb{R}^n$. Unfortunately, the size of the Gram matrix scales quadratically with the number of samples making it difficult to train using data sets with more than 10^5 samples. Instead the kernel function itself can be factorized allowing one to convert training and kernel evaluation into the corresponding operations of a linear machine by mapping data into a relatively low-dimensional randomized feature space. This idea was first introduced by Rahimi and Recht [Rah08] where they proposed that, instead of using a kernel function to implicitly lift data into a higher dimensional feature space, an explicit feature map $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}^D$ could be used to approximate k as $k(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle_{\mathbb{R}^N} \simeq \langle \varphi(\mathbf{x}), \varphi(\mathbf{y}) \rangle_{\mathbb{R}^D}$ where D is chosen so that $n \gg D$. Thus once $\varphi(\mathbf{x}_i)$ has been computed for each \mathbf{x}_i , every entry of the Gram matrix can be swiftly approximated as

$$\mathbf{K}_{ij} = \mathbf{K}_{ji} \simeq \langle \varphi(\mathbf{x}_i), \varphi(\mathbf{y}_j) \rangle_{\mathbb{R}^D}.$$

Already there have been numerous applications of this technique in GPs that have seen improved time performance with little loss in prediction accuracy [Pot21].

2.1. Theory and Computation. Contrary to the kernel trick, the Random Fourier Features (RFF) technique approximates $\langle \Phi(\cdot), \Phi(\cdot) \rangle_{\mathbb{R}^N}$ through an explicit feature mapping φ . The RFF technique hinges on Bochners theorem, stated without proof in theorem 15, which characterises positive definite functions.

Theorem 15 (Bochner's). *A continuous and shift-invariant function $k(\mathbf{x}, \mathbf{y}) = k(\mathbf{x} - \mathbf{y}) = k(\Delta)$ is positive definite (see definition 2) if and only if it can be represented as*

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

where μ_k is a positive finite measure on the frequencies of $\boldsymbol{\omega}$ [Hah33, Liu21].

The spectral distribution μ_k can be represented as finite measure induced by the Fourier transformation. Choosing a kernel for which $k(\mathbf{0}) = 1$ normalizes μ_k to a probability distribution $p(\cdot)$. For instance, the spectral distribution of the Gaussian RBF kernel is

$$(28) \quad p(\mathbf{w}) = \frac{1}{\sqrt{(2\pi)^D \left| \frac{\sigma^2}{2} \mathbb{1}_{D \times D} \right|}} \exp \left(-\frac{1}{2} \mathbf{w}^\top \left(\frac{\sigma^2}{2} \mathbb{1}_{D \times D} \right)^{-1} \mathbf{w} \right)$$

[Rah08, page 3]. One caveat in Bochner's theorem is that it requires our kernel to be shift-invariant (sometimes also referred to as stationary) as stated in definition 16.

Definition 16 (Shift-Invariant). *A kernel $k : \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{C}$ is called shift-invariant if $k(\mathbf{x}, \mathbf{y}) = g(\mathbf{x} - \mathbf{y})$ for some positive definite function $g : \mathbb{R}^N \rightarrow \mathbb{C}$ [HAe16, page 3].*

Clearly, the Gaussian RBF kernel is shift-invariant since it only relies on the bounding radius of \mathbf{x} and \mathbf{y} . Thus, from Bochner's theorem, a positive definite shift-invariant kernel with $k(\mathbf{0}) = 1$ can be computed

as

$$(29) \quad k(\mathbf{x} - \mathbf{y}) = \int_{\mathbb{C}^d} \exp(i\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle) p(\boldsymbol{\omega}) d\boldsymbol{\omega}.$$

The main idea of RFF is to approximate the integral in 29 using the following Monte-Carlo estimate

$$\begin{aligned} k(\mathbf{x} - \mathbf{y}) &= \int_{\mathbb{C}^d} \exp(i\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle) p(\boldsymbol{\omega}) d\boldsymbol{\omega} \\ &= \mathbb{E}_{\boldsymbol{\omega} \sim p(\cdot)} (\exp(i\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle)) \\ &\simeq \frac{1}{D} \sum_{j=1}^D \exp(i\langle \boldsymbol{\omega}_j, \mathbf{x} - \mathbf{y} \rangle) \\ &= \sum_{j=1}^D \left(\frac{1}{\sqrt{D}} \exp(i\langle \boldsymbol{\omega}_j, \mathbf{x} \rangle) \right) \overline{\left(\frac{1}{\sqrt{D}} \exp(i\langle \boldsymbol{\omega}_j, \mathbf{y} \rangle) \right)} \\ &= \langle \boldsymbol{\varphi}(\mathbf{x}), \boldsymbol{\varphi}(\mathbf{y}) \rangle_{\mathbb{C}^D} \end{aligned}$$

where $\boldsymbol{\omega}_i \stackrel{\text{iid}}{\sim} p(\cdot)$ using the feature map

$$(30) \quad \boldsymbol{\varphi}(\mathbf{x}) = \frac{1}{\sqrt{D}} [z(\boldsymbol{\omega}_1, \mathbf{x}), z(\boldsymbol{\omega}_2, \mathbf{x}), \dots, z(\boldsymbol{\omega}_D, \mathbf{x})]^\top$$

where for convenience of notation $z(\boldsymbol{\omega}, \mathbf{x}) = \exp(i\langle \boldsymbol{\omega}, \mathbf{x} \rangle)$. This allows the Gram matrix to be estimated as $\mathbf{K} \simeq \widetilde{\mathbf{K}} = \mathbf{Z}\mathbf{Z}^\top$ where $\mathbf{Z} = [\boldsymbol{\varphi}(\mathbf{x}_1), \boldsymbol{\varphi}(\mathbf{x}_2), \dots, \boldsymbol{\varphi}(\mathbf{x}_D)] \in \mathbb{C}^{n \times D}$ [Rah08, Liu21, HAe16]. To simplify computation in most settings both $p(\cdot)$ and $k(\Delta)$ are real valued functions meaning $\exp(i\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle)$ can be replaced with its real component $\cos(\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle)$. The vast majority of literature uses the embeddings Rahimi and Recht provide for $\cos(\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle)$ where $z(\boldsymbol{\omega}, \mathbf{x})$ satisfies equation 29. The first embedding takes the form

$$(31) \quad z(\boldsymbol{\omega}, \mathbf{x}) = [\cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle), \sin(\langle \boldsymbol{\omega}, \mathbf{x} \rangle)]^\top$$

which satisfies 29 since

$$\begin{aligned} &z(\boldsymbol{\omega}, \mathbf{x})^\top z(\boldsymbol{\omega}, \mathbf{y}) \\ &= [\cos(\langle \boldsymbol{\omega}, \mathbf{y} \rangle), \sin(\langle \boldsymbol{\omega}, \mathbf{y} \rangle)] \begin{bmatrix} \cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle) \\ \sin(\langle \boldsymbol{\omega}, \mathbf{x} \rangle) \end{bmatrix} \\ &= \cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle) \cos(\langle \boldsymbol{\omega}, \mathbf{y} \rangle) + \sin(\langle \boldsymbol{\omega}, \mathbf{x} \rangle) \sin(\langle \boldsymbol{\omega}, \mathbf{y} \rangle) \\ &= \frac{1}{2} (\cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle + \langle \boldsymbol{\omega}, \mathbf{y} \rangle) + \cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle - \langle \boldsymbol{\omega}, \mathbf{y} \rangle)) + \\ &\quad \frac{1}{2} (\cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle - \langle \boldsymbol{\omega}, \mathbf{y} \rangle) - \cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle + \langle \boldsymbol{\omega}, \mathbf{y} \rangle)) \\ &= \cos(\langle \boldsymbol{\omega}, \mathbf{x} - \mathbf{y} \rangle). \end{aligned}$$

The other embedding Rahimi and Recht give is

$$(32) \quad z(\boldsymbol{\omega}, \mathbf{x}) = \sqrt{2} \cos(\langle \boldsymbol{\omega}, \mathbf{x} \rangle + b)$$

where $b \sim U[0, 2\pi]$. Using a similar argument we can show that this embedding also satisfies 29. However, Sutherland and Schneider [DJSaJS15] argue that the Gaussian RBF kernel is better suited for the

embedding given in 31. To summarise their argument we denote

$$(33) \quad \varphi_1(\mathbf{x}) = \sqrt{\frac{2}{D}} \begin{bmatrix} \cos(\langle \boldsymbol{\omega}_1, \mathbf{x} \rangle) \\ \cos(\langle \boldsymbol{\omega}_2, \mathbf{x} \rangle) \\ \vdots \\ \cos(\langle \boldsymbol{\omega}_{D/2}, \mathbf{x} \rangle) \\ \sin(\langle \boldsymbol{\omega}_1, \mathbf{x} \rangle) \\ \vdots \\ \sin(\langle \boldsymbol{\omega}_{D/2}, \mathbf{x} \rangle) \end{bmatrix}$$

to be the feature map corresponding to embedding in equation 31 and

$$(34) \quad \varphi_2(\mathbf{x}) = \sqrt{\frac{2}{D}} \begin{bmatrix} \cos(\langle \boldsymbol{\omega}_1, \mathbf{x} \rangle + b_1) \\ \vdots \\ \cos(\langle \boldsymbol{\omega}_D, \mathbf{x} \rangle + b_D) \end{bmatrix}$$

to be the feature map corresponding to equation 32. They then show that

$$\begin{aligned} \mathbb{V}[\varphi_1(\Delta)] &= \frac{1}{D} \left(1 + k(2\Delta) - 2k(\Delta)^2 \right) \\ \mathbb{V}[\varphi_2(\Delta)] &= \frac{1}{D} \left(1 + \frac{1}{2}k(2\Delta) - k(\Delta)^2 \right) \end{aligned}$$

meaning the variance of φ_1 is smaller whenever

$$\mathbb{V}[\cos(\langle \boldsymbol{\omega}, \Delta \rangle)] = \frac{1}{2} + \frac{1}{2}k(2\Delta) - k(\Delta)^2 \leq \frac{1}{2}.$$

When using the Gaussian kernel,

$$\mathbb{V}[\cos(\langle \boldsymbol{\omega}, \Delta \rangle)] = \frac{1}{2} \left(1 - \exp\left(-\frac{2\|\Delta\|_2^2}{\sigma^2}\right) \right)^2 \leq \frac{1}{2}$$

so that $\varphi_1(\Delta) \leq \varphi_2(\Delta)$ for any $\Delta \in \mathbb{R}^d$. Their finding were indeed consistent with our preliminary results. With this in mind, an embedding of φ_1 was always used for our experiments.

Another important result Rahimi and Recht show provides a bound on the sup-norm of the difference between a Gram matrix and its RFF approximation stated in proposition 17.

Proposition 17. *Let $k(\mathbf{x}, \mathbf{y}) = k(\mathbf{x} - \mathbf{y}) = k(\Delta)$ be a continuous shift-invariant, positive definite function defined on compact subset $\mathcal{M} \subset \mathbb{R}^d$ having radius ℓ where $k(0) = 1$ such that $\nabla^2 k(0)$ exists. Then for the feature mapping defined in equation 33 let $\sigma_p^2 = \mathbb{E}_{\boldsymbol{\omega} \sim p(\cdot)} \|\boldsymbol{\omega}\|_2^2 = \text{tr } \nabla^2 k(0)$ then for any $\varepsilon \in \mathbb{R}_{>0}$, $\varepsilon \leq \sigma_p \ell$ we have*

$$\mathbb{P} \left[\sup_{\mathbf{x}, \mathbf{y} \in \mathcal{M}} |\langle \varphi(\mathbf{x}), \varphi(\mathbf{y}) \rangle_{\mathbb{R}^D} - k(\mathbf{x}, \mathbf{y})| \geq \varepsilon \right] \leq \alpha \left(\frac{\sigma_p \ell}{\varepsilon} \right)^2 \exp \left(-\frac{D\varepsilon^2}{8(d+2)} \right)$$

where $\alpha \in \mathbb{R}_{>0}$, $\alpha < \infty$ does not depend on anything [Rah08, page 3].

Rahimi and Recht prove proposition 17 for $\alpha = 2^8$ although Sutherland and Schneider improve this to $\alpha = 66$ [DJSaJS15, page 3]. Observe that this bound is somewhat determined by the ratio D/d which is why D is often chosen as a multiple of d .

