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A U S T R A L I A

OPTIMIZING PERFORMANCE  
IN GAUSSIAN PROCESSES

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## CONTENTS

ACKNOWLEDGEMENTS . . . . .	iii
SYMBOLS AND NOTATION . . . . .	iv
INTRODUCTION . . . . .	1
1. THE NYSTROM METHOD . . . . .	4
1.1. THE NYSTROM METHOD . . . . .	4
1.2. COLUMN PROBABILITIES . . . . .	8
1.3. LEVERAGE SCORES . . . . .	10
1.3.1. STATISTICAL LEVERAGE SCORES . . . . .	11
1.3.2. RANK- $k$ STATISTICAL LEVERAGE SCORES . . . . .	11
1.3.3. RIDGE LEVERAGE SCORES . . . . .	12
1.4. DATA PROBABILITIES . . . . .	13
2. KRYLOV SUBSPACE METHODS . . . . .	15
2.1. KRYLOV SUBSPACES . . . . .	15
2.2. GRAM-SCHMIDT PROCESS AND QR FACTORISATIONS . . . . .	18
2.3. ARNOLDI AND LANCZOS ALGORITHM . . . . .	20
2.4. OPTIMALITY CONDITIONS . . . . .	24
2.5. CONJUGATE GRADIENT ALGORITHM . . . . .	26
2.6. MINIMUM RESIDUAL . . . . .	31
3. APPLICATIONS AND RESULTS . . . . .	35
3.1. GAUSSIAN PROCESSES PREDICTION REVIEWED . . . . .	35
3.2. EXPERIMENTAL SETUP . . . . .	35
3.2.1. KERNEL MARTIX APPROXIMATION TESTING . . . . .	36
3.2.2. KRYLOV SUBSPACE METHODS APPROXIMATION TESTING . . . . .	37
REFERENCES . . . . .	38



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## SYMBOLS AND NOTATION

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

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

$\mathbf{A}_{(:,\cdot)}$	Index slicing to extract a submatrix from the elements of $\mathbf{A} \in \mathbb{R}^{n \times m}$ , similar to indexing slicing from the python and Matlab programming languages. Each parameter can receive a single value or a 'slice' consisting of a start and an end value separated by a semicolon. The first and second parameter describe what row and columns should be selected, respectively. A single value means that only values from the single specified row/column should be selected. A slice tells us that all rows/columns between the provided range should be selected. Additionally if now start and end values are specified in the slice then all rows/columns should be selected. For example, the slice $\mathbf{A}_{(1:3,j:j')}$ is the submatrix $\mathbb{R}^{3 \times (j'-j+1)}$ matrix containing the first three rows of $\mathbf{A}$ and columns $j$ to $j'$ . As another example, $\mathbf{A}_{(:,j)}$ is the $j^{th}$ column of $\mathbf{A}$ .
$\mathbf{A}^\dagger$	Denotes the unique psuedo inverse or Moore-Penore inverse of $\mathbf{A}$ .
$\mathbb{C}$	The complex numbers.
$C$	The classes in a classification problem.
$\text{cholesky}(\mathbf{A})$	A function to compute the Cholesky decomposition, $\mathbf{L}$ , of the matrix $\mathbf{A}$ , where $\mathbf{L}\mathbf{L}^\top = \mathbf{A}$ .
$\text{cov}(\mathbf{f})$	Gaussian process posterior covariance.
$d$	The number of features in the data set.
$D$	The dimension of the feature space of the feature mapping constructed in the Random Fourier Feature method.
$\mathcal{D}$	The dataset, $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ .
$\text{diag}(\mathbf{w})$	Vector argument, a diagonal matrix containing the elements of vector $\mathbf{w}$ .
$\text{diag}(\mathbf{W})$	Matrix argument, a vector containing the diagonal elements of the matrix $\mathbf{W}$ .
$\mathbb{E}$ or $\mathbb{E}_{q(\mathbf{x})}[z(\mathbf{x})]$	Expectation, or expectation of $z(\mathbf{x})$ where $\mathbf{x} \sim q(\mathbf{x})$ .
$\mathcal{GP}$	Gaussian process $f \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$ , the function $f$ is distributed as a Guassian process with mean function $m(\mathbf{x})$ and covariance function $k(\mathbf{x}, \mathbf{x}')$ .

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



$\mathbb{Z}$ 

The integers,  $\mathbb{Z} = \{\dots, -2, -1, 0, 1, 2, \dots\}$ .

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## INTRODUCTION

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

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

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

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

In this thesis we shall focus on a particular class of ML algorithms called Bayesian models which, unsurprisingly, makes use of Bayesian statistics to drive inference. In Bayesian models a *prior* distribution is used to quantify the uncertainty of the current state of the model before any observations are made. The model can then be updated once data is observed by using the likelihood to give a *posterior* distribution which represents the reduced uncertainty after "teaching" the model new observations. Methods of teaching a model how to change its behavior using a new set of observations often involves the use of a

loss function  $L$ . The loss function is used as an aid in deciding what action,  $a$ , should be taken in to best minimize uncertainty. The best action, roughly speaking, can be evaluated as

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

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

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

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

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

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

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

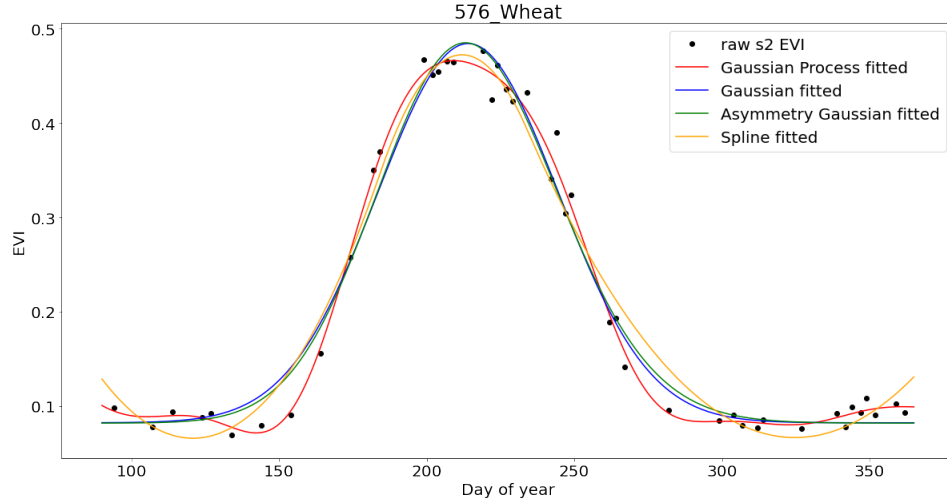


FIGURE 1. Potgieter’s team found that GPs were superior in terms of predicting a phenological timeline for a number of common seasonal crops over other parameteric models.

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

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

## 1. THE NYSTROM METHOD

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

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

[MWM11, page 13]

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

**1.1. The Nystrom Method.** Attempting to compute an entire kernel matrix can be a computational headache prompting an investigation of estimative alternatives. The approximation techniques studied in this chapter have been spurred on by the John-Lindenstrauss lemma stated in Lemma 1.

**Lemma 1** (John-Lindenstrauss). *Given  $0 < \varepsilon < 1$ , any set of  $n$  points,  $X$ , in a high dimensional Euclidean space can be embedded into a  $\ell$ -dimensional Euclidean space where  $\ell = \mathcal{O}(\ln(n))$  via some linear map  $\Omega \in \mathbb{R}^{n \times \ell}$  which satisfies*

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

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

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

$$\|\mathbf{A} - \mathbf{Q}\mathbf{Q}^* \mathbf{A}\|_F \leq \varepsilon$$

which can be expressed in a more short hand notation as

$$(1) \quad \mathbf{A} \simeq \mathbf{Q}\mathbf{Q}^* \mathbf{A}.$$

This is commonly called the *fixed precision approximation problem*. To simplify algorithmic development, a value of  $k$  is specified in advance (instead of  $\varepsilon$ , thus removing  $k$ 's dependence on  $\varepsilon$ ) which is instead given the name *fixed rank problem*. Within the fixed rank problem framework, when  $\mathbf{A}$  is hermitian, the

matrix  $QQ^*$  acts as a good projection for both the columns and row space of  $A$  so that we have both  $A \simeq QQ^*A$  and  $A \simeq AQQ^*$  meaning

$$(2) \quad A \simeq QQ^*(A) \simeq QQ^*AQQ^*.$$

Furthermore, if  $A$  is positive semi-definite we can improve the quality of our approximation of our approximation at almost no additional cost [Hal11, page 32]. Using the approximation from 2

$$(3) \quad \begin{aligned} A &\simeq Q(Q^*AQ)Q^* \\ &= Q(Q^*AQ)(Q^*AQ)^\dagger(Q^*AQ)Q^* \\ &\simeq (AQ)(Q^*AQ)^\dagger(Q^*A). \end{aligned}$$

This is known as the Nystrom method. Since any Gram matrix is positive semi-definite, we can always applied the Nystrom method to find an approximation to it. A general Nystrom framework is presented in Algorithm 1.

---

**Algorithm 1:** General Nystrom Framework

---

**input :** A positive semi-definite matrix  $A \in \mathbb{R}^{n \times m}$ , a matrix  $Q \in n \times k$  that satisfies 1.

**output:** A rank  $k$  approximation  $\bar{A} \simeq A$ .

1  $C = AQ$

2  $W = Q^*C$

3 **return**  $CW^\dagger C^*$

---

However, Algorithm 1 assumes that  $Q$  has already been computed. Naturally, the next question is then how to efficiently construct a suitable matrix  $Q$  that satisfies equation 1? We can do this through a very popular column sampling technique ubiquitous in numerical linear algebra literature. This technique has been driven by Theorem 2.

**Theorem 2.** Every  $A \in \mathbb{R}^{n \times m}$  matrix contains a  $k$ -column submatrix  $C$  for which

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

where  $A_k$  is the best rank- $k$  approximation of  $A$  [Hal11, page 11].

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

$$(4) \quad A = \sum_{i=1}^I A_i.$$

The basic idea is to consider a Monte-Carlo approximation of equation 4 that randomly selects  $A_i$  according to the distribution  $\{p_i\}_{i=1}^I$  to give an estimate

$$(5) \quad A \simeq \frac{1}{c} \sum_{t=1}^c p_{t_i}^{-1} A_{t_i}$$

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

$$AB = \sum_{i=1}^I A_{(:,i)} B_{(i,:)}$$

[FR20,Dri06]. A straight forward way to approximate this using the Monte-Carlo estimate is to simply set each  $A_i$  in 4 to the corresponding rank-1 outer product summand  $A_{(:,i)} B_{(i,:)}$ . This justifies the random matrix multiplication algorithm seen in Algorithm 2 [PDaMWM17, page 16].

