Semi-Infinite Linear Regression and Its Applications

Paz Fink Shustin and Haim Avron

October 27, 2021

Abstract

Finite linear least squares is one of the core problems of numerical linear algebra, with countless applications across science and engineering. Consequently, there is a rich and ongoing literature on algorithms for solving linear least squares problems. In this paper, we explore a variant in which the system’s matrix has one infinite dimension (i.e., it is a quasimatrix). We call such problems semi-infinite linear regression problems. As we show, the semi-infinite case arises in several applications, such as supervised learning and function approximation, and allows for novel interpretations of existing algorithms. We explore semi-infinite linear regression rigorously and algorithmically. To that end, we give a formal framework for working with quasimatrices, and generalize several algorithms designed for the finite problem to the infinite case. Finally, we suggest the use of various sampling methods for obtaining an approximate solution.

1 Introduction

Consider the classical linear least squares problem: given an \( m \times n \) matrix \( A \), and a vector \( b \), we seek to compute:

\[
x^* = \arg \min_{x \in \mathbb{R}^n} \| Ax - b \|_2.
\] (1)

The problem of solving Eq. (1) is one of the most fundamental problems of numerical linear algebra, and it has countless applications throughout scientific computing and data science. As such, there is a rich literature on algorithms for solving Eq. (1). In particular, there are algorithms that: compute an approximate solution [16], compute a near exact solution [38, 5, 28], are designed for the over-determined case [5], designed for the under-determined case [28], consider also the presence of a regularizer [2, 36], and replace the two-norm with some other norm [10]. The previous list is far from exhaustive. Finding efficient algorithms for solving Eq. (1) is an active research field.

In this paper, we explore a variant of Eq. (1) in which \( A \) is no longer a matrix, but a quasimatrix, that is a matrix in which one of the two dimensions is infinite (while the other dimension is finite). We call such problems 'semi-infinite linear regression'. As we show, the semi-infinite case arises in several applications, such as supervised learning and function approximation, and allows for novel interpretations of existing algorithms. In contrast to the rich literature on the finite (i.e., matrix) variant of Eq. (1), the semi-infinite case has been hardly treated in the literature (the only exception we aware of is [44]).

The goal of this paper is to explore semi-infinite linear regression rigorously and algorithmically. To that end, we first define the notion of quasimatrix formally, and give the needed framework for working with quasimatrices, both mathematically and algorithmically. The use of the term 'quasimatrix' as a matrix which has columns or rows that are functions first appears in the literature in [41, 44], but has so far been informal. Once we have the mathematical foundations, we define semi-infinite regression formally, and discuss applications.

We then proceed to proposing algorithms for solving semi-infinite linear regression problems. First, we discuss direct methods, which factorize a quasimatrix \( A \) into a product of quasimatrices. Even though most
of the algorithms we present are straightforward generalizations of classical methods for finite linear least squares problems, we also show how in some cases the use of quasimatrix operations can be sidestepped.

Next, we discuss iterative methods. It is possible to devise a wide array of iterative methods for solving semi-infinite linear regression by generalizing iterative methods for the finite case. However, for conciseness we show a representative algorithm from each of the two approaches: Krylov subspace methods and stochastic optimization. For Krylov methods, we show how LSMR \cite{18} can be generalized to solve semi-infinite linear regression. For stochastic optimization, we adapt a method based on stochastic variance reduce gradient descent (SVRG) \cite{23, 48}. Unlike LSMR, the adaptation of SVRG is less straightforward, and requires generalizing it to work with integrable sums.

Motivated by recent literature on Randomized Numerical Linear Algebra (RandNLA), we discuss algorithms that are based on sampling the semi-infinite linear regression problem. We discuss both randomized sampling and deterministic sampling. For randomized sampling, we discuss a sampling technique which we term as natural sampling. Conceptually, natural sampling is analogous to uniformly sampling rows or columns from $A$ when dealing with finite linear least-squares problems, though for semi-infinite linear regression problems, uniform sampling is not always well defined. It is well known from the RandNLA literature that it is better to sample based on the so-called leverage scores. For quasimatrices, the analogous operation is sampling using the leverage function, a generalization of leverage scores. Similar results have been shown before for restricted cases \cite{3, 12, 4}. We also propose a deterministic sampling method based on Gauss-Legendre quadrature. Interestingly, this method does not have any finite analogue.

Most of the methods we present are based on existing algorithms for the finite linear least squares case to some degree (the only exception is the quadrature sampling). The main contribution of the paper is in the rigorous and systematic treatment of the subject. We hope that our systematic treatment of semi-infinite linear regression will spur additional interest and research on this problem.

## 2 Quasimatrices

The term ‘quasimatrix’ appears in the literature as a name for matrices in which one of their dimensions is infinite \cite{41}. The term was later adapted by the chebfun library \cite{8} and a variety of papers related to that package, and other literature, use it, e.g. \cite{41, 31, 33, 25, 22}. In previous literature, quasimatrices were defined and treated informally as matrices which have columns or rows that are functions. For our purposes, a more formal treatment is needed, and we provide it here. Our approach is in many ways similar to the one taken by \cite{15} to defining fundamental notions such as rank and basis as ones derived from linear maps in which the domain is finite dimensional vectors.