These results justify the RFF procedure seen in algorithm 3, which was used to approximate a Gram matrix for the data set \mathbf{X} using the feature map from 33.

Algorithm 3: RFF Algorithm

input : $\mathbf{X} \in \mathbb{R}^{n \times d}$, the dimension of the feature space D .
output: $\widetilde{\mathbf{K}} \simeq \mathbf{K}$ where \mathbf{K} is the Gram matrix corresponding to \mathbf{X} .
Construct $\mathbf{W} \triangleq [\omega_1, \dots, \omega_D]^\top \in \mathbb{R}^{D \times d}$ where $\omega_i \stackrel{\text{iid}}{\sim} p(\cdot)$
 $\mathbf{Z} = \frac{1}{\sqrt{D}} [\cos(\mathbf{W}\mathbf{X}^\top), \sin(\mathbf{W}\mathbf{X}^\top)]^\top$
 $\widetilde{\mathbf{K}} = \mathbf{Z}\mathbf{Z}^\top$
return $\widetilde{\mathbf{K}}$

Algorithm 3 of course assumes an appropriate construction of \mathbf{W} , commonly called the transformation matrix, and thus has access to a routine which allows one to sample from $p(\cdot)$. When using the RBF Gaussian kernel, the spectral distribution given in equation 28 corresponds to a multivariate Gaussian distribution with mean $\mathbf{0}$ and covariance matrix $\left(\frac{\sigma}{\sqrt{2}}\right)^{-2} \mathbb{1}_{D \times D}$. This means \mathbf{W} can simply be constructed as $\mathbf{W} = \left(\frac{\sigma}{\sqrt{2}}\right)^{-1} [\omega_1, \dots, \omega_D]^\top$ where $\omega_i \stackrel{\text{iid}}{\sim} \mathcal{N}(\mathbf{0}, \mathbb{1}_{D \times D})$. Transformations matrices constructed in this manner are given the notation \mathbf{W}_{RFF} . It can be shown that if \mathbf{W}_{RFF} is used as the transformation matrix in algorithm 3 then it produces an unbiased estimate, $\widetilde{\mathbf{K}}_{\text{RFF}}$, for the Gram matrix. This stated more precisely in lemma 18.

Lemma 18. $\widetilde{\mathbf{K}}_{\text{RFF}}$ is an unbiased estimate of \mathbf{K} , that is

$$\mathbb{E} \left[\left(\widetilde{\mathbf{K}}_{\text{RFF}} \right)_{ij} \right] = \exp \left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma^2} \right)$$

[Yu16, page 3].

Unfortunately, constructing the transformation matrix using \mathbf{W}_{RFF} does not scale well as the dimension of the feature space increases. Thus the focus of the upcoming sections will be to highlight a few of the more popular alternative methods used in the literature for the construction of the transformation matrix.

2.2. Orthogonal Random Features. In the previous chapter algorithm 3 assumed some sort of mechanism for producing the transformation matrix \mathbf{W} . The construction presented in 2.1 involved sampling $\omega_i \stackrel{\text{iid}}{\sim} p(\cdot)$. For the Gaussian RBF kernel this meant sampling from the multivariate Gaussian distribution $\mathcal{N}(\mathbf{0}, \mathbb{1}_{D \times D})$. The transformation matrix constructed in this manner was denoted \mathbf{W}_{RFF} . Recently, there has been a buzz in the literature exploring alternative constructs for the transformation matrix described in section 2.1 [Liu21]. We shall consider the two methods proposed by Yu *et al.* [Yu16]; the first method here and the second in the following section (2.3). The first method from Yu *et al.* is the Orthogonal Random Features (ORF) method with imposes orthogonality on the transformation matrix. To do this a Gaussian matrix $\mathbf{G} \in \mathbb{R}^{D \times d}$ is first produced, much like in \mathbf{W}_{RFF} . An orthogonal matrix \mathbf{Q} is then created by taking the QR-factorization (see section 3.2) of \mathbf{G} . However, the random orthogonal matrix, \mathbf{Q} , will not give an unbiased estimate of the kernel matrix. To fix this, the following common probabilistic

identity is employed

$$\|z\|_2^2 \sim \chi_k^2, \text{ where } z \sim \mathcal{N}(\mathbf{0}, \mathbb{1}_{k \times k})$$

where χ_k^2 is the chi-squared distribution with k degrees of freedom [Bro91, page 41]. This identity is easily demonstrated by equating a shared moment generating function of $(1 - 2t)^{-\frac{k}{2}}$ for $t < \frac{1}{2}$. Taking the square root of both sides gives $\|z\|_2 \sim \chi_k$ where χ_k is the chi distribution with k degrees of freedom. In the RFF method, each $\omega_i \in \mathbb{R}^D$ was independently taken from the multivariate normal Gaussian distribution meaning that using the identity provided above $\|\omega_i\|_2 \sim \chi_D$. The ORF method augments \mathbf{Q} by scaling its rows by iid χ_D values which can be accomplished through right multiplication with $\mathbf{S} = \text{diag}(\psi_1, \psi_2, \dots, \psi_D)$ where $\psi_i \stackrel{\text{iid}}{\sim} \chi_D$. This means

$$\left\| (\mathbf{S}\mathbf{Q})_{(i)} \right\|_2 = \left\| \psi_i \mathbf{Q}_{(i)} \right\|_2 = \psi_i \sim \chi_D$$

so that the row norms of \mathbf{G} and $\mathbf{S}\mathbf{Q}$ have the same distribution. Thus the transformation matrix for the ORF method is

$$(35) \quad \mathbf{W}_{\text{ORF}} = \left(\frac{\sigma}{\sqrt{2}} \right)^{-1} \mathbf{S}\mathbf{Q}.$$

The main downside the the ORF method is that the QR-factorization brings a computational cost of $\mathcal{O}(Dd)$. Fortunately when using \mathbf{W}_{ORF} as our transformation matrix in algorithm 3 the approximate Gram matrix $\widetilde{\mathbf{K}}_{\text{RFF}}$ is an unbiased estimate of \mathbf{K} , stated more formally in theorem 19.

Theorem 19. $\widetilde{\mathbf{K}}_{\text{ORF}}$ is an unbiased estimate of \mathbf{K} , that is

$$\mathbb{E} \left[\left(\widetilde{\mathbf{K}}_{\text{ORF}} \right)_{ij} \right] = \exp \left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma^2} \right)$$

[Yu16, page 3].

Furthermore, the variance of $\left(\widetilde{\mathbf{K}}_{\text{ORF}} \right)_{ij}$ is bounded by

$$\mathbb{V} \left[\left(\widetilde{\mathbf{K}}_{\text{ORF}} \right)_{ij} \right] - \mathbb{V} \left[\left(\widetilde{\mathbf{K}}_{\text{RFF}} \right)_{ij} \right] = \frac{1}{D} \left(\frac{g(\tau)}{d} - \frac{(d-1)e^{-\tau^2}\tau^4}{2d} \right)$$

where $\tau = \|\mathbf{x}_i - \mathbf{x}_j\|_2 / \frac{\sigma}{\sqrt{2}}$ and

$$g(\tau) = \frac{e^{\tau^2}(\tau^8 + 6\tau^6 + 7\tau^4 + \tau)}{4} + \frac{e^{\tau^2}\tau^4(\tau^6 + 2\tau^4)}{2d}$$

[Liu21, page 8]. This shows that there are scenarios for which $\mathbb{V} \left[\left(\widetilde{\mathbf{K}}_{\text{ORF}} \right)_{ij} \right] < \mathbb{V} \left[\left(\widetilde{\mathbf{K}}_{\text{RFF}} \right)_{ij} \right]$, namely when d is large and τ is small. Also, the ratio in variance between $\widetilde{\mathbf{K}}_{\text{ORF}}$ and $\widetilde{\mathbf{K}}_{\text{RFF}}$ for large d can be approximated as

$$\frac{\mathbb{V} \left[\left(\widetilde{\mathbf{K}}_{\text{ORF}} \right)_{ij} \right]}{\mathbb{V} \left[\left(\widetilde{\mathbf{K}}_{\text{RFF}} \right)_{ij} \right]} \simeq 1 - \frac{(s-1)e^{-\tau^2}\tau^4}{d(1 - e^{-\tau^2})^2}$$

[Liu21, page 8].

2.3. Random Ortho-Matrices and Structured Orthogonal Random Matrices. The second method we shall consider for producing a transformation matrix also originates from Yu’s *et al.* paper, which Choromanski *et al.* [Cho17] generalized as Random Ortho-Matrices (ROM). This second class of methods is underpinned by transformation matrices with the same variance reductions as ORF with the added benefit of time and memory savings. The transformation matrices generated using ROM take the form

$$(36) \quad \mathbf{W}_{\text{ROM}} = \sqrt{d} \prod_{i=1}^k \mathbf{S} \mathbf{D}_i$$

where $\mathbf{S} \in \mathbb{R}^{D \times D}$ has orthogonal rows and $\mathbf{D} = \text{diag}(\delta_1, \dots, \delta_D) \in \mathbb{R}^{D \times D}$ where $\delta_i \stackrel{\text{iid}}{\sim} U(\{-1, 1\})$. This matrix can be forced into a $\mathbb{R}^{D \times d}$ sized matrix by simply extracting the first d columns of \mathbf{D}_1 . The matrix to take the role of \mathbf{S} in virtually every application of ROM is the Hadamard matrix, defined in 20, which facilitates a fast $m \log(n)$ matrix multiplication with a size $m \times n$ and is known as Fast Walsh-Hadamard transform (FWHT) [FaA76].

Definition 20 (Hadamard Matrix). *The Hadamard matrix $\mathbf{H}_i \in \mathbb{R}^{(2^{i-1} \times 2^{i-1})}$ is defined recursively as*

$$\mathbf{H}_i = \begin{cases} [1] & , i = 1 \\ \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{H}_{i-1} & \mathbf{H}_{i-1} \\ \mathbf{H}_{i-1} & -\mathbf{H}_{i-1} \end{bmatrix} & , i > 1 \end{cases} .$$

Note that while Hadamard matrices are only defined for dimensions of exact powers of 2, although other sizes can be constructed by removing portions of the matrix given in definition 20 or by padding with 0. This provides a concrete means for which one can generate a transformation matrix

$$(37) \quad \sqrt{d} \prod_{i=1}^k \mathbf{H} \mathbf{D}_i$$

where \mathbf{H} is an appropriately sized Hadamard matrix. It is easy to check that the matrix generated by equation 37 shares the same expected rows norm lengths as \mathbf{W}_{ORF} and thus enjoys the same variance reduction benefits. Moreover, since matrix multiplication with \mathbf{H} can be performed in $\mathcal{O}(D \log(d))$ time (using FWHT) and multiplication with \mathbf{H} can be performed in $\mathcal{O}(D)$ time, the ROM method has the added benefit of improved run time complexity $\mathcal{O}(D \log(d))$ using only $\mathcal{O}(D)$ extra memory. Table 1 gives a comparison of the time and space complexities for the methods mentioned so far.

TABLE 1. A comparison of various methods for computing a suitable transformation matrix with the Random Fourier Features paradigm. Typically the dimension of the feature space, D , is chosen as some multiple of the dimension of data, d .

<i>Method</i>	<i>Time</i>	<i>Extra Space</i>
RFF [Rah08]	$\mathcal{O}(Dd)$	$\mathcal{O}(Dd)$
ORF [Yu16]	$\mathcal{O}(Dd)$	$\mathcal{O}(Dd)$
ROM (SORF) [Cho17, Yu16]	$\mathcal{O}(D \log(d))$	$\mathcal{O}(D)$

Despite the wide use of the ROM method in various machine learning tasks [Cho17, And15, Cho20, Liu21] a number of high-interest theoretical properties remain unsolved, leaving many aspects of this

method shrouded in mystery. Instead, much of what we understand about ROM's estimate capabilities comes from empirical analysis. Nonetheless, we shall still cover a smaller number of important results that have been established.

