



THE UNIVERSITY OF QUEENSLAND
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. APPLICATIONS AND RESULTS	4
1.1. GAUSSIAN PROCESSES PREDICTION REVIEWED	4
1.2. EXPERIMENTAL SETUP	4
1.2.1. KERNEL MARTIX APPROXIMATION TESTING	5
1.2.2. KRYLOV SUBSPACE METHODS APPROXIMATION TESTING	6
1.3. DISCUSSION	6
1.3.1. KERNEL MATRIX APPROXIMATION	6
1.3.2. KRYLOV SUBSPACE METHODS	8
REFERENCES	10
APPENDIX A. SUPPLEMENTARY RESULTS	14
A.1. GRAM MATRIX SPECTRAL VALUES	14
A.2. NYSTROM SCORES	17
A.3. PROBABILITY CONSTRUCTION TIMES FOR NYSTROM METHODS	20
A.4. RIDGE LEVERAGE SCORES	23
A.5. NYSTROM ERRORS	26
A.6. NYSTROM ERRORS	32
A.7. KERNEL COMPARISONS	36

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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.
$ 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.
x^T, X^T	The transpose operator.
x^*, X^*	The hermitian operator.
$a.*b$ or $A.*B$	Element-wise vector (matrix) multiplication, similar to Matlab.
\propto	Proportional to.
∇ or ∇_f	The partial derivative (with respect to f).
$\nabla\nabla$	The Hessian.
\sim	Distributed according to, example $x \sim \mathcal{N}(0, 1)$
0 or 0_n or $0_{n \times m}$	The zero vector (matrix) of appropriate length (size) or the zero vector of length n or the zero matrix with dimensions $n \times m$.
1 or 1_n or $1_{n \times m}$	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. The identity matrix in the case $n = m$.

$\mathbf{A}_{(.,.)}$	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 $\mathbb{R}^{3 \times (j'-j+1)}$ submatrix 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 $\mathbb{E}_{q(x)}[z(x)]$	Expectation, or expectation of $z(x)$ where $x \sim q(x)$.
\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, $\{\sum_{k=1}^n \lambda_k \mathbf{x}_k \mid \lambda_k \in \mathbb{R}\}$.
$\mathbf{K}_{WW'}$	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 $\mathbf{K}_{WW'} \in \mathbb{R}^{n \times n'}$ has elements $(\mathbf{K}_{WW'})_{i,j} = k(\mathbf{w}_i, \mathbf{w}'_j)$.
$\text{lin-solve}(\mathbf{A}, \mathbf{B})$	A function used to solve $\mathbf{X} = \mathbf{A}^{-1} \mathbf{B}$ for the linear system $\mathbf{AX} = \mathbf{B}$.
$\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ 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 is a member of $\mathcal{O}(g)$ 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^{th} training input.

\mathbb{Z}

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

INTRODUCTION

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

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

Interestingly, the best action does not rely so much on the model's internalized parameters but rather on the predictive distribution $p(y_* | \mathbf{x}_*, \mathbf{X}, \mathbf{y})$ [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

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

[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^{th} nearest neighbors and ridge regression) are still overshadowed by their neural network cousins, GPs have made a quiet comeback in the ML community [Cao18].

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

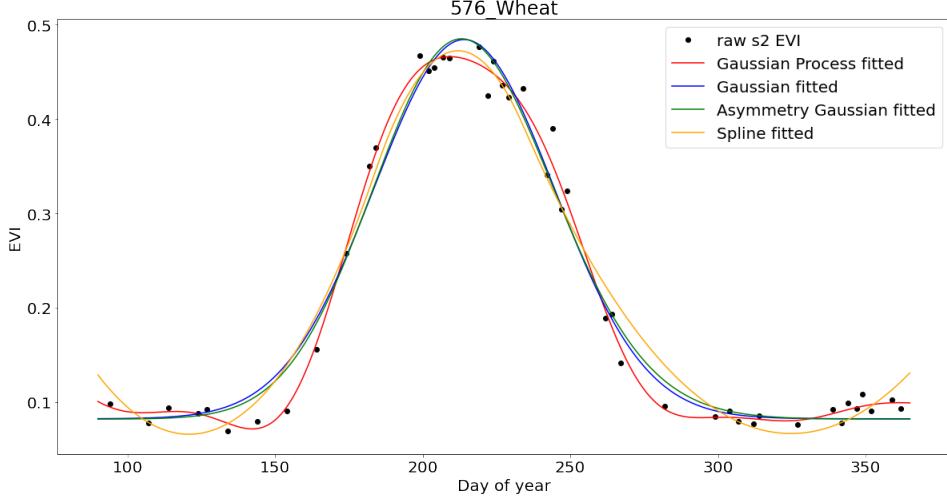


FIGURE 1. Potgieter’s team found that GPs were superior in terms of predicting a phenological timeline for a number of common seasonal crops over other parametric models.

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 ?? and ?? will cover techniques for approximating a large matrix used with GPs that provides information on how similar each observation is to one other. Chapter ?? then gives alternative methods for solving linear systems, an essential component required for the GP algorithm to work.

1. 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 faster methods, at the expense of small amounts of accuracy. 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 model.

1.1. 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, this will scale very poorly where most modern desktops would not be able to feasibly perform training with datasets having more than 10^5 samples [WJMaSKaAGW21, page 2]. The Gaussian Process classifier from ?? suffers for the exact same reasons as GPR. To mitigate the computational burden of these bottle necks, we can replace these procedures with their inexact counterparts discussed in Chapters ??, ?? and ??.

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 solves 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, as this is rather counterintuitive if approximations are used earlier on within the algorithm.

1.2. 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

1.2.1. *Kernel Matrix 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 [PDAWM05] and RFF according to [Rah08] and [Liu21]. Each method was used to compute approximations for kernel matrices for each of the above data sets for a fixed σ 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 $\|K_{XX} - \widehat{K}_{XX}\|_\infty / \|K_{XX}\|_\infty = \|K_{XX} - \widehat{K}_{XX}\|_\infty$ (in the case of the RBF kernel) was recorded, using the notation that \widehat{K}_{XX} represents an approximated kernel matrix. The values of σ used were 0.1, 1.0 and 10.0, although a σ value of 2.1 was also used for the Wine data set to compare with [PDAWM05] 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 $4/5^{ths}$ 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 for 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 to their approximations of the form $\widehat{\mathbf{K}}_{\mathbf{X}\mathbf{X}} = \mathbf{U}\mathbf{W}^\dagger\mathbf{U}^\top$ we can make 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 σ was used to create predictions for each dataset. The value of σ chosen corresponds to the best value of σ out of 0.1, 2.1, 1.0 and 10.0 when an exact GP algorithm was used to provide predictions (a value of 2.1 was used to help compare with the results from [PDAWMW05]). 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.

1.2.2. 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 for 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 σ was used to create predictions for each dataset, that being the value of σ that provided the best predictions results using exacts methods. Each method was used to train a Gaussian process with $4/5^{ths}$ 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 metrics such as prediction error, time and memory ususage were recorded for every experiment and averaged across repetitions for each dataset and method.

1.3. Discussion.

1.3.1. Kernel Matrix Approximation. Starting with the performance of the Nystrom methods, assessing Figures 26 to 37, overall the rls method is certainly the best methods among the sampling distributions as it virtually always is among the top three methods for any combination of dataset, k or σ . Interestingly,

non-uniform sampling techniques performed better with datasets for which the spectrum of the corresponding kernel matrix was also non-uniform. For example the spectrum for the kernel matrices of the magic04 and Stocks dataset (see Figures 4 and 5) are relatively uniform and from Figures 30 and 32 we find that the non-uniform sampling techniques give rather poor approximations and generally behave just as bad, or even worse, than the naive uniform sampling distribution. In contrast, non-uniform methods very much shine for datasets such as the 3DSN and Wine datasets where some of the better methods could provide almost exact kernel matrix approximations (refer to Figures 26, 27, 36 and 37) after a few thousand samples. This phenomena is likely due to the fact that when the spectrum of a matrix is less uniform, it decays faster, meaning that the matrix can be better expressed as a low-rank approximation. Evidently, the majority of non-uniform sampling distributions are intelligent enough to select columns that are best representative in this low rank approximation, most of the time. What is especially interesting about the Abalone dataset is, despite the rls sampling distribution being almost uniform (compared to other sampling distributions, see Figures 9 and 21), the rls methods seems to perform significantly better than uniform selection, shown in Figure 28. The small amount of variation in the rls sampling distribution presumably gives it an edge over the uniform method in selecting columns that better provides information to the lower rank approximation.

Looking at the RFF methods, we find that the ORF and SORF methods do not really live up to their acclaimed theoretical error bounds. While the ORF and SORF methods do occasionally produce better errors over the standard transformation matrix sampling (see Figures 38 to 49), it is hard to argue using either of these methods as neither them offer no obvious advantage in terms of time and memory saving (see Figures TODO). This may come as a surprise for most with the SORF method under deliverance, even with a JIT compiler was used to speed up various parts of the algorithm. This dissonance between the theoretical bounds presented in ?? and these "real world" experiments is that the single line of code to produce the i.i.d. Gaussian matrix for the standard transformation matrix using the numpy python library has been incredibly well engineered and optimized to produce matrix samples brilliantly fast and is designed to cope with large scaling. When given large enough datasets, the SORF method likely will overtake the "basic" sampling method proposed by Rami and Recht. Unfortunately, due to the memory constraints of the computers used for this project, such large data sets could not be experimented with.

To make a fair comparison in kernel matrix approximation between the RFF and Nystrom methods, the time that each method used to build an approximation was graphed along side the corresponding relative error. In this setup, we can think about each method having some sort of time budget and that its task is to produce the best approximation it can within this time limit, regardless of how many samples it requires or how big of a feature space it uses. Comparing the methods in this manner, the Nystrom family is superior in lowering the Frobenius error in the approximations it produces, while the RFF methods provide approximations with smaller infinity errors (see Figures 50 to 61). In other words, Nystrom methods produce approximations where entries are *on average* closer to the true matrix compared to RFF methods, while RFF methods produce approximations where entries are *in the worst case* closer to the true matrix compared to the Nystrom methods. This makes sense since much of the theory in the Nystrom methods was aimed towards lowering the Frobenius errors, while the theory behind the RFF methods was aimed towards lowering the infinity errors. One final point worth mentioning is that RFF methods

seemed to require much larger amounts of memory to produce their approximations, sometimes double or even triple the amount of memory the Nyström methods used (refer to Figures TODO).

Next, two methods from the nyström class and one method from the RFF class, that we deemed to be the best among the respective families, were used within Gaussian Process algorithm (replacing exact kernel matrix creation) to help form predictions. The rls and data columns methods were chosen to represent the best of the nyström family while the Rami and Recht's "basic" RFF method was chosen to represent the best of the RFF techniques. Similar to relative error comparisons, the time that each method used to an approximation was graphed along side the corresponding prediction error. Looking at the results, no method seemed to be a clear winner. In general Rami and Recht's RFF method usually delivered the best predictions with smaller time budgets were the rls generally caught up and overtook it when a larger time budget was allowed. Moreover, the data columns method, overall, yields the poorest predictions errors among the selected methods. Thus, the RFF method would probably be the best method to use in practice for two main reasons. The first reason is, if one was to select an inexact method for kernel matrix production, it likely means that they do not have a large time budget to begin with so that RFF's ability to produce the best approximation within shorter timeframes makes it highly desirable to use. Furthermore, the time taken to construct probability distributions used in the nyström methods are not included in Figure TODO (and can instead be found in ...) making it harder to justify using the rls method if the probability distribution is not already available since a much larger time budget would be required to deliver the same level of prediction accuracy.

1.3.2. Krylov Subspace Methods. The CG and MINRES methods where also used within the Gaussian Process algorithm to see which one of the two would provide better predictions. The number of iterations that each method used to form an approximation was graphed along side the corresponding prediction error produced. Differences in execution time per iteration were nominal between the two methods. Looking at the results in Figures TODO, it seems that the MINRES method performs just as well and, occasionally, even better than CG. This becomes very apparent from the prediction errors produced from the abalone and 3DSN datasets. In particular, the MINRES method seems to give better results even of the quadratic dataset. The quadratic dataset is an artificial dataset constructed using a Gaussian process with a quadratic mean function $x^2 + y^2$ and some amount of variance. The purpose of this dataset was to check if applied method was prone to overfitting. The fact that, overall, MINRES gave better error indicates that it is also more robust against overfitting compared to CG. To understand why MINRES may produce better errors for regression tasks, recall that the mean square error is computed in the following manner

$$\begin{aligned} \text{MSE}(\bar{\mathbf{f}}_*) &= \frac{1}{n} \|\bar{\mathbf{f}}_* - \mathbf{y}_*\|_2^2 \\ &= \frac{1}{n} \|\mathbf{K}_{\mathbf{X}_* \mathbf{X}} \text{lin-solve}(\mathbf{K}_{\mathbf{X} \mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}, \mathbf{y}) - \mathbf{y}_*\|_2^2 \\ &\leq \frac{1}{n} (\|\mathbf{K}_{\mathbf{X}_* \mathbf{X}}\|_2^2 \|\text{lin-solve}(\mathbf{K}_{\mathbf{X} \mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}, \mathbf{y})\|_2^2 + \|\mathbf{y}_*\|_2^2). \end{aligned}$$

From the above result, we find that the mean square error is bounded above by the Euclidean norm of $\text{lin-solve}(\mathbf{K}_{\mathbf{X} \mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}, \mathbf{y})$. The MINRES method seeks to solve $\text{lin-solve}(\mathbf{K}_{\mathbf{X} \mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}, \mathbf{y})$ by

finding vectors, \mathbf{x}_k , that successively minimize the Euclidean-distance that is

$$\mathbf{x}_k = \arg \min_{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_k} \|[\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}] \mathbf{x} - \mathbf{y}\|_2.$$

In contrast, CG instead seeks vectors that successively minimize $\|\mathbf{r}_k\|_{[\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}]^{-1}}$, which we are not so interested in when comparing and contrasting test accuracies across different methods. Thus, the success of MINRES is likely owed to its ability to more directly lower the Euclidean distance of lin-solve $(\mathbf{K}_{\mathbf{X}\mathbf{X}} + \sigma_n^2 \mathbb{1}_{n \times n}, \mathbf{y})$.

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APPENDIX A. SUPPLEMENTARY RESULTS

Additional results that may have not been included in the main text for conciseness.

A.1. Gram Matrix Spectral Values.

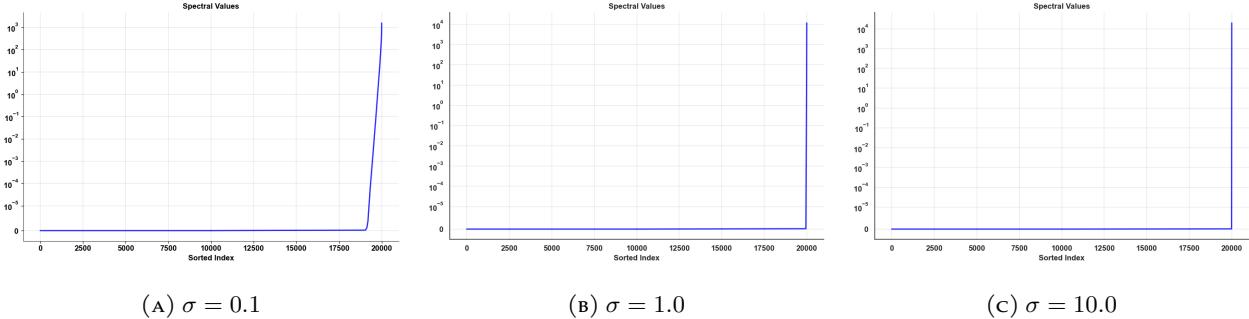


FIGURE 2. Spectral values for 3D-spatial network data.

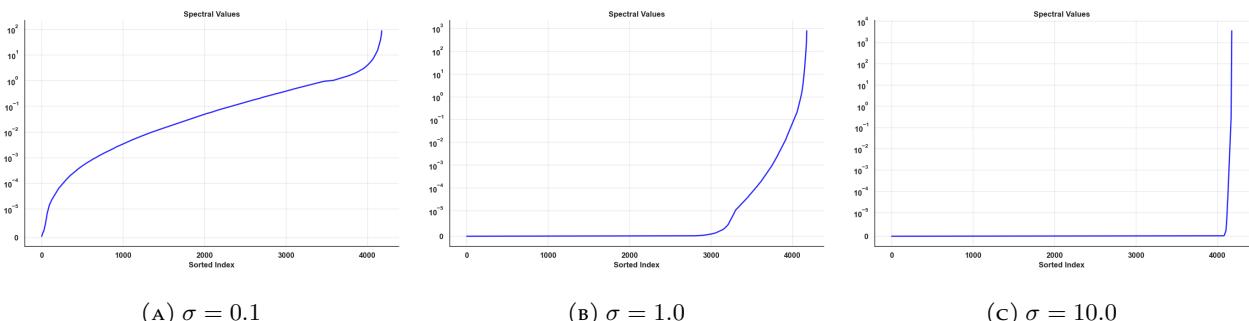


FIGURE 3. Spectral values for abalone data.

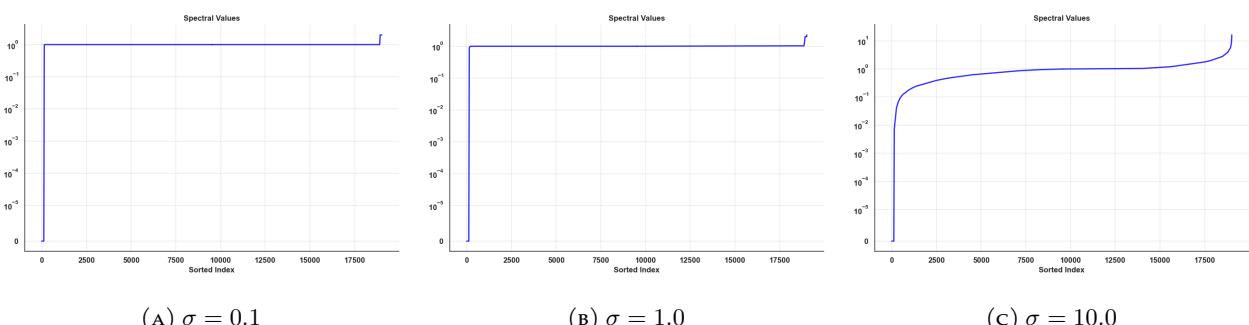


FIGURE 4. Spectral values for magic04 data.