---

**Algorithm 2:** Random Matrix Multiplication

---

**input :**  $A \in \mathbb{R}^{n \times I}$  and  $B \in \mathbb{R}^{I \times m}$ , the number of samples  $1 \leq c \leq I$  and a probability distribution over  $I$ ,  $\{p_i\}_{i=1}^I$ .

**output:** Matrices  $C \in \mathbb{R}^{n \times c}$  and  $R \in \mathbb{R}^{c \times m}$  such that  $CR \simeq AB$ .

- 1 **for**  $t = 1, \dots, c$  **do**
- 2     Pick  $i_t \in \{1, \dots, I\}$  with  $\mathbb{P}[i_t = k] = p_k$ , independently and with replacement.
- 3      $C_{(:,t)} = \frac{1}{\sqrt{cp_{i_t}}} A_{(:,i_t)}$
- 4      $R_{(:,t)} = \frac{1}{\sqrt{cp_{i_t}}} B_{(i_t,:)}$
- 5 **end**
- 6 **return**  $CR = \sum_{t=1}^c \frac{1}{cp_{i_t}} A_{(:,i_t)} B_{(i_t,:)}$

---

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

$$AB \simeq \sum_{t=1}^c \frac{1}{cp_{i_t}} A_{(:,i_t)} B_{(i_t,:)}$$

Equivalently, the above can be restated as the product of two matrices  $CR$  formed by Algorithm 2, where  $C$  consists of  $c$  randomly selected rescaled columns of  $A$  and  $R$  is  $c$  randomly selected rescaled rows of  $B$ . Notice that

$$CR = \sum_{t=1}^c C_{(:,i_t)} R_{(i_t,:)} = \sum_{t=1}^c \left( \frac{1}{\sqrt{cp_{i_t}}} A_{(:,i_t)} \right) \left( \frac{1}{\sqrt{cp_{i_t}}} B_{(i_t,:)} \right) = \frac{1}{c} \sum_{t=1}^c \frac{1}{p_{i_t}} A_{(:,i_t)} B_{(i_t,:)}$$

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

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

so that

$$(6) \quad \mathbf{CR} = \mathbf{ASS}^\top \mathbf{B} \simeq \mathbf{AB}.$$

Notice that  $\mathbf{S}$  is generally a very sparse matrix and therefore is generally not constructed explicitly and instead the matrix products  $\mathbf{AS}$  and  $\mathbf{S}^\top \mathbf{B}$  are done through row and column rescaling [PDaMWM17, page 17]. Lemma 3 provides some bounds on  $\mathbf{CR}$  as an estimate for  $\mathbf{AB}$ .

**Lemma 3.** *Let  $\mathbf{C}$  and  $\mathbf{R}$  be constructed as described in Algorithm 2, then*

$$\mathbb{E}[(\mathbf{CR})_{ij}] = (\mathbf{AB})_{ij}.$$

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

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

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

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

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

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

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

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

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

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

□

So how does this help us with the Nystrom method? Consider using the random matrix multiplication algorithm to approximate the matrix multiplication of a Gram matrix  $\mathbf{K} \in \mathbb{R}^{n \times n}$  and  $\mathbf{1}_{n \times n}$ . Equation 6 gives

$$\mathbf{KSS}^\top \mathbf{1}_{n \times n} = \mathbf{KSS}^\top \simeq \mathbf{K}.$$

We see now that the sketching matrix produced by Algorithm 2 provides a sketching matrix  $\mathbf{S}$  that satisfies the properties of  $\mathbf{Q}$  from equation 1 meaning that  $\mathbf{S}$  can be used in place of  $\mathbf{Q}$  within the Nystrom estimate from equation 3. These ideas are used together in Algorithm 3 that uses the column sampling



technique from Algorithm 2 together with the general Nystrom framework (Algorithm 1) to provide a new column sampling Nystrom method to approximate a Gram matrix for a provided dataset and probability distribution [PDaMWM05, AGaMWM13].

---

**Algorithm 3:** Nystrom Method via Column Sampling

---

**input :** Data matrix  $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]^\top \in \mathbb{R}^{n \times d}$ , the number of samples  $1 \leq c \leq n$  and a probability distribution over  $n$ ,  $\{p_i\}_{i=1}^n$ .

**output:** An approximation of the Gram matrix corresponding to  $\mathbf{X}$ , that is  $\overline{\mathbf{K}} \simeq \mathbf{K}$  where  $\mathbf{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$ .

- 1 Initialize  $\mathbf{C}$  as an empty  $n \times c$  matrix.
- 2 Pick  $c$  columns with the probability of choosing the  $k^{th}$  column ( $1 \leq k \leq n$ ) as  $\mathbb{P}[k = i] = p_i$ , independently and with replacement and let  $I$  a list of indices of the sampled columns.
- 3 **for**  $i \in I$  **do**
- 4      $\mathbf{K}_{(:,i)} = [k(\mathbf{x}_1, \mathbf{x}_i), \dots, k(\mathbf{x}_n, \mathbf{x}_i)]^\top$
- 5      $\mathbf{C}_{(:,i)} = \mathbf{K}_{(:,i)} / \sqrt{cp_i}$
- 6 **end**
- 7  $\mathbf{W} = \mathbf{K}_{(I,I)} \in \mathbb{R}^{c \times c}$
- 8 Rescale each entry of  $\mathbf{W}$ ,  $\mathbf{W}_{ij}$ , by  $1/c\sqrt{p_i p_j}$ .
- 9 Compute  $\mathbf{W}^\dagger$
- 10 **return**  $\mathbf{C}\mathbf{W}^\dagger\mathbf{C}^*$

---

As we can tell from the algorithms inputs, this requires some sort of probability distribution to select the columns. As seen in Lemma 3 any probability distribution will provide an unbiased estimate. However, some probability distributions can be used to lower the variance faster than others. Naively, we could just employ uniform sampling where each column is selected with equal probability although it should be cautioned that this is seldom a good idea since uniform sampling tends to over sample landmarks from one large cluster while under sampling or even missing entire small but important clusters. As a result, the approximation for  $\mathbf{K}$  will decline [CMaCM17, page 3]. This is demonstrated in graphic form in Figure 2.

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

**1.2. Column Probabilities.** Recall that the Nystrom method from Algorithm 3 is largely dependent on the random matrix multiplication algorithm (Algorithm 2) to produce a suitable sketching matrix. Moreover, improvements in the sketching matrix produced by the random matrix multiplication algorithm are reflected as smaller errors in the Nystrom approximation. Now, consider using the random matrix multiplication algorithm to approximate  $\mathbf{A}\mathbf{A}^\top$  by setting  $\mathbf{B} = \mathbf{A}$ . The output is an approximation of the

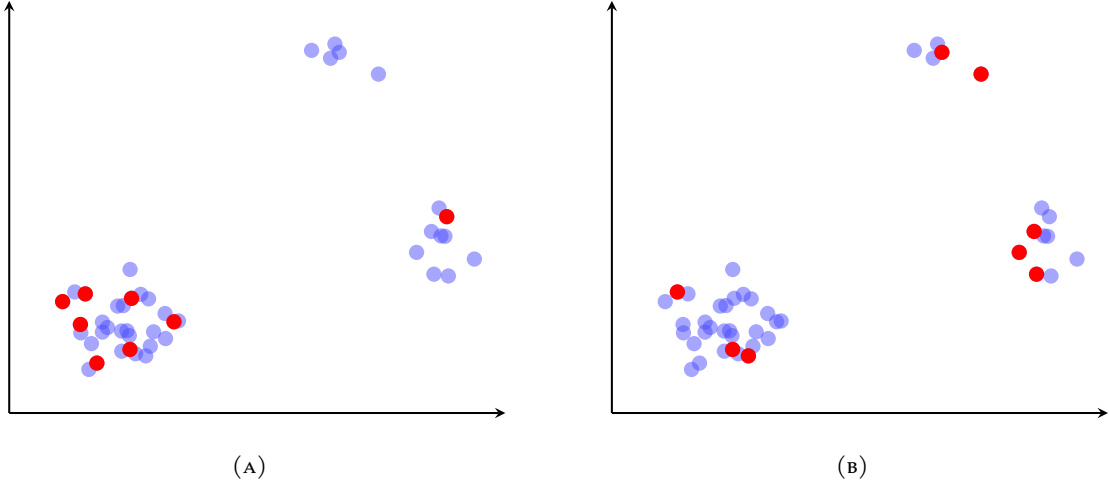


FIGURE 2. Employing uniform sampling in the column sampling Nystrom estimate can lead to oversampling from denser parts of the data set (Panel (A)). Instead data dependent probability densities are commonly used to better cover the relevant data (Panel (B)). Example taken from [CMaCM17, page 4].

form

$$\mathbf{A}\mathbf{A}^\top \simeq \mathbf{C}\mathbf{C}^\top = \mathbf{C}\mathbf{R}.$$

The probability distribution

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

aims to minimize the error between  $\mathbf{A}\mathbf{A}^\top$  and the approximation  $\mathbf{C}\mathbf{C}^\top$ . As a result, we should expect that  $\mathbf{C}$  becomes a better estimate for  $\mathbf{A}\mathbf{S}$ , implying that the sketching matrix,  $\mathbf{S}$ , is using a better sampling and landmark selection criteria. Drineas and Mahoney give a precise bound on this error presented in Theorem 4 [PDaMWM05, page 2158].

**Theorem 4.** Given  $\mathbf{A} \in \mathbb{R}^{n \times I}$ ,  $1 \leq c \leq I$  and the probability distribution  $\{p_i\}_{i=1}^I$  described in equation 1.2. Construct  $\mathbf{C}$  using Algorithm 2, then

$$\mathbb{E} [\|\mathbf{A}\mathbf{A}^\top - \mathbf{C}\mathbf{C}^\top\|_F] \leq \frac{1}{\sqrt{c}} \|\mathbf{A}\|_F^2$$

[PDaMWM05, page 2158].

To show Theorem 4, we can actually prove something a little more general.

**Lemma 5.** Given  $\mathbf{A} \in \mathbb{R}^{n \times I}$ ,  $\mathbf{B} \in \mathbb{R}^{I \times m}$ ,  $1 \leq c \leq I$  and the probability distribution  $\{p_i\}_{i=1}^I$  as follows

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

Construct  $\mathbf{C}$  using Algorithm 2, using the probability distribution described above, then

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

This choice of probability distribution minimises  $\mathbb{E} [\| \mathbf{AB} - \mathbf{CR} \|_F]$  among all possible sampling probabilities [Dri06, pages 9-12].