Choromanski *et al.* [Cho17] show that there are diminishing returns (estimate wise) for choosing larger values of k in equation 37. They also show that choosing odd values of k in 37 provides better estimates than its even-parity $k - 1$ and $k + 1$ counterparts. For this reason a k value of 3 is usually chosen which gives rise to the transformation matrix estimate given in equation 38. The method for constructing transformation matrices in this manner is referred to as Structured Orthogonal Random Features (SORF).

$$(38) \quad \mathbf{W}_{\text{SORF}} = \sqrt{d} \mathbf{H} \mathbf{D}_3 \mathbf{H} \mathbf{D}_2 \mathbf{H} \mathbf{D}_1$$

This is the same transformation matrix estimate that Yu *et al.* provides. Unfortunately using the SORF method in algorithm 3 does not produce an unbiased estimate of the Gram matrix; however, it does satisfy an asymptotic unbiased property

$$\left| \mathbb{E} \left[\left(\widetilde{\mathbf{K}}_{\text{SORF}} \right)_{ij} \right] - \mathbb{E} \left[\left(\widetilde{\mathbf{K}}_{\text{RFF}} \right)_{ij} \right] \right| \leq \frac{6\tau}{\sqrt{d}}$$

where τ is again $\|x_i - x_j\|_2 / \frac{\sigma}{\sqrt{2}}$ [Liu21, page 8].

Bojarski *et al.* [Boj16, page 4] give an intuitive explanation for the roles of each of the different blocks $\mathbf{H} \mathbf{D}_1$, $\mathbf{H} \mathbf{D}_2$ and $\mathbf{H} \mathbf{D}_3$. The first block can be shown to satisfy

$$\mathbb{P} \left[\|\mathbf{H} \mathbf{D}_1 \mathbf{x}\|_\infty > \frac{\log D}{\sqrt{D}} \right] \leq 2d \exp \left(-\frac{\log^2 D}{8} \right), \quad \mathbf{x} \in \mathbb{R}^D$$

[Liu21, page 8] so that it can be thought as a "balancer" leaving no single dimension bearing too much of the l^2 norm. For the second block, the cost of using a structured matrix is the loss of independence. The purpose of the second block is to mitigate this effect by making similar input vectors near-orthogonal. Finally the third block controls the capacity of the entire structure by providing a vector of parameters. Near-independence is now implied by the near-orthogonality (achieved by $\mathbf{H} \mathbf{D}_2$) and the fact that the projections of the Gaussian vector or Radamacher vector onto "almost orthogonal directions" are "close to independent". These roles are portrayed visually in Figure 6.

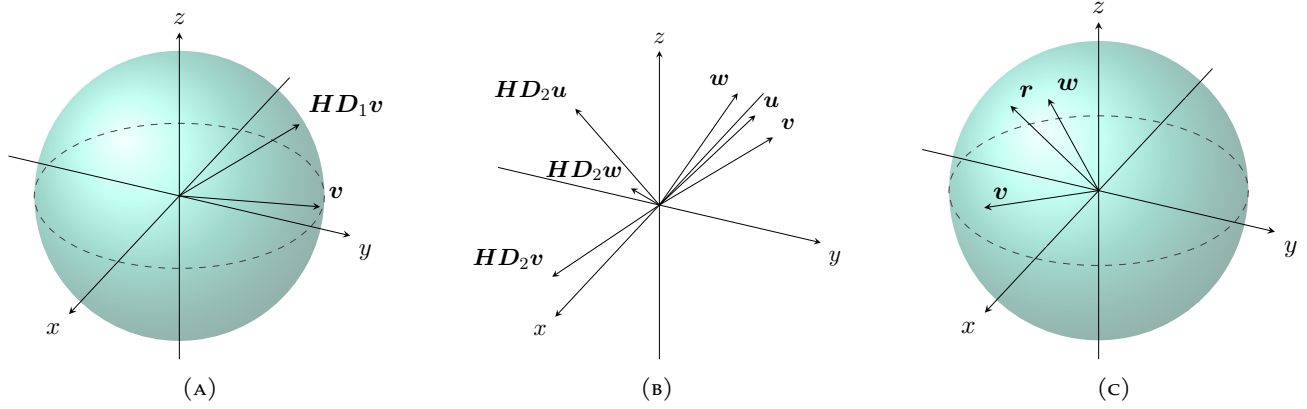


FIGURE 6. A visual representation for the roles of each matrix block in the SORF method. The first block HD_1 rotates v so that single dimension bears too much of the l^2 norm seen in panel (A). In panel (B) the second block HD_2 transforms vectors so that their image is near-orthogonal. Panel (C) shows that the projection of a random vector r onto two near-orthogonal vector v, w yields a near-independent vector.

3. KRYLOV SUBSPACE METHODS

In this section we will focus on how iterative methods, in particular a class of iterative methods called Krylov Subspace methods, may be used to solve a linear system $Ax = b$. While non-iterative methods exist to solve such systems virtually all of them carry an unwieldy runtime of $\mathcal{O}(n^3)$ for a system of n parameters. Even for current computer systems, this renders many common matrix problems untractable. Consequently the focus of solving linear systems has shifted towards iterative methods. While iterative methods typically demand certain structural properties of the matrices, such as symmetry and positive definiteness, this generally is not a problem since the majority of large matrix problems that, by mature, endow these systems with the desired properties. For example, in the context of this paper the Gram matrices used to solve linear systems in Gaussian Processes possess both symmetry and positive definiteness. There are also a number of other properties of iterative methods which make them rather attractive to users. To start, iterative Krylov subspace methods are guranteed to converge to an exact solution within a finite number of iterations and even if the method is prematurely stopped before reaching an exact solution, the approximation obtained on the final iteration will in some sense be a good enough estimate of our exact solution. Furthermore, unlike most non-iterative methods, Krylov subspace methods do not require an explicit form of the matrix A and instead only requires some routine or process for computing Ax .

3.1. Krylov Subspaces. We will motivate the Krylov subspaces by observing their usefullness in solving linear systems. To this end, consider the problem of solving the linear system

$$(39) \quad Ax^* = b$$

where no explicit form of \mathbf{A} is available and instead one must draw information from \mathbf{A} solely through a routine that can evaluate $\mathbf{A}\mathbf{v}$ for any \mathbf{v} . How could this routine be utilized in such a manner to provide with a solution to equation 39? Before answering this, consider the following theorem

Theorem 21. For $\mathbf{A} \in \mathbb{K}^{n \times n}$ if $\|\mathbf{A}\| = q < 1$ then $\mathbb{1} - \mathbf{A}$ is invertible and its inverse admits the following representation

$$(\mathbb{1} - \mathbf{A})^{-1} = \sum_{k=0}^{\infty} \mathbf{A}^k.$$

[Ber96]

Consider a matrix for which $\|\mathbf{A}\| < 2$, it follows that $\|\mathbb{1} - \mathbf{A}\| < 1$ meaning $\mathbb{1} - (\mathbb{1} - \mathbf{A})$ is invertible and $\mathbf{A}^{-1} = (\mathbb{1} - (\mathbb{1} - \mathbf{A}))^{-1} = \sum_{k=0}^{\infty} (\mathbb{1} - \mathbf{A})^k$. Thinking back to equation 39 for any $x_0 \in \mathbb{K}^n$ we have

$$\begin{aligned} \mathbf{x}^* &= \mathbf{A}^{-1}\mathbf{b} = \mathbf{A}^{-1}(\mathbf{A}\mathbf{x}^* - \mathbf{A}\mathbf{x}_0 + \mathbf{A}\mathbf{x}_0) \\ &= \mathbf{x}_0 + \mathbf{A}^{-1}\mathbf{r}_0 \\ &= \mathbf{x}_0 + \sum_{k=0}^{\infty} (\mathbb{1} - \mathbf{A})^k \end{aligned}$$

where $\mathbf{r}_0 = \mathbf{A}\mathbf{x}^* - \mathbf{A}\mathbf{x}_0$. A natural question that arises is that can we find a closed form solution of the above equation? To answer this question we need to enlist the help of the Cayley-Hamilton theorem.

Theorem 22 (Cayley-Hamilton). Let $p_n(\lambda) = \sum_{i=0}^n c_i \lambda^i$ be the characteristic polynomial of the matrix $\mathbf{A} \in \mathbb{K}^{n \times n}$, then $p_n(\mathbf{A}) = \mathbf{0}$. **THIS NEEDS A CITATION**

The Cayley-Hamilton theorem implies that

$$\begin{aligned} 0 &= c_0 + c_1 \mathbf{A} + \dots + c_{n-1} \mathbf{A}^{n-1} + c_n \mathbf{A}^n \\ 0 &= \mathbf{A}^{-1} c_0 + c_1 + \dots + c_{n-1} \mathbf{A}^{n-2} + c_n \mathbf{A}^{n-1} \\ \mathbf{A}^{-1} &= \alpha_0 + c_1 + \dots + \alpha_{n-1} \mathbf{A}^{n-2} + \alpha_n \mathbf{A}^{n-1} \end{aligned}$$

where $\alpha_i = -c_i/c_0$. This demonstrates that \mathbf{A}^{-1} can be represented as a matrix polynomial of degree $n - 1$. This means that $\sum_{k=0}^{\infty} (\mathbb{1} - \mathbf{A})^k$ indeed possess a closed form solution namely

$$\mathbf{x}^* = \mathbf{x}_0 + \mathbf{A}^{-1}\mathbf{r}_0 = \alpha_0 + c_1 + \dots + \alpha_{n-1} \mathbf{A}^{n-2} + \alpha_n \mathbf{A}^{n-1}.$$

This also shows that $\mathbf{x}^* \in \text{l.s}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \dots, \mathbf{A}^{n-1}\mathbf{r}_0\}$. One idea for finding a solution to equation 39 is to use our routine for evaluating $\mathbf{A}\mathbf{v}$ to iteratively compute new basis elements for the space generated by $\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \dots, \mathbf{A}^{n-1}\mathbf{r}_0\}$ and at each step carefully choosing a \mathbf{x}_k such that \mathbf{x}_k approaches \mathbf{x}^* , in some form. The subspace constructed using this technique is so important that it has its own name.

Definition 23 (Krylov Subspace). The Krylov Subspace of order k generated by the matrix $\mathbf{A} \in \mathbb{K}^{n \times n}$ and the vector $\mathbf{v} \in \mathbb{K}$ is defined as

$$\mathcal{K}_k(\mathbf{A}, \mathbf{v}) = \text{l.s}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \dots, \mathbf{A}^{k-1}\mathbf{r}_0\}$$

for $k \geq 1$ and $\mathcal{K}_k(\mathbf{A}, \mathbf{v}) = \{\mathbf{0}\}$.

For the purposes of solving equation 39 it is of much interest to understand how $\mathcal{K}_k(\mathbf{A}, \mathbf{v})$ grows for larger and larger k since a solution for equation 39 will be present in a Krylov Subspace that cannot be

grown any larger. In other words, an exact solution can be constructed once we have extracted all the information from \mathbf{A} through multiplication of \mathbf{r}_0 . The following theorem provides information on how exactly the Krylov Subspace grows as k increases.

Theorem 24. *There is a positive called the grade of \mathbf{v} with respect to \mathbf{A} , denoted $t_{\mathbf{v},\mathbf{A}}$, where*

$$\dim(\mathcal{K}_k(\mathbf{A}, \mathbf{v})) = \begin{cases} k, & k \leq t \\ t, & k \geq t \end{cases}$$

Theorem 24 essentially tells us that for $k \leq t_{\mathbf{v},\mathbf{A}}$ that $\mathbf{A}^k \mathbf{v}$ is linearly independent to $\mathbf{A}^i \mathbf{v}$ for $0 \leq i \leq k-1$ meaning $\{\mathbf{v}, \mathbf{A}\mathbf{v}, \mathbf{A}^2\mathbf{v}, \dots, \mathbf{A}^{k-1}\mathbf{v}\}$ serves as a basis for $\mathcal{K}_k(\mathbf{A}, \mathbf{v})$ and that $\mathcal{K}_{k-1}(\mathbf{A}, \mathbf{v}) \subsetneq \mathcal{K}_k(\mathbf{A}, \mathbf{v})$. Conversely, any new vectors formed beyond $t_{\mathbf{v},\mathbf{A}}$ will be linearly independent meaning $\mathcal{K}_k(\mathbf{A}, \mathbf{v}) \subsetneq \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{v})$ for $k \geq t_{\mathbf{v},\mathbf{A}}$. While $t_{\mathbf{v},\mathbf{A}}$ clearly plays a role in determining a suitable basis for which $\mathbf{A}^{-1}\mathbf{b}$ lies in its importance is made abundantly clear in the following corollary.