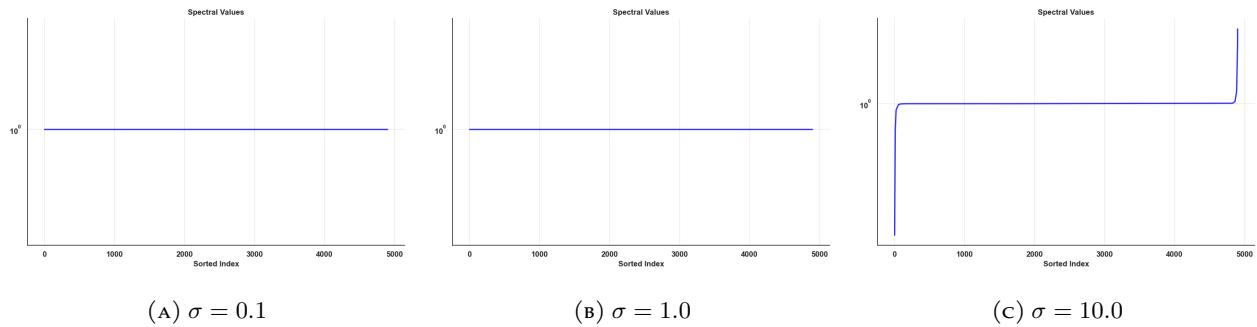


FIGURE 5. Spectral values for stock market data.

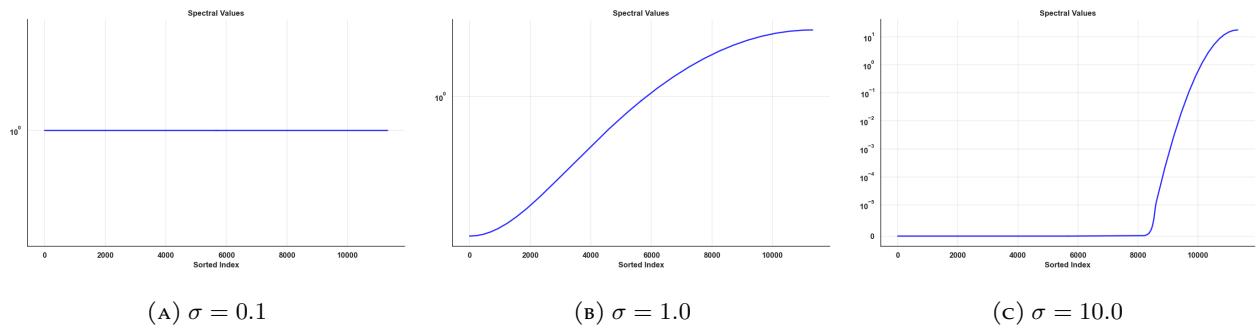


FIGURE 6. Spectral values for temperature data.

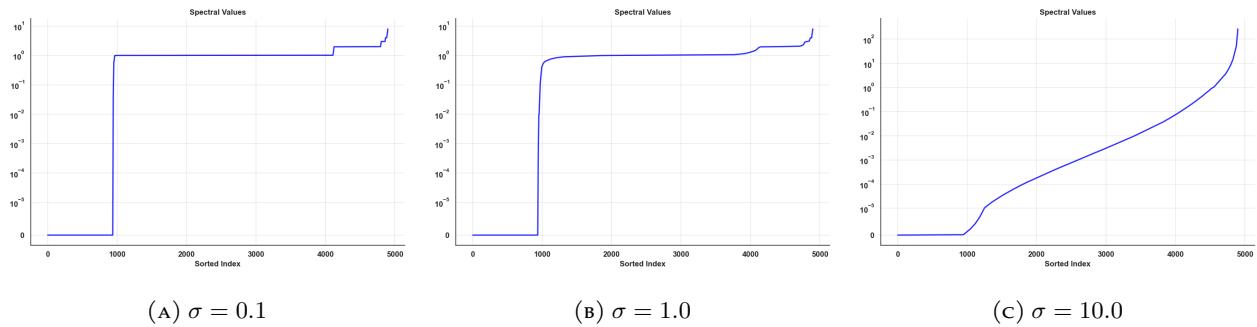


FIGURE 7. Spectral values for wine data.

A.2. Nystrom Scores.

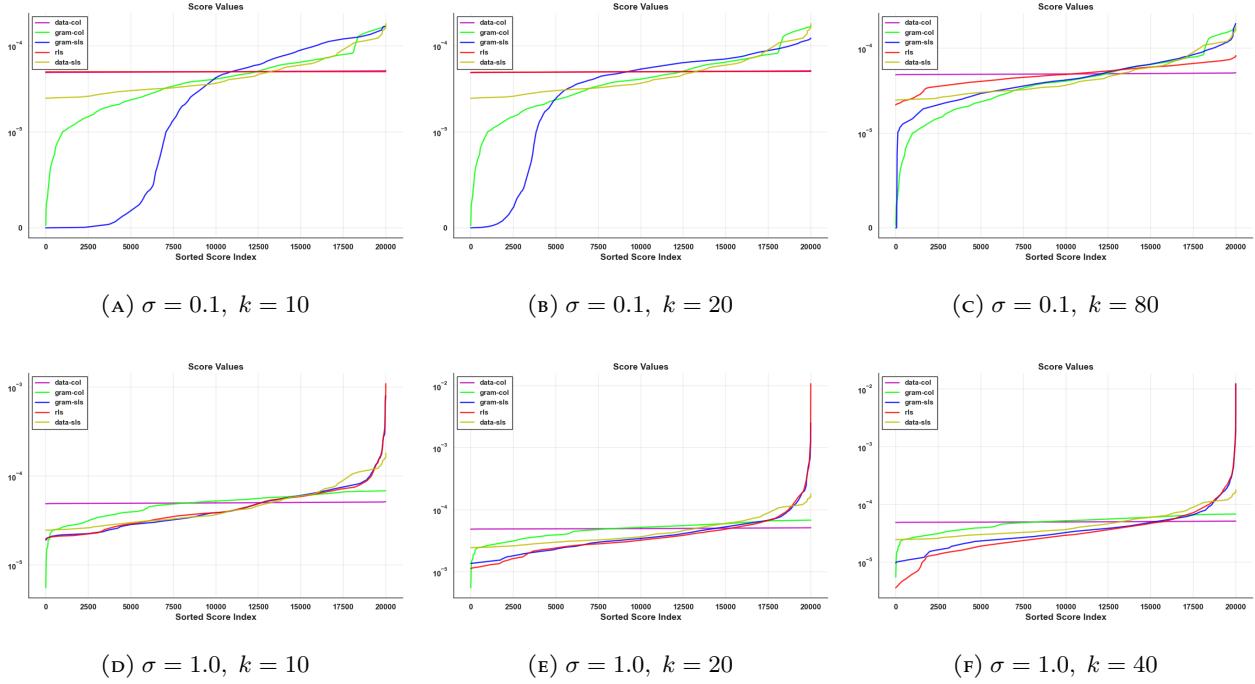


FIGURE 8. Nystrom scores for the 3D-spatial network data set.

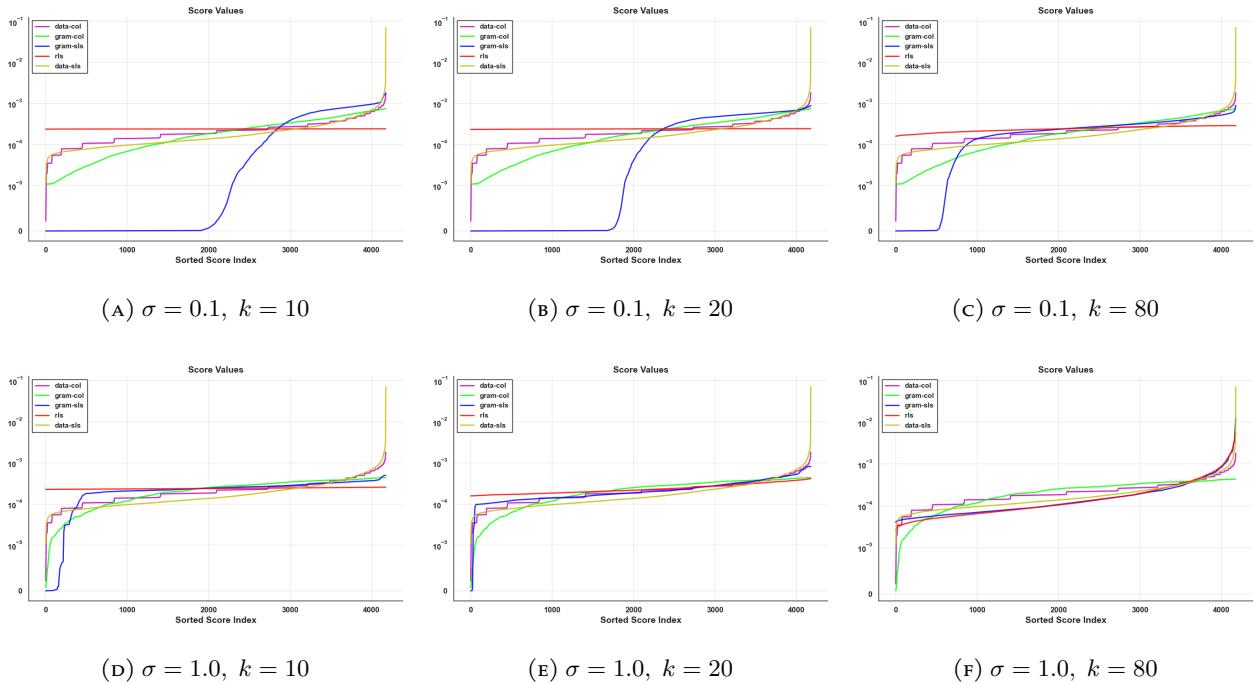


FIGURE 9. Nystrom scores for the Abalone data set.

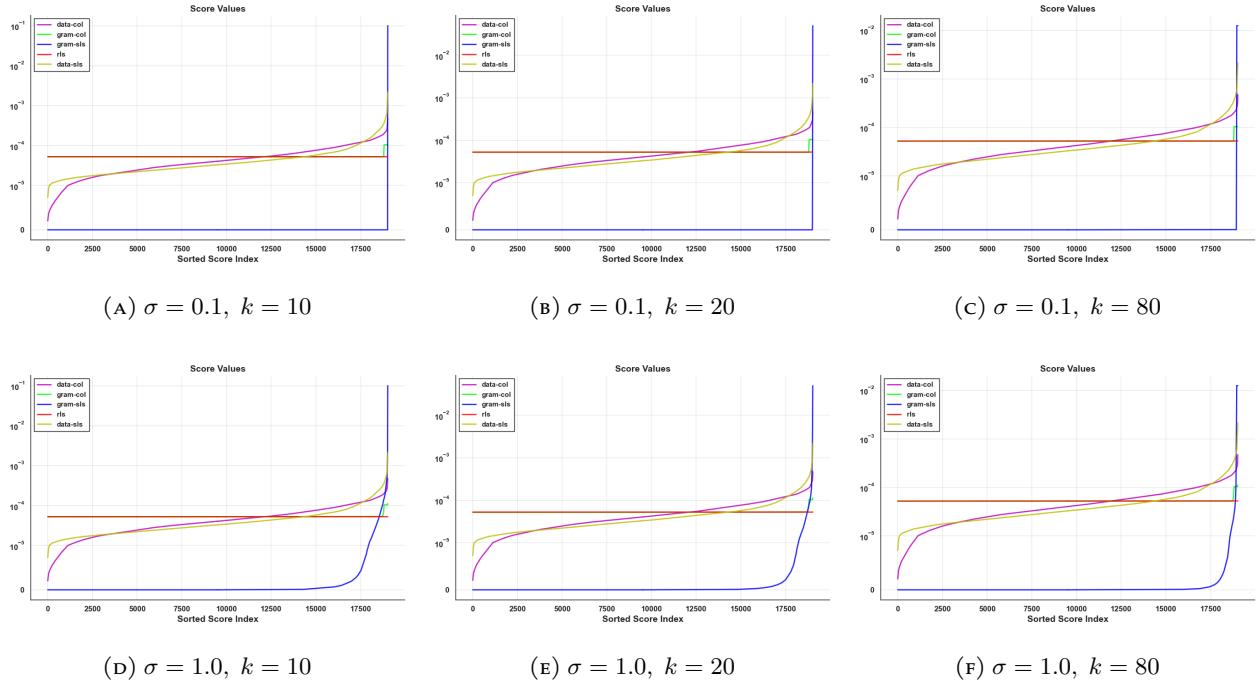


FIGURE 10. Nystrom scores for the Magic data set.

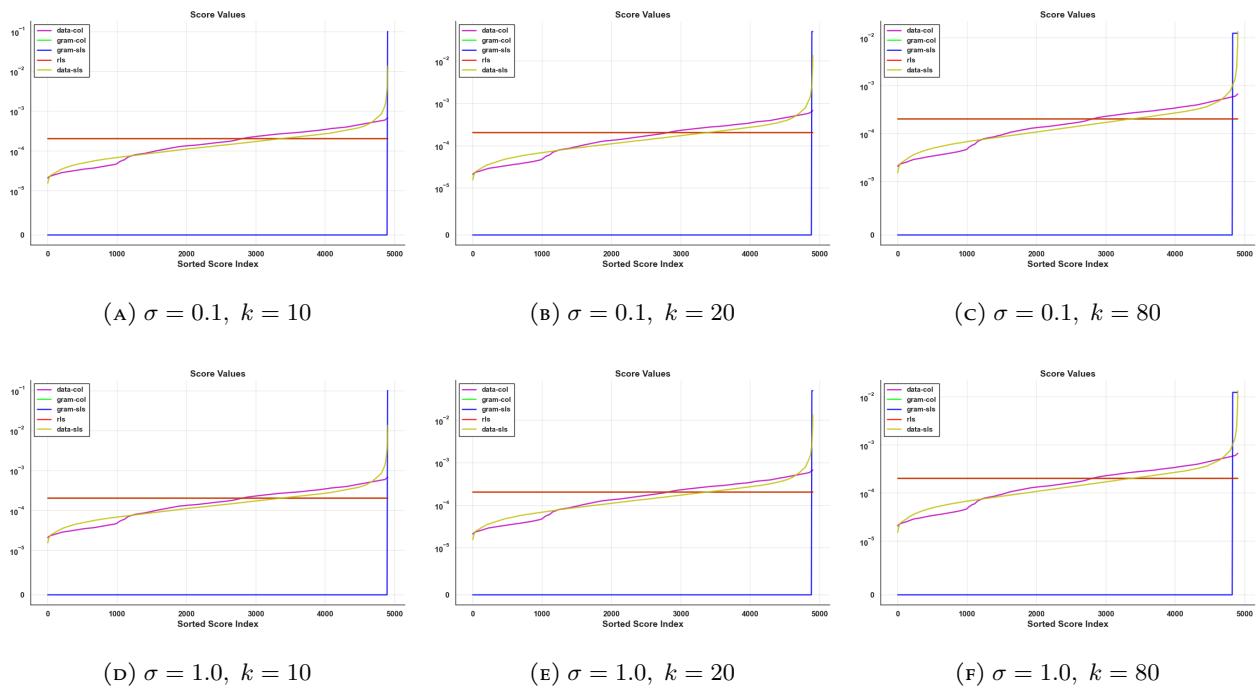


FIGURE 11. Nystrom scores for the stock market data set.

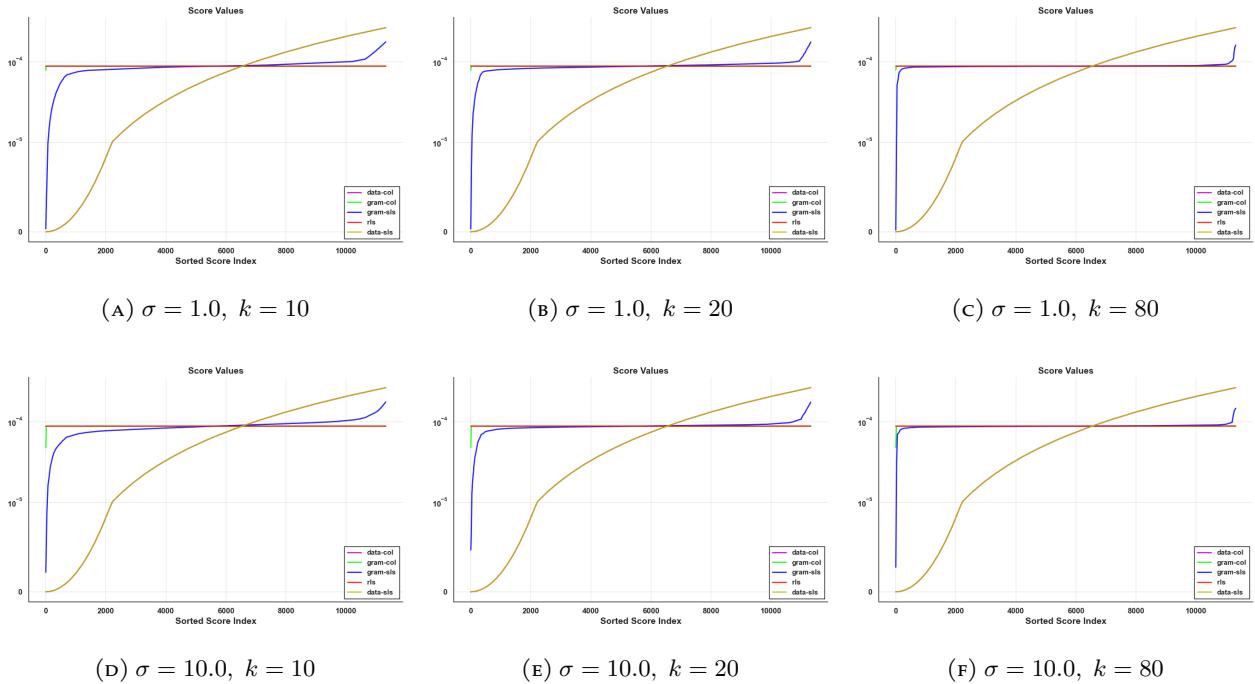


FIGURE 12. Nystrom scores for the temperature data set.