*Proof.* First note that

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

Thus from Lemma 3, it follows that

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

Substituting in a probability of

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

yields

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

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

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

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

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

The minimum is then

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

Thus

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

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

### 1.3. Leverage Scores.

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

$$\mathbf{x}_{opt} = \arg \min_x \|\mathbf{Ax} - \mathbf{b}\|$$

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

$$\mathbf{H} = \mathbf{A} (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top$$

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

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

$$\begin{aligned} \mathbf{H}_{ii} &= \left( \mathbf{A} (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \right)_{ii} \\ &= \left( \mathbf{U} \mathbf{\Sigma}^2 (\mathbf{\Sigma}^2)^{-1} \mathbf{U} \right)_{ii} \\ &= \|\mathbf{U}_{(i,:)}\|_2^2. \end{aligned}$$

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

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

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

Here  $\mathbf{U}_1$  contains the first  $k \leq r$  columns of  $\mathbf{U}$ ,  $\mathbf{V}_1$  the first  $k$  rows of  $\mathbf{V}$  and  $\mathbf{\Sigma}_1$  is a  $k \times k$  matrix containing the top  $k$  singular values across its diagonal. The matrix  $\mathbf{A}_k = \mathbf{U}_1 \mathbf{\Sigma}_1 \mathbf{V}_1$  serves as the best rank- $k$  approximation to  $\mathbf{A}$ . The statistical leverage scores relative to the best rank- $k$  approximation are again  $\mathbf{H}_{ii}$ , but this time  $\mathbf{H}$  is computed only using the best rank- $k$  approximation of  $\mathbf{A}$ , that is  $\mathbf{A}_k$ . These low

rank scores can be evaluated as

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

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

**1.3.3. Ridge Leverage Scores.** The low rank leverage scores we saw in equation 1.3.2 will not always be unique and can be sensitive to perturbations [MBCaCMaCM15, page 6]. Consequently these scores can vary drastically when  $\mathbf{A}$  is modified slightly or when we only have access to partial information on the matrix. This undermines the possibility of computing good quality low rank approximations from statistical leverage scores. This shortcoming is addressed in the next class of leverage score, that is, ridge leverage scores. Ridge leverage scores are similar to statistical leverage scores although a ridge regression term (hence the name) is added to the hat matrix with a regularization parameter  $\lambda$ . The  $\lambda$ -ridge leverage score is defined as

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

A regularization parameter of

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

is typically used since this choice of  $\lambda$  will guarantee that the sum of the ridge leverage scores (keep in mind that the raw ridge leverage scores do not necessarily form a probability distribution) is bounded by  $2k$ , stated more formally in Lemma 6.

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

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

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

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

$$\begin{aligned} \sum_{i=1}^n r_i^\lambda &= \text{tr} \left( \mathbf{A}^\top \mathbf{U} \bar{\Sigma}^{-2} \mathbf{U}^\top \mathbf{A} \right) \\ &= \text{tr} \left( \mathbf{V} \Sigma \bar{\Sigma}^{-2} \Sigma \mathbf{V}^\top \right) \\ &= \text{tr} \left( \Sigma^2 \bar{\Sigma}^{-2} \right). \end{aligned}$$

Here we have

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

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

$$\text{tr}(\Sigma^2 \bar{\Sigma}^{-2}) = k + \sum_{i=k+1}^n \frac{\sigma_i^2(\mathbf{A})}{\sigma_i^2(\mathbf{A}) + \frac{\|\mathbf{A} - \mathbf{A}_k\|_F^2}{k}} \leq k + \sum_{i=k+1}^n \frac{\sigma_i^2(\mathbf{A})}{\frac{\|\mathbf{A} - \mathbf{A}_k\|_F^2}{k}} = k + \frac{\sum_{i=k+1}^n \sigma_i^2(\mathbf{A})}{\frac{\|\mathbf{A} - \mathbf{A}_k\|_F^2}{k}} \leq k + k.$$

□

From now on (unless otherwise stated) the regularization parameter seen in 1.3.3 will always be used for ridge leverage scores where the notation

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

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

**1.4. Data Probabilities.** Here we present two novel Nystrom probability sampling distributions that make use of the data matrix,  $\mathbf{X}$ , directly without requiring any knowledge of the associated kernel matrix. The first of these two methods is the data-column sampling distribution defined simply as

$$p_i = \|\mathbf{X}_{(i,:)}\|_2 / \|\mathbf{X}\|_F^2.$$

This sampling distribution can be thought of as the data-column dual of the kernel column sampling probabilities seen in Section 1.2. The second sampling method is the  $\mathbf{Q}$  matrix column sampling distribution defined as

$$p_i = \|\mathbf{Q}_{(i,:)}\|_2 / \|\mathbf{Q}\|_F^2.$$

where  $\mathbf{X} = \mathbf{Q}\mathbf{R}$  is the  $\mathbf{QR}$  factorisation (see Theorem 14) of  $\mathbf{X}$ . This sampling technique can be thought of as the data matrix equivalent of leverage score sampling. There are numerous benefits computing the sampling probabilities using the data matrix directly without needing any knowledge about the corresponding matrix. To start, the obvious benefit is that no properties or elements (along with their corresponding calculations) of the kernel matrix are required saving large amounts of computation time. Second, if the parameters of the kernel function are changed, or an entirely different kernel function is used altogether, then the data-column sampling probabilities need not be re-evaluated.

The main grounds for the theoretical justification for using the data matrix directly to produce a sampling distribution comes from a result shown in [Kar10], presented below.

**Theorem 7** (Inner Product of Kernel Matrices). *Let us assume that we observe  $n$  i.i.d. random vectors,  $X_i \in \mathbb{R}^p$ . let us consider the kernel matrix  $\mathbf{M}$  with entries*

$$M_{ij} = f\left(\frac{\mathbf{X}_i^\top \mathbf{X}_j}{p}\right).$$

*We assume that*

- (a) an apple*
- (b) a banana*
- (c) a carrot*
- (d) a durian*

[[Kar10](#), page 9].

## 2. KRYLOV SUBSPACE METHODS

In this section we will focus on how iterative methods and, in particular a class of iterative methods known as Krylov Subspace methods, may be used to solve a linear system  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . 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 computation intractable. 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 by nature endow these systems with these desired properties. For example, 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 guaranteed to converge to an exact solution within a finite number of iterations. Even if the method is prematurely stopped before reaching an exact solution, the solution obtained on the final iteration will, in some sense, be a good enough estimate. Additionally, unlike most non-iterative methods, Krylov subspace methods do not require an explicit form of the matrix  $\mathbf{A}$  and instead only requires some routine for computing  $\mathbf{A}\mathbf{x}$ .

**2.1. Krylov Subspaces.** The main usefulness of Krylov subspaces come from their ability in assisting us to solving linear systems. To this end, consider the problem of solving the linear system

$$(7) \quad \mathbf{A}\mathbf{x}^* = \mathbf{b}$$

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 7? Before answering this, consider the following theorem.

**Theorem 8.** For  $\mathbf{A} \in \mathbb{C}^{n \times n}$  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, page 287].

*Proof.* Let us show that the sequence  $\mathbf{S}_n = \sum_{k=0}^n \mathbf{A}^k$  (where  $n$  is some natural number) of partial sums of the series on the right-hand side of Theorem 8 is fundamental in  $\mathbb{C}^{n \times n}$ . Indeed, by using the fact that  $\|\mathbf{A}\mathbf{B}\| \leq \|\mathbf{A}\|\|\mathbf{B}\|$  for any  $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{n \times n}$ , we conclude that

$$\|\mathbf{S}_{n+p} - \mathbf{S}_n\| \leq \|\mathbf{A}^{n+1}\| + \dots + \|\mathbf{A}^{n+p}\| \leq q^{n+1} + \dots + q^{n+p}$$

for all  $n, p \in \mathbb{N}$ . Since  $q < 1$ , this yields the desired result. Since  $\mathbb{C}^{n \times n}$  is a Banach space, the sequence  $\{\mathbf{S}_n\}_n^\infty$  uniformly converges to an operator  $\mathbf{S} \in \mathbb{C}^{n \times n}$ . Let us show that  $\mathbf{S}(\mathbb{1}_{n \times n} - \mathbf{A}) = (\mathbb{1}_{n \times n} - \mathbf{A})\mathbf{S} = \mathbb{1}_{n \times n}$ . To this end, we note that

$$\|(\mathbb{1}_{n \times n} - \mathbf{A})\mathbf{S}_n - (\mathbb{1}_{n \times n} - \mathbf{A})\mathbf{S}\| \leq \|\mathbb{1}_{n \times n} - \mathbf{A}\| \cdot \|\mathbf{S} - \mathbf{S}_n\| \rightarrow 0$$



as  $n \rightarrow \infty$ . Therefore, it suffices to show that the sequence  $\{(\mathbb{1}_{n \times n} - \mathbf{A}) \mathbf{S}_n\}_{n=1}^{\infty}$  uniformly converges to the identity operator. We have

$$\mathbf{S}_n (\mathbb{1}_{n \times n} - \mathbf{A}) = (\mathbb{1}_{n \times n} - \mathbf{A}) \mathbf{S}_n = \sum_{k=0}^n \mathbf{A}^k - \sum_{k=1}^{n+1} \mathbf{A}^k = \mathbb{1}_{n \times n} - \mathbf{A}^{n+1},$$

that is,  $\|(\mathbb{1}_{n \times n} - \mathbf{A}) \mathbf{S}_n - \mathbb{1}_{n \times n}\| = \|\mathbf{A}^{n+1}\| \leq q^{n+1}$ , which vanishes as  $n \rightarrow \infty$ . Thus  $\mathbf{S} = (\mathbb{1}_{n \times n} - \mathbf{A})^{-1}$ .  $\square$

Consider a matrix for which  $\|\mathbf{A}\| < 2$ , it follows that  $\|\mathbb{1}_{n \times n} - \mathbf{A}\| < 1$  meaning  $\mathbb{1}_{n \times n} - (\mathbb{1}_{n \times n} - \mathbf{A})$  is invertible and  $\mathbf{A}^{-1} = (\mathbb{1}_{n \times n} - (\mathbb{1}_{n \times n} - \mathbf{A}))^{-1} = \sum_{k=0}^{\infty} (\mathbb{1}_{n \times n} - \mathbf{A})^k$ . Returning to equation 7 for any  $\mathbf{x}_0 \in \mathbb{R}^n$  we have