Corollary 25.

$$t_{\mathbf{v},\mathbf{A}} = \min \{k \mid \mathbf{A}^{-1}\mathbf{v} \in \mathcal{K}_k(\mathbf{A}, \mathbf{v})\}$$

Proof. Recall from Cayley-Hamilton (theorem 22) that

$$\mathbf{A}^{-1}\mathbf{v} = \sum_{i=0}^{n-1} \alpha_i \mathbf{A}^i \mathbf{v}$$

But since $\mathcal{K}_k(\mathbf{A}, \mathbf{v}) = \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{v})$ for $k \geq t_{\mathbf{v},\mathbf{A}}$

$$\mathbf{A}^{-1}\mathbf{v} = \sum_{i=0}^{t-1} \beta_i \mathbf{A}^i \mathbf{v}$$

meaning $\mathbf{A}^{-1}\mathbf{v} \in \mathcal{K}_k(\mathbf{A}, \mathbf{v})$ for $k \geq t_{\mathbf{v},\mathbf{A}}$. Suppose for the sake of contradiction that this also holds for $k = t_{\mathbf{v},\mathbf{A}} - 1$, that is, $\mathbf{A}^{-1}\mathbf{v} = \sum_{i=0}^{t-2} \gamma_i \mathbf{A}^i \mathbf{v}$. However, this gives

$$\mathbf{v} = \sum_{i=0}^{t-2} \gamma_i \mathbf{A}^{i+1} \mathbf{v} = \sum_{i=0}^{t-1} \gamma_{i-1} \mathbf{A}^i \mathbf{v}$$

implying $\{\mathbf{v}, \mathbf{A}\mathbf{v}, \mathbf{A}^2\mathbf{v}, \dots, \mathbf{A}^{t-1}\mathbf{v}\}$ are linearly dependent which means that $\dim(\mathcal{K}_k(\mathbf{A}, \mathbf{v})) < t$, which provides us with our contradiction. \square

This machinery allows us to make a much stronger statement on the whereabouts of \mathbf{x}^* in relation to the Krylov Subspaces.

Corollary 26. *For any \mathbf{x}_0 , we have*

$$\mathbf{x}^* \in \mathbf{x}_0 + \mathcal{K}_{t_{\mathbf{r}_0},\mathbf{A}}(\mathbf{A}, \mathbf{r}_0)$$

where $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$.

3.2. Gram-Schmidt Process and QR factorisations. Many areas of linear algebra involving studying the column space of matrices. The QR factorisation provides us with a powerful tool to better understand the column space of a matrix as well as serving as an important factorisation mechanism for many numerical methods. Suppose that a matrix $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n] \in \mathbb{K}^{n \times n}$ has full rank. The idea of a QR factorisation is to find an alternative orthonormal basis for $(\mathbf{a}_i)_{i=1}^n$, say $(\mathbf{q}_i)_{i=1}^n$, and to somehow relate the original matrix \mathbf{A} to a new matrix whose columns are $(\mathbf{q}_i)_{i=1}^n$. Consider the following procedure that allows us to find an orthonormal basis $(\mathbf{q}_i)_{i=1}^n$ for which $\text{l.s}\{(\mathbf{a}_i)_{i=1}^n\} = \text{l.s}\{(\mathbf{q}_i)_{i=1}^n\}$. First set $\mathbf{q}_1 = \frac{\mathbf{a}_1}{\|\mathbf{a}_1\|}$, clearly $\text{l.s}\{\mathbf{a}_1\} = \text{l.s}\{\mathbf{q}_1\}$. Next, construct a vector $\mathbf{q}'_2 = \mathbf{a}_2 - r_{1,2} \cdot \mathbf{q}_1$ so that $\mathbf{q}'_2 \perp \mathbf{q}_1$. This means

$$\begin{aligned} 0 &= \langle \mathbf{q}_1, \mathbf{q}'_2 \rangle \\ 0 &= \langle \mathbf{q}_1, \mathbf{a}_2 - r_{1,2} \cdot \mathbf{q}_1 \rangle \\ 0 &= \langle \mathbf{q}_1, \mathbf{a}_2 \rangle - r_{1,2} \cdot \langle \mathbf{q}_1, \mathbf{q}_1 \rangle \\ r_{1,2} &= \langle \mathbf{q}_1, \mathbf{a}_2 \rangle \end{aligned}$$

Since \mathbf{q}'_2 may not be a unit vector we set $\mathbf{q}_2 = \frac{\mathbf{q}'_2}{\|\mathbf{q}'_2\|}$ where $\text{l.s}\{\mathbf{a}_1, \mathbf{a}_2\} = \text{l.s}\{\mathbf{q}_1, \mathbf{q}_2\}$. Continuing the vector \mathbf{q}'_3 is constructed so that

$$\mathbf{q}'_3 = \mathbf{a}_3 - r_{1,3}\mathbf{q}_1 - r_{2,3}\mathbf{q}_2$$

are chosen so that \mathbf{q}'_3 is orthogonal to both \mathbf{q}_2 and \mathbf{q}_1 . This amounts to setting $r_{1,3} = \langle \mathbf{q}_1, \mathbf{a}_3 \rangle$ and $r_{2,3} = \langle \mathbf{q}_2, \mathbf{a}_3 \rangle$. Similarly, \mathbf{q}'_3 is normalized so that $\mathbf{q}_3 = \frac{\mathbf{q}'_3}{\|\mathbf{q}'_3\|}$ and $\text{l.s}\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} = \text{l.s}\{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\}$. Continuing in this fashion the k^{th} vector in our orthonormal basis is computed as

$$(40) \quad \mathbf{q}_k = \frac{\mathbf{a}_k - \sum_{i=1}^{k-1} r_{i,k} \cdot \mathbf{q}_i}{r_{k,k}}$$

where $r_{i,k} = \langle \mathbf{q}_i, \mathbf{a}_k \rangle$, $r_{k,k} = \|\mathbf{a}_k - \sum_{i=1}^{k-1} r_{i,k} \cdot \mathbf{q}_i\|$ and $\text{l.s}\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_k\} = \text{l.s}\{\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_k\}$. This procedure is famously known as the Gram-Schmidt process [Ber96, Tre97, Dem97] and is summarized in the following algorithm.

Algorithm 4: Classical Gram-Schmidt

input : A basis $(\mathbf{a}_i)_{i=1}^n$.

output: An orthonormal basis $(\mathbf{q}_i)_{i=1}^n$ such that $\text{l.s}\{(\mathbf{a}_i)_{i=1}^n\} = \text{l.s}\{(\mathbf{q}_i)_{i=1}^n\}$

for $k = 1$ **to** n **do**

$\mathbf{q}'_k = \mathbf{a}_k$

for $i = 1$ **to** $k - 1$ **do**

$r_{i,k} = \langle \mathbf{q}_i, \mathbf{a}_k \rangle$

$\mathbf{q}'_k = \mathbf{q}'_k - r_{i,k}\mathbf{q}_i$

end

$r_{k,k} = \|\mathbf{q}'_k\|$

$\mathbf{q}_k = \mathbf{q}'_k / r_{k,k}$

end

return $(\mathbf{q}_i)_{i=1}^n$

Relating the column space of \mathbf{A} to the orthonormal basis $(\mathbf{q}_i)_{i=1}^n$ in a matrix form

$$[\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n] = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n] \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,n} \\ & r_{2,2} & & \vdots \\ & & \ddots & \vdots \\ & & & r_{n,n} \end{bmatrix}$$

or more succinctly

$$(41) \quad \mathbf{A} = \mathbf{Q}\mathbf{R}$$

where $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n]$ and $(\mathbf{R})_{i,j} = r_{i,j}$ for $i \leq j$ and $(\mathbf{R})_{i,j} = 0$ for $i > j$. This is exactly the QR factorisation for a full rank matrix. Note that $\text{Range}(\mathbf{A}) = \text{Range}(\mathbf{Q})$. In general, any square matrix $\mathbf{A} \in \mathbb{K}^{m \times n}$ may be decomposed as $\mathbf{A} = \mathbf{Q}\mathbf{R}$ where $\mathbf{Q} \in \mathbb{K}^{m \times m}$ is an orthogonal matrix and $\mathbf{R} \in \mathbb{K}^{m \times n}$ is an upper triangular matrix. This is known as a full QR factorisation. Since bottom $(m - n)$ rows of this \mathbf{R} consists entirely of zeros, it is often useful to partition the full QR factorisation in the following manner to shed vacuous entries

$$\mathbf{A} = \mathbf{Q}\mathbf{R} = \mathbf{Q} \begin{bmatrix} \hat{\mathbf{R}} \\ \mathbf{0}_{(m-n) \times n} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{Q}} & \mathbf{Q}' \end{bmatrix} \begin{bmatrix} \hat{\mathbf{R}} \\ \mathbf{0}_{(m-n) \times n} \end{bmatrix} = \hat{\mathbf{Q}}\hat{\mathbf{R}}.$$

This alternate decomposition is called the reduced (or sometimes the thin) QR -factorization. We shall state the following two theorems on the QR -factorization are stated without proof.

Theorem 27. Every $\mathbf{A} \in \mathbb{K}^{m \times n}$, $(m \geq n)$ has a full QR factorisation, hence also a reduced QR factorisation. [Tre97]

Theorem 28. Each $\mathbf{A} \in \mathbb{K}^{m \times n}$, $(m \geq n)$ of full rank has a unique reduced QR factorisation $\mathbf{A} = \hat{\mathbf{Q}}\hat{\mathbf{R}}$ with $r_{k,k} > 0$. [Tre97]

In practice the classical Gram-Schmidt process described in algorithm 4 is rarely used as the procedure becomes numerically unstable if $(\mathbf{a}_i)_{i=1}^n$ are almost linearly dependent. Before looking for ways to resolve these numerical instabilities a quick recap of projectors has been devised. A square matrix \mathbf{P}_G acting on a Hilbert space H that sends $\mathbf{x} \in H$ to its projection onto a subspace G is called the projector onto G . If $(\mathbf{q}_k)_{k=1}^m$ is an orthonormal basis in G then

$$\mathbf{P}_G = \mathbf{Q}\mathbf{Q}^*$$

where $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_m, 0, \dots, 0] \in \mathbb{K}^{n \times n}$. A special class of projectors which isolates the components of a given vector onto a one dimensional subspace spanned by a single unit vector \mathbf{q} called a rank one orthogonal projector, denoted as \mathbf{P}_q . Each k in the classical Gram-Schmidt process \mathbf{q}'_k using the following orthogonal projection

$$(42) \quad \mathbf{q}'_k = \mathbf{P}_{A_k^\perp} \mathbf{a}_k$$

where $A_k = \text{l.s}\{\mathbf{a}_i\}_{i=1}^k$ and $\mathbf{P}_{A_k^\perp} = \mathbb{1}$ for convenience. A modified version of the Gram-Schmidt process performs the same orthogonal projection broken up as $k - 1$ orthogonal projections of rank $n - 1$ as so

$$\begin{aligned} \mathbf{q}'_k &= \mathbf{P}_{A_k^\perp} \mathbf{a}_k \\ &= (\mathbb{1} - \mathbf{Q}_k \mathbf{Q}_k^*) \mathbf{a}_k \end{aligned}$$

$$\begin{aligned}
&= \left(\prod_{i=1}^{k-1} (\mathbb{1} - \mathbf{q}_i \mathbf{q}_i^*) \right) \mathbf{a}_k \\
&= (\mathbb{1} - \mathbf{q}_1 \mathbf{q}_1^*) (\mathbb{1} - \mathbf{q}_1 \mathbf{q}_1^*) \cdots (\mathbb{1} - \mathbf{q}_{k-1} \mathbf{q}_{k-1}^*) \mathbf{a}_k \\
&= P_{\mathbf{q}_k^\perp} \cdots P_{\mathbf{q}_1^\perp} \mathbf{a}_k
\end{aligned}$$

While its clear that $P_{A_k^\perp} \mathbf{a}$ and $P_{\mathbf{q}_k^\perp} \cdots P_{\mathbf{q}_1^\perp} \mathbf{a}_k$ used for computing \mathbf{q}'_k are algebraically, they differ arithmetically as the latter expression evaluates \mathbf{q}'_k using the follow procedure

$$\begin{aligned}
\mathbf{q}_k^{(1)} &= \mathbf{a}_k \\
\mathbf{q}_k^{(2)} &= P_{\mathbf{q}_1^\perp} \mathbf{q}_k^{(1)} \\
\mathbf{q}_k^{(3)} &= P_{\mathbf{q}_2^\perp} \mathbf{q}_k^{(2)} \\
&\vdots \\
\mathbf{q}'_k &= \mathbf{q}_k^{(k)} = P_{\mathbf{q}_{k-1}^\perp} \mathbf{q}_k^{(k-1)}
\end{aligned}$$

Applying projections sequentially in this manner produces smaller numerical errors. The modified Gram-Schmidt process [Tre97, Dem97] is summarized in the following algorithm.