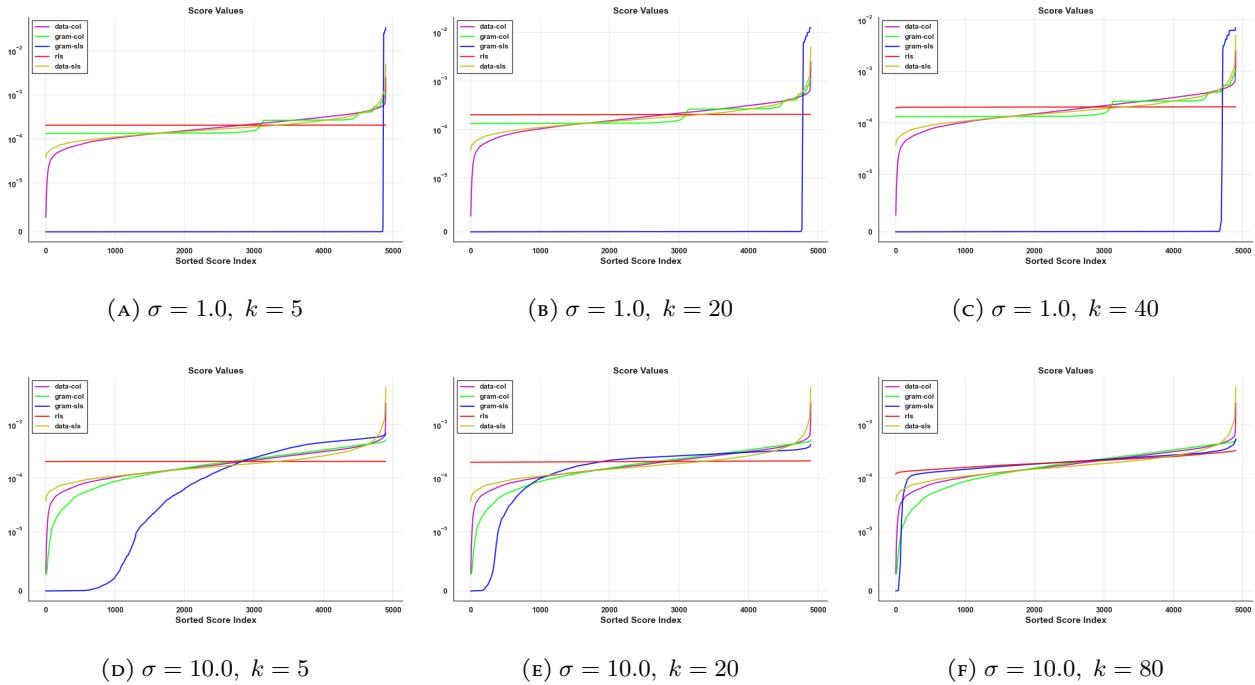


FIGURE 13. Nystrom scores for the wine data set.

A.3. Probability Construction Times for Nystrom Methods.

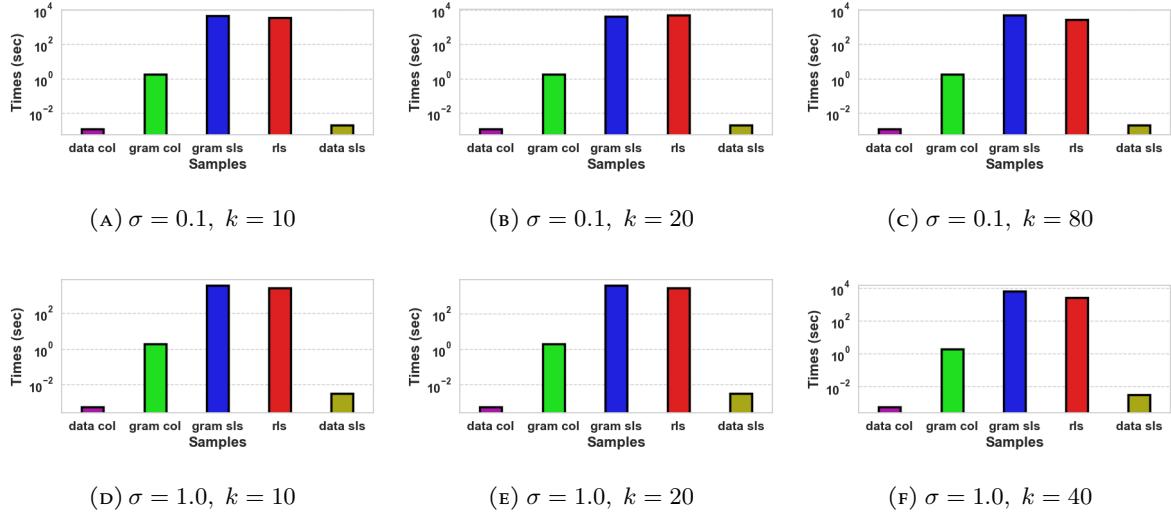


FIGURE 14. Probability construction times for the 3D-spatial network data set.

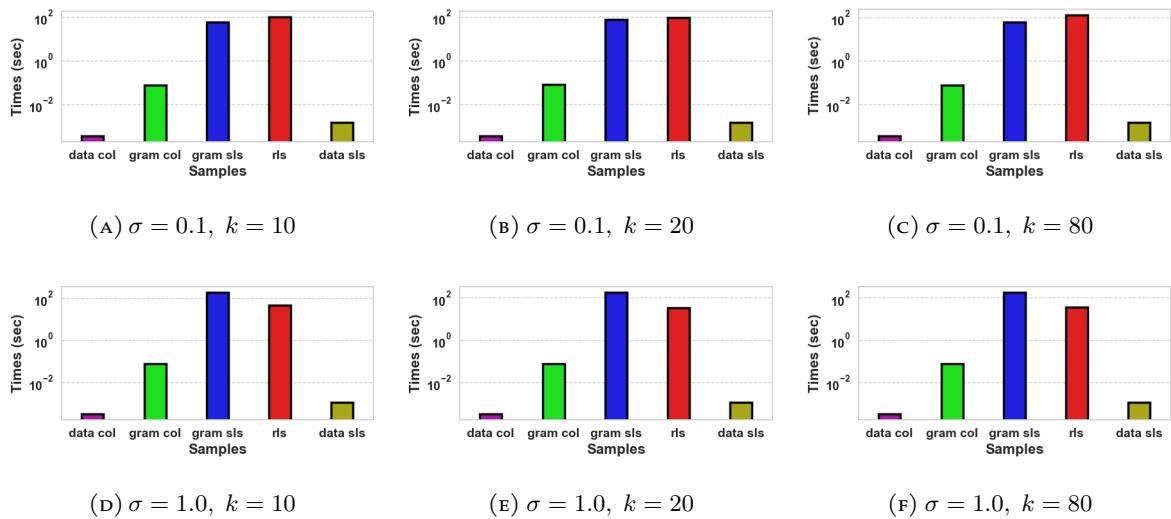


FIGURE 15. Probability construction times for the Abalone data set.

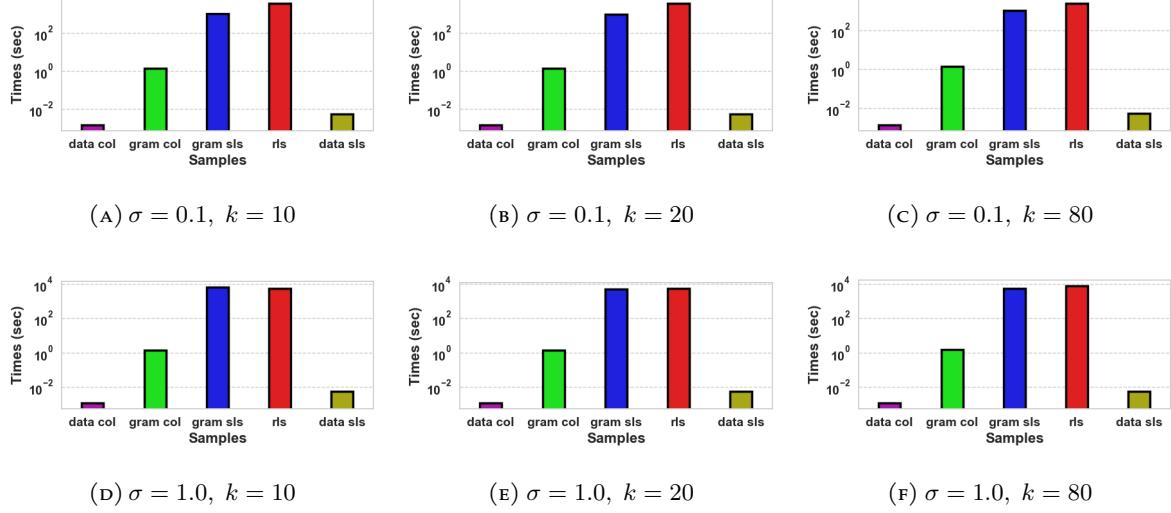


FIGURE 16. Probability construction times for the Magic data set.

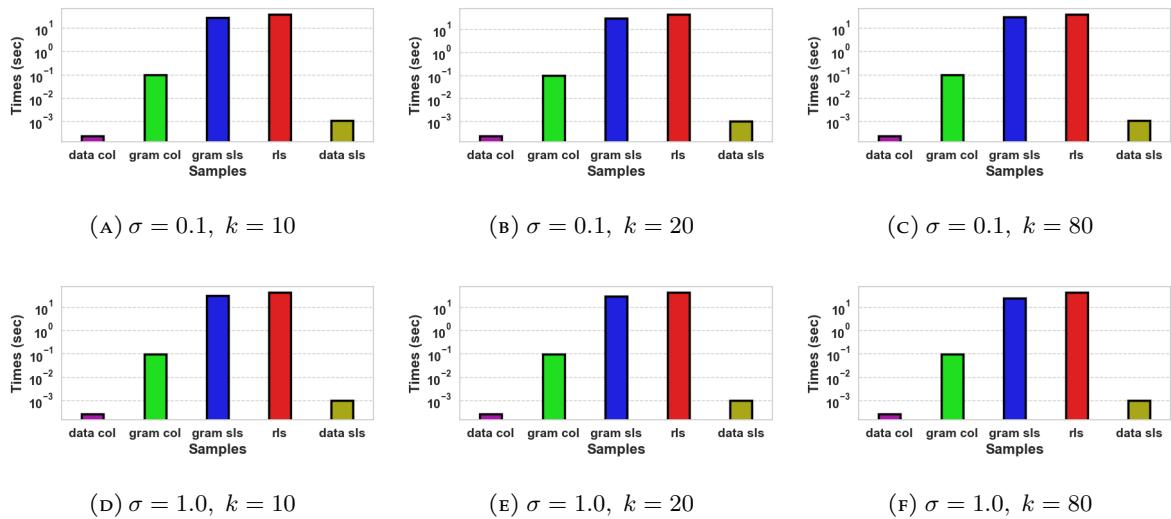


FIGURE 17. Probability construction times for the stock market data set.

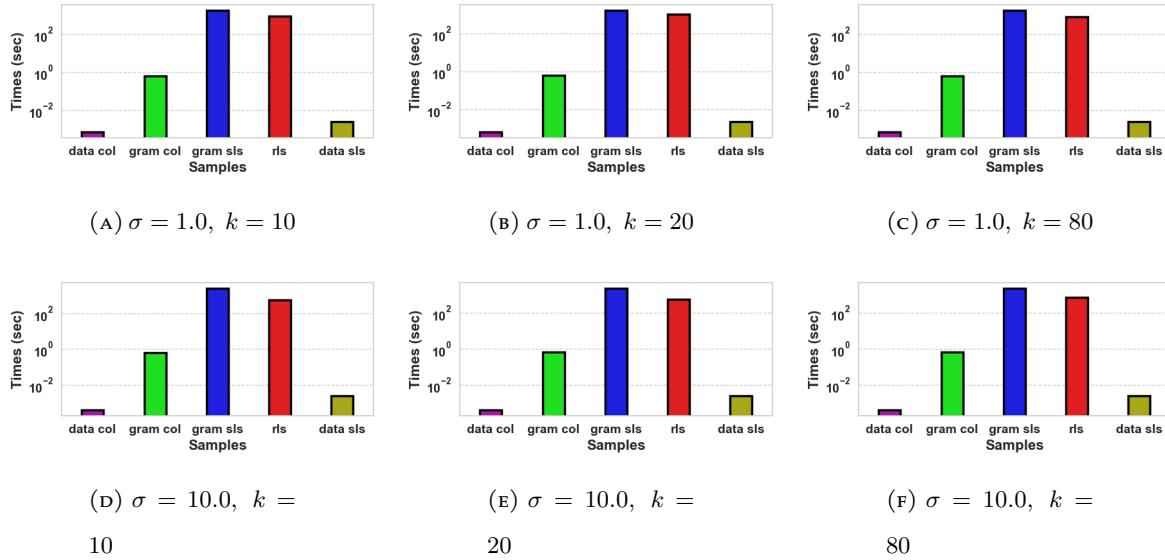


FIGURE 18. Probability construction times for the temperature data set.

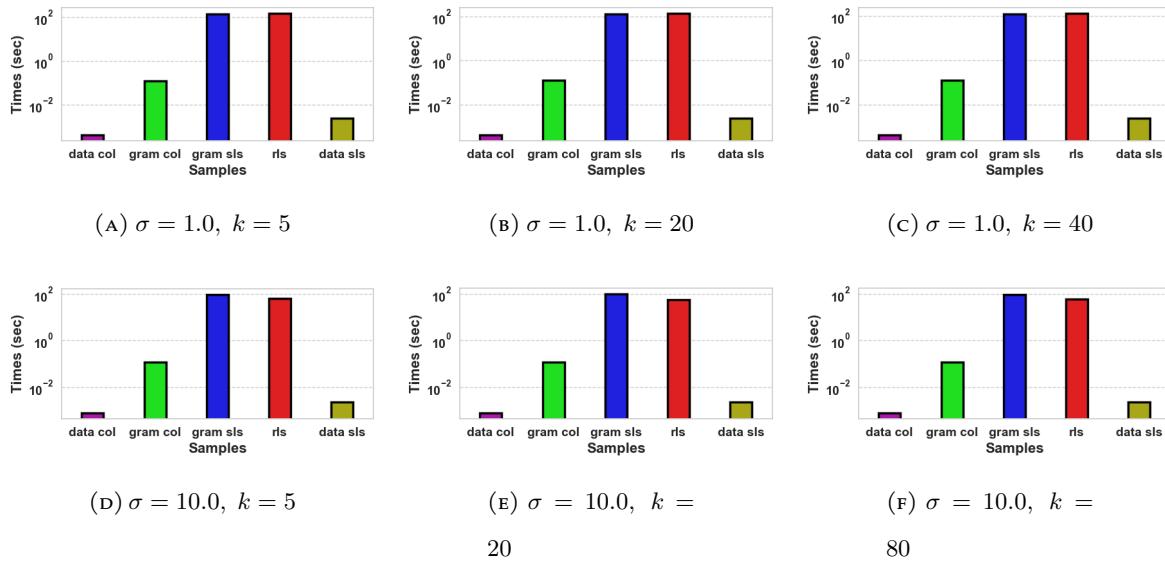


FIGURE 19. Probability construction times for the wine data set.

A.4. Ridge Leverage Scores.

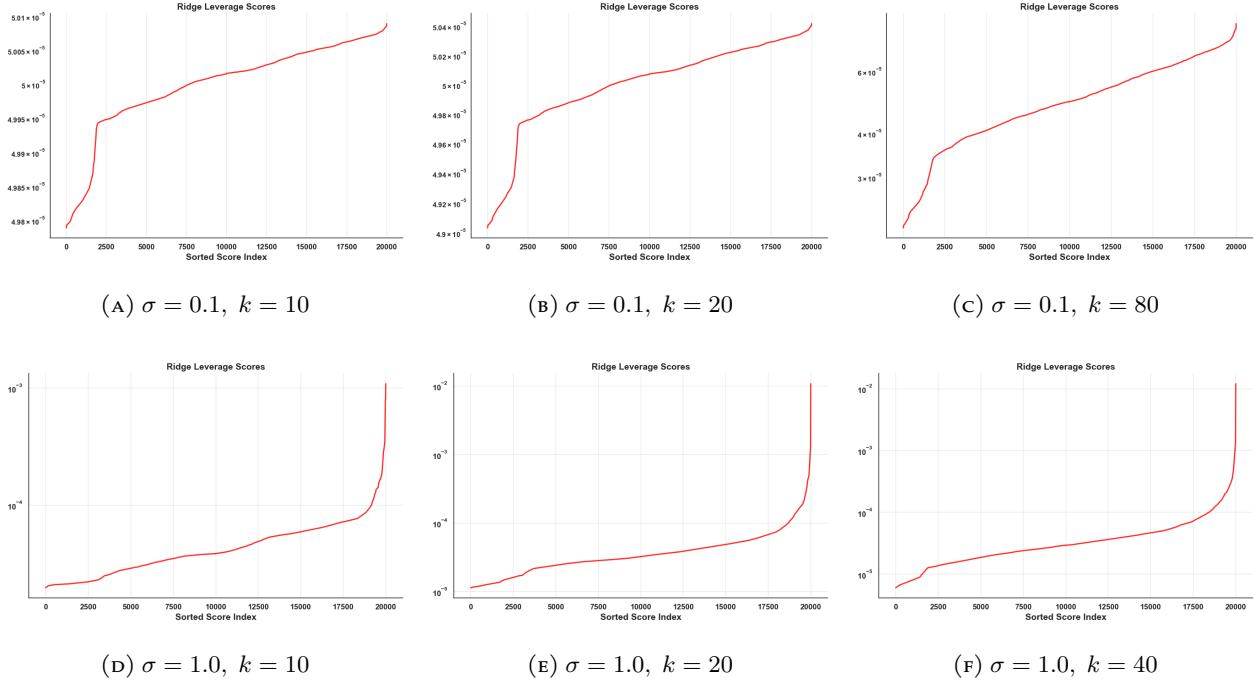


FIGURE 20. Ridge Leverage scores for the 3D-spatial network data set.