**Notations and Basic Terminology.** For an integer $n$, we denote $[n] = \{1, \ldots, n\}$. Scalars are denoted by lower-case Greek letters or by $x, y, \ldots$. Given two Banach spaces, $X$ and $Y$, we denote by $B(X,Y)$ the Banach space of bounded linear operators from $X$ to $Y$. Given a Banach space $X$, $X^*$ denotes the topological dual space of $X$, i.e. the space of continuous linear functionals from $X$ to $\mathbb{R}$ or $\mathbb{C}$. So, $X^* = B(X, \mathbb{R})$ or $X^* = B(X, \mathbb{C})$ (depending on the context). Vectors are denoted by $x, y, \ldots$ and considered as column vectors (unless otherwise stated), and matrices are denoted by $A, B, \ldots$ or upper-case Greek letters. Quasimatrices are denoted by $x, y, \ldots$ if they are lying in a Hilbert space and otherwise by $A, B, \ldots$ (defined later in this paper). For a vector $x$ or a matrix $A$, the notation $x^*$ or $A^*$ denotes the Hermitian transpose. The $n \times n$ identity matrix is denoted by $I_n$. We use $e_1, e_2, \ldots$ to denote the unit vectors and assume that their dimensions are clear from the context. All vectors are considered as columns vectors, which can be of finite or infinite dimension.

We use $L_2(\Omega, d\mu)$ to denote the space of complex-valued square integrable functions over $\Omega$ with respect \footnote{See \url{http://www.chebfun.org/docs/guide/guide06.html}}.
to the measure µ, i.e. the inner product in $L_2(\Omega, d\mu)$ is
\[
(f, g)_{L_2(\Omega, d\mu)} := \int_\Omega \overline{f(\eta)} g(\eta) d\mu(\eta).
\]

2.1 Quasimatrix Algebra

A matrix is a mapping from two indexes to a scalar. Alternatively, a matrix can be viewed as mapping from a finite index set to finite dimensional vectors, where the index set is either the column index or the row index. For a quasimatrix we drop the condition that the mapped vectors are finite dimensional, and instead require them to be from a Hilbert space.

**Definition 1.** Let $n$ be a positive integer and let $\mathcal{H}$ be an Hilbert space over $\mathbb{R}$ or $\mathbb{C}$. A tall quasimatrix is a mapping from $[n]$ to $\mathcal{H}$. A wide quasimatrix is a mapping from $[n]$ to $\mathcal{H}^\ast$.

We generally omit the adjectives tall and wide when the text refers to both types, or when the relevant type is clear from the context. We say the size of a tall quasimatrix is $m \times n$ if $m$ is the dimension of the Hilbert space $\mathcal{H}$. We generally write $\infty \times n$ if $\mathcal{H}$ has infinite dimension. A similar notion of size applies for wide quasimatrices. To avoid clutter, henceforth we assume that $\mathcal{H}$ is defined over $\mathbb{C}$, and leave for the reader to deduce how some of the description is somewhat simplified for the real case.

For a tall quasimatrix $A$, we refer to the values at the various indexes as the columns of the quasimatrix. We use the following notation
\[
A = \begin{bmatrix} a_1 & \cdots & a_n \end{bmatrix}
\]
to denote the tall quasimatrix $A$ which maps $j \in [n]$ to $a_j$, where $a_1, \ldots, a_n \in \mathcal{H}$.

Let $b_1, \ldots, b_m \in \mathcal{H}$, and $b_1^*, \ldots, b_m^* \in \mathcal{H}^\ast$ their adjoints. We denote
\[
B = \begin{bmatrix} b_1^* \\ \vdots \\ b_m^* \end{bmatrix}
\]
for the wide quasimatrix $B$ which maps $j \in [m]$ to $b_j^\ast$. If a wide quasimatrix $B$ maps $j$ to $x \in \mathcal{H}^\ast$, the Riesz Representation Theorem implies that there exists a $b \in \mathcal{H}$ such that $x = b^\ast$, so every wide quasimatrix can be written in this way. For a wide quasimatrix $B$, we refer to the adjoints of the values at the indexes as the rows of the quasimatrix. Note that both the columns of a tall quasimatrix, and the rows of a wide quasimatrix, are vectors in $\mathcal{H}$.

In the rest of Section 2 $A$ is a tall quasimatrix with columns $a_1, \ldots, a_n$, and $B$ is a wide quasimatrix with rows $b_1^*, \ldots, b_m^*$.

The conjugate transpose of a tall quasimatrix $A$ is the wide quasimatrix $B$ whose coordinates are the adjoints of the corresponding coordinates of $A$. The conjugate transpose of a wide quasimatrix $B$ is the tall quasimatrix $A$ whose coordinates are the adjoints of the corresponding coordinates of $B$, which corresponds to removing the adjoints. These definitions are consistent with the notations above.