Algorithm 5: Modified Gram-Schmidt

input : A basis $\{\mathbf{a}_i\}_{i=1}^n$.
output: An orthornormal basis $\{\mathbf{q}_i\}_{i=1}^n$ such that l.s $\{\mathbf{a}_i\}_{i=1}^n = \text{l.s } \{\mathbf{q}_i\}_{i=1}^n$

for $k = 1$ **to** n **do**
 $\mathbf{q}'_k = \mathbf{a}_k$
end
for $k = 1$ **to** n **do**
 $r_{k,k} = \|\mathbf{q}'_k\|$
 $\mathbf{q}_k = \mathbf{q}'_k / r_{k,k}$
 for $i = k + 1$ **to** n **do**
 $r_{i,k} = \langle \mathbf{q}_k, \mathbf{q}'_i \rangle$
 $\mathbf{q}_i = \mathbf{q}_i - r_{i,k} \mathbf{q}_k$
 end
end
return $\{\mathbf{q}_i\}_{i=1}^n$

3.3. Arnoldi and Lanczos Algorithm. As a quick reminder, we are in search of an iterative process to solve the linear system $\mathbf{A} \mathbf{x}^* = \mathbf{b}$ where no explicit form of \mathbf{A} is available and we may only rely on a routine that computes $\mathbf{A} \mathbf{v}$ for any \mathbf{v} to extract information on \mathbf{A} . In section 3.1 it wa discovered that $\mathbf{x}^* \in \mathcal{K}_{t_{r_0, \mathbf{A}}}(\mathbf{A}, \mathbf{r}_0)$. With many iterative methods, computing an exact value for \mathbf{x}^* is out the question with the view that $t_{r_0, \mathbf{A}}$ is impractically large. We must instead resort to approximating \mathbf{x}^* by \mathbf{x}_k for

which $\mathbf{x}^k \in \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$ where $k \ll t_{\mathbf{r}_0}$. To find an appropriate value for \mathbf{x}_k , a good start would be to find a basis $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$. Definition 23 showed us that $\{\mathbf{A}^{i-1}\mathbf{r}_0\}_{i=1}^k$ serves as a basis for $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$. However, for numerical reasons this is a poor choice of basis since each consecutive term becomes closer and closer to being linearly dependent. From now on, for more convenient notation we shall set $n = t_{\mathbf{r}_0, \mathbf{A}}$ so that $\mathbf{x}^* \in \mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$. To search for a more appropriate basis let $\mathbf{K} \in \mathbb{K}^{n \times n}$ be the invertible matrix

$$\mathbf{K} = [\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \dots, \mathbf{A}^{n-1}\mathbf{r}_0].$$

Since \mathbf{K} is invertible we can compute $\mathbf{c} = -\mathbf{K}^{-1}\mathbf{A}^n\mathbf{r}_0$ so that

$$\begin{aligned} \mathbf{A}\mathbf{K} &= [\mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \dots, \mathbf{A}^n\mathbf{r}_0] \\ \mathbf{A}\mathbf{K} &= \mathbf{K} \cdot [\mathbf{e}_2, \mathbf{e}_3, \dots, \mathbf{e}_n, -\mathbf{c}] \triangleq \mathbf{K}\mathbf{C} \end{aligned}$$

or, in a more verbose form

$$\mathbf{K}^{-1}\mathbf{A}\mathbf{K} = \mathbf{C} = \begin{bmatrix} 0 & 0 & \cdots & 0 & -c_1 \\ 1 & 0 & \cdots & 0 & -c_2 \\ 0 & 1 & \cdots & 0 & \vdots \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & -c_n \end{bmatrix}.$$

Note here that \mathbf{C} is upper Hessenberg. While this form is simple, it is of little practical use since the matrix \mathbf{K} is very likely to be ill-conditioned. To remedy this we can replace \mathbf{K} with an orthogonal matrix which spans the same space. These are exactly the properties that the \mathbf{Q} matrix offers in the QR -factorisation of \mathbf{K} . With this in mind let $\mathbf{K} = \mathbf{Q}\mathbf{R}$ be the full QR -factorisation of \mathbf{K} . Then

$$\begin{aligned} \mathbf{A}\mathbf{Q}\mathbf{R} &= \mathbf{A}\mathbf{K} \\ \mathbf{A}\mathbf{Q} &= \mathbf{A}\mathbf{K}\mathbf{R}^{-1} \\ \mathbf{A}\mathbf{Q} &= \mathbf{K}\mathbf{C}\mathbf{R}^{-1} \\ \mathbf{A}\mathbf{Q} &= \mathbf{Q}\mathbf{R}\mathbf{C}\mathbf{R}^{-1} \\ \mathbf{A}\mathbf{Q} &\triangleq \mathbf{Q}\mathbf{H}. \end{aligned}$$

Since \mathbf{R} and \mathbf{R}^{-1} are both upper triangular and \mathbf{C} is upper Hessenberg, \mathbf{H} is also upper Hessenberg. This form provides us with a \mathbf{Q} such that the range of \mathbf{Q} is $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$ and

$$(43) \quad \mathbf{Q}^\top \mathbf{A}\mathbf{Q} = \mathbf{H}.$$

Again, in practice, it may be very difficult to compute this entire expression forcing us to search for approximative alternatives. Consider equation 43 for which the only first k columns of \mathbf{Q} have been computed. Let $\mathbf{Q}_k = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_k]$ and $\mathbf{Q}_u = [\mathbf{q}_{k+1}, \mathbf{q}_{k+2}, \dots, \mathbf{q}_n]$. Then

$$\begin{aligned} \mathbf{Q}^\top \mathbf{A}\mathbf{Q} &= \mathbf{H} \\ [\mathbf{Q}_k, \mathbf{Q}_u]^\top \mathbf{A} [\mathbf{Q}_k, \mathbf{Q}_u] &= \begin{bmatrix} \mathbf{H}_k & \mathbf{H}_{u,k} \\ \mathbf{H}_{k,u} & \mathbf{H}_u \end{bmatrix} \\ \begin{bmatrix} \mathbf{Q}_k^\top \mathbf{A}\mathbf{Q}_k & \mathbf{Q}_k^\top \mathbf{A}\mathbf{Q}_u \\ \mathbf{Q}_u^\top \mathbf{A}\mathbf{Q}_k & \mathbf{Q}_u^\top \mathbf{A}\mathbf{Q}_u \end{bmatrix} &= \begin{bmatrix} \mathbf{H}_k & \mathbf{H}_{u,k} \\ \mathbf{H}_{k,u} & \mathbf{H}_u \end{bmatrix} \end{aligned}$$

where H_k , $H_{u,k}$, $H_{k,u}$ and H_u are the relevant sub matrices. This provides us with the equality

$$(44) \quad Q_k^\top A Q_k = H_k$$

noting that H_k is upper Hessenberg for the same reason that H is. We know that when $n = t_{r_0, A}$ we can find a $Q \in \mathbb{K}^{n \times n}$ and $H \in \mathbb{K}^{n \times n}$ that satisfies $AQ = QH$. However, in general, we may not be so fortunate in finding a $Q_k \in \mathbb{K}^{n \times k}$ and $H_k \in \mathbb{K}^{n \times k}$ so satisfy $AQ_k = Q_k H_k$ for any $k < n$. Instead we can adjust this equality by adding an error $E_k \in \mathbb{K}^{n \times k}$ so that we do get equality. Our expression now becomes

$$(45) \quad Q_k^\top A Q_k = H_k + E_k.$$

A careful choice of E_k must be made to also retain equality in equation 44, meaning $Q_k^\top E_k = 0$. Since $\{q_i\}_{i=1}^k$ forms an orthonormal basis for $\mathcal{K}_n(A, r_0)$, consider the following choice of E_k ,

$$E_k = q_{k+1} h_k^\top$$

where h_k is any vector in \mathbb{K}^k . Notice that

$$Q_k^\top E = Q^\top (q_{k+1} h_k) = (Q^\top q_{k+1}) h_k^\top = 0.$$

Since this holds for any $h_k \in \mathbb{K}^k$, to preserve sparsity and to keep this form as simple as possible we can set $h_k = [0, 0, \dots, h_{k+1,k}]^\top$. This means AQ_k can be written as

$$(46) \quad A Q_k = Q_k H_k + q_{k+1} h_k^\top$$

where

$$Q_k H_k = [q_1, q_2, \dots, q_k] \begin{bmatrix} h_{1,1} & \cdots & \cdots & \cdots & h_{1,k} \\ h_{2,1} & \cdots & \cdots & \cdots & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & h_{k,k-1} & h_{k,k} \\ 0 & \cdots & 0 & 0 & 0 \end{bmatrix}.$$

Equating the j^{th} columns of equation 46 yields

$$A q_j = \sum_{i=1}^{j+1} h_{i,j} q_i.$$

Again since $\{q_i\}_{i=1}^n$ form an orthonormal basis, multiplying both sides by q_m for $1 \leq m \leq j$ gives

$$q_m^\top A q_j = \sum_{i=1}^{j+1} h_{i,j} q_m^\top q_i = h_{m,j}$$

and so

$$(47) \quad h_{j+1,j} q_{j+1} = A q_j - \sum_{i=1}^j h_{i,j} q_i.$$

From equation 47 we find that q_{j+1} can be computed using a recurrence involving its previous Krylov factors. Notice this bears a striking resemblance to equation 40 having a virtually an identical setup to computing an orthonormal basis using the modified Gram-Schmidt process (algorithm 5). As such,

values for \mathbf{q}_{j+1} and $h_{j+1,j}$ can be evaluated using a procedure very similar to the modified Gram-Schmidt process better known as the Arnoldi algorithm [Tre97, Dem97], presented in algorithm 6.

Algorithm 6: Arnoldi Algorithm

input : \mathbf{A} , \mathbf{r}_0 and k , the number of columns of \mathbf{Q} to compute.

output: $\mathbf{Q}_k, \mathbf{H}_k$.

$\mathbf{q}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\|$

for $j = 1$ **to** k **do**

$\mathbf{z} = \mathbf{A}\mathbf{q}_j$

for $i = 1$ **to** j **do**

$h_{i,j} = \langle \mathbf{q}_i, \mathbf{z} \rangle$

$\mathbf{z} = \mathbf{z} - h_{i,j}\mathbf{q}_i$

end

$h_{j+1,j} = \|\mathbf{z}\|$

if $h_{j+1,j} = 0$ **then**

return $\mathbf{Q}_k, \mathbf{H}_k$

end

$\mathbf{q}_{j+1} = \mathbf{z} / h_{j+1,j}$

end

return $\mathbf{Q}_k, \mathbf{H}_k$

When \mathbf{A} is symmetric then $\mathbf{H} = \mathbf{T}$ becomes a tridiagonal matrix, simplifying a large amount of the Arnoldi algorithm since the matrix elements from \mathbf{T} can be written as

$$\mathbf{T} = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix}.$$

As before, equating the j^{th} columns of $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{T}$ yields

$$(48) \quad \mathbf{A}\mathbf{q}_j = \beta_{j-1}\mathbf{q}_{j-1} + \alpha_j\mathbf{q}_j + \beta_j\mathbf{q}_{j+1}.$$

Again since $\{\mathbf{q}_i\}_{i=1}^n$ form an orthonormal basis, multiplying both sides of equation 48 by \mathbf{q}_j gives $\mathbf{q}_j\mathbf{A}\mathbf{q}_j = \alpha_j$. A simplified version of the Arnoldi algorithm can be devised can be used to compute $\{\mathbf{q}_i\}_{i=1}^n$ and \mathbf{T} for symmetric matrices known as the Lanczos algorithm [Dem97]. The Lanczos algorithm is presented in algorithm 7.

Algorithm 7: Lanczos Algorithm

input : A, r_0 and k , the number of columns of Q to compute.

output: Q_k, T_k .