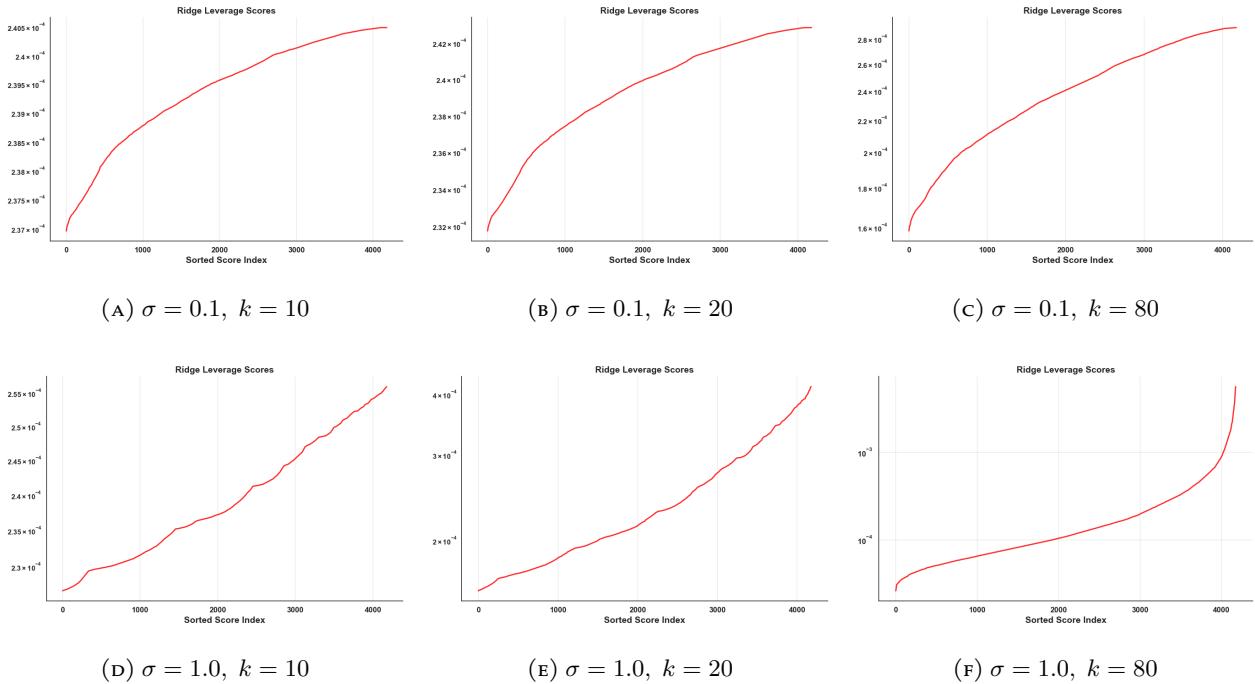


FIGURE 21. Ridge Leverage scores for the Abalone data set.

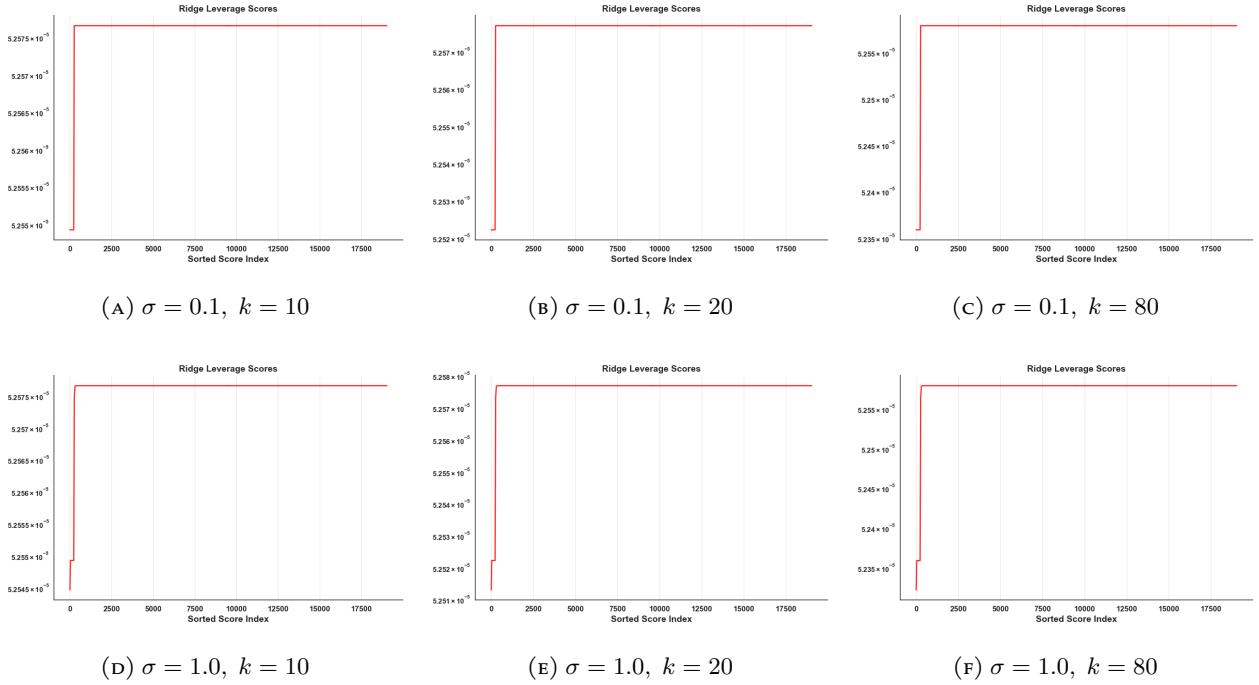


FIGURE 22. Ridge Leverage scores for the Magic data set.

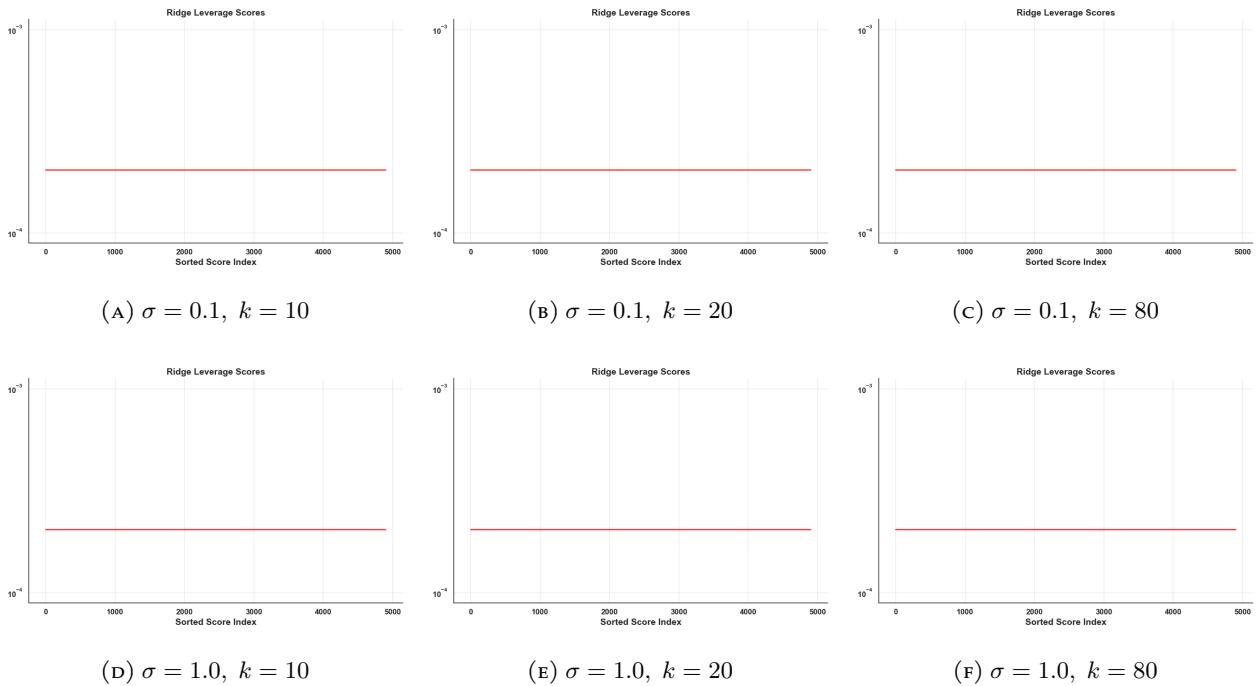


FIGURE 23. Ridge Leverage scores for the stock market data set.

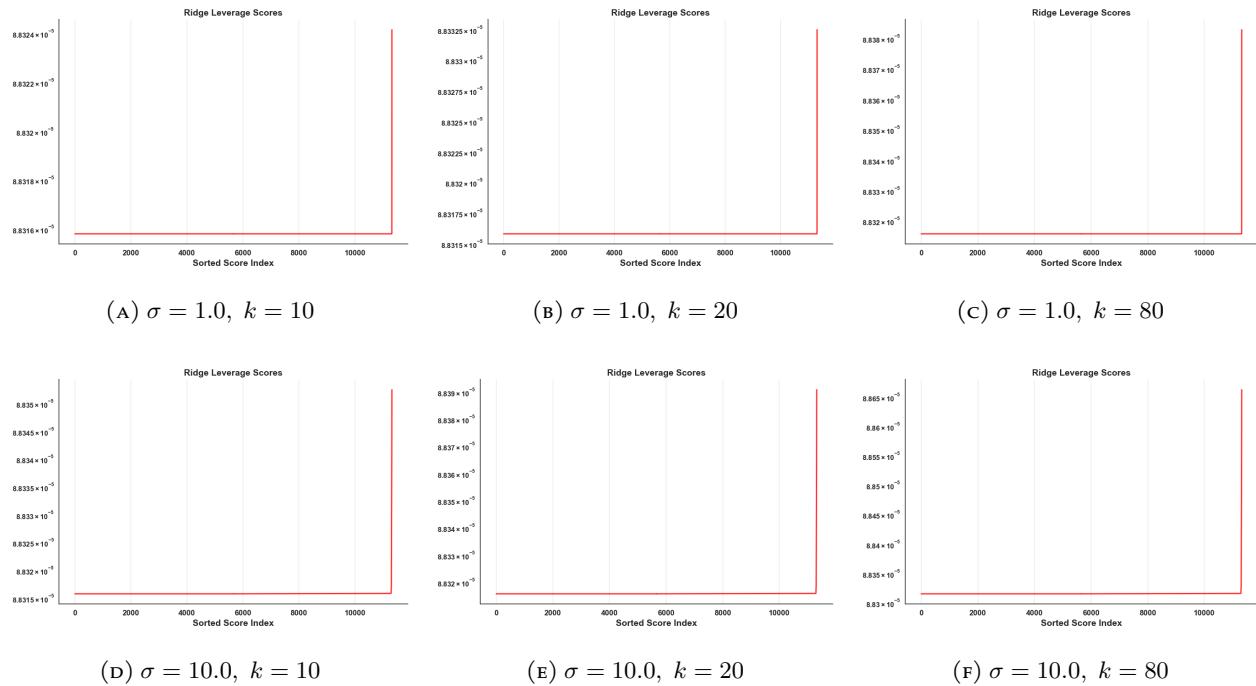


FIGURE 24. Ridge Leverage scores for the temperature data set.

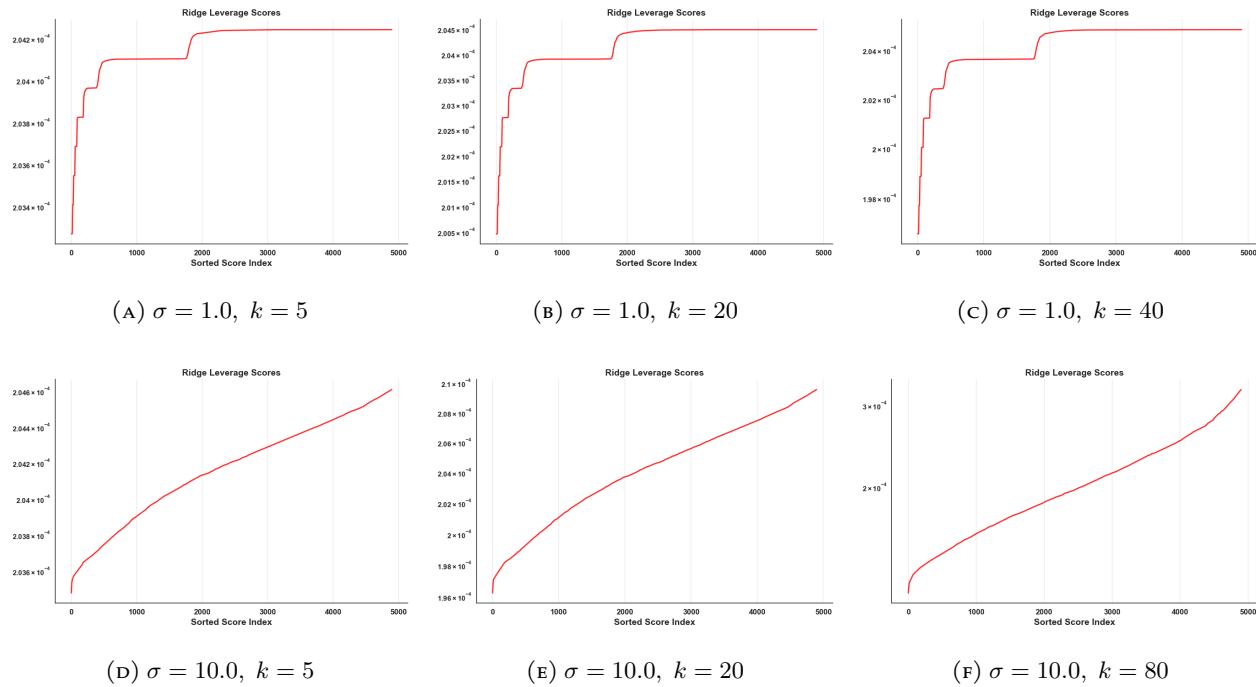


FIGURE 25. Ridge Leverage scores for the wine data set.

A.5. Nystrom Errors.

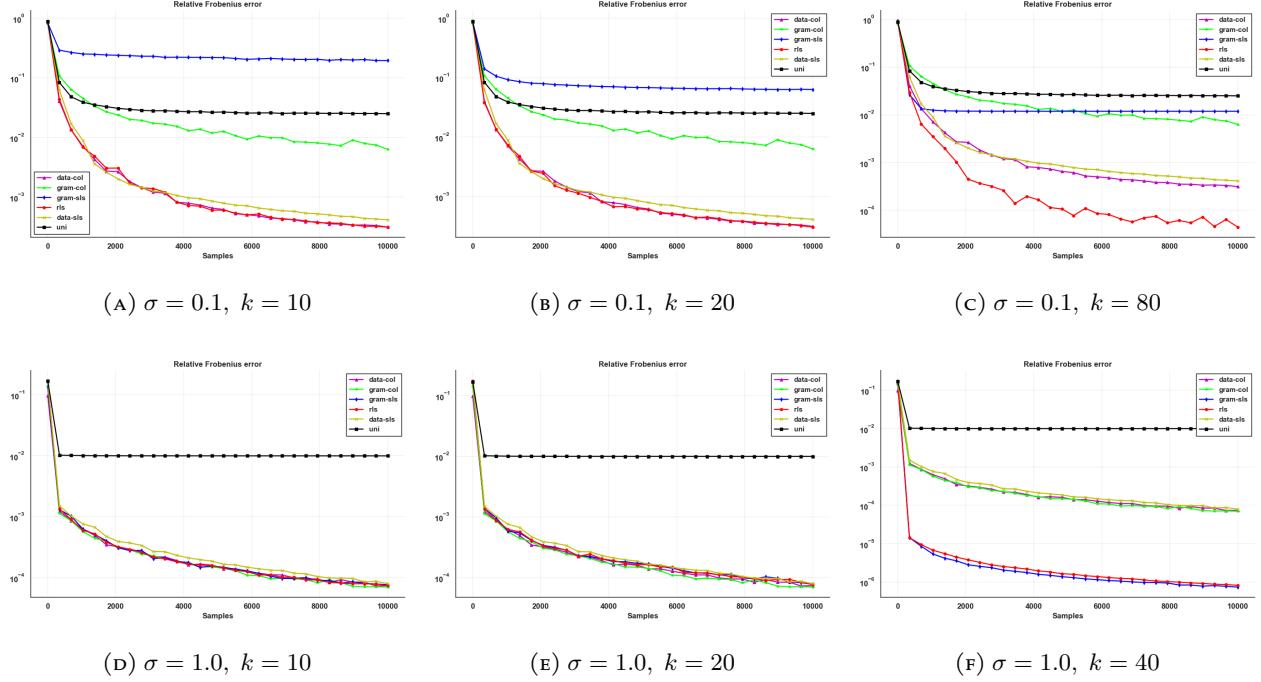


FIGURE 26. Nystrom Frobenius errors for the 3DSN data set.

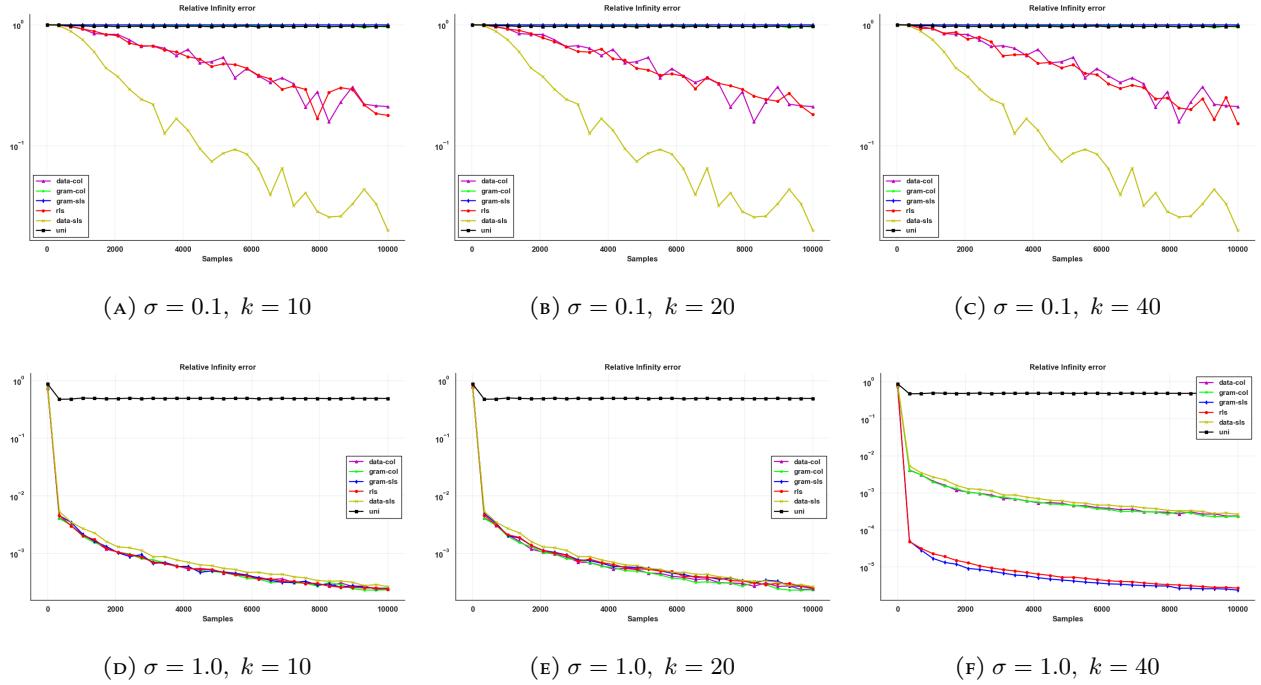


FIGURE 27. Nystrom infinity errors for the 3DSN data set.