Given a tall quasimatrix $A$ and a vector $x \in \mathbb{C}^n$, we define the product of $A$ and $x$ as $Ax = \sum_{j=1}^n x_j a_j$.

This definition naturally extends to the definition of a product $AX$, where $X \in \mathbb{C}^{n \times k}$, as the tall quasimatrix whose columns are $Ax_1, \ldots, Ax_k$ (where $x_1, \ldots, x_n$ are the columns of $X$). Given a wide quasimatrix $B$ and a $x \in \mathcal{H}$ we define
\[
Bx = \begin{bmatrix} b_1^* x \\ \vdots \\ b_m^* x \end{bmatrix}.
\]
This definition naturally extends to the definition of a product of $B$ and $A$ as the $m \times n$ matrix whose columns are $Ba_1, \ldots, Ba_n$. 
We now define the left product. Given a tall quasimatrix $A$ and a vector $x \in H$, we define $x^* A = (A^* x)^*$. This definition is consistent with viewing $x^*$ as a $1 \times \infty$ quasimatrix, and the previous definition of $BA$. Similarly, $x^* B = (B^* x)^*$ for $x \in R^m$. These definitions naturally extend to the left product of a matrix and a quasimatrix. The product algebra we have defined over matrices and quasimatrices is associative (but, of course, not commutative).

It is well known that a $m \times n$ complex matrix is, in fact, a coordinate representation of a linear transformation from $C^n$ to $C^m$ under the standard basis, and that choosing a different basis leads to a different matrix (coordinate) representation. Similar to finite matrices, quasimatrices define bounded linear transformations between finite-dimensional Euclidean spaces and $H$. Concretely, for a tall quasimatrix $A$, we can define the transformation $A : x \in C^n \mapsto Ax \in H$. Conversely, given a bounded linear transformation $A : C^n \mapsto H$, for the tall quasimatrix $A = [ Ae_1 \cdots Ae_n ]$, the corresponding linear transformation is $A$. Thus, we can abuse notation and use $A$ to denote both the quasimatrix and the linear transformation it defines. Likewise, every wide quasimatrix $B$ defines a bounded linear transformation $B : x \in H \mapsto Bx \in R^m$, likewise abusing notation (this is well justified by the Riesz Representation Theorem). Taking the conjugate transpose of a tall or wide quasimatrices produces a quasimatrix which represents the adjoint of the transformation defined by the original quasimatrix, thus our notation is consistent with that operation as well.

Similarly to the finite dimensional matrix case, the extended product algebra over matrices and quasimatrices is consistent with composition in the transformation spaces. That is, given two matrices or quasimatrices $X$ and $Y$, with sizes or underlying Hilbert space such that the product $XY$ is defined, the transformation defined by $XY$ (which is a matrix or a quasimatrix) is exactly the same as the transformation obtained by $X$ composed with $Y$. However, we remark that if $X$ is a tall quasimatrix and $Y$ is a wide quasimatrix, then we can certainly define the transformation from $H$ to $H$ by composing $X$ with $Y$, but that transformation is not represented by a quasimatrix.

We have defined columns of a tall quasimatrix and rows of a wide quasimatrix. Defining the rows of a tall quasimatrix or the columns of a wide quasimatrix is less straightforward, and in some senses impossible. Intuitively, if $H$ is a space of functions over some index set $\Omega \subseteq R^n$, then row $\eta$ of a tall quasimatrix is simply the evaluation of the columns at a location $\eta \in \Omega$ (and likewise for wide quasimatrices). However, requiring $H$ to be a space of functions is somewhat restrictive. In particular, note that $L^2$ spaces are, strictly speaking, spaces of equivalence classes of functions, and point-wise evaluation is not really well-defined.

However, note that if $H$ is a reproducing kernel Hilbert space (RKHS), then we can define the notion of rows (or columns) of a tall (wide) quasimatrix in a way that is consistent with the use of identity vectors in finite matrices. If $H$ is a RKHS over $R^d$ then for every $\eta \in R^d$ the point-wise evaluation $f \in H \mapsto f(\eta)$ is a bounded linear transformation. Thus, there is a unique $e_\eta \in H$ such that for every $f \in H$ we have $e^*_\eta f = f(\eta)$. Thus, we define row $\eta$ of a $\infty \times n$ quasimatrix $A$ over a RKHS $H$ as $e^*_\eta A \in R^{1 \times n}$. For a $m \times \infty$ quasimatrix $B$, column $\eta$ is defined as $Be_\eta$.

Many notions related to matrices can be easily generalized to quasimatrices. For example, the rank is the dimension of space spanned by the columns (rows) of a tall (wide) quasimatrix. Obviously, the rank cannot be larger then the size of the finite dimension, and similar properties of matrix rank can be shown for quasimatrix rank.

2.2 Numerical Computing with Quasimatrices

In subsequent sections, we describe algorithms that “operate” on quasimatrices and functions. Such algorithms assume a model of computation in which functions are primitive types, and certain operations between functions are allowed (e.g., taking the integral of a function). Of course, such computations are not supported in hardware by general purpose computing machines. However, the software package chebfun\footnote{http://www.chebfun.org/} does provide this abstraction in software \cite{8}. Thus, we refer to this model of computation as the chebfun model.
In numerical computing, it is customary to regard floating-point operations (FLOPs) as the costly operations, and thus runtime analysis focuses on counting FLOPs. In the chebfun model, arguably the costly operations are operations on functions. Thus, when analyzing algorithms in the chebfun model we count FUNction OPerations (FUNOPs).