$q_1 = r_0 / \|r_0\|, \beta_0 = 0, q_0 = 0$

for $j = 1$ **to** k **do**

$z = Aq_j$

$\alpha_j = \langle q_j, z \rangle$

$z = z - \alpha_j q_j - \beta_{j-1} q_{j-1}$

$\beta_j = \|z\|$

if $\beta_j = 0$ **then**

 | **return** Q_k, T_k

end

$q_{j+1} = z / \beta_j$

end

return Q_k, T_k

For the Lanczos algorithm, equation 46 can be re-written in the a more compact form as

$$(49) \quad AV_k = V_k T_{k+1,k}$$

where $T_{k+1,k} = T_k + v_{k+1} t_k^\top$.

3.4. Optimality Conditions. So far we have shown that $x^* \in \mathcal{K}_{t_{r_0}, A}(A, r_0)$ where $n = t_{r_0}$ is the grade of r_0 with respect to A . Moreover from section 3.3 we found ways to construct a basis for $\mathcal{K}_{t_{r_0}, A}(A, r_0)$ allowing us to generate vectors with these affine spaces, namely the Arnoldi algorithm (algorithm 6) and Lanczos algorithm (algorithm 7) for non-symmertic and symmertic systems respectively. From now on $\mathcal{K}_{t_{r_0}, A}(A, r_0)$ will be abbreviated to $\mathcal{K}_{t_{r_0}, A}$ when the context is clear. The question still remains however, how should one choose an x_k that best approximates x^* satisfying equation 39? Here are a few of the most well known methods for selecting a suitable x_k .

- (1) Select an $x_k \in x_0 + \mathcal{K}_k$ which minimizes $\|x_k - x^*\|_2$. While this method seems like the most intuitive and natural way to select x_k , it is unfortunately of no practical use since there is not enough information in the Krylov subspace to find an x_k which matches this specification.
- (2) Select an $x_k \in x_0 + \mathcal{K}_k$ which minimizes $\|r_k\|_2$ (recall this is the residual of x_k , that is, $r_k = b - Ax_k$). This method is possible to implement. Two well known algorithms stem from this class of methods, namely MINRES (minimum residual) and GMRES (general minimum residual) which solve linear systems for symmetric and non-symmertic A respectively.
- (3) When A is a positive definite matrix it defines a norm $\|r\|_A = (r^\top A r)^{\frac{1}{2}}$, called the energy norm. Select an $x_k \in x_0 + \mathcal{K}_k$ which minimizes $\|r\|_{A^{-1}}$ which is equivalent to minimizing $\|x_k - x\|_A$. This technique is known as the CG (conjugate gradient) algorithm.
- (4) Select an $x_k \in x_0 + \mathcal{K}_k$ for which $r_k \perp \mathcal{W}_k$ where \mathcal{W}_k is some k -dimensional subspace. Two well known algorithms that belong to this family of methods are SYMMLQ (Symmetric LQ Method) and a variant of GMRES used for solving symmetric and non-symmetric methods respectively.

Interestingly, when A is symmetric positive definite and $\mathcal{W}_k = \mathcal{K}_k$ the last two selection methods are equivalent. This is stated more precisely in theorem 29 without proof.

Theorem 29. *In the context of the above selection method, if $A \succ 0$ and $\mathcal{W}_k = \mathcal{K}_k$ in method (4) then it produces the same x_k in method (3) [Dem97].*

In fact the very last method can be used to bring together a number of different analytical aspects and unify them in a general framework known as projection methods. Selecting an x_k from our Krylov subspace allows k degrees of freedom meaning k constraints must be used to determine a unique x_k for selection. As seen in method (4) already, typically orthogonality constraints are imposed on the residual r_k . Specifically we would like to find a $x_k \in x_0 + \mathcal{K}_k$ where $r_k \perp \mathcal{W}_k$. This is sometimes referred to as the Petrov-Galerkin (or just Galerkin) conditions. Projection methods for which $\mathcal{W}_k = \mathcal{K}_k$ are known as orthogonal projections while methods for which $\mathcal{W}_k = A\mathcal{K}_k$ are known as oblique projections. If we set $x_k = x_0 + z_k$ for some $z_k \in \mathcal{K}_k$ then the Petrov-Galerkin conditions imply $r_0 - Az_k \perp \mathcal{W}_k$, or alternatively $\langle r_0 - Az_k, w \rangle = 0$ for every $w \in \mathcal{W}_k$. To impose these conditions it will help to have an appropriate basis for \mathcal{K} and \mathcal{W} . Suppose we have access to such a basis where $\{q_i\}_{i=1}^k$ and $\{w_i\}_{i=1}^k$ are basis elements for \mathcal{K} and \mathcal{W} respectively. Let

$$K_k \triangleq [v_1, v_2, \dots, v_k] \in \mathbb{K}^{n \times k}$$

$$W_k \triangleq [w_1, w_2, \dots, w_k] \in \mathbb{K}^{n \times k}$$

then the Petrov-Galerkin conditions can be imposed as follows

$$K_k y_k = z_k, \quad \text{for some } y_k \in \mathbb{K}^k$$

$$W_k^\top (r_0 - AK_k y_k) = 0.$$

Moreover if $W_k^\top AK_k$ is invertible then x_k can be expressed as

$$(50) \quad x_k = x_0 + K_k (W_k^\top AK_k)^{-1} W_k^\top r_0.$$

This justifies a general form of the projection method algorithm presented in algorithm 8.

Algorithm 8: General Projection Method

output: An approximation of x^* , x_k .

for $k = 1, \dots$ **until convergence do**

 Select \mathcal{K}_k and \mathcal{W}_k

 Form K_k and W_k

 Solve $(W_k^\top AK_k) y_k = W_k^\top r_0$

$x_k = x_0 + K_k y_k$

end

return x_k

3.5. Conjugate Gradient Algorithm. From section 3.4 that the Petrov-Galerkin conditions for the CG algorithm used an orthogonal projection and the matrix A was assumed to be positive definite. To derive the CG algorithm we can start by using some machinery that the Lanczos algorithm provides us with. Recall, the Lanczos algorithm produces the form $AQ_k = Q_k T_k + q_{k+1} t_k^\top$ where $t_k \triangleq [0, 0, \dots, 0, \beta_k]^\top \in \mathbb{K}^k$

and the columns of \mathbf{Q}_k span \mathcal{K}_k . Recall that \mathbf{x}_k can be expressed as $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{K}_k (\mathbf{W}_k^\top \mathbf{A} \mathbf{K}_k)^{-1} \mathbf{W}_k \mathbf{r}_0$ (equation 50) when $\mathbf{W}_k^\top \mathbf{A} \mathbf{K}_k$ is invertible. For the CG algorithm $\mathcal{K} = \mathcal{W}$ and $\mathbf{A} \succ \mathbf{0}$. Under these conditions we can easily show that $\mathbf{W}_k^\top \mathbf{A} \mathbf{K}_k$ is indeed invertible. This means the approximate vector can be expressed as $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{z}_k$ where $\mathbf{z}_k \in \mathcal{K}_k$. In terms of the Petrov-Galerkin conditions this means that \mathbf{z}_k must satisfy $\mathbf{r}_0 - \mathbf{A} \mathbf{z}_k \perp \mathcal{W}_k$. Furthermore since $\mathcal{K}_k = \text{Range}(\mathbf{Q}_k)$ where \mathbf{Q}_k has full column rank then \mathbf{z}_k can be represented as $\mathbf{z}_k = \mathbf{Q}_k \mathbf{y}$ for a unique $\mathbf{y} \in \mathbb{K}^k$ so that

$$(51) \quad \mathbf{x}_k = \mathbf{x}_0 + \mathbf{Q}_k \mathbf{y}.$$

Coupling this with the Petrov-Galerkin conditions means

$$(52) \quad \begin{aligned} \mathbf{Q}_k^\top (\mathbf{r}_0 - \mathbf{A} \mathbf{Q}_k \mathbf{y}) &= \mathbf{0} \\ \mathbf{Q}_k^\top \mathbf{A} \mathbf{Q}_k \mathbf{y} &= \mathbf{Q}_k^\top \mathbf{r}_0 \\ \mathbf{T}_k \mathbf{y} &= \|\mathbf{r}_0\| \mathbf{e}_1. \end{aligned}$$

In the CG algorithm \mathbf{x}_{k+1} is computed as the recurrence of the following three sets of vectors

- (1) The approximate solutions \mathbf{x}_k
- (2) The residual vectors \mathbf{r}_k
- (3) The conjugate gradient vectors \mathbf{p}_k

The conjugate gradient vectors are given the name gradient since the attempt to find the direction of steepest descent that minimizes $\|\mathbf{r}_k\|_{\mathbf{A}^{-1}}$. They are also given the name conjugate since $\langle \mathbf{p}_k, \mathbf{A} \mathbf{p}_j \rangle = 0$ for $i \neq j$, that is, vectors \mathbf{p}_i and \mathbf{p}_j are mutually \mathbf{A} -conjugate.

Since \mathbf{A} is symmetric positive definite then so is $\mathbf{T}_k = \mathbf{Q}_k \mathbf{A} \mathbf{Q}_k$. We can take the Cholesky decomposition of \mathbf{T}_k to get

$$(53) \quad \mathbf{T}_k = \mathbf{L}_k \mathbf{D}_k \mathbf{L}_k^\top$$

where \mathbf{L}_k is a unit lower bidiagonal matrix and \mathbf{D}_k is diagonal written as

$$\mathbf{L}_k = \begin{bmatrix} 1 & & & \\ l_1 & \ddots & & \\ & \ddots & \ddots & \\ & & l_{k-1} & 1 \end{bmatrix}, \quad \mathbf{D}_k = \begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_k \end{bmatrix}.$$

Combining equations 51, 52 and 53

$$\begin{aligned} \mathbf{x}_k &= \mathbf{x}_0 + \mathbf{Q}_k \mathbf{y} \\ \mathbf{x}_k &= \mathbf{x}_0 + \|\mathbf{r}_0\| \mathbf{Q}_k \mathbf{T}_k^{-1} \mathbf{e}_1 \\ \mathbf{x}_k &= \mathbf{x}_0 + \|\mathbf{r}_0\| \mathbf{Q}_k (\mathbf{L}_k \mathbf{D}_k \mathbf{L}_k^\top)^{-1} \mathbf{e}_1 \\ \mathbf{x}_k &= \mathbf{x}_0 + \left(\mathbf{Q}_k \mathbf{L}_k^{-\top} \right) (\|\mathbf{r}_0\| \mathbf{D}_k^{-1} \mathbf{L}_k^{-1} \mathbf{e}_1) \\ \mathbf{x}_k &\triangleq \mathbf{x}_0 + \tilde{\mathbf{P}}_k \tilde{\mathbf{y}}_k \end{aligned}$$

where $\tilde{\mathbf{P}}_k = \mathbf{Q}_k \mathbf{L}_k^{-\top}$ and $\tilde{\mathbf{y}}_k = \|\mathbf{r}_0\| \mathbf{D}_k^{-1} \mathbf{L}_k^{-1} \mathbf{e}_1$. The matrix $\tilde{\mathbf{P}}_k$ can be written as $\tilde{\mathbf{P}}_k = [\tilde{\mathbf{p}}_1, \tilde{\mathbf{p}}_2, \dots, \tilde{\mathbf{p}}_k]$. Lemma 30 shows that the columns of $\tilde{\mathbf{P}}_k$ are \mathbf{A} -conjugate.