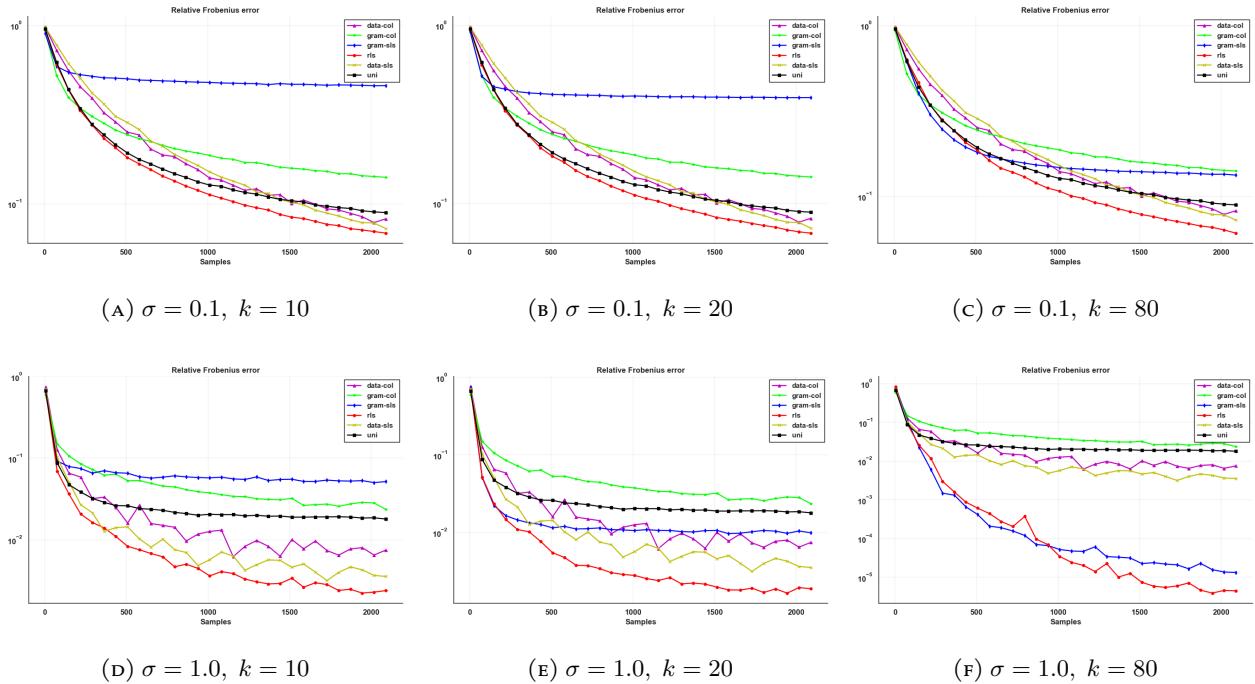


FIGURE 28. Nystrom Frobenius errors for the Abalone data set.

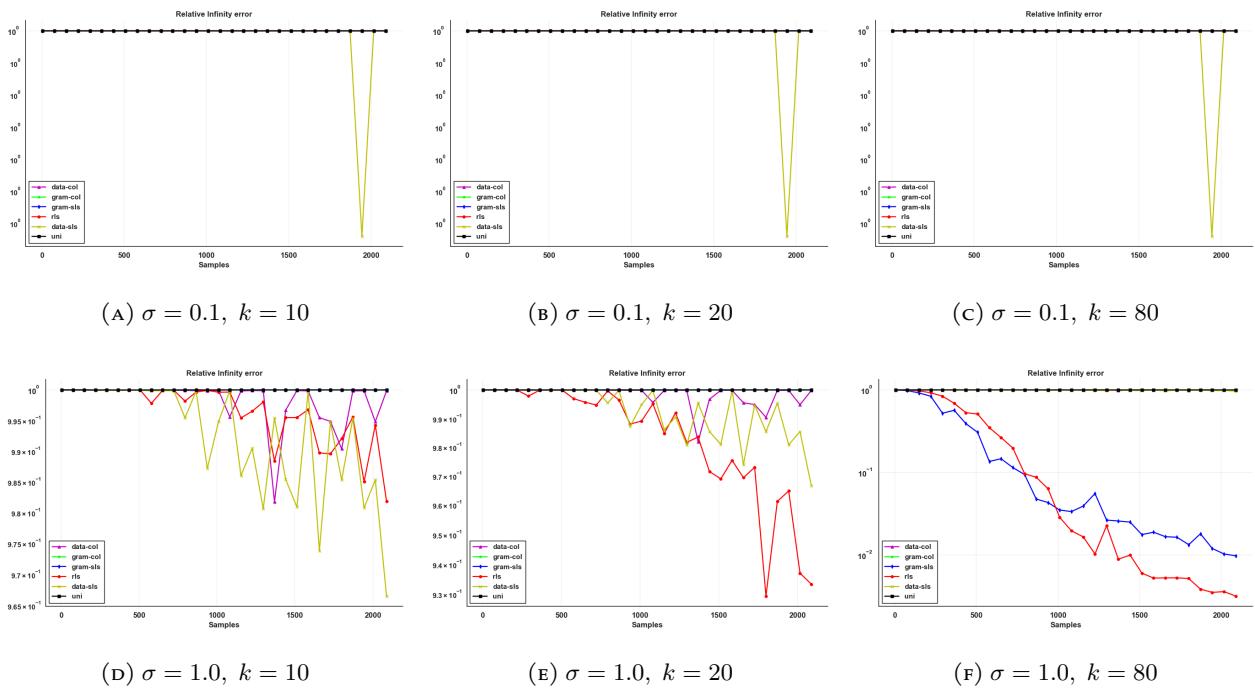


FIGURE 29. Nystrom infinity errors for the Abalone data set.

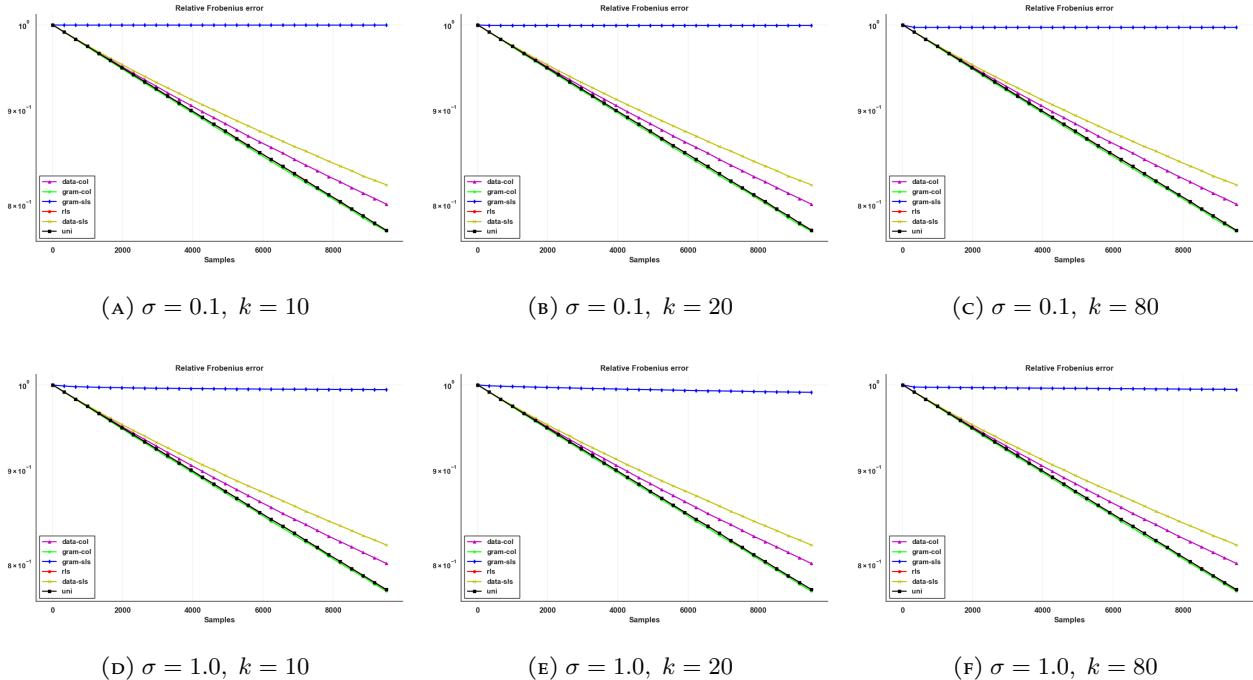


FIGURE 30. Nystrom Frobenius errors for the Magic data set.

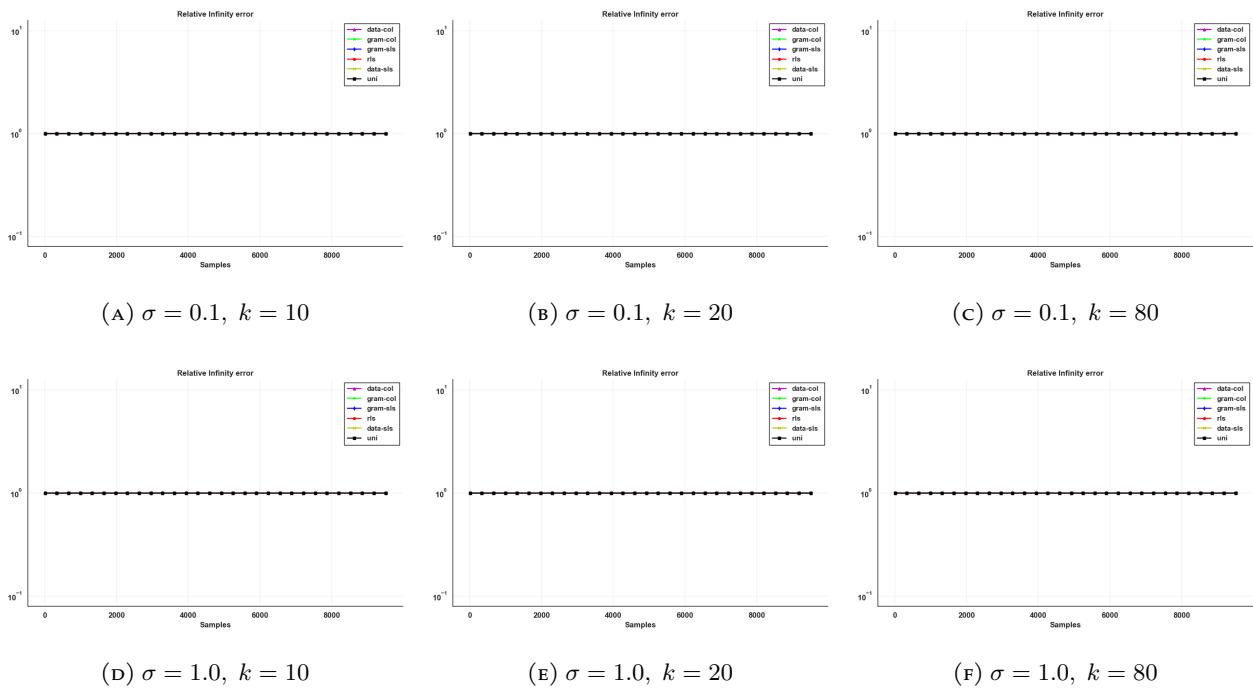


FIGURE 31. Nystrom infinity errors for the Magic data set.

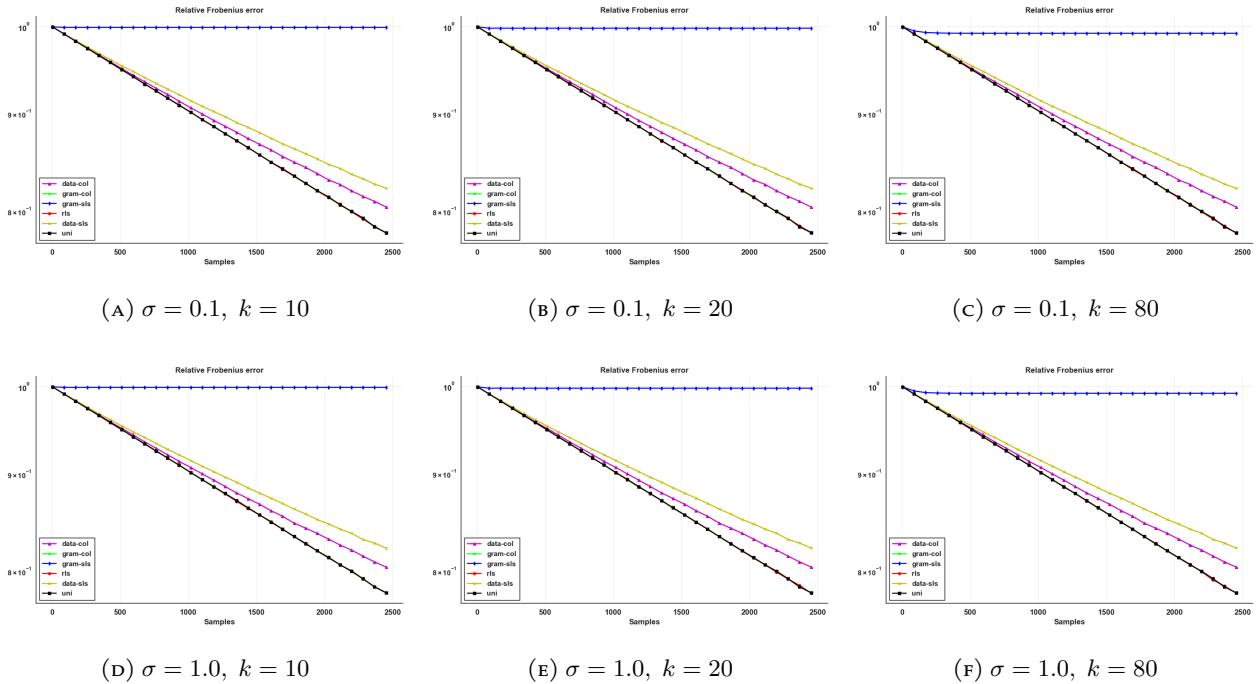


FIGURE 32. Nystrom Frobenius errors for the Stocks data set.

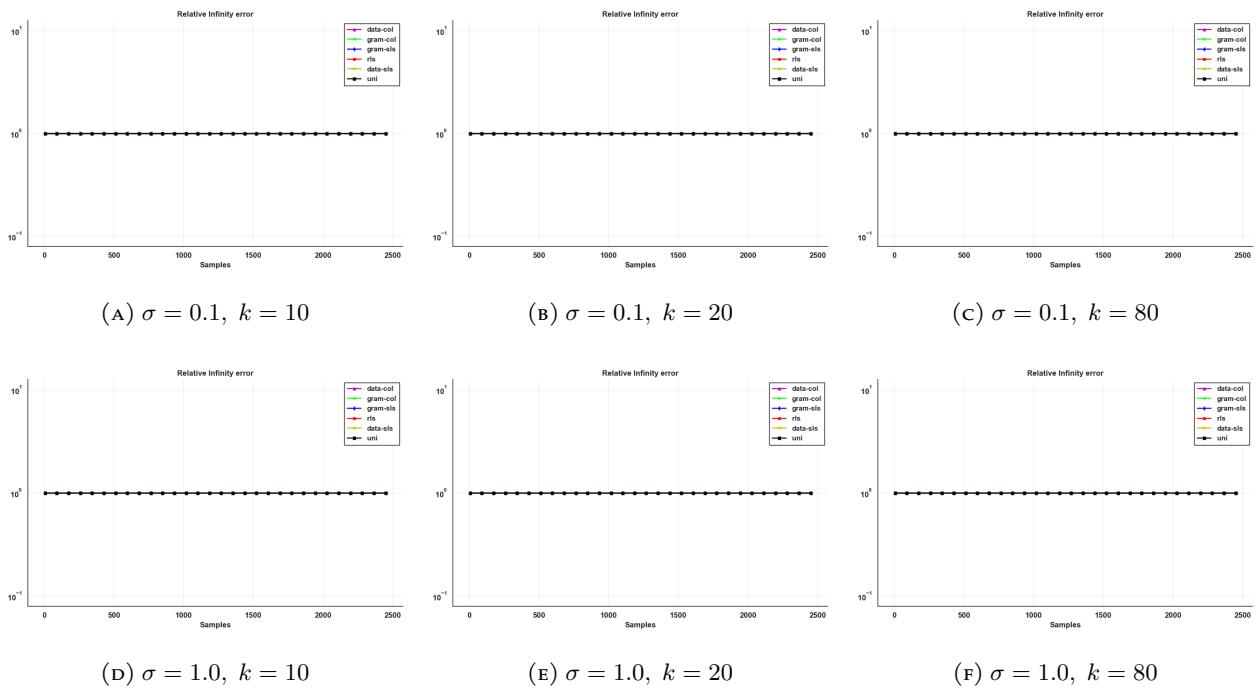


FIGURE 33. Nystrom infinity errors for the Stocks data set.

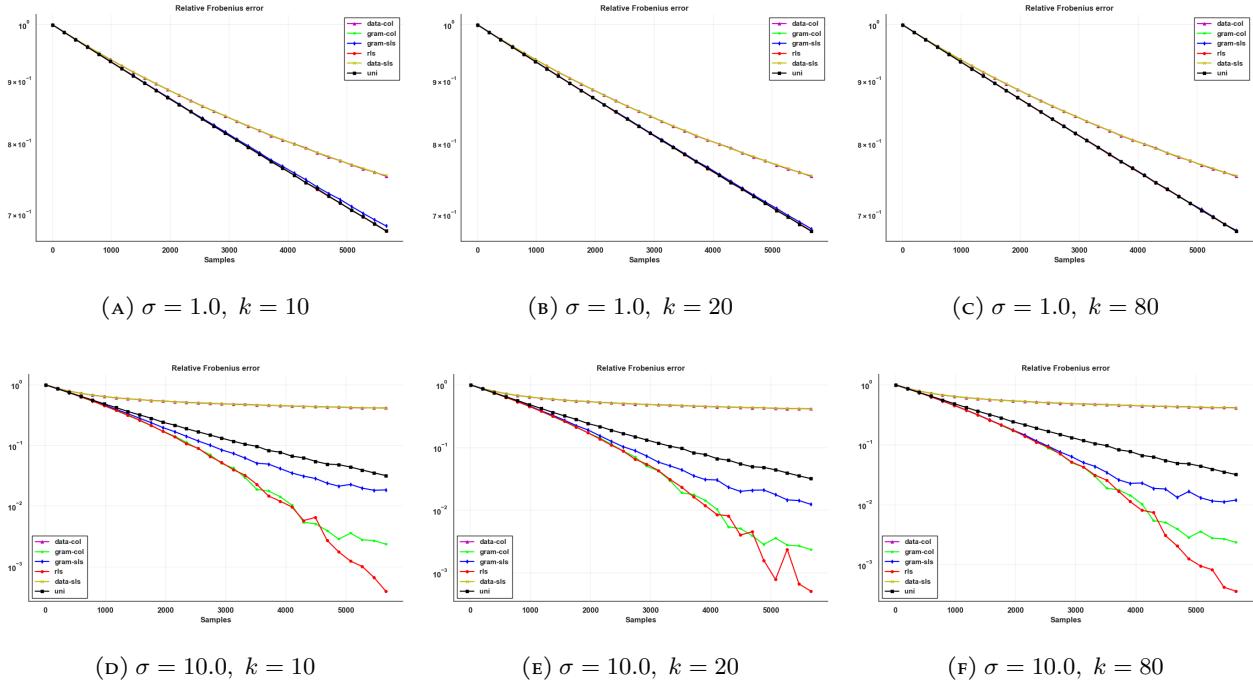


FIGURE 34. Nystrom Frobenius errors for the Temp data set.