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

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

**Theorem 9** (Cayley-Hamilton). *Let  $p_n(\lambda) = \sum_{i=0}^n c_i \lambda^i$  be the characteristic polynomial of the matrix  $\mathbf{A} \in \mathbb{C}^{n \times n}$ , then  $p_n(\mathbf{A}) = \mathbf{0}$ . **THIS NEEDS A CITATION***

The Cayley-Hamilton Theorem implies that

$$\begin{aligned} \mathbf{0} &= c_0 + c_1 \mathbf{A} + \dots + c_{n-1} \mathbf{A}^{n-1} + c_n \mathbf{A}^n \\ \mathbf{0} &= \mathbf{A}^{-1} c_0 + c_1 + \dots + c_{n-1} \mathbf{A}^{n-2} + c_n \mathbf{A}^{n-1} \\ \mathbf{A}^{-1} &= \alpha_1 \mathbb{1}_{n \times n} + \dots + \alpha_{n-1} \mathbf{A}^{n-2} + \alpha_n \mathbf{A}^{n-1} \end{aligned}$$

where  $\alpha_i = -c_i/c_0$ . The above 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

$$(8) \quad \mathbf{x}^* = \mathbf{x}_0 + \mathbf{A}^{-1} \mathbf{r}_0 = \mathbf{x}_0 + \alpha_1 \mathbf{r}_0 + \dots + \alpha_{n-1} \mathbf{A}^{n-2} \mathbf{r}_0 + \alpha_n \mathbf{A}^{n-1} \mathbf{r}_0.$$

This also shows that  $\mathbf{x}^* \in \mathbf{x}_0 + \text{l.s}\{\mathbf{r}_0, \mathbf{A} \mathbf{r}_0, \mathbf{A}^2 \mathbf{r}_0, \dots, \mathbf{A}^{n-1} \mathbf{r}_0\}$ . One idea for finding a solution to equation 7 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 10** (Krylov Subspace). *The Krylov Subspace of order  $k$  generated by the matrix  $\mathbf{A} \in \mathbb{C}^{n \times n}$  and the vector  $\mathbf{v} \in \mathbb{C}^n$  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  $\mathcal{K}_0(\mathbf{A}, \mathbf{v}) = \{\mathbf{0}\}$  [Tre97, page 245].

For the purposes of solving equation 7 it is important to understand how  $\mathcal{K}_k(\mathbf{A}, \mathbf{v})$  grows for larger and larger  $k$  since a solution for equation 7 will be present in a Krylov Subspace that cannot be grown any larger, according to equation 8. 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 11.** *There is a positive called the grade of  $\mathbf{v}$  with respect to  $\mathbf{A}$ , denoted  $t_{\mathbf{v}, \mathbf{A}}$ , where*

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

Theorem 11 essentially tells us 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  $\mathcal{K}_{k-1}(\mathbf{A}, \mathbf{v}) \subsetneq \mathcal{K}_k(\mathbf{A}, \mathbf{v})$ . 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  $t_{\mathbf{v}, \mathbf{A}}$  obviously plays a central role in determining a suitable basis whose span contains  $\mathbf{A}^{-1}\mathbf{b}$ , its importance is made abundantly clear in the following corollary.

**Corollary 12.**

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

*Proof.* Recall from Cayley-Hamilton (Theorem 9) 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 allows us to make a much stronger statement on the whereabouts of  $\mathbf{x}^*$  in relation to the Krylov Subspaces.

**Corollary 13.** *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  $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ .

**2.2. Gram-Schmidt Process and QR factorisations.** Many areas of linear algebra involving studying the column space of matrices. The  $QR$  factorisation both provides a powerful tool to better understand the column space of a matrix and serves as an important factorisation mechanism for many numerical methods. Suppose that a matrix  $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n] \in \mathbb{R}^{n \times n}$  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 in this fashion, the vector  $\mathbf{q}'_3$  is constructed so that

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

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  $k^{\text{th}}$  vector in our orthonormal basis is computed as

$$(9) \quad \mathbf{q}_k = \frac{\mathbf{a}_k - \sum_{i=1}^{k-1} r_{i,k} \cdot \mathbf{q}_i}{r_{k,k}}$$

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 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  $\text{l.s}\{\{\mathbf{a}_i\}_{i=1}^n\} = \text{l.s}\{\{\mathbf{q}_i\}_{i=1}^n\}$

---

```

1 for  $k = 1$  to  $n$  do
2    $\mathbf{q}'_k = \mathbf{a}_k$ 
3   for  $i = 1$  to  $k - 1$  do
4      $r_{i,k} = \langle \mathbf{q}_i, \mathbf{a}_k \rangle$ 
5      $\mathbf{q}'_k = \mathbf{q}'_k - r_{i,k}\mathbf{q}_i$ 
6   end
7    $r_{k,k} = \|\mathbf{q}'_k\|$ 
8    $\mathbf{q}_k = \mathbf{q}'_k / r_{k,k}$ 
9 end
10 return  $\{\mathbf{q}_i\}_{i=1}^n$ 

```

---

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

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

or more written succinctly as

$$(10) \quad \mathbf{A} = \mathbf{Q}\mathbf{R}$$

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 the 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. The following two theorems on the  $QR$  factorization are stated without proof.

**Theorem 14.** 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 15.** 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 at ways to resolve these numerical instabilities, a quick recap of projectors is useful. 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  $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_m, \mathbf{0}, \dots, \mathbf{0}] \in \mathbb{R}^{n \times n}$ . 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 creates  $\mathbf{q}'_k$  using the following orthogonal projection

$$(11) \quad \mathbf{q}'_k = \mathbf{P}_{A_k^\perp} \mathbf{a}_k$$

where  $A_k = \text{span}\{\mathbf{a}_i\}_{i=1}^k$  and  $\mathbf{P}_{A_k^\perp} = \mathbb{1}_{n \times n}$  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

$$\mathbf{q}'_k = \mathbf{P}_{A_k^\perp} \mathbf{a}_k$$

$$\begin{aligned}
&= (\mathbb{1}_{n \times n} - \mathbf{Q}_k \mathbf{Q}_k^*) \mathbf{a}_k \\
&= \left( \prod_{i=1}^{k-1} (\mathbb{1}_{n \times n} - \mathbf{q}_i \mathbf{q}_i^*) \right) \mathbf{a}_k \\
&= (\mathbb{1}_{n \times n} - \mathbf{q}_1 \mathbf{q}_1^*) (\mathbb{1}_{n \times n} - \mathbf{q}_2 \mathbf{q}_2^*) \cdots (\mathbb{1}_{n \times n} - \mathbf{q}_{k-1} \mathbf{q}_{k-1}^*) \mathbf{a}_k \\
&= \mathbf{P}_{\mathbf{q}_k^\perp} \cdots \mathbf{P}_{\mathbf{q}_1^\perp} \mathbf{a}_k
\end{aligned}$$

where  $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_k, 0, \dots, 0]$ . While its clear that  $\mathbf{P}_{\mathbf{A}_k^\perp} \mathbf{a}$  and  $\mathbf{P}_{\mathbf{q}_k^\perp} \cdots \mathbf{P}_{\mathbf{q}_1^\perp} \mathbf{a}_k$  used for computing  $\mathbf{q}'_k$  are algebraically equivalent, they differ arithmetically as the latter expression evaluates  $\mathbf{q}'_k$  using the follow procedure

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

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  $\text{l.s}\{\mathbf{a}_i\}_{i=1}^n = \text{l.s}\{\mathbf{q}_i\}_{i=1}^n$

```

1 for  $k = 1$  to  $n$  do
2    $\mathbf{q}'_k = \mathbf{a}_k$ 
3 end
4 for  $k = 1$  to  $n$  do
5    $r_{k,k} = \|\mathbf{q}'_k\|$ 
6    $\mathbf{q}_k = \mathbf{q}'_k / r_{k,k}$ 
7   for  $i = k + 1$  to  $n$  do
8      $r_{i,k} = \langle \mathbf{q}_k, \mathbf{q}'_i \rangle$ 
9      $\mathbf{q}_i = \mathbf{q}_i - r_{i,k} \mathbf{q}_k$ 
10  end
11 end
12 return  $\{\mathbf{q}_i\}_{i=1}^n$ 

```

---

**2.3. 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 2.1 it was shown 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  $k \ll t_{r_0}$ . 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 10 indicated 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  $n = t_{r_0, \mathbf{A}}$  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 other terms

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

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  $\mathbf{V}$  matrix offers in the  $QR$ -factorisation of  $\mathbf{K}$ . With this in mind let  $\mathbf{K} = \mathbf{V}\mathbf{R}$  be the full  $QR$ -factorisation of  $\mathbf{K}$ . Then

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

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  $\mathbf{V}$  such that the range of  $\mathbf{V}$  is  $\mathcal{K}_n(\mathbf{A}, \mathbf{r}_0)$  and

$$(12) \quad \mathbf{V}^\top \mathbf{A}\mathbf{V} = \mathbf{H}.$$

Again, in practice, it may be very difficult to compute this entire expression forcing us to search for approximative alternatives. Consider equation 12 for which the only first  $k$  columns of  $\mathbf{V}$  have been computed. Let  $\mathbf{V}_k = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k]$  and  $\mathbf{V}_u = [\mathbf{v}_{k+1}, \mathbf{v}_{k+2}, \dots, \mathbf{v}_n]$ . Then

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

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

where  $\mathbf{H}_k$ ,  $\mathbf{H}_{u,k}$ ,  $\mathbf{H}_{k,u}$  and  $\mathbf{H}_u$  are the relevant sub matrices. This provides us with the equality

$$(13) \quad \mathbf{V}_k^\top \mathbf{A} \mathbf{V}_k = \mathbf{H}_k$$

noting that  $\mathbf{H}_k$  is upper Hessenberg for the same reason that  $\mathbf{H}$  is. We know that when  $n = t_{r_0, \mathbf{A}}$  we can find a  $\mathbf{V} \in \mathbb{K}^{n \times n}$  and  $\mathbf{H} \in \mathbb{K}^{n \times n}$  that satisfies  $\mathbf{A} \mathbf{V} = \mathbf{V} \mathbf{H}$ . However, in general, we may not be so fortunate in finding a  $\mathbf{V}_k \in \mathbb{K}^{n \times k}$  and  $\mathbf{H}_k \in \mathbb{K}^{n \times k}$  to satisfy  $\mathbf{A} \mathbf{V}_k = \mathbf{V}_k \mathbf{H}_k$  for any  $k < n$ . Instead we can adjust this equality by adding an error  $\mathbf{E}_k \in \mathbb{K}^{n \times k}$  to force an equality. Our expression now becomes

$$(14) \quad \mathbf{V}_k^\top \mathbf{A} \mathbf{V}_k = \mathbf{H}_k + \mathbf{E}_k.$$