Lemma 30. *The columns of $\tilde{\mathbf{P}}_k$ are A -conjugate, in otherwise $\tilde{\mathbf{P}}_k^\top \mathbf{A} \tilde{\mathbf{P}}_k$ is diagonal.*

Proof. We compute

$$\begin{aligned}
 \tilde{\mathbf{P}}_k^\top \mathbf{A} \tilde{\mathbf{P}}_k &= \left(\mathbf{Q}_k \mathbf{L}_k^{-\top} \right)^\top \mathbf{A} \left(\mathbf{Q}_k \mathbf{L}_k^{-\top} \right) \\
 &= \mathbf{L}_k^{-1} \left(\mathbf{Q}_k^\top \mathbf{A} \mathbf{Q}_k \right) \mathbf{L}_k^{-\top} \\
 &= \mathbf{L}_k^{-1} \left(\mathbf{T}_k \right) \mathbf{L}_k^{-\top} \\
 &= \mathbf{L}_k^{-1} \left(\mathbf{L}_k \mathbf{D}_k \mathbf{L}_k^\top \right) \mathbf{L}_k^{-\top} \\
 &= \mathbf{D}_k
 \end{aligned}$$

(equation 53)

as wanted. □

Since \mathbf{L}_k is a lower bidiagonal, setting $\mathbf{a} \triangleq l_{k-1} \mathbf{e}_{k-1}$, it can be written in the form

$$\mathbf{L}_k = \begin{bmatrix} \mathbf{L}_{k-1} & \mathbf{0} \\ \mathbf{a}^\top & 1 \end{bmatrix}$$

meaning

$$\mathbf{L}_k^{-1} = \begin{bmatrix} \mathbf{L}_{k-1}^{-1} & \mathbf{0} \\ \star & 1 \end{bmatrix}.$$

With this a recurrence for the columns of $\tilde{\mathbf{P}}_k$ can now be derived in terms of \mathbf{y}_k . To start we can show that the first $k-1$ entries of $\tilde{\mathbf{y}}_k$ shares the first $k-1$ entries with $\tilde{\mathbf{y}}_{k-1}$ and that $\tilde{\mathbf{P}}_k$ and $\tilde{\mathbf{P}}_{k-1}$ share the same first $k-1$ columns. To start we can compute a recurrence for $\tilde{\mathbf{y}}_k$ as follows

$$\begin{aligned}
 \tilde{\mathbf{y}}_k &= \|\mathbf{r}_0\| \mathbf{D}_k^{-1} \mathbf{L}_k^{-1} \mathbf{e}_1^k \\
 &= \|\mathbf{r}_0\| \begin{bmatrix} \mathbf{D}_{k-1}^{-1} & \mathbf{0} \\ \mathbf{0} & d_k^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{L}_{k-1}^{-1} & \mathbf{0} \\ \star & 1 \end{bmatrix} \mathbf{e}_1^k \\
 &= \|\mathbf{r}_0\| \begin{bmatrix} \mathbf{D}_{k-1}^{-1} \mathbf{L}_{k-1}^{-1} & \mathbf{0} \\ \star & d_k^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{e}_1^k \\ 0 \end{bmatrix} \\
 &= \begin{bmatrix} \tilde{\mathbf{y}}_{k-1} \\ \eta_k \end{bmatrix}
 \end{aligned}$$

To get a recurrence for the columns of $\tilde{\mathbf{P}}_{k-1} = [\tilde{\mathbf{p}}_1, \tilde{\mathbf{p}}_2, \dots, \tilde{\mathbf{p}}_k]$ since \mathbf{L}_{k-1}^\top is upper triangular then so is $\mathbf{L}_{k-1}^{-\top}$, thus forming the leading $(k-1) \times (k-1)$ submatrix of $\mathbf{L}_k^{-\top}$. This means that $\tilde{\mathbf{P}}_{k-1}$ is identical to the leading $k-1$ columns of

$$\tilde{\mathbf{P}}_k = \mathbf{Q}_k \mathbf{L}_k^{-\top} = [\mathbf{Q}_{k-1}, \mathbf{q}_k] \begin{bmatrix} \mathbf{L}_{k-1}^{-1} & \mathbf{0} \\ \star & 1 \end{bmatrix} = [\mathbf{Q}_{k-1} \mathbf{L}_{k-1}^{-1}, \tilde{\mathbf{p}}_k] = [\tilde{\mathbf{P}}_{k-1}, \tilde{\mathbf{p}}_k].$$

Moreover rearranging $\tilde{\mathbf{P}}_k = \mathbf{Q}_k \mathbf{L}_k^{-\top}$ we get $\tilde{\mathbf{P}}_k \mathbf{L}_k^\top = \mathbf{Q}_k$. Equating the k^{th} column yields

$$(54) \quad \tilde{\mathbf{p}}_k = \mathbf{q}_k - l_{k-1} \tilde{\mathbf{p}}_{k-1}.$$

Finally we can use

$$(55) \quad \mathbf{x}_k = \mathbf{x}_0 + \tilde{\mathbf{P}}_k \tilde{\mathbf{y}}_k = \mathbf{x}_0 + \begin{bmatrix} \tilde{\mathbf{P}}_{k-1} & \tilde{\mathbf{p}}_k \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{y}}_{k-1} \\ \eta_k \end{bmatrix} = \mathbf{x}_0 + \tilde{\mathbf{P}}_{k-1} \tilde{\mathbf{y}}_{k-1} + \eta_k \tilde{\mathbf{p}}_k = \mathbf{x}_{k-1} + \eta_k \tilde{\mathbf{p}}_k$$

as a recurrence for \mathbf{x}_k . A recurrence for \mathbf{r}_k is easily computed as

$$(56) \quad \mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k = \mathbf{b} - \mathbf{A}(\mathbf{x}_{k-1} + \eta_k \tilde{\mathbf{p}}_k) = (\mathbf{b} - \mathbf{A}\mathbf{x}_{k-1}) - \eta_k \mathbf{A}\tilde{\mathbf{p}}_k = \mathbf{r}_{k-1} - \eta_k \mathbf{A}\tilde{\mathbf{p}}_k$$

Altogether we are left with recurrences for \mathbf{q}_k from Lanczos, $\tilde{\mathbf{p}}_k$ (equation 54), the residual \mathbf{r}_k (equation 54), and for the approximate solution \mathbf{x}_k (equation 55). However, further simplification can be made for a more efficient algorithm. Recall from section 3.3 that $\mathbf{A}\mathbf{Q}_k = \mathbf{Q}_k \mathbf{T}_k + \mathbf{q}_{k+1} \mathbf{t}_k^\top$ where $\mathbf{t}_k = [0, 0, \dots, 0, \beta_k]^\top \in \mathbb{K}^k$ meaning

$$\mathbf{r}_k = \mathbf{r}_0 - \mathbf{A}\mathbf{Q}_k \mathbf{y}_k = \mathbf{r}_0 - \mathbf{Q}_k \mathbf{T}_k \mathbf{y}_k - \langle \mathbf{t}_k, \mathbf{y} \rangle \mathbf{q}_{k+1} = -\beta_k \mathbf{y}_k \mathbf{q}_{k+1}.$$

This tells us that \mathbf{r}_k is parallel to \mathbf{q}_{k+1} and orthogonal to all \mathbf{q}_i , $1 \leq i \leq k$. This further implies that \mathbf{r}_k is orthogonal to all \mathbf{r}_i , $1 \leq i \leq k-1$ since they are just \mathbf{q}_i scaled by some constant factor. So replacing \mathbf{r}_{k-1} with \mathbf{q}_k/η_k and defining $\mathbf{p}_k \triangleq \tilde{\mathbf{p}}_k/\gamma_k$ gives us a new set of recurrences

$$\begin{aligned} \mathbf{x}_k &= \mathbf{x}_{k-1} + \alpha_k \mathbf{p}_k \\ \mathbf{r}_k &= \mathbf{r}_{k-1} - \alpha_k \mathbf{A}\mathbf{p}_k \\ \mathbf{p}_k &= \mathbf{r}_{k-1} + \beta_k \mathbf{p}_{k-1} \end{aligned}$$

where $\alpha_k = \eta_k/\gamma_k$. From theorem 30 we have shown that the columns of $\tilde{\mathbf{P}}_k$ are A -conjugate (that is $\langle \tilde{\mathbf{p}}_i, \mathbf{A}\tilde{\mathbf{p}}_j \rangle = 0$, $i \neq j$) and that $\tilde{\mathbf{P}}_k^\top \mathbf{A}\tilde{\mathbf{P}}_k = \mathbf{D}_k$. This also means that $\langle \mathbf{r}_i, \mathbf{r}_j \rangle = 0$, $i \neq j$. Now note that from our recurrence for $\mathbf{p}_k = \mathbf{r}_{k-1} + \beta_k \mathbf{p}_{k-1}$ that

$$\langle \mathbf{A}\mathbf{p}_k, \mathbf{p}_k \rangle = \langle \mathbf{A}\mathbf{p}_k, \mathbf{r}_{k-1} + \beta_k \mathbf{p}_{k-1} \rangle = \langle \mathbf{A}\mathbf{p}_k, \mathbf{r}_{k-1} \rangle.$$

We can now find an expression for α_k as

$$\begin{aligned} \langle \mathbf{r}_{k-1}, \mathbf{r}_k \rangle &= \langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} - \alpha_k \mathbf{A}\mathbf{p}_k \rangle \\ \langle \mathbf{r}_{k-1}, \mathbf{r}_k \rangle &= \langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle - \alpha_k \langle \mathbf{r}_{k-1}, \mathbf{A}\mathbf{p}_k \rangle \\ \alpha_k &= \frac{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}{\langle \mathbf{p}_k, \mathbf{A}\mathbf{p}_k \rangle}. \end{aligned}$$

Similarly, using the recurrence for \mathbf{p}_k , an expression for β_k can be computed as

$$\begin{aligned} \langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{p}_k \rangle &= \langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{r}_{k-1} + \beta_k \mathbf{p}_{k-1} \rangle \\ \langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{p}_k \rangle &= \langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{r}_{k-1} \rangle + \beta_k \langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{p}_{k-1} \rangle \\ \beta_k &= -\frac{\langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{r}_{k-1} \rangle}{\langle \mathbf{A}\mathbf{p}_{k-1}, \mathbf{p}_{k-1} \rangle}. \end{aligned}$$

This formula requires an additional dot product which was not present before. Fortunately, this dot product can be eliminated using our recurrence for \mathbf{r}_k

$$\begin{aligned} \langle \mathbf{r}_k, \mathbf{r}_k \rangle &= \langle \mathbf{r}_k, \mathbf{r}_{k-1} - \alpha_k \mathbf{A}\mathbf{p}_k \rangle \\ \langle \mathbf{r}_k, \mathbf{r}_k \rangle &= \langle \mathbf{r}_k, \mathbf{r}_{k-1} \rangle - \alpha_k \langle \mathbf{r}_k, \mathbf{A}\mathbf{p}_k \rangle \\ \alpha_k &= -\frac{\langle \mathbf{r}_k, \mathbf{r}_k \rangle}{\langle \mathbf{r}_k, \mathbf{A}\mathbf{p}_k \rangle}. \end{aligned}$$

Equating the two expressions for \mathbf{a}_k yields

$$\begin{aligned} -\frac{\langle \mathbf{r}_k, \mathbf{r}_k \rangle}{\langle \mathbf{r}_k, \mathbf{A}\mathbf{p}_k \rangle} &= \frac{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}{\langle \mathbf{p}_k, \mathbf{A}\mathbf{p}_k \rangle} \\ -\frac{\langle \mathbf{r}_k, \mathbf{r}_k \rangle}{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle} &= \frac{\langle \mathbf{r}_k, \mathbf{A}\mathbf{p}_k \rangle}{\langle \mathbf{p}_k, \mathbf{A}\mathbf{p}_k \rangle}. \end{aligned}$$

This means that

$$\beta_k = \frac{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}{\langle \mathbf{r}_{k-2}, \mathbf{r}_{k-2} \rangle}.$$

These recurrences are computed iteratively to form the basis of the CG algorithm, seen in Algorithm 9.

Algorithm 9: CG Algorithm

input : $\mathbf{A} \succ \mathbf{0}$, \mathbf{b} and an initial guess \mathbf{x}_0 .

output: An approximation of \mathbf{x}^* , \mathbf{x}_k .