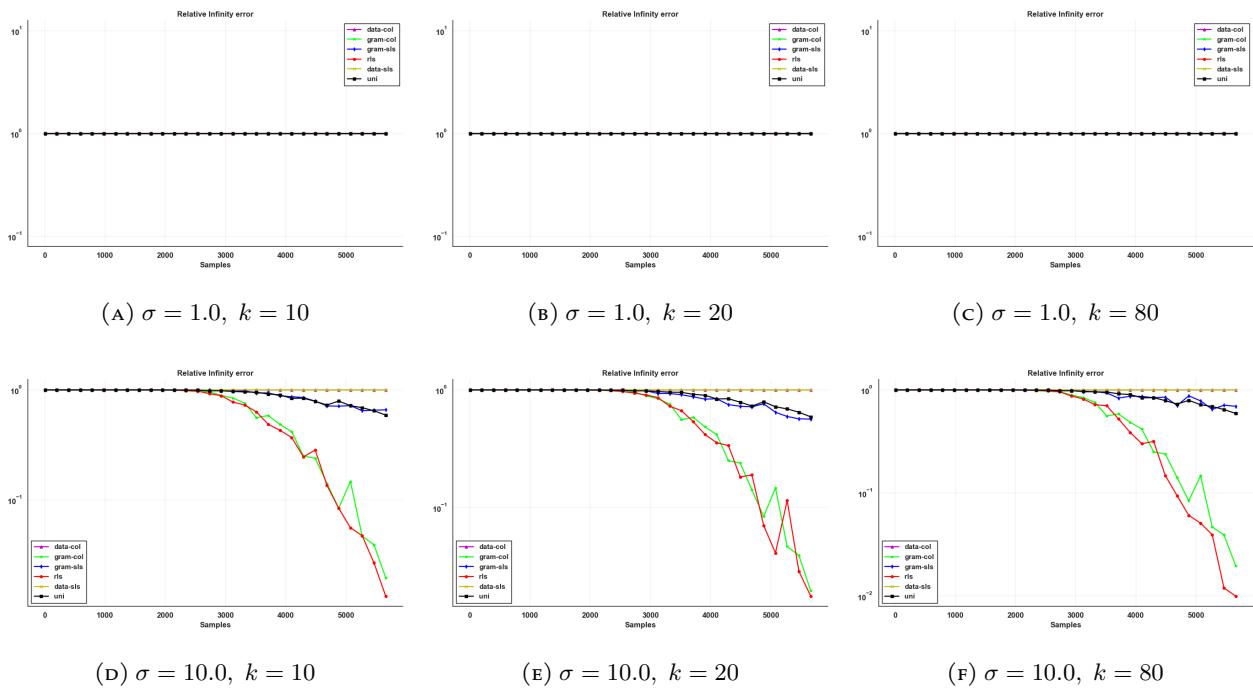


FIGURE 35. Nystrom infinity errors for the Temp data set.

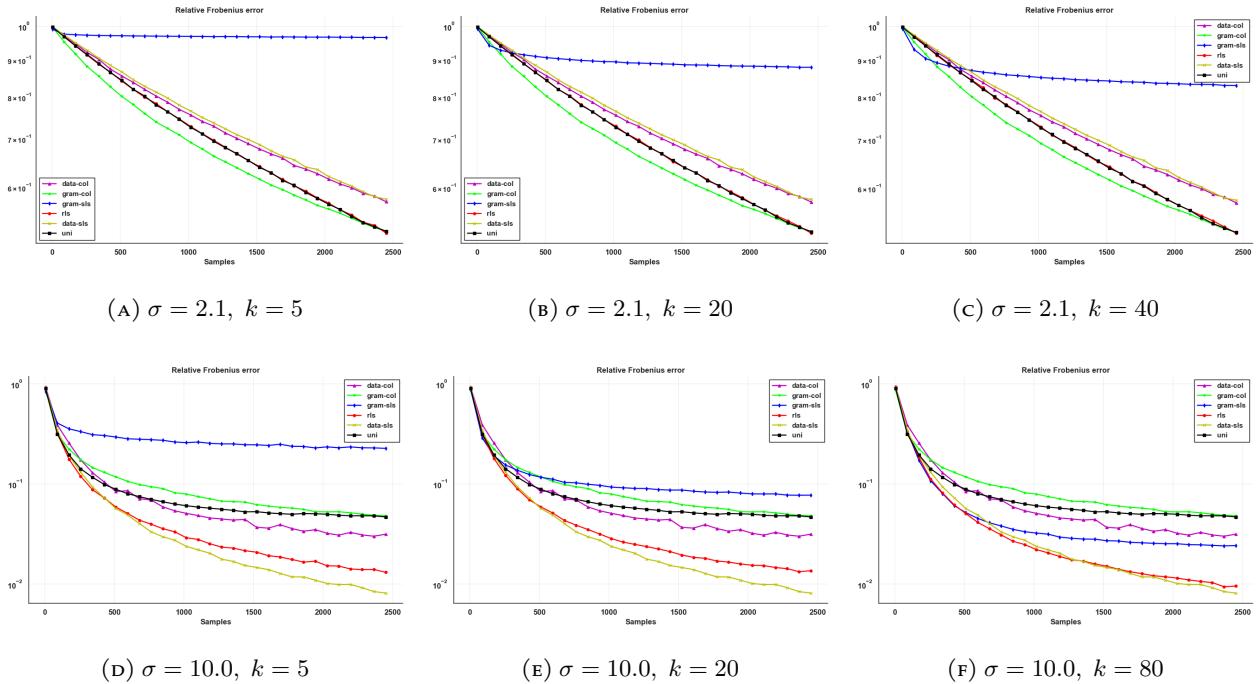


FIGURE 36. Nystrom Frobenius errors for the wine data set.

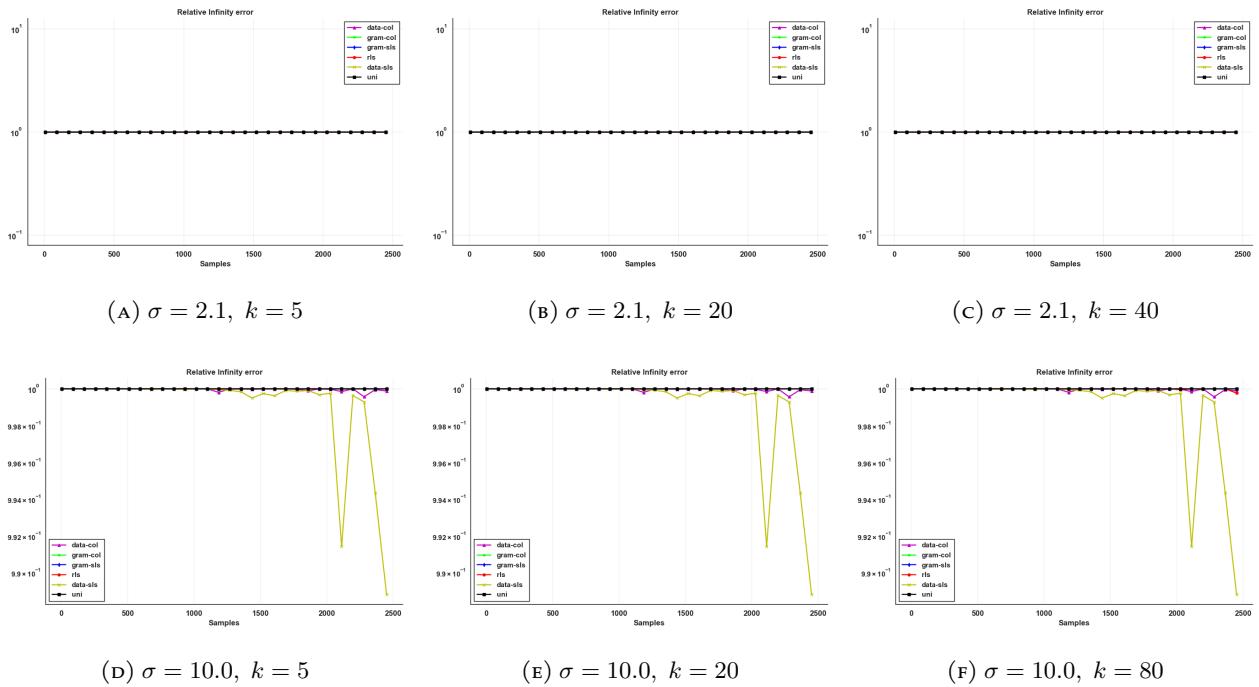


FIGURE 37. Nystrom infinity errors for the wine data set.

A.6. Nyström Errors.

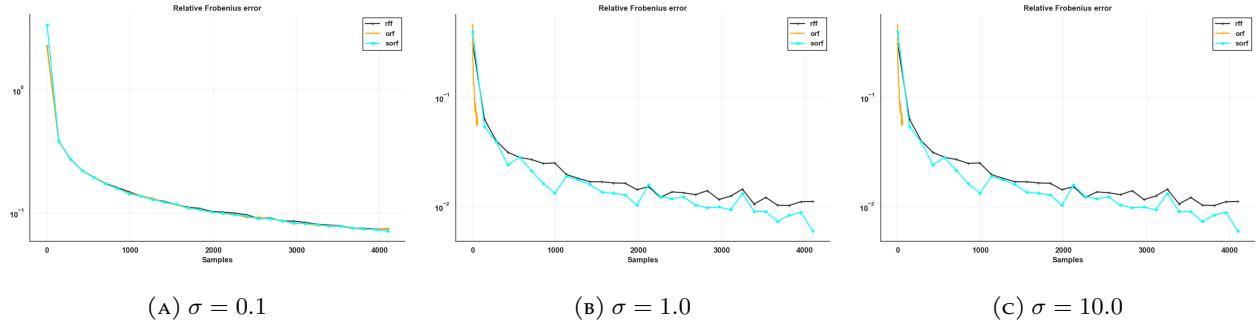


FIGURE 38. RFF Frobenius errors for the 3DSN data set.

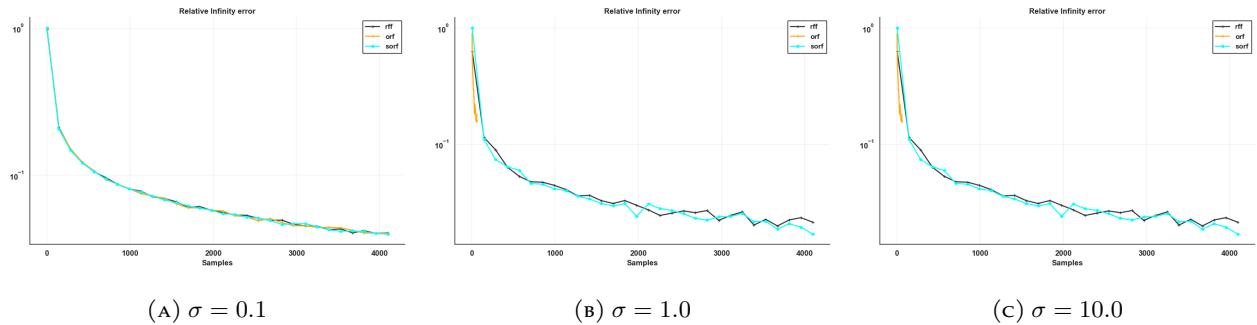


FIGURE 39. RFF absolute errors for the 3DSN data set.

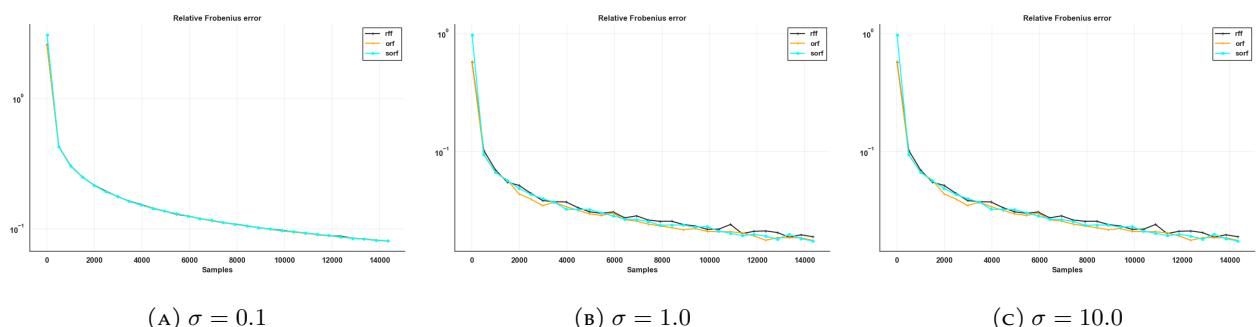


FIGURE 40. RFF Frobenius errors for the Abalone data set.

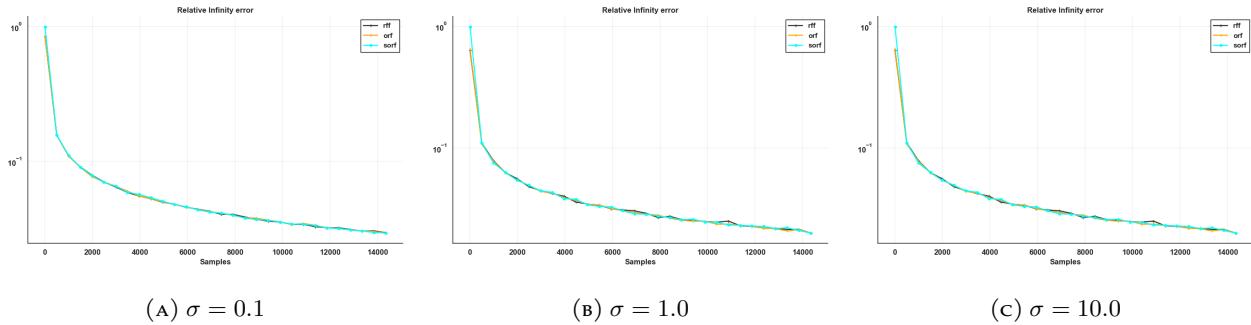


FIGURE 41. RFF infinity errors for the Abalone data set.

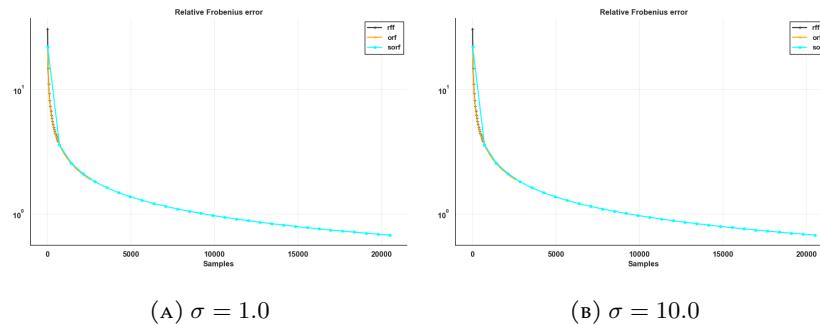


FIGURE 42. RFF Frobenius errors for the magic04 data set.

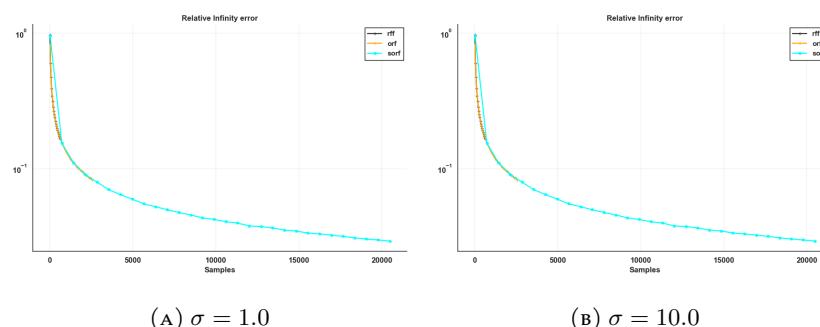


FIGURE 43. RFF infinity errors for the magic04 data set.

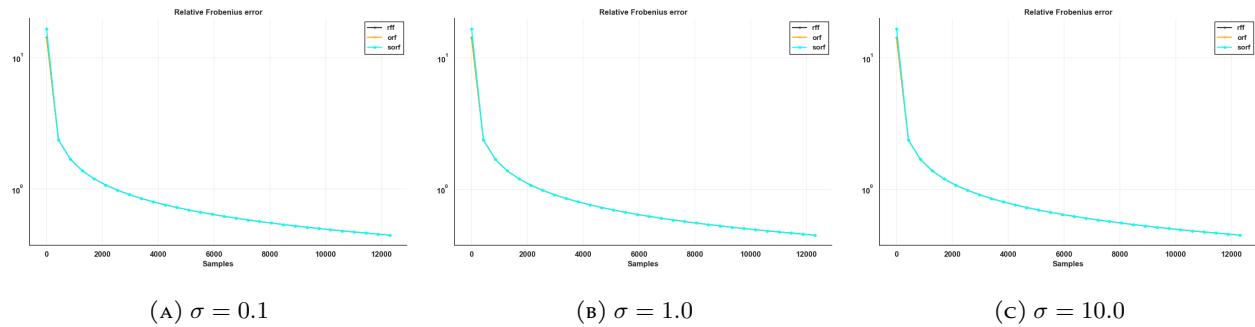


FIGURE 44. RFF Frobenius errors for the Stocks data set.