A judicious choice of  $\mathbf{E}_k$  must be made to also retain equality in equation 13, meaning  $\mathbf{V}_k^\top \mathbf{E}_k = \mathbf{0}$ . Since  $\{\mathbf{v}_i\}_{i=1}^k$  forms an orthonormal basis for  $\mathcal{K}_n(\mathbf{A}, r_0)$ , consider the following choice of  $\mathbf{E}_k$ ,

$$\mathbf{E}_k = \mathbf{v}_{k+1} \mathbf{h}_k^\top$$

where  $\mathbf{h}_k$  is any vector in  $\mathbb{K}^k$ . Notice that

$$\mathbf{V}_k^\top \mathbf{E} = \mathbf{V}^\top (\mathbf{v}_{k+1} \mathbf{h}_k) = (\mathbf{V}^\top \mathbf{v}_{k+1}) \mathbf{h}_k^\top = \mathbf{0}.$$

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

$$(15) \quad \mathbf{A} \mathbf{V}_k = \mathbf{V}_k \mathbf{H}_k + \mathbf{v}_{k+1} \mathbf{h}_k^\top$$

where

$$\mathbf{V}_k \mathbf{H}_k = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k] \begin{bmatrix} h_{1,1} & \cdots & \cdots & \cdots & h_{1,k} \\ h_{2,1} & \cdots & \cdots & \cdots & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & h_{k,k-1} & h_{k,k} \\ 0 & \cdots & 0 & 0 & 0 \end{bmatrix}.$$

Equating the  $j^{\text{th}}$  columns of equation 15 yields

$$\mathbf{A} \mathbf{v}_j = \sum_{i=1}^{j+1} h_{i,j} \mathbf{v}_i.$$

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

$$\mathbf{v}_m^\top \mathbf{A} \mathbf{v}_j = \sum_{i=1}^{j+1} h_{i,j} \mathbf{v}_m^\top \mathbf{v}_i = h_{m,j}$$

and so

$$(16) \quad h_{j+1,j} \mathbf{v}_{j+1} = \mathbf{A} \mathbf{v}_j - \sum_{i=1}^j h_{i,j} \mathbf{v}_i.$$

From equation 16 we find that  $\mathbf{v}_{j+1}$  can be computed using a recurrence involving its previous Krylov factors. This bears a striking resemblance to equation 9 having a virtually identical setup to computing

an orthonormal basis using the modified Gram-Schmidt process (Algorithm 5). As such, values for  $\mathbf{v}_{j+1}$  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  $\mathbf{V}$  to compute.

**output:**  $\mathbf{V}_k, \mathbf{H}_k$ .

```

1  $\mathbf{v}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\|$ 
2 for  $j = 1$  to  $k$  do
3    $\mathbf{z} = \mathbf{A}\mathbf{v}_j$ 
4   for  $i = 1$  to  $j$  do
5      $h_{i,j} = \langle \mathbf{v}_i, \mathbf{z} \rangle$ 
6      $\mathbf{z} = \mathbf{z} - h_{i,j}\mathbf{v}_i$ 
7   end
8    $h_{j+1,j} = \|\mathbf{z}\|$ 
9   if  $h_{j+1,j} = 0$  then
10    return  $\mathbf{V}_k, \mathbf{H}_k$ 
11  end
12   $\mathbf{v}_{j+1} = \mathbf{z} / h_{j+1,j}$ 
13 end
14 return  $\mathbf{V}_k, \mathbf{H}_k$ 
```

---

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  $\mathbf{A}\mathbf{V} = \mathbf{V}\mathbf{T}$  yields

$$(17) \quad \mathbf{A}\mathbf{v}_j = \beta_{j-1}\mathbf{v}_{j-1} + \alpha_j\mathbf{v}_j + \beta_j\mathbf{v}_{j+1}.$$

Again since  $\{\mathbf{v}_i\}_{i=1}^n$  form an orthonormal basis, multiplying both sides of equation 17 by  $\mathbf{v}_j$  gives  $\mathbf{v}_j\mathbf{A}\mathbf{v}_j = \alpha_j$ . A simplified version of the Arnoldi algorithm can be devised to compute  $\{\mathbf{v}_i\}_{i=1}^n$  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 :**  $\mathbf{A}$ ,  $\mathbf{r}_0$  and  $k$ , the number of columns of  $\mathbf{V}$  to compute.

**output:**  $\mathbf{V}_k, \mathbf{T}_k$ .

```

1  $\mathbf{v}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\|, \beta_0 = 0, \mathbf{v}_0 = 0$ 
2 for  $j = 1$  to  $k$  do
3    $\mathbf{z} = \mathbf{A}\mathbf{v}_j$ 
4    $\alpha_j = \langle \mathbf{v}_j, \mathbf{z} \rangle$ 
5    $\mathbf{z} = \mathbf{z} - \alpha_j \mathbf{v}_j - \beta_{j-1} \mathbf{v}_{j-1}$ 
6    $\beta_j = \|\mathbf{z}\|$ 
7   if  $\beta_j = 0$  then
8     return  $\mathbf{V}_k, \mathbf{T}_k$ 
9   end
10   $\mathbf{v}_{j+1} = \mathbf{z} / \beta_j$ 
11 end
12 return  $\mathbf{V}_k, \mathbf{T}_k$ 

```

---

For the Lanczos algorithm, equation 15 can be re-written in the a more compact form as

$$(18) \quad \mathbf{A}\mathbf{V}_k \triangleq \mathbf{V}_k \mathbf{T}_{k+1,k}$$

where  $\mathbf{T}_{k+1,k} = \mathbf{T}_k + \mathbf{v}_{k+1} \mathbf{t}_k^\top$ .

**2.4. Optimality Conditions.** So far we have shown that  $\mathbf{x}^* \in \mathcal{K}_{t_{\mathbf{r}_0}, \mathbf{A}}(\mathbf{A}, \mathbf{r}_0)$  where  $n = t_{\mathbf{r}_0}$  is the grade of  $\mathbf{r}_0$  with respect to  $\mathbf{A}$ . Moreover from Section 2.3 we found ways to construct a basis for  $\mathcal{K}_{t_{\mathbf{r}_0}, \mathbf{A}}(\mathbf{A}, \mathbf{r}_0)$  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  $\mathcal{K}_{t_{\mathbf{r}_0}, \mathbf{A}}(\mathbf{A}, \mathbf{r}_0)$  will be abbreviated to  $\mathcal{K}_{t_{\mathbf{r}_0}, \mathbf{A}}$  when the context is clear. The question still remains however, how should one choose an  $\mathbf{x}_k$  that best approximates  $\mathbf{x}^*$  satisfying equation 7? The following are some of the most well known methods for selecting a suitable  $\mathbf{x}_k$ .

- (a) Select an  $\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k$  which minimizes  $\|\mathbf{x}_k - \mathbf{x}^*\|_2$ . While this method seems like the most intuitive and natural way to select  $\mathbf{x}_k$ , it is unfortunately of no practical use since there is not enough information in the Krylov Subspace to find an  $\mathbf{x}_k$  which matches this profile.
- (b) Select an  $\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k$  which minimizes  $\|\mathbf{r}_k\|_2$  (recall this is the residual of  $\mathbf{x}_k$ , that is,  $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$ ). 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  $\mathbf{A}$  respectively.
- (c) When  $\mathbf{A}$  is a positive definite matrix it defines a norm  $\|\mathbf{r}\|_{\mathbf{A}} = (\mathbf{r}^\top \mathbf{A} \mathbf{r})^{\frac{1}{2}}$ , called the energy norm. Select an  $\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k$  which minimizes  $\|\mathbf{r}_k\|_{\mathbf{A}^{-1}}$  which is equivalent to minimizing  $\|\mathbf{x}_k - \mathbf{x}\|_{\mathbf{A}}$ . This technique is known as the CG (conjugate gradient) algorithm.

- (d) Select an  $\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k$  for which  $\mathbf{r}_k \perp \mathcal{W}_k$  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  $\mathbf{A}$  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 16 without proof.

**Theorem 16.** *In the context of the above selection method, if  $\mathbf{A} \succ \mathbf{0}$  and  $\mathcal{W}_k = \mathcal{K}_k$  in method (4) then it produces the same  $\mathbf{x}_k$  in method (3) [Dem97].*

In fact the 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  $\mathbf{x}_k$  from our Krylov subspace allows  $k$  degrees of freedom meaning  $k$  constraints must be used to determine a unique  $\mathbf{x}_k$  for selection. As seen in method (4) already, typically orthogonality constraints are imposed on the residual  $\mathbf{r}_k$ . Specifically we would like to find a  $\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k$  where  $\mathbf{r}_k \perp \mathcal{W}_k$ . 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  $\mathcal{W}_k = \mathbf{A}\mathcal{K}_k$  are known as oblique projections. If we set  $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{z}_k$  for some  $\mathbf{z}_k \in \mathcal{K}_k$  then the Petrov-Galerkin conditions imply  $\mathbf{r}_0 - \mathbf{A}\mathbf{z}_k \perp \mathcal{W}_k$ , or alternatively  $\langle \mathbf{r}_0 - \mathbf{A}\mathbf{z}_k, \mathbf{w} \rangle = 0$  for every  $\mathbf{w} \in \mathcal{W}_k$ . 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  $\{\mathbf{v}_i\}_{i=1}^k$  and  $\{\mathbf{w}_i\}_{i=1}^k$  are basis elements for  $\mathcal{K}$  and  $\mathcal{W}$  respectively. Let

$$\mathbf{K}_k \triangleq [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k] \in \mathbb{K}^{n \times k}$$

$$\mathbf{W}_k \triangleq [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_k] \in \mathbb{K}^{n \times k}$$

then the Petrov-Galerkin conditions can be imposed as follows

$$\mathbf{K}_k \mathbf{y}_k = \mathbf{z}_k, \quad \text{for some } \mathbf{y}_k \in \mathbb{K}^k$$

$$\mathbf{W}_k^\top (\mathbf{r}_0 - \mathbf{A}\mathbf{K}_k \mathbf{y}_k) = \mathbf{0}.$$

Moreover if  $\mathbf{W}_k^\top \mathbf{A}\mathbf{K}_k$  is invertible then  $\mathbf{x}_k$  can be expressed as

$$(19) \quad \mathbf{x}_k = \mathbf{x}_0 + \mathbf{K}_k (\mathbf{W}_k^\top \mathbf{A}\mathbf{K}_k)^{-1} \mathbf{W}_k^\top \mathbf{r}_0.$$