Specifically, we assume the following operations are supported, each costing one FUNOP: multiplying a function by a scalar, adding or subtracting two functions, evaluating a function at a point, and taking the inner product of two functions.

Of course, wherever possible we attempt to describe algorithms that operate under the standard model of computation (no FUNOPs). Such algorithms usually require additional assumptions on the quasimatrices involved.

2.3 Coordinate Representation of Quasimatrices over $L_2$ Spaces

As explained in the previous sections, the rows of a of a tall quasimatrix or the columns of a quasimatrix cannot be defined for quasimatrices over $L_2$ spaces. For most algorithms we describe that use the chebfun model this is not an issue. However, when we discuss algorithms that perform sampling and operate in the standard model, we need access to rows/columns so they can be sampled. In such cases we need to assume that the algorithm, when applied to quasimatrices over $L_2$, has additional information in the form of a coordinate representation of the quasimatrix it operates on.

**Definition 2.** Suppose $A$ is a quasimatrix over $L_2(\Omega, d\mu)$ whose finite dimension is $n$. A coordinate representation of $A$ is a function $z : \Omega \to \mathbb{C}^n$ such that

$$\int_{\Omega} \|z(\eta)\|_2^2 d\mu(\eta) < \infty$$

and:

1. If $A$ is tall, for every $x \in \mathbb{C}^n$,

$$Ax = \sum_{i=1}^n x_i \overline{z(\cdot)_i}$$

   where the above equality should be interpreted in the $L_2(\Omega, d\mu)$ sense and $z(\eta)_i$ is coordinate $i$ of $z(\eta)$ (for $\eta \in \Omega$).

2. If $A$ is wide, for every $x \in L_2(\Omega, d\mu)$ and $j \in [n]$,

$$e_j^*Ax = (\overline{z(\cdot)_j}, x)_{L_2(\Omega, d\mu)}.$$

The definition implies that if $z$ is a coordinate representation of $A$ then it is also a coordinate representation of $A^*$. Essentially, for a tall quasimatrix with a coordinate representation $z$, column $i$ is $\overline{z(\cdot)_i}$, and for a wide quasimatrix with a coordinate representation $z$, row $i$ is $\overline{z(\cdot)_i}$. If the quasimatrix is defined over $L_2(\Omega, d\mu)$, we say that $\Omega$ is the index set of the infinite dimension. We now say that for an index $\eta \in \Omega$, row $\eta$ of a tall quasimatrix with coordinate representation $z$ is $z(\eta)^*$, and column $\eta$ of a wide quasimatrix with coordinate representation $z$ is $z(\eta)$.

Note that the definition also implies the following. For $A$ we have,

$$A^*A = \begin{bmatrix} (\overline{z_A(\cdot)_1}, z_A(\cdot)_1)_{L_2(\Omega, d\mu)} & \cdots & (\overline{z_A(\cdot)_1}, z_A(\cdot)_n)_{L_2(\Omega, d\mu)} \\ \vdots & \ddots & \vdots \\ (\overline{z_A(\cdot)_n}, z_A(\cdot)_1)_{L_2(\Omega, d\mu)} & \cdots & (\overline{z_A(\cdot)_n}, z_A(\cdot)_n)_{L_2(\Omega, d\mu)} \end{bmatrix} = \int_{\Omega} z_A(\eta)z_A(\eta)^* d\mu(\eta)$$

and similarly for the product $BB^*$. 

5
Table 1: Factorizations of a tall Quasimatrix $A$ with $n$ columns over $H$.

| Factorization Form | Reference | FUNOPs in the chebfun model |
|--------------------|-----------|-----------------------------|
| Reduce QR using Gram-Schmidt | $A = QR$ $Q \in \mathbb{R}^{\infty \times n}$, $Q^*Q = I_n$ $R_{ij} = \{(a_i, a_j)_H \mid j \geq i \}$ | $n(n + 1)$ |
| Reduce QR using Householder Triangulation | $A = QR$ $Q = H_1H_2\cdots H_nES$ $S \in \mathbb{R}^{n \times n}$ diagonal sign matrix $R_{ij} = (e_i^H, a_j)_H$ | $(3n(3n-1)/2 + 6n)$ |
| SVD | $A = U\Sigma V^*$ $U \in \mathbb{R}^{\infty \times n}$, $U^*U = I_n$ $V \in \mathbb{R}^{n \times \infty}$, $V^*V = I_n$ $\Sigma \in \mathbb{R}^{n \times n}$ non-negative diagonal matrix | [8, 7, 26, 24, 25, 44] QR cost $(2n - 1)n$ |

2.4 Quasimatrix Factorizations

Matrix factorizations such as QR and SVD are used to define direct methods for solving linear regression problems (and more generally, in matrix analysis at large). Thus, it is no surprising that they can be used to solve semi-infinite linear regression problems as well, as was already noted in [44]. Various quasimatrix factorizations are already mentioned in [45, 8, 44], and are further developed in [43]. They can be formulated in our formal quasimatrix framework (previous aforementioned works used quasimatrices in an informal manner). In Table 1 we detail a few key quasimatrix factorizations of a tall quasimatrix $A$. Factorizations for a wide quasimatrix $B$ can be obtained by taking the conjugate transpose of a factorization of $B^*$. We also detail in Table 1 the FUNOPs cost of forming the various quasimatrix factorization.