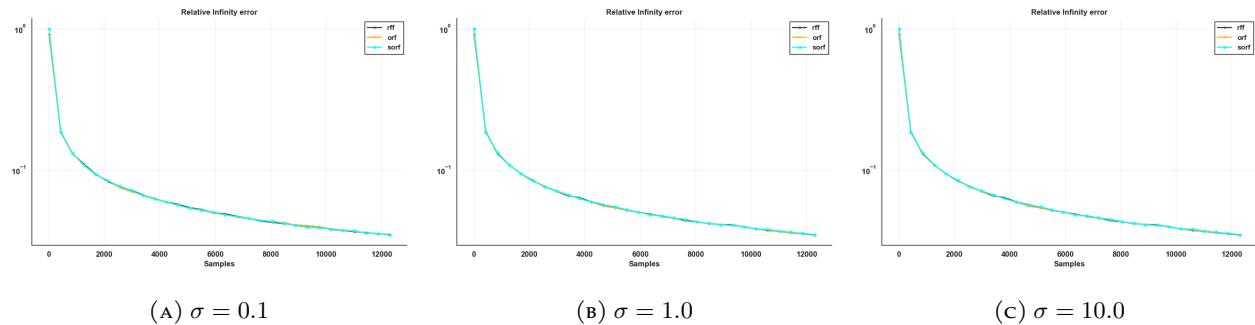


FIGURE 45. RFF infinity errors for the Stocks data set.

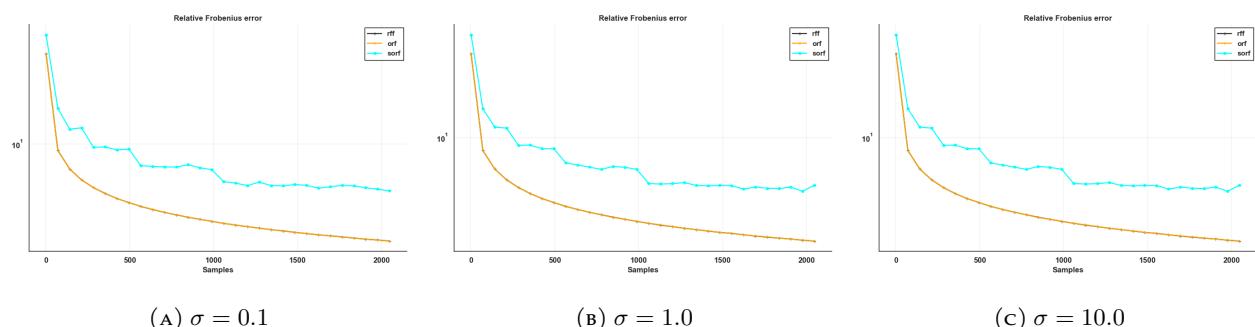


FIGURE 46. RFF Frobenius errors for the Temp data set.

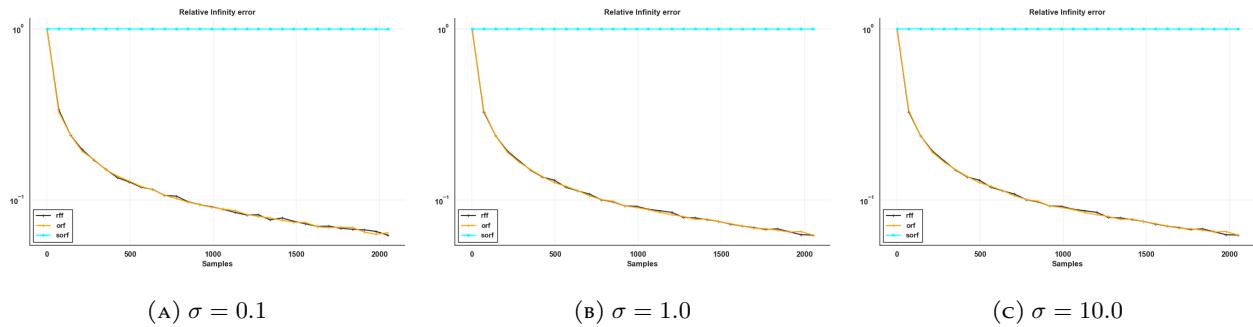


FIGURE 47. RFF infinity errors for the Temp data set.

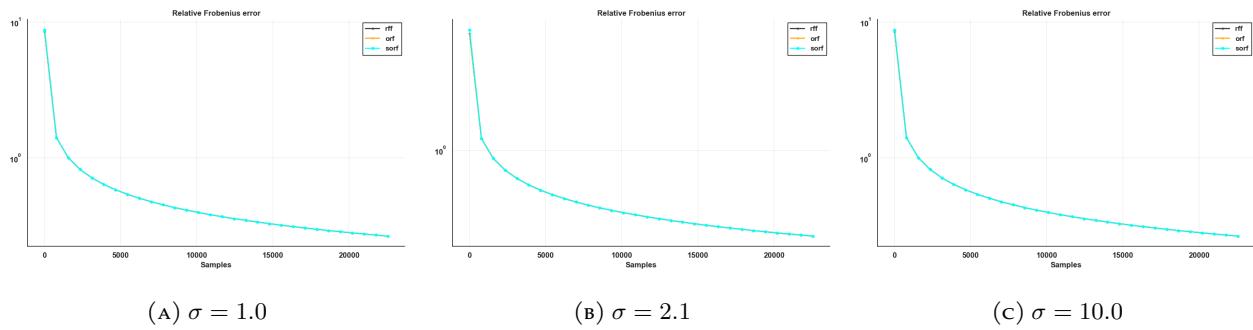


FIGURE 48. RFF Frobenius errors for the Wine data set.

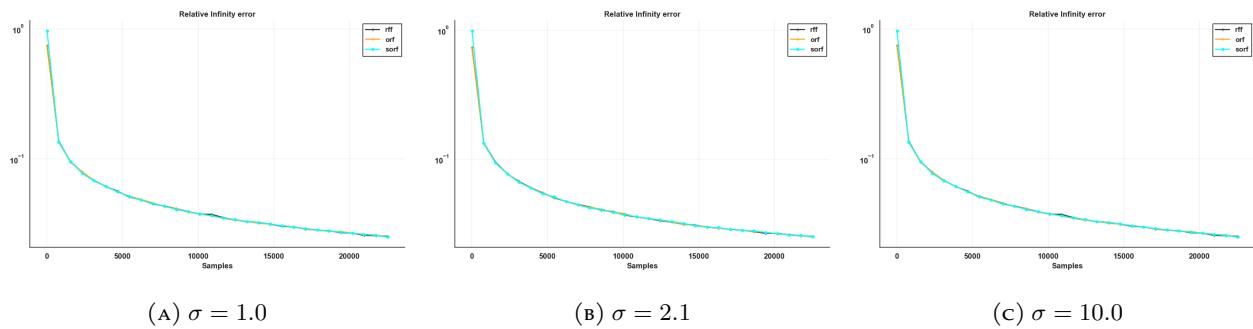


FIGURE 49. RFF infinity errors for the Wine data set.

A.7. Kernel Comparisons.

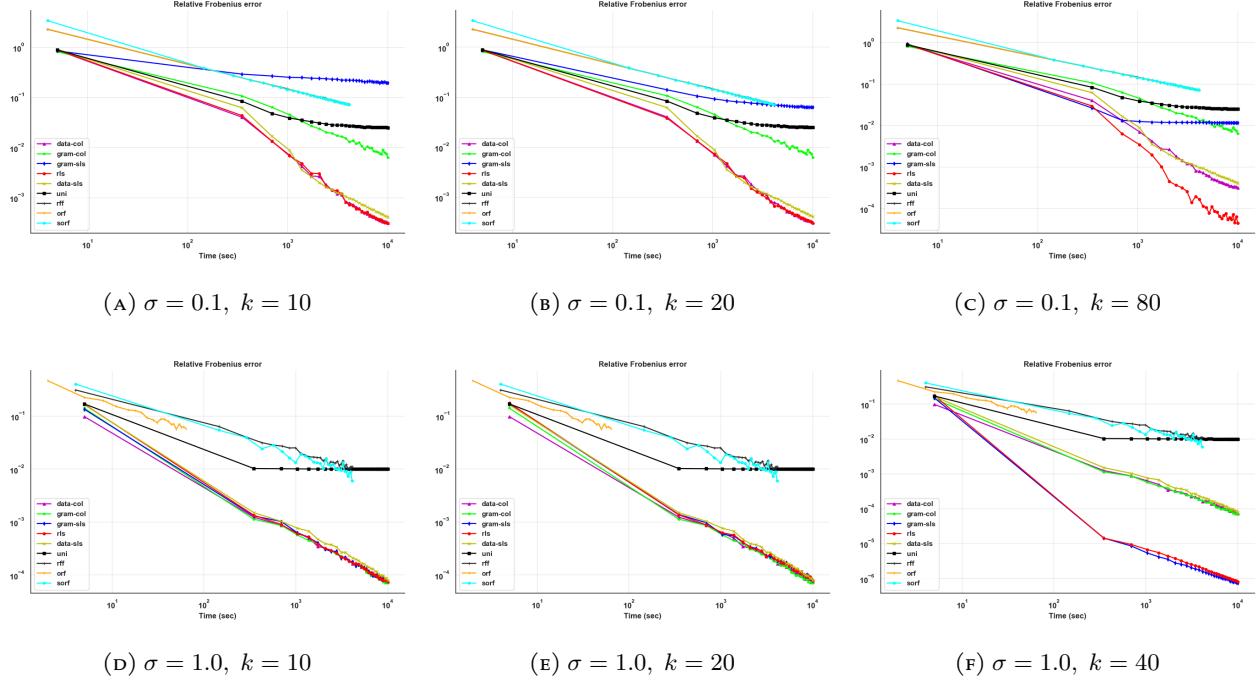


FIGURE 50. Comparing Frobenius errors of kernel methods for the 3DSN data set.

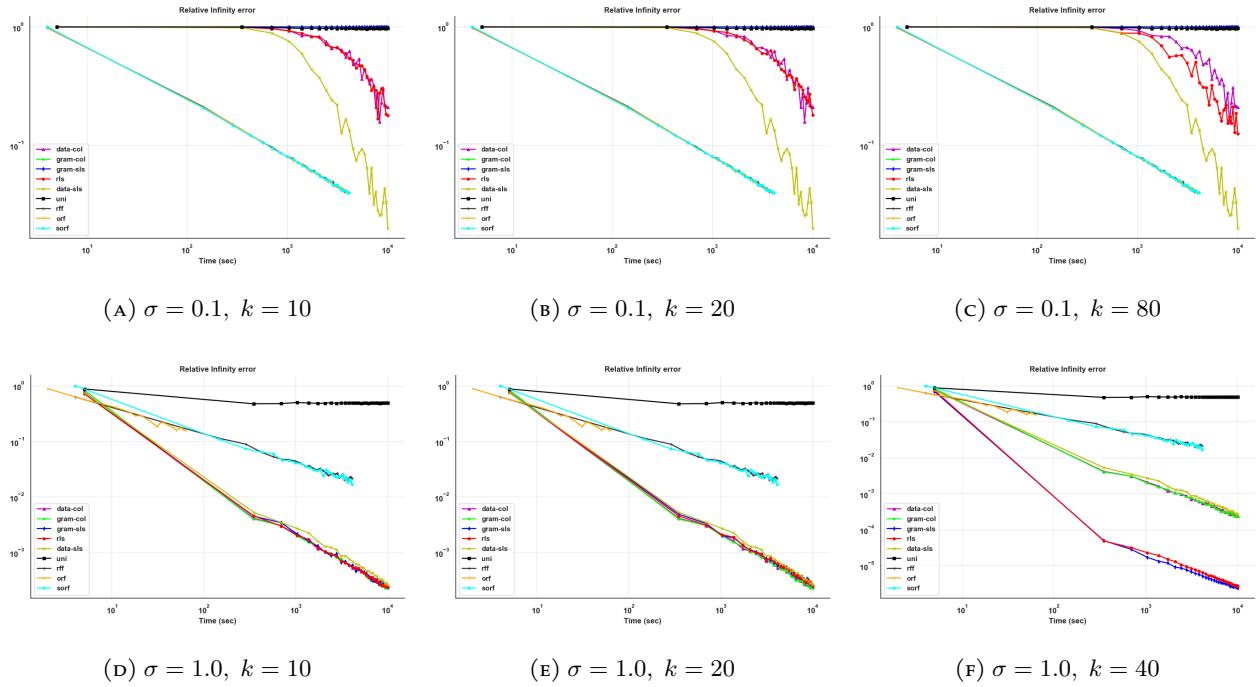


FIGURE 51. Comparing infinity errors of kernel methods for the 3DSN data set.

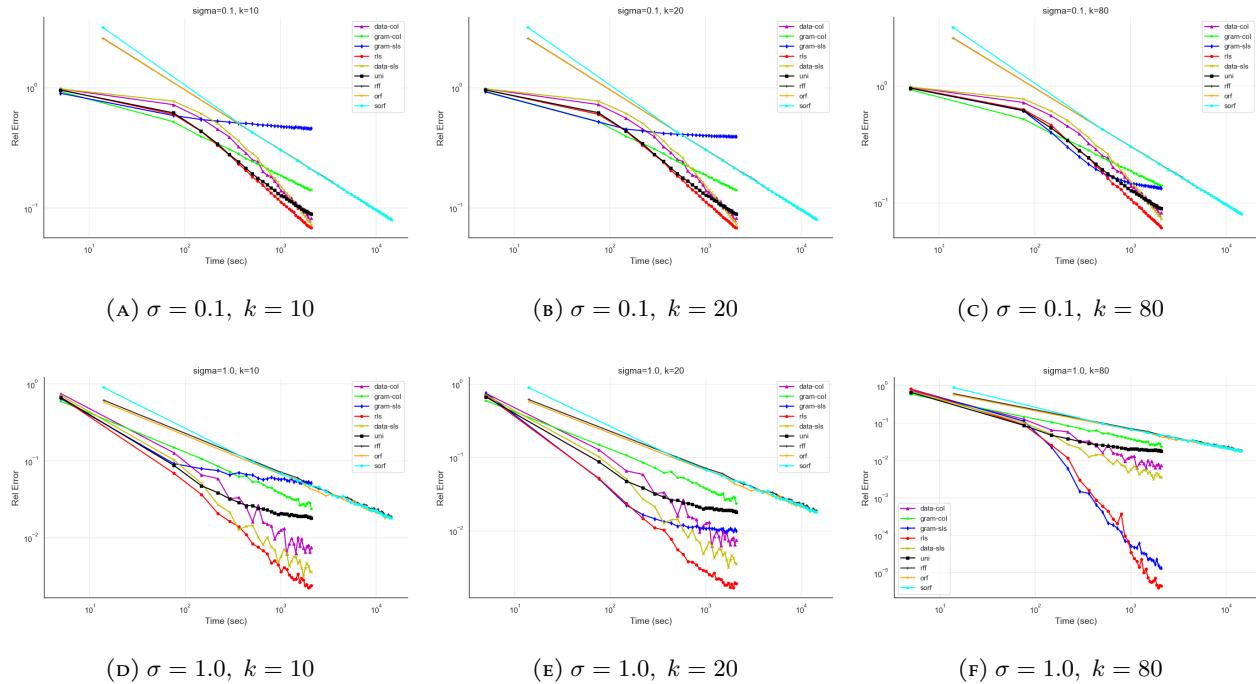


FIGURE 52. Comparing Frobenius errors of kernel methods for the Abalone data set.

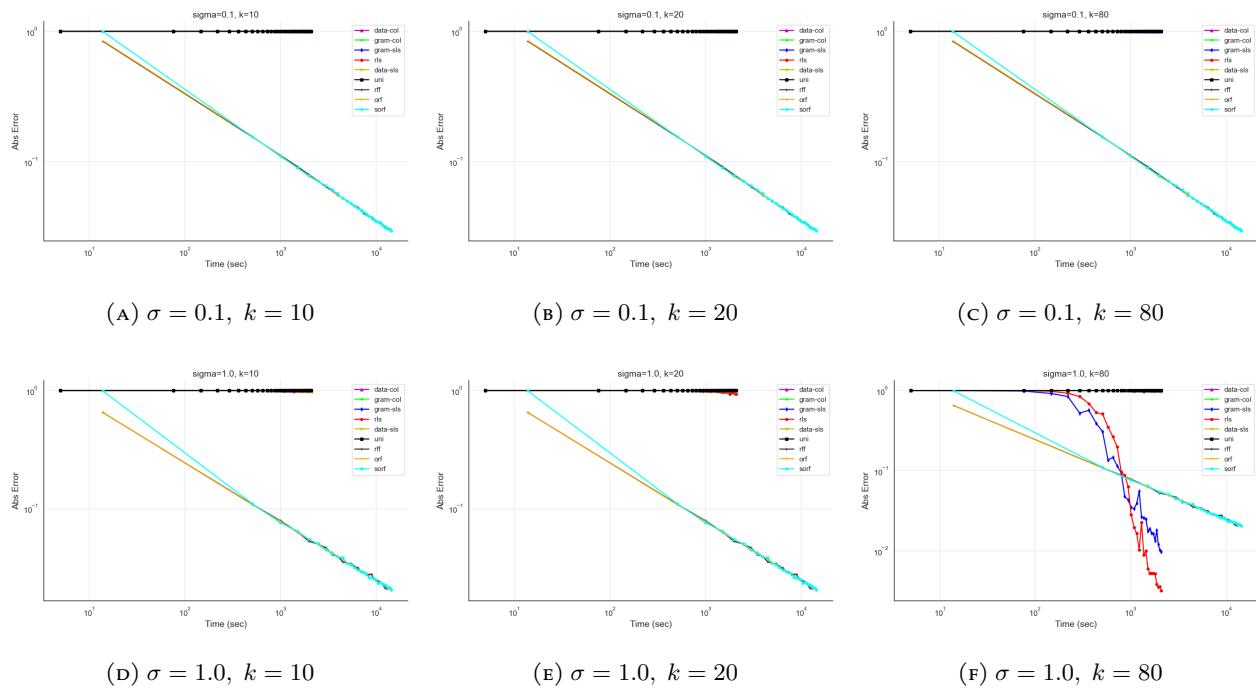


FIGURE 53. Comparing infinity errors of kernel methods for the Magic data set.

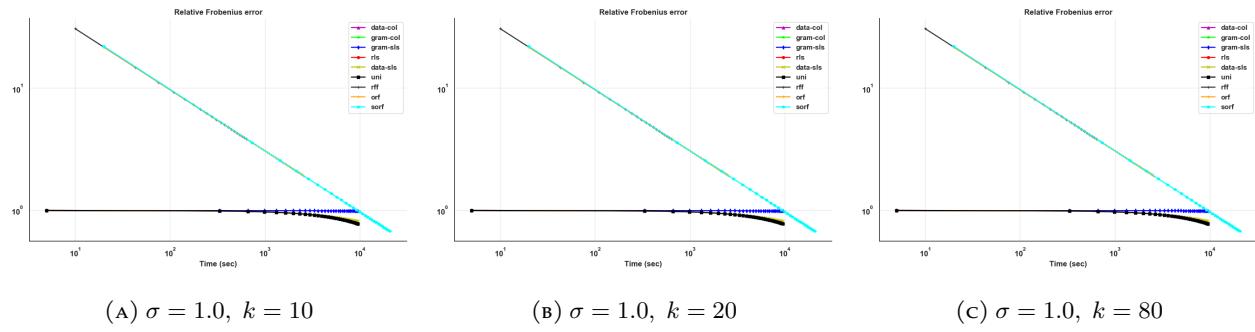


FIGURE 54. Comparing Frobenius errors of kernel methods for the Magic data set.