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$, $\mathbf{p}_1 = \mathbf{r}_0$

for $k = 1, \dots$ **until** $\|\mathbf{r}_{k-1}\| \leq \tau$ **do**

$$\alpha_k = \frac{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}{\langle \mathbf{p}_k, \mathbf{A}\mathbf{p}_k \rangle}$$

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_k \mathbf{p}_k$$

$$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{A}\mathbf{p}_k$$

$$\beta_{k+1} = \frac{\langle \mathbf{r}_k, \mathbf{r}_k \rangle}{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}$$

$$\mathbf{p}_{k+1} = \mathbf{r}_k + \beta_{k+1} \mathbf{p}_k$$

end

return \mathbf{x}_k

3.6. Minimum Residual. In contrast to CG, MINRES is applicable to a wider range of linear systems and is used for solving symmetric indefinite systems. From section 3.4 we saw that MINRES minimizes the residual \mathbf{r}_k with respect to the Euclidean norm at each iteration (hence the name), that is \mathbf{x}_k is chosen so that

$$(57) \quad \mathbf{x}_k = \arg \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2.$$

It can be shown that this is equivalent setting $\mathcal{W} = \mathbf{A}\mathcal{K}_k$ in the Petrov-Galerkin conditions where $\det(\mathbf{A}) \neq 0$, in other words MINRES is an oblique projection method. We can also show that when $\det(\mathbf{A}) \neq 0$ and $\mathcal{W} = \mathbf{A}\mathcal{K}_k$ the matrix $\mathbf{W}^\top \mathbf{A}\mathbf{K}$ is non-singular. So under the conditions of MINRES, using a similar argument used for CG, \mathbf{x}_k can be expressed as $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{V}_k \mathbf{y}_k$. Using equation 49 produced by the Lanczos algorithm in 3.3 we can manipulate our optimality condition 57 as follows

$$\begin{aligned} \mathbf{x}_k &= \arg \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 \\ \iff \mathbf{y}_k &= \arg \min_{\mathbf{y} \in \mathbb{R}^k} \|\mathbf{A}(\mathbf{x}_0 + \mathbf{V}_k \mathbf{y}) - \mathbf{b}\|_2 \\ &= \arg \min_{\mathbf{y} \in \mathbb{R}^k} \|-(\mathbf{b} - \mathbf{A}\mathbf{x}_0) + \mathbf{A}\mathbf{V}_k \mathbf{y}\|_2 \\ &= \arg \min_{\mathbf{y} \in \mathbb{R}^k} \|\mathbf{V}_k \mathbf{T}_{k+1,k} \mathbf{y} - \mathbf{r}_0\|_2 \end{aligned}$$

$$\begin{aligned}
&= \arg \min_{\mathbf{y} \in \mathbb{R}^k} \|\mathbf{T}_{k+1,k} \mathbf{y} - \mathbf{V}_k^\top \mathbf{r}_0\|_2 \\
&= \arg \min_{\mathbf{y} \in \mathbb{R}^k} \|\mathbf{T}_{k+1,k} \mathbf{y} - \beta_0 \mathbf{e}_1\|_2
\end{aligned}$$

[Gre97, page 43]. Using the general project method procedure 8 as a guide, this gives the following high-level description of the MINRES algorithm [Tre97, page 268].

Algorithm 10: High-Level MINRES

output: An approximation of \mathbf{x}^* , \mathbf{x}_k .

for $k = 1, \dots$ **until convergence do**

 Lanczos-Step (\mathbf{A} , \mathbf{v}_k , \mathbf{v}_{k-1} , β_k) $\rightarrow \alpha_k, \beta_{k+1}, \mathbf{v}_{k+1}$

 Find \mathbf{y} to minimize $\|\mathbf{T}_{k+1,k} \mathbf{y} - \beta_0 \mathbf{e}_1\|_2$

$\mathbf{x}_k = \mathbf{V}_k \mathbf{y}$

end

return \mathbf{x}_k

At each step solving \mathbf{y} is a matter of solving a $(n+1) \times n$ least squares problem with Hessenberg structure. This can be done by performing a QR-factorisation on the successive $\mathbf{T}_{k+1,k}$ matrices, whats more using a clever bit of thinking, we can actually compute the QR-factorisation of $\mathbf{T}_{k+1,k}$ from the QR-factorisation of $\mathbf{T}_{k,k-1}$ using a inexpensive $\mathcal{O}(n)$ Householder reflection [Tre97, page 268]. Computing the QR-factorisation of $\mathbf{T}_{k,k-1}$ yields

$$(58) \quad \mathbf{Q}_k \mathbf{T}_{k,k+1} = \begin{bmatrix} \mathbf{R}_k \\ 0 \end{bmatrix} = \begin{bmatrix} \gamma_1^{(1)} & \delta_2^{(1)} & \varepsilon_3^{(1)} & & & & \\ & \gamma_1^{(2)} & \delta_3^{(2)} & \varepsilon_4^{(1)} & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & \ddots & \ddots & \varepsilon_k^{(1)} \\ & & & & & \ddots & \gamma_k^{(2)} \\ & & & & & & \delta_k^{(2)} \\ & & & & & & & 0 \end{bmatrix}$$

where $\mathbf{Q}_k = \prod_{i=1}^k \mathbf{Q}_{i,i+1}$ is the product of Householder reflections designed to annihilate the β_i s in the subdiagonal of $\mathbf{T}_{k,k+1}$ [Cho07, page 25] where each $\mathbf{Q}_{i,i+1}$ is defined as

$$\mathbf{Q}_{i,i+1} \triangleq \begin{bmatrix} \mathbb{1}_{(i-1) \times (i-1)} & & \\ & c_i & s_{i-1} \\ & & \mathbb{1}_{(k-i) \times (k-i)} \end{bmatrix}$$

[Cho07, page 22]. As mentioned for each i , $\mathbf{Q}_{i,i+1}$ is orthogonal, symmetric and constructed to annihilate β_{k+1} that is the bottom right element of $\mathbf{T}_{k,k+1}$. To see this better we can alternatively write $\mathbf{Q}_k \mathbf{T}_{k,k+1}$ as $\mathbf{Q}_{k,k+1} \cdot \mathbf{Q}_{2,3} \mathbf{Q}_{1,2} \mathbf{T}_{k,k+1}$. Notice however that $\mathbf{Q}_{k,k+1}$ is the only rotation matrix that will involve β_{k+1} in its matrix multiplication with $\mathbf{T}_{k,k+1}$. To study the influence of $\mathbf{Q}_{k,k+1}$ in a more compact way we only need to consider the matrix vector product

$$(59) \quad \begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} \begin{bmatrix} \gamma_k^{(1)} & \delta_{k+1}^{(1)} & 0 \\ \beta_{k+1} & \alpha_{k+1} & \beta_{k+1} \end{bmatrix}.$$

To annihilate β_{k+1} , we find the appropriate choice of c_k and s_k are

$$\rho_k = \sqrt{\gamma_k^{(1)^2} + \beta_{k+1}^2}, \quad c_k \triangleq \frac{\gamma_k^{(1)}}{\rho_k}, \quad s_k \triangleq \frac{\beta_{k+1}}{\rho_k}$$

so that 59 becomes

$$\begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} \begin{bmatrix} \gamma_k^{(1)} & \delta_{k+1}^{(1)} & 0 \\ \beta_{k+1} & \alpha_{k+1} & \beta_{k+1} \end{bmatrix} = \begin{bmatrix} \gamma_k^{(2)} & \delta_{k+1}^{(2)} & \varepsilon_{k+2}^{(1)} \\ 0 & \gamma_{k+1}^{(1)} & \delta_{k+2}^{(1)} \end{bmatrix}.$$

Furthermore, if we set

$$\begin{aligned} \mathbf{Q}_k(\beta_0 \mathbf{e}_1) &= \prod_{i=1}^k \mathbf{Q}_{i,i+1}(\beta_0 \mathbf{e}_1) \\ &= \beta_0 \mathbf{Q}_{k,k+1} \cdots \mathbf{Q}_{2,3} \begin{bmatrix} c_1 \\ s_1 \\ \mathbf{0}_{k-1} \end{bmatrix} \\ &= \beta_0 \mathbf{Q}_{k,k+1} \cdots \mathbf{Q}_{3,4} \begin{bmatrix} c_1 \\ s_1 c_1 \\ s_1 s_2 \\ \mathbf{0}_{k-2} \end{bmatrix} \\ &= \beta_0 \mathbf{Q}_{k,k+1} \begin{bmatrix} c_1 \\ s_1 c_1 \\ \vdots \\ s_1 \cdots s_{k-1} \\ 0 \end{bmatrix} \\ &= \mathbf{Q}_{k,k+1} \begin{bmatrix} \mathbf{t}_{k-1} \\ \phi_{k-1} \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{t}_k \\ \phi_{k-1} \end{bmatrix} \end{aligned}$$

where $\mathbf{t}_k = [\tau_1, \tau_2, \dots, \tau_k]^\top$ then our optimality condition becomes

$$\mathbf{y}_k = \arg \min_{\mathbf{y} \in \mathbb{R}^k} \left\| \begin{bmatrix} \mathbf{R}_k \\ 0 \end{bmatrix} \mathbf{y} - \begin{bmatrix} \mathbf{t}_k \\ \phi_{k-1} \end{bmatrix} \right\|_2$$

which can be used to formulate subproblems [Cho07, page 25]. From the new optimality condition it is obvious that the optimal solution will satisfy $\mathbf{R}_k \mathbf{y}_k = \mathbf{t}_k$. However, instead of solving for \mathbf{y}_k directly, MINRES solves

$$(60) \quad \mathbf{R}_k^\top \mathbf{D}_k^\top = \mathbf{V}_k^\top$$

where $\mathbf{D}_k = [\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_k] \triangleq \mathbf{V}_k \mathbf{R}_k^{-1}$. This is done by forward substitution obtaining the last column \mathbf{d}_k of \mathbf{D}_k at iteration k . At the same time \mathbf{x}_k is updated as

$$\begin{aligned} \mathbf{x}_k &= \mathbf{V}_k \mathbf{y}_k = \mathbf{D}_k \mathbf{R}_k \mathbf{y}_k = \mathbf{D}_k \mathbf{t}_k \\ &= [\mathbf{D}_{k-1}, \mathbf{d}_k] \begin{bmatrix} \mathbf{t}_{k-1} \\ \tau_t \end{bmatrix} \\ (61) \quad &= \mathbf{x}_{k-1} + \tau_k \mathbf{d}_k. \end{aligned}$$

The d_j in equation 61 can be found as

$$\begin{cases} \mathbf{d}_1 = \mathbf{v}_1 / \gamma_1 \\ \mathbf{d}_2 = (\mathbf{v}_2 - \delta_2 \mathbf{d}_1) / \gamma_2^{(2)} \\ \mathbf{d}_j = (\mathbf{v}_j - \delta_j^{(2)} \mathbf{d}_{j-1} - \varepsilon_j \mathbf{d}_{j-2}) / \gamma_j^{(2)}, \quad j = 3, \dots, k \end{cases}$$

from equation 60 [CHO11, page 4]. The final form of the MINRES is presented in algorithm 11.

Algorithm 11: MINRES Algorithm

input : \mathbf{A} where $\mathbf{A} = \mathbf{A}^\top$, \mathbf{b} and an initial guess \mathbf{x}_0 .

output: An approximation of \mathbf{x}^* , \mathbf{x}_k .

$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$, $\tau_0 = \beta_0 = \|\mathbf{r}_0\|$, $\mathbf{v}_1 = \mathbf{r}_0 / \beta_0$, $\delta_1^{(1)} = 0$, $\mathbf{v}_0 = \mathbf{d}_0 = \mathbf{d}_{-1} = \mathbf{0}$

for $k = 1, \dots$ **until convergence do**

Lanczos-Step ($\mathbf{A}, \mathbf{v}_k, \mathbf{v}_{k-1}, \beta_k$) $\rightarrow \alpha_k, \beta_{k+1}, \mathbf{v}_{k+1}$

$$\begin{bmatrix} \delta_k^{(2)} & \varepsilon_{k+1}^{(1)} \\ \gamma_k^{(1)} & \delta_{k+1}^{(1)} \end{bmatrix} = \begin{bmatrix} c_{k-1} & s_{k-1} \\ s_{k-1} & -c_{k-1} \end{bmatrix} \begin{bmatrix} \delta_k^{(1)} & 0 \\ \alpha_k & \beta_{k+1} \end{bmatrix}$$

$$\rho_k = \sqrt{\gamma_k^{(1)2} + \beta_{k+1}^2}, \quad c_k = \frac{\gamma_k^{(1)}}{\rho_k}, \quad s_k = \frac{\beta_{k+1}}{\rho_k}$$

$$\gamma_k^{(2)} = c_k \gamma_k^{(1)}$$

$$\tau_k = c_k \phi_{k-1}, \quad \phi_k = s_k \phi_{k-1}$$

$$\mathbf{d}_k = (\mathbf{v}_k - \delta_k^{(2)} \mathbf{d}_{k-1} - \varepsilon_k \mathbf{d}_{k-2}) / \gamma_k^{(2)}$$

$$\mathbf{x}_k + \tau_k \mathbf{d}_k$$

end

return \mathbf{x}_k

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