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

---

**Algorithm 8:** General Projection Method

---

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

---

```

1 for  $k = 1, \dots$  until convergence do
2   | Select  $\mathcal{K}_k$  and  $\mathcal{W}_k$ 
3   | Form  $\mathbf{K}_k$  and  $\mathbf{W}_k$ 
4   | Solve  $(\mathbf{W}_k^\top \mathbf{A}\mathbf{K}_k) \mathbf{y}_k = \mathbf{W}_k^\top \mathbf{r}_0$ 
5   |  $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{K}_k \mathbf{y}_k$ 
6 end
7 return  $\mathbf{x}_k$ 
```

---

**2.5. Conjugate Gradient Algorithm.** From Section 2.4 that the Petrov-Galerkin conditions for the CG algorithm used an orthogonal projection and the matrix  $\mathbf{A}$  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  $\mathbf{A}\mathbf{V}_k = \mathbf{V}_k\mathbf{T}_k + \mathbf{v}_{k+1}\mathbf{t}_k^\top$  where  $\mathbf{t}_k \triangleq [0, 0, \dots, 0, \beta_k]^\top \in \mathbb{K}^k$  and the columns of  $\mathbf{V}_k$  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 19) 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. Thus 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  $\mathcal{K}_k = \text{Range}(\mathbf{V}_k)$  where  $\mathbf{V}_k$  has full column rank then  $\mathbf{z}_k$  can be represented as  $\mathbf{z}_k = \mathbf{V}_k \mathbf{y}$  for a unique  $\mathbf{y} \in \mathbb{R}^k$  so that

$$(20) \quad \mathbf{x}_k = \mathbf{x}_0 + \mathbf{V}_k \mathbf{y}.$$

Coupling this with the Petrov-Galerkin conditions ensures

$$(21) \quad \begin{aligned} \mathbf{V}_k^\top (\mathbf{r}_0 - \mathbf{A}\mathbf{V}_k \mathbf{y}) &= \mathbf{0} \\ \mathbf{V}_k^\top \mathbf{A} \mathbf{V}_k \mathbf{y} &= \mathbf{V}_k^\top \mathbf{r}_0 \\ \mathbf{T}_k \mathbf{y} &= \|\mathbf{r}_0\| \mathbf{e}_1. \end{aligned}$$

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

- (a) The approximate solutions  $\mathbf{x}_k$
- (b) The residual vectors  $\mathbf{r}_k$
- (c) The conjugate gradient vectors  $\mathbf{p}_k$

The conjugate gradient vectors include the word 'gradient' since the attempt to find the direction of steepest descent that minimizes  $\|\mathbf{r}_k\|_{\mathbf{A}^{-1}}$ . It also includes the word '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 (shown in Lemma 17).

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

$$(22) \quad \mathbf{T}_k = \mathbf{L}_k \mathbf{D}_k \mathbf{L}_k^\top$$

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 20, 21 and 22

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

$$\mathbf{x}_k \triangleq \mathbf{x}_0 + \tilde{\mathbf{P}}_k \tilde{\mathbf{y}}_k$$

where  $\tilde{\mathbf{P}}_k = \mathbf{V}_k \mathbf{L}_k^{-\top}$  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 17 shows that the columns of  $\tilde{\mathbf{P}}_k$  are  $A$ -conjugate.

**Lemma 17.** *The columns of  $\tilde{\mathbf{P}}_k$  are  $A$ -conjugate, in otherwords  $\tilde{\mathbf{P}}_k^\top \mathbf{A} \tilde{\mathbf{P}}_k$  is diagonal.*

*Proof.* We compute

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

(equation 22)

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

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

where the elements of  $\star$  are of no importance. 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  $k-1$  entires 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. We can begin by computing a recurrence for  $\tilde{\mathbf{y}}_k$  as follows

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

where  $\mathbf{e}_i^k$  is the  $i^{th}$  unit vector with  $k$  dimensions. To get a recurrence for the columns of  $\tilde{\mathbf{P}}_{k-1} = [\tilde{\mathbf{p}}_1, \tilde{\mathbf{p}}_2, \dots, \tilde{\mathbf{p}}_{k-1}]$  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  $\mathbf{L}_k^{-\top}$ . In effect,  $\tilde{\mathbf{P}}_{k-1}$  is identical to the leading  $k-1$  columns of

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

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

$$(23) \quad \tilde{\mathbf{p}}_k = \mathbf{v}_k - l_{k-1} \tilde{\mathbf{p}}_{k-1}.$$

Finally we can use

$$(24) \quad \mathbf{x}_k = \mathbf{x}_0 + \tilde{\mathbf{P}}_k \tilde{\mathbf{y}}_k = \mathbf{x}_0 + [\tilde{\mathbf{P}}_{k-1}, \tilde{\mathbf{p}}_k] \begin{bmatrix} \tilde{\mathbf{y}}_{k-1} \\ \eta_k \end{bmatrix} = \mathbf{x}_0 + \tilde{\mathbf{P}}_{k-1} \tilde{\mathbf{y}}_{k-1} + \eta_k \tilde{\mathbf{p}}_k = \mathbf{x}_{k-1} + \eta_k \tilde{\mathbf{p}}_k$$

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

$$(25) \quad \mathbf{r}_k = b - \mathbf{A} \mathbf{x}_k = b - \mathbf{A} (\mathbf{x}_{k-1} + \eta_k \tilde{\mathbf{p}}_k) = (b - \mathbf{A} \mathbf{x}_{k-1}) - \eta_k \mathbf{A} \tilde{\mathbf{p}}_k = \mathbf{r}_{k-1} - \eta_k \mathbf{A} \tilde{\mathbf{p}}_k$$

Altogether we are left with recurrences for  $\mathbf{v}_k$  from Lanczos,  $\tilde{\mathbf{p}}_k$  (equation 23), the residual  $\mathbf{r}_k$  (equation 23), and for the approximate solution  $\mathbf{x}_k$  (equation 24). However, further simplifications can be made to bring about a more efficient algorithm. Recall from Section 2.3 that  $\mathbf{A} \mathbf{V}_k = \mathbf{V}_k \mathbf{T}_k + \mathbf{v}_{k+1} \mathbf{t}_k^\top$  where  $\mathbf{t}_k = [0, 0, \dots, 0, \beta_k]^\top \in \mathbb{R}^k$  meaning

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

This tells us that  $\mathbf{r}_k$  is parallel to  $\mathbf{v}_{k+1}$  and orthogonal to all  $\mathbf{v}_i$ ,  $1 \leq i \leq k$ . This further implies that  $\mathbf{r}_k$  is orthogonal to all  $\mathbf{r}_i$ ,  $1 \leq i \leq k-1$  since they are just  $\mathbf{v}_i$  scaled by some constant factor. So replacing  $\mathbf{r}_{k-1}$  with  $\mathbf{v}_k / \eta_k$  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 Lemma 17 we have shown that the columns of  $\tilde{\mathbf{P}}_k$  are  $\mathbf{A}$ -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  $\langle \mathbf{r}_i, \mathbf{r}_j \rangle = 0$ ,  $i \neq j$ . Note that from our recurrence for  $\mathbf{p}_k = \mathbf{r}_{k-1} + \beta_k \mathbf{p}_{k-1}$  we have

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

We can now find an expression for  $\alpha_k$  as

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

Similarly, using the recurrence for  $\mathbf{p}_k$ , an expression for  $\beta_k$  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  $\mathbf{r}_k$

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

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

Equating the two expressions for  $\alpha_k$  affords

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

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  $\mathbf{x}^*$ ,  $\mathbf{x}_k$ .

---

```

1  $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ ,  $\mathbf{p}_1 = \mathbf{r}_0$ 
2 for  $k = 1, \dots$  until  $\|\mathbf{r}_{k-1}\| \leq \tau$  do
3    $\alpha_k = \frac{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}{\langle \mathbf{p}_k, \mathbf{A}\mathbf{p}_k \rangle}$ 
4    $\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_k \mathbf{p}_k$ 
5    $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{A}\mathbf{p}_k$ 
6    $\beta_{k+1} = \frac{\langle \mathbf{r}_k, \mathbf{r}_k \rangle}{\langle \mathbf{r}_{k-1}, \mathbf{r}_{k-1} \rangle}$ 
7    $\mathbf{p}_{k+1} = \mathbf{r}_k + \beta_{k+1} \mathbf{p}_k$ 
8 end
9 return  $\mathbf{x}_k$ 
```

---

The next few theorems pertain to the rate of convergence of the CG algorithm.

**Theorem 18.** *Let the CG iteration (Algorithm 9) be applied to a symmetric positive definite matrix problem  $\mathbf{A}\mathbf{x} = \mathbf{b}$ . As long as the iteration has not yet converged (that is,  $\mathbf{r}_{n-1} \neq \mathbf{0}$ ), the algorithm proceeds without divisions by zero, and we have the following identities of subspaces:*

$$(26) \quad \mathcal{K}_n = \text{l.s} \{ \mathbf{x}_i \}_{i=1}^n = \text{l.s} \{ \mathbf{p}_i \}_{i=0}^{n-1} = \text{l.s} \{ \mathbf{r}_i \}_{i=0}^{n-1} = \text{l.s} \{ \mathbf{A}^i \mathbf{b} \}_{i=0}^{n-1}.$$

Moreover the residuals are orthogonal,

$$\langle \mathbf{r}_n, \mathbf{r}_j \rangle = 0 \quad (j < n)$$

and the search directions are  $\mathbf{A}$ -conjugate [Tre97, page 295].

*Proof.* The orthogonality of the residuals has already been shown within the derivation of the CG algorithm. Seeing that the search directions are  $\mathbf{A}$ -conjugate is a very straight forward application of Lemma 17. To show Equation (26) we can induct on  $k$ . From the initial guess  $\mathbf{x}_0$  and the expression  $\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_k \mathbf{p}_k$ , using an induction argument it follows that  $\mathbf{x}_k$  belongs to  $\text{l.s} \{ \mathbf{p}_i \}_{i=0}^{k-1}$ . Similarly, from

$\mathbf{p}_k = \mathbf{r}_{k-1} + \beta_k \mathbf{p}_{k-1}$  it follows that this belongs to  $\text{l.s}\{\mathbf{r}_i\}_{i=0}^{n-1}$ . Finally, from  $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{A} \mathbf{p}_k$  that this belongs to  $\text{l.s}\{\mathbf{A}^i \mathbf{b}\}_{i=0}^{n-1}$ .  $\square$

It is fairly straight forward to confirm that CG minimizes error at each step.