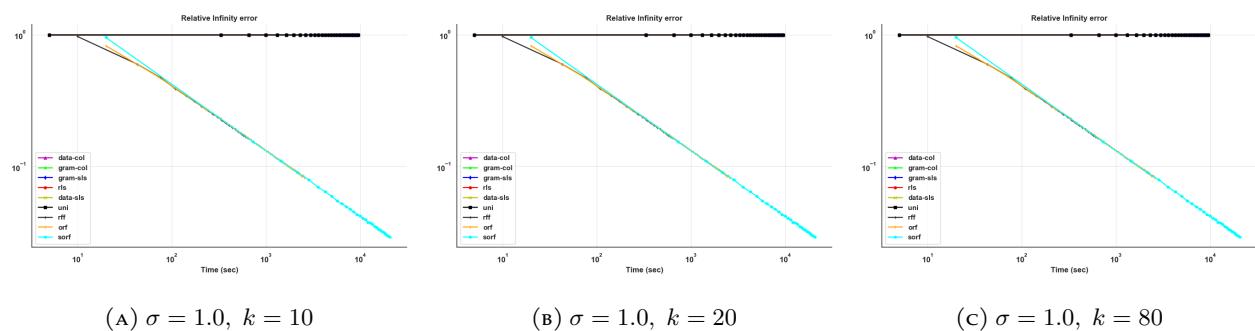


FIGURE 55. Comparing infinity errors of kernel methods for the Magic data set.

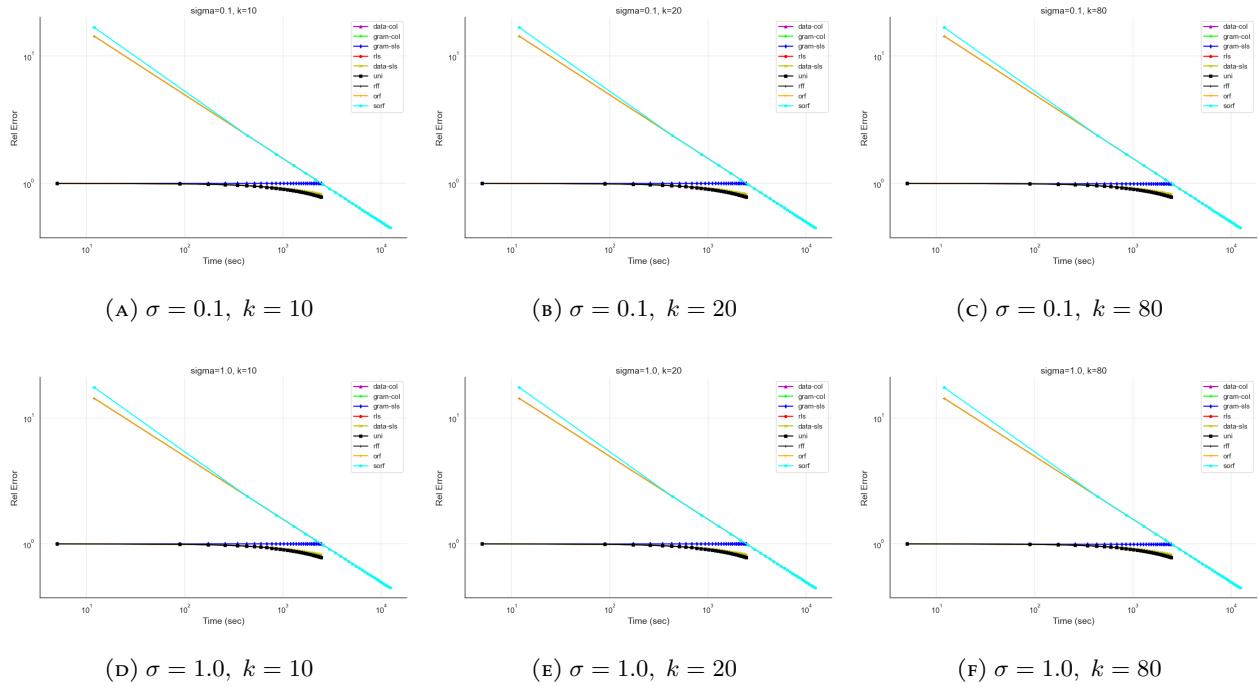


FIGURE 56. Comparing Frobenius errors of kernel methods for the Stocks data set.

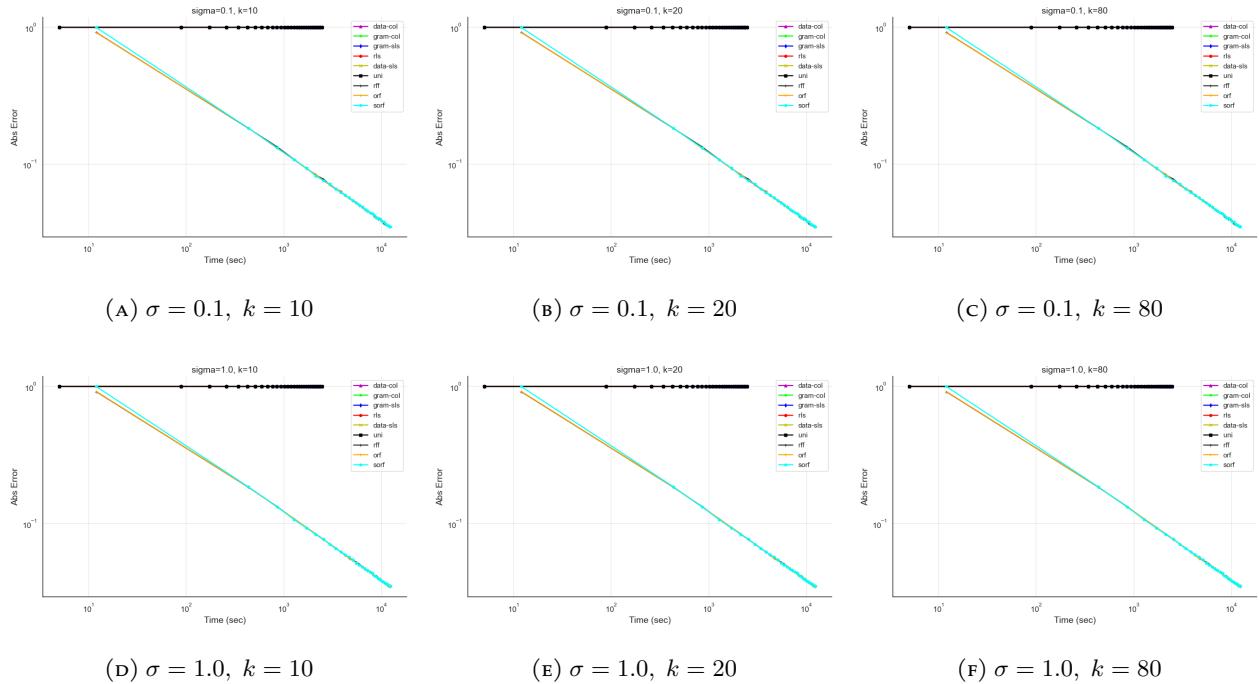


FIGURE 57. Comparing infinity errors of kernel methods for the Stocks data set.

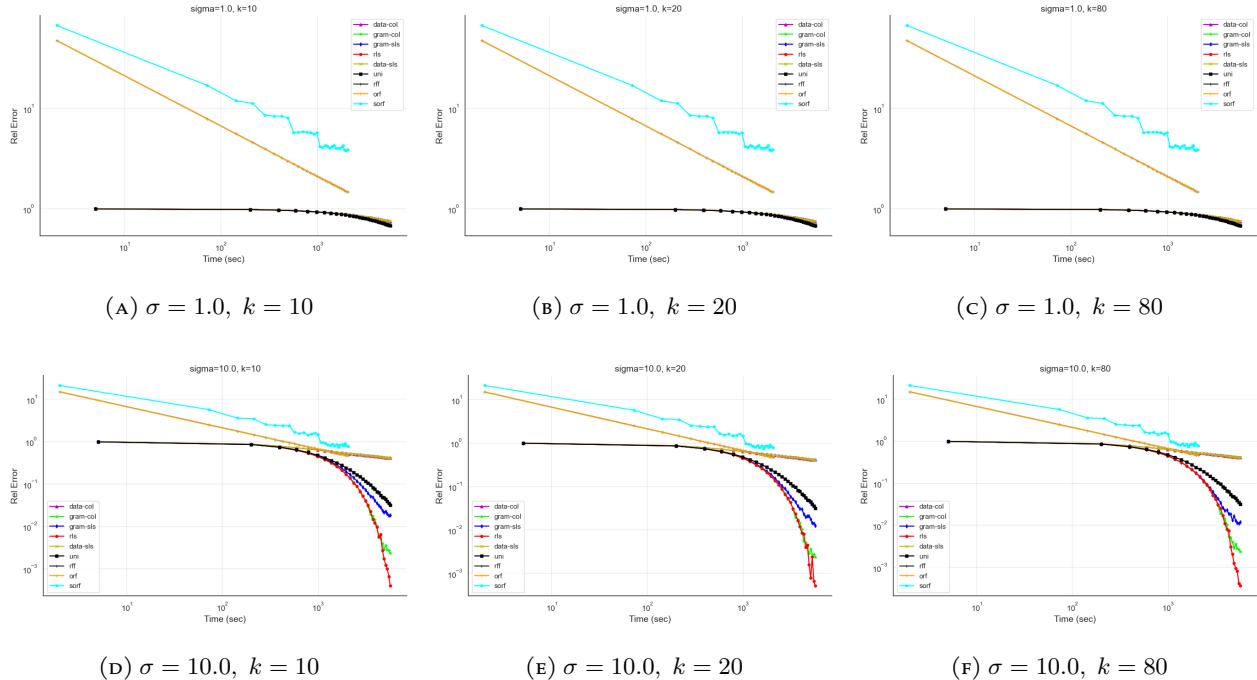


FIGURE 58. Comparing Frobenius errors of kernel methods for the Temp data set.

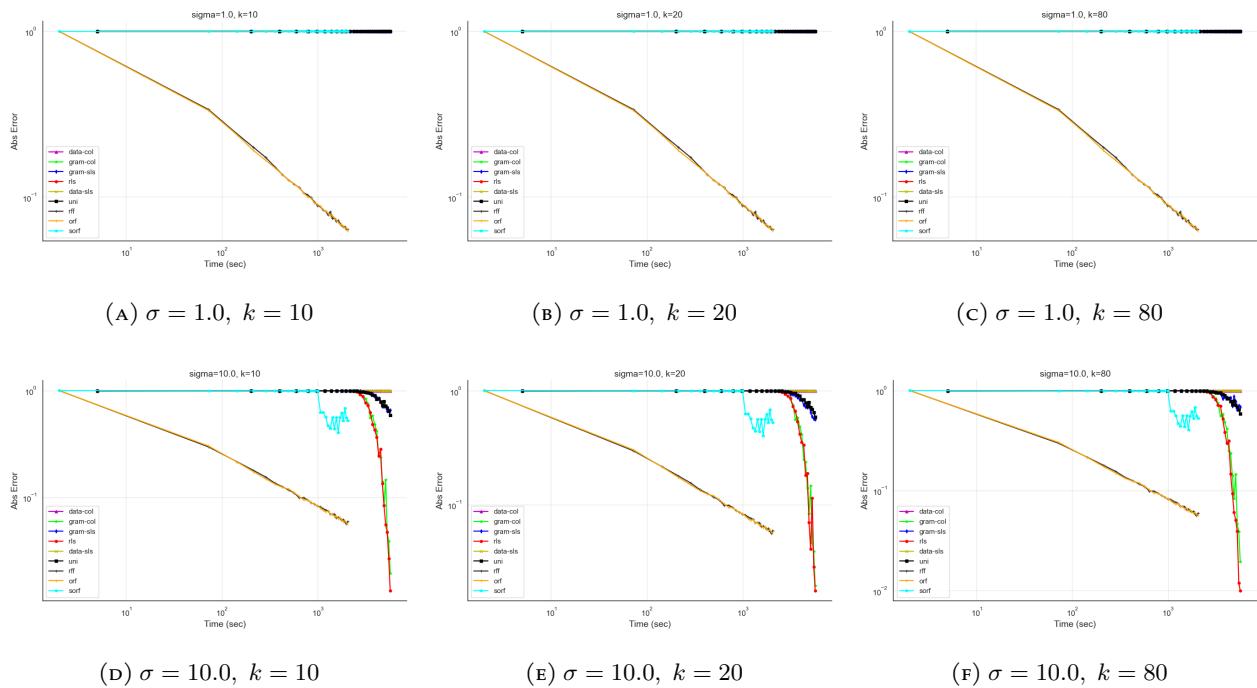


FIGURE 59. Comparing infinity errors of kernel methods for the Temp data set.

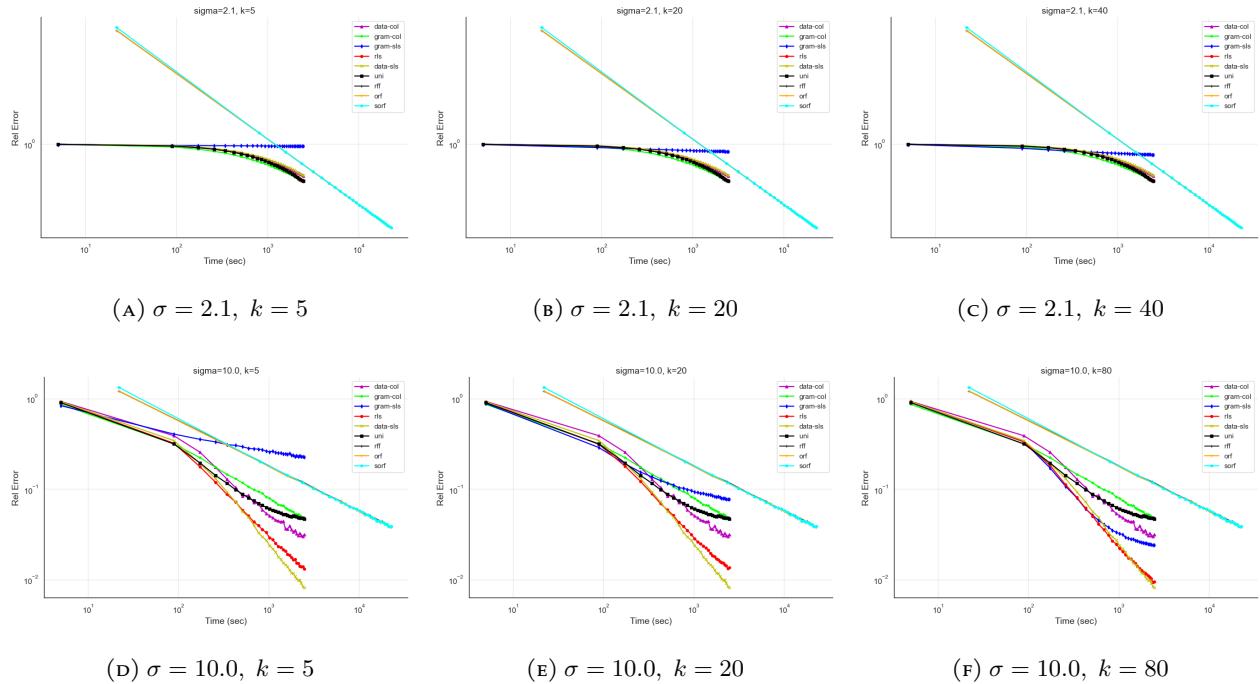


FIGURE 60. Comparing Frobenius errors of kernel methods for the wine data set.

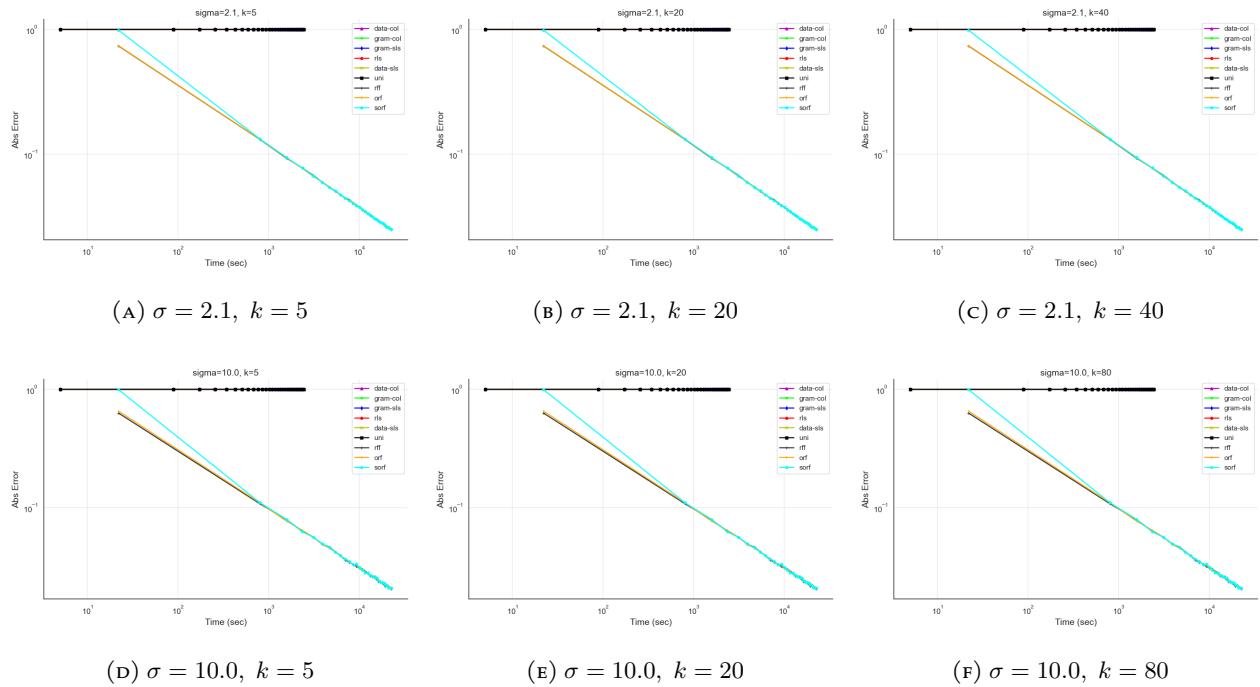


FIGURE 61. Comparing infinity errors of kernel methods for the wine data set.