Using the SVD factorization, we define the condition number of a quasi-matrix to be $\kappa(A) := \sigma_1/\sigma_n$ where $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$ in the SVD factorization.

3 Semi-Infinite Linear Regression: Problem Statement and Examples

In this paper, we are mainly concerned with the solution of regularized linear least squares regression problems with quasimatrices. We specifically consider ridge regularization (also called Tikhonov regularization). We call such problems Semi-Infinite Linear Regression (SILR). Both the overdetermined case and the underdetermined case are considered. In the overdetermined case, we are given a $\infty \times n$ quasimatrix $A$ over $H$, a target $b \in H$, and a regularization parameter $\lambda \geq 0$. The goal of SILR is to find $x \in \mathbb{C}^n$ such that

$$\|Ax - b\|_H^2 + \lambda \|x\|_2^2 = \text{minimum}. \quad (2)$$

In the underdetermined case, we are given a $n \times \infty$ quasimatrix $A$ over $H$, a target $b \in \mathbb{C}^n$, and a regularization parameter $\lambda \geq 0$. Our goal is to find a $x \in H$ such that

$$\|Ax - b\|_2^2 + \lambda \|x\|_2^2 = \text{minimum}. \quad (3)$$
Suppose we are given a function $f \in H = L_2([-1, 1], d\lambda)$ (or any other Hilbert space), and a finite dimensional subspace $V$ of $H$ (e.g., the space of polynomials up to a certain degree). We want to find the optimal approximation (in the $H$ sense) of $f$ in $V$, which we denote by $f_V$. Denote by $n$ the dimension of $V$, and let $v_1, \ldots, v_n$ be a basis for $V$. Define the $\infty \times n$ quasimatrix $A = [v_1 \ \cdots \ v_n]$. Then, $f_V = Ax^*$ where

$$x^* = \arg \min_{x \in \mathbb{R}^n} \|Ax - f\|^2_H. \tag{4}$$

A closely related problem is the problem of reconstructing an unknown function $f$ on a domain $X$ from samples at randomly chosen points $\{x_i\}$. In this problem setting we are given $y_i = f(x_i) + \epsilon_i$ at $m$ given data points $x_1, \ldots, x_m$ sampled i.i.d from some distribution $\rho$ on $X$ (we do not assume we have an explicit formula for $\rho$, or that we can produce additional samples; we only assume such a distribution exists). The scalars $\epsilon_1, \ldots, \epsilon_n$ are noise terms, which might be zero in the noiseless case. We can connect this problem to Eq. (4) in the following way, originally discussed in [11]. We setup a finite dimensional subspace $V$ and try to approximate $f_V$ via sampling. Specifically, let $A_s \in \mathbb{R}^{m \times n}$ be a “rows sample” of the quasimatrix $A$, i.e., defined by $(A_s)_{ij} = v_j(x_i)$, and let

$$\hat{x} = \arg \min_{x \in \mathbb{R}^n} \|A_s x - y\|^2_2. \tag{5}$$

The approximation is $\hat{f}_V = \hat{A} \hat{x}$. In [11] the authors provide a criterion on $s$ that describes the needed amount of samples to ensure that the least squares method is stable and that its accuracy is comparable to the best approximation error of $f$ by elements from $V$. Note that Eq. (5) is a sampled version of Eq. (4). We discuss solving SILR problems using sampling in Section 6.

### 3.2 Kernel Ridge Regression

Kernel ridge regression is an important method for supervised learning. Recall the problem of supervised learning: given training data $(x_1, y_1), \ldots, (x_n, y_n) \in X \times Y$, where $X \subseteq \mathbb{R}^d$ is an input domain and $Y \subseteq \mathbb{R}$ is an output domain, we wish to infer some functional dependency between the outputs and the inputs [14]. In kernel ridge regression, one starts with a positive definite kernel function $k : X \times X \to \mathbb{R}$. The kernel is associated with a reproducing kernel Hilbert space (RKHS) $H_k$ which is the completion of the function space

$$\left\{ \sum_{i=1}^m \alpha_i k(x_i, \cdot) \mid x_i \in X, \alpha_i \in \mathbb{R}, m \in \mathbb{Z}_+ \right\}$$

equipped with the inner product

$$\langle \sum_{i=1}^m \alpha_i k(x_i, \cdot), \sum_{j=1}^n \beta_j k(x_j, \cdot) \rangle_{H_k} = \sum_{i=1}^m \sum_{j=1}^n \alpha_i \beta_j k(x_i, x_j).$$