**Theorem 19.** *Let the CG iteration be applied to a symmetric positive definite matrix  $\mathbf{A} \mathbf{x} = \mathbf{b}$ . If the iteration has not already converged (that is,  $\|\mathbf{r}_{k-1}\| > 0$ ), then  $\mathbf{x}_k$  is the unique point in  $\mathcal{K}_k$  that minimizes  $\|\mathbf{x}^* - \mathbf{x}_k\|_{\mathbf{A}}$ . The convergence is the monotonic,*

$$\|\mathbf{x}^* - \mathbf{x}_k\|_{\mathbf{A}} \leq \|\mathbf{x}^* - \mathbf{x}_{k-1}\|_{\mathbf{A}}$$

and  $\|\mathbf{x}^* - \mathbf{x}_k\|_{\mathbf{A}} = 0$  is achieved for some  $k \leq n$  [Tre97, page 296].

*Proof.* From Theorem 18 we know that  $\mathbf{x}_k$  belongs to  $\mathcal{K}_k$ . To show that it is the unique point in  $\mathcal{K}_k$  that minimizes the error, consider an arbitrary point  $\mathbf{z} = \mathbf{x}_k - \Delta \mathbf{z} \in \mathcal{K}_k$ , with error  $\mathbf{e} = \mathbf{x}_* - \mathbf{z} = \mathbf{e}_k + \Delta \mathbf{x}$ . Note in this context  $\mathbf{e}_k = \mathbf{x}_* - \mathbf{x}_k$ , and does not represent standard basis vectors. We calculate

$$\begin{aligned} \|\mathbf{e}\|_{\mathbf{A}}^2 &= (\mathbf{e}_k + \Delta \mathbf{x})^\top \mathbf{A} (\mathbf{e}_k + \Delta \mathbf{x}) \\ &= \mathbf{e}_k^\top \mathbf{A} \mathbf{e}_k + (\Delta \mathbf{x})^\top \mathbf{A} (\Delta \mathbf{x}) + 2\mathbf{e}_k^\top \mathbf{A} (\Delta \mathbf{x}). \end{aligned}$$

The final term of this expression is  $2\mathbf{r}_k^\top (\Delta \mathbf{x})$ , an inner product of  $\mathbf{r}_k$  with a vector in  $\mathcal{K}_k$ , and by Theorem 19, any such inner product is zero. Effectively, this means

$$\|\mathbf{e}\|_{\mathbf{A}}^2 = \mathbf{e}_k^\top \mathbf{A} \mathbf{e}_k + (\Delta \mathbf{x})^\top \mathbf{A} (\Delta \mathbf{x}).$$

Only the second of these terms depends on  $\Delta \mathbf{x}$ , since  $\mathbf{A}$  is positive definite, that term is greater than or equal to 0, attaining the value of 0 if and only if  $\Delta \mathbf{x} = \mathbf{0}$ , that is,  $\mathbf{x}_k = \mathbf{x}$ . Thus  $\|\mathbf{e}\|_{\mathbf{A}}$  is minimal if and only if  $\mathbf{x}_k = \mathbf{x}$ , as claimed.  $\square$

As seen in Equation (8) Krylov subspace methods, in some sense, aim to find a polynomial  $p_n \in P_n$  which minimizes  $\|p_n(\mathbf{A})\| = \|\sum_{k=0}^{n-1} \alpha_{k+1} \mathbf{A}^k \mathbf{r}_0\|$ , where  $P_n$  is the set of polynomials with degree less than or equal to  $n$  with  $p(\mathbf{0}) = \mathbf{1}$ . In the context of the CG algorithm, this is equivalent to finding a polynomial  $p_n \in P_n$  which instead minimizes

$$(27) \quad \|p_n(\mathbf{A}) \mathbf{e}_0\|_{\mathbf{A}}.$$

From Theorem 18, we can derive the following convergence theorem.

**Theorem 20.** *If the CG iteration has not already converged before step  $k$  (that is,  $\|\mathbf{r}_{k-1}\| > 0$ ), then Equation (27) has a unique solution  $p_n \in P_n$ , and the iterate  $\mathbf{x}_k$  has error  $\mathbf{e}_k = p_n(\mathbf{A}) \mathbf{e}_0$  for this same polynomial  $p_n$ . Consequently we have*

$$(28) \quad \frac{\|\mathbf{e}_k\|_{\mathbf{A}}}{\|\mathbf{e}_0\|_{\mathbf{A}}} = \inf_{p \in P_n} \frac{\|p(\mathbf{A}) \mathbf{e}_0\|_{\mathbf{A}}}{\|\mathbf{e}_0\|_{\mathbf{A}}} \leq \inf_{p \in P_n} \max_{\lambda \in \Lambda(\mathbf{A})} |p(\lambda)|$$

[Tre97, page 298].

*Proof.* From Theorem 18 it follows that  $\mathbf{e}_k = p(\mathbf{A}) \mathbf{e}_0$  for some  $p \in P_n$ . The equality in 28 is a consequence of this and Theorem 19. As for the inequality in 28, if  $\mathbf{e}_0 = \sum_{j=1}^m a_j \mathbf{v}_j$  is an expansion of  $\mathbf{e}_0$  in orthonormal

eigenvectors of  $\mathbf{A}$ , then we have  $p(\mathbf{A})\mathbf{e}_0 = \sum_{j=1}^m a_j p(\lambda_j) \mathbf{v}_j$  and thus

$$\|\mathbf{e}_0\|_{\mathbf{A}}^2 = \sum_{j=1}^m a_j^2 \lambda_j, \quad \|p(\mathbf{A})\mathbf{e}_0\|_{\mathbf{A}}^2 = \sum_{j=1}^m a_j^2 \lambda_j (p(\lambda_j))^2.$$

These identities indicate  $\|p(\mathbf{A})\mathbf{e}_0\|_{\mathbf{A}}^2 / \|\mathbf{e}_0\|_{\mathbf{A}}^2 \leq \max_{\lambda \in \Lambda(\mathbf{A})} |p(\lambda)|^2$ , which implies the inequality in question.  $\square$

**2.6. Minimum Residual.** In contrast to CG, MINRES is applicable to a wider range of linear systems, namely symmetric indefinite systems. From Section 2.4 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

$$(29) \quad \mathbf{x}_k = \arg \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2.$$

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 for CG,  $\mathbf{x}_k$  can be expressed as  $\mathbf{x}_k = \mathbf{x}_0 + \mathbf{V}_k \mathbf{y}_k$ . Employing equation 18 produced by the Lanczos algorithm in 2.3 we can manipulate our optimality condition 29 as follows

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

[Gre97, page 43]. Under the general project method procedure 8, this affords the following high-level description of the MINRES algorithm [Tre97, page 268].

---

**Algorithm 10:** High-Level MINRES

---

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

---

```

1 for  $k = 1, \dots$  until convergence do
2   | Lanczos-Step ( $\mathbf{A}, \mathbf{v}_k, \mathbf{v}_{k-1}, \beta_k$ )  $\rightarrow \alpha_k, \beta_{k+1}, \mathbf{v}_{k+1}$ 
3   | Find  $\mathbf{y}$  to minimize  $\|\mathbf{T}_{k+1,k} \mathbf{y} - \beta_0 \mathbf{e}_1\|_2$ 
4   |  $\mathbf{x}_k = \mathbf{V}_k \mathbf{y}$ 
5 end
6 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  $T_{k+1,k}$  from the  $QR$  factorisation of  $T_{k,k-1}$  using an inexpensive  $\mathcal{O}(n)$  Householder reflection [Tre97, page 268]. Computing the  $QR$  factorisation of  $T_{k,k-1}$  yields

$$(30) \quad Q_k T_{k,k+1} = \begin{bmatrix} R_k \\ 0 \end{bmatrix} = \begin{bmatrix} \gamma_1^{(1)} & \delta_2^{(1)} & \varepsilon_3^{(1)} & & & \\ & \gamma_1^{(2)} & \delta_3^{(2)} & \varepsilon_4^{(1)} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \varepsilon_k^{(1)} \\ & & & & \ddots & \gamma_k^{(2)} \\ & & & & & \delta_k^{(2)} \\ & & & & & 0 \end{bmatrix}$$

where  $Q_k = \prod_{i=1}^k Q_{i,i+1}$  is the product of Householder reflections designed to annihilate the  $\beta_i$ s in the subdiagonal of  $T_{k,k+1}$  [Cho07, page 25] where each  $Q_{i,i+1}$  is defined as

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

[Cho07, page 22]. As mentioned for each  $i$ ,  $Q_{i,i+1}$  is orthogonal, symmetric and constructed to annihilate  $\beta_{k+1}$  that is the bottom right element of  $T_{k,k+1}$ . To see this better an alternative way of writing  $Q_k T_{k,k+1}$  is  $Q_{k,k+1} \cdot Q_{2,3} Q_{1,2} T_{k,k+1}$ . Notice however that  $Q_{k,k+1}$  is the only rotation matrix that will involve  $\beta_{k+1}$  in its matrix multiplication with  $T_{k,k+1}$ . To study the influence of  $Q_{k,k+1}$  in a more compact way we only need to consider the matrix product

$$(31) \quad \begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} \begin{bmatrix} \gamma_k^{(1)} & \delta_{k+1}^{(1)} & 0 \\ \beta_{k+1} & \alpha_{k+1} & \beta_{k+1} \end{bmatrix}.$$

To annihilate  $\beta_{k+1}$ , 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 31 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

$$\begin{aligned} Q_k(\beta_0 \mathbf{e}_1) &= \prod_{i=1}^k Q_{i,i+1}(\beta_0 \mathbf{e}_1) \\ &= \beta_0 Q_{k,k+1} \cdots Q_{2,3} \begin{bmatrix} c_1 \\ s_1 \\ \mathbf{0}_{k-1} \end{bmatrix} \end{aligned}$$

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

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 becomes 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

$$(32) \quad \mathbf{R}_k^\top \mathbf{D}_k^\top = \mathbf{V}_k^\top$$

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

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

The  $\mathbf{d}_j$  in equation 33 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 32 [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  $\mathbf{x}^*$ ,  $\mathbf{x}_k$ .

```

1  $\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$ ,  $\tau_0 = \beta_0 = \|\mathbf{r}_0\|$ ,  $\mathbf{v}_1 = \mathbf{r}_0/\beta_0$ ,  $\delta_1^{(1)} = 0$ ,  $\mathbf{v}_0 = \mathbf{d}_0 = \mathbf{d}_{-1} = \mathbf{0}$ 
2 for  $k = 1, \dots$  until convergence do
3   Lanczos-Step ( $\mathbf{A}, \mathbf{v}_k, \mathbf{v}_{k-1}, \beta_k$ )  $\rightarrow \alpha_k, \beta_{k+1}, \mathbf{v}_{k+1}$ 
4    $\begin{bmatrix} \delta_k^{(2)} & \varepsilon_{k+1}^{(1)} \\ \gamma_k^{(1)} & \delta_{k+1}^{(1)} \end{bmatrix} = \begin{bmatrix} c_{k-1} & s_{k-1} \\ s_{k-1} & -c_{k-1} \end{bmatrix} \begin{bmatrix} \delta_k^{(1)} & 0 \\ \alpha_k & \beta_{k+1} \end{bmatrix}$ 
5    $\rho_k = \sqrt{\gamma_k^{(1)2} + \beta_{k+1}^2}$ ,  $c_k = \frac{\gamma_k^{(1)}}{\rho_k}$ ,  $s_k = \frac{\beta_{k+1}}{\rho_k}$ 
6    $\gamma_k^{(2)} = c_k \gamma_k^{(1)}$ 
7    $\tau_k = c_k \phi_{k-1}$ ,  $\phi_k = s_k \phi_{k-1}$ 
8    $\mathbf{d}_k = (\mathbf{v}_k - \delta_k^{(2)} \mathbf{d}_{k-1} - \varepsilon_k \mathbf{d}_{k-2}) / \gamma_k^{(2)}$ 
9    $\mathbf{x}_k + \tau_k \mathbf{d}_k$ 
10 end
11 return  $\mathbf{x}_k$ 

```

---

### 3. APPLICATIONS AND RESULTS

So far we have discussed a number of different approximation techniques to use to speed up some of the bottle necks within our Gaussian Process regression and classification algorithms. Here, we shall see how they can be used within the naive implementations from ?? to provide implementations that produce much faster predictions, at the expense of slightly less accurate results. We shall also go through an extensive treatment of how the various methods reviewed in previous chapters were implemented and the setup of the experiments used to make comparisons to determine the most successful method.

**3.1. Gaussian Processes Prediction Reviewed.** In chapter ??, a naive implementation for Gaussian Process prediction was presented in ?. While this does provide a simple and convenient way to produce predictions for a regression task, it is not quite all smooth sailing from here. Unfortunately, there are a number of problems with this algorithm in terms of scalability. For convenience, this algorithm has been restated below but this time with its various bottlenecks highlighted in red.

---

**Algorithm 1:** Unoptimized GPR

---

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

- 1  $\mathbf{L} = \text{cholesky}(\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbf{1}_{n \times n})$
- 2  $\boldsymbol{\alpha} = \text{lin-solve}(\mathbf{L}^\top, \text{lin-solve}(\mathbf{L}, \mathbf{y}))$
- 3  $\bar{f}_* = \mathbf{K}_{\mathbf{x}_*\mathbf{X}} \boldsymbol{\alpha}$
- 4  $\mathbf{v} = \text{lin-solve}(\mathbf{L}, \mathbf{K}_{\mathbf{x}_*\mathbf{X}})$
- 5  $\mathbb{V}[f_*] = \mathbf{K}_{\mathbf{x}_*\mathbf{x}_*} - \mathbf{v}^\top \mathbf{v}$
- 6 **return**  $\bar{f}_*, \mathbb{V}[f_*]$

---

To start computing the kernel matrix,  $\mathbf{K}_{\mathbf{X}\mathbf{X}}$ , on line 1 carries an  $\mathcal{O}(n^2)$  runtime since  $\mathcal{O}(n^2)$  pairwise kernel evaluations must be made. Moreover, solving linear systems using a cholesky decomposition (seen on lines 1, 2 and 4) will incur a runtime of  $\mathcal{O}(n^3)$ . While this quadratic scaling may not be much of an issue for smaller datasets, however this will scale very poorly for larger datasets making and training sets larger than  $10^5$  infeasible to use on most modern work stations [WJMaSKaAGW21, page 2]. The Gaussian Process classifier from ?? suffers for the exact same reasons as GPR. To mitigate this computation burden of these bottle necks, we can replace these procedures with their approximative counterparts discussed in Chapters 1, ?? and 2.

To start, computing the kernel matrix can be done using either the Nystrom method or the RFF technique, both of which provide better asymptotic runtimes. Similarly, the Cholesky decomposition and linear solvers can be replaced with either CG or MINRES to, again, improve runtime performance. This especially makes sense approximating the kernel matrix as the Cholesky decomposition will provide an almost-exact solution to solving these linear system, although this is rather counterproductive if approximations are used earlier on within the algorithm.

**3.2. Experimental Setup.** Each method was implemented in python3 and run using the python3.8.5 interpreter distributed by the official python website. Various scientific computing python libraries, such

as numpy, pandas and scipy, were used to help implement methods to enhance runtime performance. A just-in-time compiler was also used to improve the performance of the FWHT and Krylov-Subspace methods as fast runtime is critically important for the success of both these methods. Experiments were carried out on a variety of different datasets listed in Table 2.

TABLE 2. Descriptions and sources for each of the datasets used in experiments.

<i>Name</i>	<i>Description</i>	<i>d</i>	<i>n</i>	<i>Source</i>
3DSN	The 3D Spatial Network (3DSN) dataset was constructed by adding elevation information to a 2D road network in North Jutland, Denmark (covering a region of $185 \times 135 km^2$ ).	2	2000	UCI
Abalone	Physical measurements of abalones.	7	4177	UCI
magic04	Simulated registration of high energy gamma particles in a ground-based atmospheric Cherenkov gamma telescope.	10	19020	UCI
Wine	Chemical measurements of wine.	11	4898	UCI
Temp	Weather station data from rural Queensland.	1	11324	Qld Gov
Stocks	Daily stock prices spanning 2000 to 2019.	4	4904	tiskw

3.2.1. *Kernel Martix Approximation Testing.* To test the various kernel matrix approximation techniques, each method was used to construct an estimate of the actual kernel matrix with varying sample sizes. The definition of samples changes depending of which family of approximation technique is considered. For the Nystrom technique, the number of samples refers to  $s$ , that is the number of columns sampled. For the RFF technique the samples refer to  $D$ , that being the dimension of the constructed feature space. The Nystrom technique was implemented according to [PDaMWM05] and RFF according to [Rah08] and [Liu21]. To see how well each technique was at approximating the kernel matrix by itself, each method was used to compute approximations for kernel matrices for each of the above data sets for a fixed  $\sigma$  and sample size. This was repeated 30 times for each dataset. For every method the relative Frobenius error  $\|K_{XX} - \widehat{K}_{XX}\|_F / \|K_{XX}\|_F$  and relative infinity error  $\|K_{XX} - \widehat{K}_{XX}\|_\infty / \|K_{XX}\|_\infty = \|\widehat{K}_{XX} - K_{XX}\|_\infty / \|K_{XX}\|_\infty$  (in the case of the RBF kernel) was recorded, using the notation that  $\widehat{K}_{XX}$  represents an approximated kernel matrix. The values of  $\sigma$  used were 0.1, 1.0 and 10.0, although a  $\sigma$  value of 2.1 was also used for the Wine data set to compare with [PDaMWM05] results. Additionally, computation time and memory usage for each kernel approximation was also recorded. It should be noted, however, that the time and memory spent on constructing probabilities for the Nystrom methods are not included in the kernel construction time and have instead been recorded separately in TODO. This is because the probabilities are typically known prior to kernel matrix construction and are simply used to provide an approximation to the kernel matrix instead on needing to save the entire data kernel matrix for new prediction. Thus they act as an efficient means to quickly save and rebuild the data kernel matrix. The errors, time and memory were average across the repetitions for each experiment.

To understand how well each kernel matrix approximation method performs in terms of providing predictions, each method was used to train a Gaussian process with  $4/5^{th}$  of each data set and required to predict the remaining  $1/5^{th}$ . Predictions for each data set was repeated 15 times across various sample sizes. The Mean Square Error (MSE) and Classification Error was captured to regression and classification tasks respectively. To make comparisons between different approximation methods as fair as possible, the matrix  $(\widehat{\mathbf{K}}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})^{-1}$  was directly inverted to eliminate any error an in-exact linear system solver might introduce. To do this efficiently, since both the Nystrom and RFF methods produce decompositions of their approximations in the form  $\widehat{\mathbf{K}}_{\mathbf{X}\mathbf{X}} = \mathbf{U}\mathbf{W}^\dagger\mathbf{U}^\top$  we can employ the use of the matrix inversion lemma (see ??) to compute

$$\begin{aligned} (\widehat{\mathbf{K}}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n})^{-1} &= (\mathbf{U}\mathbf{W}\mathbf{U}^\top + \sigma_n^2 \mathbb{1}_{n \times n})^{-1} \\ &= \sigma_n^{-2} \mathbb{1}_{n \times n} + \sigma_n^{-2} \mathbb{1}_{n \times n} \mathbf{U} (\mathbf{W}^\dagger + \mathbf{U}^\top \sigma_n^{-2} \mathbb{1}_{n \times n} \mathbf{U})^{-1} \mathbf{U}^\top \sigma_n^{-2} \mathbb{1}_{n \times n}. \end{aligned}$$

Only a single value of  $\sigma$  was used to create predictions for each dataset. The value of  $\sigma$  chosen corresponds to the best value of  $\sigma$  out of 0.1, 1.0 and 10.0 (as well as 2.1 for the Wine dataset) when an exact GP algorithm was used to provide predictions. The time and memory of performing the matrix inverse using the above was recorded. Again, errors, time and memory were average across the repetitions for each different sample.

**3.2.2. Krylov Subspace Methods Approximation Testing.** Similar to the kernel matrix approximation setup, to see how well CG and MINRES compare in providing predictions each method was used to solve the linear system

$$(\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}) \boldsymbol{\alpha} = \mathbf{y}$$

within the GPR algorithm and

$$(\mathbf{K}_{\mathbf{X}\mathbf{X}} + \mathbf{W}^{-1}) \boldsymbol{\alpha} = \mathbf{K}_{\mathbf{x}_* \mathbf{X}}^\top$$

within the GPC algorithm in terms of  $\boldsymbol{\alpha}$ . As before, predictions for each data set was repeated 15 times across various samples. The Mean Square Error (MSE) and Classification Error was captured to regression and classification tasks respectively. To allow for a fair comparison between the different linear solvers, the kernel matrix was constructed in an exact manner to ensure no error was introduced through any other part of the prediction process. As with the kernel matrix approximation prediction set up, only a single value of  $\sigma$  was used to create predictions for each dataset, that being the value of  $\sigma$  that provided the best predictions results using exacts methods. Each method was used to train a Gaussian process with  $4/5^{th}$  of each data set and required to predict the remaining  $1/5^{th}$  over all the different datasets and was repeated 15 times for each dataset with a varying number of maximum iterations. The usual statistics such as prediction error, time and memory usage were recorded for every experiment and averaged across repetitions for each dataset and method.

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