For some $\lambda > 0$, the kernel ridge regression estimator is

$$f^* = \arg \min_{f \in H_k} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \|f\|^2_{H_k}. \tag{6}$$
The celebrated Representer Theorem [39] guarantees that $f^*$ can be written as
\[ f^*(x) = \sum_{i=1}^{n} \alpha_i^* k(x_i, x) \] 
for some $\alpha_1^*, \ldots, \alpha_n^* \in \mathbb{R}$ (note that $k(x_i, \cdot) \in \mathcal{H}_k$ so $\sum_{i=1}^{n} \alpha_i^* k(x_i, \cdot) \in \mathcal{H}_k$). Simple linear algebra now implies that we can find $\alpha_1, \ldots, \alpha_n$ by solving the linear system
\[ (K + \lambda I_n)\alpha = y \] 
where $K \in \mathbb{R}^{n \times n}$ is the matrix defined by $K_{ij} = k(x_i, x_j)$ and $y = [y_1 \cdots y_n]^T \in \mathbb{R}^n$.

3.2.1 KRR as Semi-Infinite Linear Regression

We now show how Eq. (6) can be written as a SILR problem. Define the $n \times \infty$ quasimatrix $A$ over $\mathcal{H}_k$:
\[ A = \begin{bmatrix} k(\cdot, x_1)^* \\ \vdots \\ k(\cdot, x_n)^* \end{bmatrix}. \]

Due to the reproducing property of RKHS, $(f, k(\cdot, x_j))_{\mathcal{H}_k} = f(x_j) = (Af)_j$ and we have
\[ f^* = \arg \min_{f \in \mathcal{H}_k} \|Af - y\|_2^2 + \lambda\|f\|_{\mathcal{H}_k}^2. \]

Thus, the kernel ridge regression estimator is the solution to an underdetermined SILR problem. In fact, using Eq. (8) to solve Eq. (9) is an instance of a direct method for solving underdetermined SILR problems; see Section 4.2.

In Eq. (9), the quasimatrix $A$ is defined over a RKHS. In certain cases, the problem can be cast as a SILR problem with quasimatrices defined over a $L_2$ space, and this leads to approximation methods based on sampling. The following is based on the seminal work of Rahimi and Recht on random Fourier features [37]. Suppose that $k$ is a shift-invariant positive definite function, that is $k(x, z) = k(x - z)$ for some positive definite $k(\cdot)$ (note that we abuse notation in denoting by $k$ both the kernel and the positive definite function that defines it). Further assume that $k$ is normalized in the sense that $k(x, x) = 1$. According to Bochner’s Theorem, there exists a probability measure $\mu$ such that
\[ k(x, z) = \int_{\mathbb{R}^d} e^{-2\pi i (x - z)^T \eta} d\mu(\eta). \]

Define the function $\varphi : \mathcal{X} \times \mathbb{R}^d \to \mathbb{C}$:
\[ \varphi(x, \eta) = e^{2\pi i x^T \eta}. \]

For fixed $x, z \in \mathcal{X}$ we have
\[ (\varphi(x, \cdot), \varphi(z, \cdot))_{L_2(\mathbb{R}^d, d\mu)} = \int_{\mathbb{R}^d} e^{-2\pi i (x - z)^T \eta} d\mu(\eta) = \int_{\mathbb{R}^d} e^{-2\pi i (x - z)^T \eta} p(\eta) d\eta = k(x, z) \]
so $\varphi(x, \cdot) \in L_2(\mathbb{R}^d, d\mu)$ for every $x \in \mathcal{X}$. Let us now define the $n \times \infty$ quasimatrix $B$ over $L_2(\mathbb{R}^d, d\mu)$:
\[ B = \begin{bmatrix} \varphi(x_1, \cdot)^* \\ \vdots \\ \varphi(x_n, \cdot)^* \end{bmatrix}. \]
Lemma 3. Assuming that $K$ is full rank or $\lambda > 0$, the following holds:

$$f^*(x) = (\varphi(x, \cdot), w^*)_{L_2(\mathbb{R}^d, d\mu)}$$

where

$$w^* = \arg \min_{w \in L_2(\mathbb{R}^d, d\mu)} \|Bw - y\|_2^2 + \lambda \|w\|_2^2_{L_2(\mathbb{R}^d, d\mu)}.$$  \hfill (11)

Proof. Let

$$w^* = \arg \min_{w \in L_2(\mathbb{R}^d, d\mu)} \|Bw - y\|_2^2 + \lambda \|w\|_{L_2(\mathbb{R}^d, d\mu)}.$$  

Since \text{range}(B^*) is a a closed linear subspace of $\mathcal{H}$, there exists $v^* \in \mathbb{R}^n$ such that $w^* = B^*v^* + z$ where $z \perp \text{range}(B^*)$. Since $B$, viewed as an operator, is bounded, \text{null}(B) = (\text{range}(B^*))^\perp$, so $Bz = 0$. Now, since $z \neq 0$ can only increase $\lambda \|w\|_{L_2(\mathbb{R}^d, d\mu)}^2$ we conclude that $z = 0$. Thus, $w^* = B^*v^*$ and we can write

$$\min_{w \in L_2(\mathbb{R}^d, d\mu)} \|Bw - y\|_2^2 + \lambda \|w\|_{L_2(\mathbb{R}^d, d\mu)} = \min_{v \in \mathbb{R}^n} \|BB^*v - y\|_2^2 + \lambda \|B^*v\|_{L_2(\mathbb{R}^d, d\mu)}^2 = \min_{v \in \mathbb{R}^n} \|Kv - y\|_2^2 + \lambda v^TKv$$

where $K = BB^* \in \mathbb{R}^{n \times n}$ is the kernel matrix previously defined. The optimal solution is $v^* = (K + \lambda I_n)^{-1}y$, i.e., $v^* = \alpha^*$, so $w^* = \sum_{j=1}^n \alpha_j^* \varphi(x_j, \cdot)$. We now have

$$(\varphi(x, \cdot), w^*)_{L_2(\mathbb{R}^d, d\mu)} = \int_{\mathbb{R}^d} \varphi(x, \eta)w^*(\eta)d\mu(\eta)$$

$$= \int_{\mathbb{R}^d} e^{-2\pi i x^T \eta} \left( \sum_{j=1}^n \alpha_j^* e^{2\pi i x_j^T \eta} \right) d\mu(\eta)$$

$$= \sum_{j=1}^n \alpha_j^* \int_{\mathbb{R}^d} e^{-2\pi i (x - x_j)^T \eta} d\mu(\eta)$$

$$= \sum_{j=1}^n \alpha_j^* k(x, x_j) = f^*(x).$$

The quasimatrix $B$ is over complex-valued $L_2$ spaces. It is possible to actually define an equivalent SILR problem with a quasimatrix over a real-valued $L_2$ space. Let $\Omega = \mathbb{R}^d \times [0, 2\pi]$ and $\hat{\mu} = \mu \times U(0, 2\pi)$ where $U(0, 2\pi)$ is the uniform measure on $[0, 2\pi]$. Now, let $L_2(\hat{\Omega}, d\hat{\mu})$ denote the space of \textit{real-valued} square integrable functions with respect to the measure $\hat{\mu}$. Define the function $\hat{\varphi} : \mathcal{X} \times \hat{\Omega} \rightarrow \mathbb{R}$:

$$\hat{\varphi}(x, (\eta, b)) = \sqrt{2} \cos(x^T \eta + b).$$

Now, let

$$C = \begin{bmatrix} \hat{\varphi}(x_1, \cdot)^* \\ \vdots \\ \hat{\varphi}(x_n, \cdot)^* \end{bmatrix}.$$  

Then,

$$f^*(x) = (\hat{\varphi}(x, \cdot), u^*)_{L_2(\hat{\Omega}, d\hat{\mu})}$$

where

$$u^* = \arg \min_{u \in L_2(\hat{\Omega}, d\hat{\mu})} \|Cu - y\|_2^2 + \lambda \|u\|_2^2_{L_2(\hat{\Omega}, d\hat{\mu})}.$$  

See [37].
3.2.2 Approximating KRR using Quasimatrix Sampling

Computing the exact KRR estimator is costly (since $K$ is typically dense, finding $\alpha$ in Eq. (8) costs $O(n^3)$ using direct methods; computing $f^*(x)$ for some $x$ using Eq. (7) costs $O(nd)$; since computing $f^*$ requires storing the entire training set, storage requirements for holding a representation of $f^*$ is $O(nd)$), which motivates looking for some approximation schemes. In this section we show how to perform approximate KRR by sampling the quasimatrix $B$ defined in the previous subsection. The resulting method is actually identical to approximating KRR using random Fourier features, one of the most popular approximation of KRR, though the presentation as a sampling method for finding an approximate solution to a SILR problem is new.

Consider the wide quasimatrix $B$ defined in the previous subsection. A coordinate representation of $B$ is

$$z(\eta) = \begin{bmatrix}
\varphi(x_1, \eta) \\
\vdots \\
\varphi(x_n, \eta)
\end{bmatrix}.$$

This allows us to discuss column sampling of $B$. For $s \leq n$, consider the matrix $B_\eta \in \mathbb{C}^{n \times s}$ obtained by column sampling $B$ according to $\mu$. That is, we sample $\eta_1, \ldots, \eta_s$ according to $\mu$ and define the matrix

$$B_\eta = \begin{bmatrix}
z(\eta_1) & z(\eta_2) & \cdots & z(\eta_s)
\end{bmatrix} = \begin{bmatrix}
\varphi(x_1, \eta_1) & \cdots & \varphi(x_s, \eta_1) \\
\vdots & \ddots & \vdots \\
\varphi(x_1, \eta_s) & \cdots & \varphi(x_n, \eta_s)
\end{bmatrix}.$$

Let

$$w^*_\eta = \arg \min_{w \in \mathbb{C}^s} \| B_\eta w - y \|_2^2 + \lambda \| w \|_2^2.$$ 

Finding $w^*_\eta$ amounts to solving a finite linear least squares problem, and can be accomplished using $O(ns^2)$ arithmetic operations (and, notably, without performing any FUNOPs). The approximate KRR estimator is

$$f_\eta(x) = \sum_{i=1}^s \varphi(x, \eta_i)(w^*_\eta)_i,$$

where $(w^*_\eta)_i$ denotes entry $i$ of $w^*_\eta$. In a sense, the vector $w^*_\eta$ is an approximation of the function $w^*$ that is obtained by solving a sampled version of Eq. (11), and $f_\eta$ approximates the inner product $(\varphi(x, \cdot), w^*)_{L_2(X,d\mu)}$.

3.3 Stretching a Finite Linear Least Squares Problem

Since numerical computing is typically done with numbers and not with functions, it is natural to find an approximate solution to SILR problems by sampling the quasimatrix. Here, we show that it is also possible to go the other way, and “stretch” a finite linear least squares problem to a SILR problem. This process is interesting since it yields a novel interpretation to the use of the Johnson-Lindenstrauss sketch in order to approximately solve a linear regression problem.

Suppose that $X \in \mathbb{R}^{n \times d}$ is a full rank matrix with $n \gg d$, and that $y \in \mathbb{R}^n$. Consider finding $w^*$ that minimizes $\|Xw - y\|_2^2$. Define the function

$$\varphi(x, \eta) = \eta^T x,$$

and let $p$ denote the standard Gaussian density over $\mathbb{R}^n$. We have

$$\int_{\mathbb{R}^n} \varphi(x, \eta)^2 p(\eta) d\eta = x^T \left( \int_{\mathbb{R}^n} \eta \eta^T p(\eta) d\eta \right) x = x^T x,$$
so for \( x \in \mathbb{R}^n \) it holds that \( \varphi(x, \cdot) \in L_2(\mathbb{R}^n, d\mu) \) where \( d\mu \) denotes the standard Gaussian distribution. Denote by \( x_1, \ldots, x_d \) the columns of \( X \). Define the \( \infty \times d \) quasimatrix \( A \) over \( L_2(\mathbb{R}^n, d\mu) \): \( A = [ \varphi(x_1, \cdot) \cdots \varphi(x_d, \cdot) ] \). We now show that

\[
\mathbf{w}^* = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \| A\mathbf{w} - \varphi(y, \cdot) \|_{L_2(\mathbb{R}^n, d\mu)}^2.
\]

Indeed, for every \( \mathbf{w} \in \mathbb{R}^d \) we have

\[
\| A\mathbf{w} - \varphi(y, \cdot) \|_{L_2(\mathbb{R}^n, d\mu)}^2 = \int_{\mathbb{R}^n} \left( \sum_{i=1}^d (\eta^T x_i) w_i - \eta^T y \right)^2 p(\eta) d\eta
= \int_{\mathbb{R}^n} (\eta^T (X\mathbf{w} - y))^2 p(\eta) d\eta
= \| X\mathbf{w} - y \|_2^2.
\]

Thus, we have converted the finite linear least squares problem to a SILR problem.

Let us now consider approximately solving Eq. (12) by sampling “rows” from \( A \) and the corresponding entries from \( \varphi(y, \cdot) \). Since \( A \) is a quasimatrix over a \( L_2 \) space, we need a coordinate representation to meaningfully talk about sampling rows from \( A \). A coordinate representation of \( A \) is \( z(\eta) = X^T \eta \) where the index set is \( \Omega = \mathbb{R} \). We can now sample Eq. (12) as follows. We sample \( \eta_1, \ldots, \eta_s \in \mathbb{R}^n \) independently according to \( p \) and form the matrix

\[
A_\eta = \begin{bmatrix}
  z(\eta_1)^T \\
  z(\eta_2)^T \\
  \vdots \\
  z(\eta_s)^T
\end{bmatrix}
\]

and the vector \( y_\eta = (\eta_i^T y)_{i=1}^s \). The sampled problem (which is again a finite linear least squares problem) is

\[
\hat{\mathbf{w}} = \| A_\eta \mathbf{w} - y_\eta \|_2^2.
\]

One may ask, whether \( \hat{\mathbf{w}} \) is close to a be a minimizer of \( \| X\mathbf{w} - y \|_2^2 \). Let \( S \) be the \( s \times n \) matrix whose rows are \( \eta_1, \ldots, \eta_s \), then \( A_\eta = SX \) and \( y_\eta = Sy \). Using known results on subspace embedding \[17\] we conclude that if \( s = \Omega(d/\epsilon^2) \) then with high probability

\[
\| X\hat{\mathbf{w}} - y \|_2 \leq (1 + \epsilon) \| X\mathbf{w}^* - y \|_2.
\]

The random matrix \( S \) is a Johnson-Lindenstrauss sketching matrix, and we have demonstrated that applying the Johnson-Lindenstrauss sketch corresponds to stretching the linear least squares problem and then applying plain row sampling. A surprising aspect of this observation is the fact that only \( O(d/\epsilon^2) \) samples are sufficient. Indeed, standard techniques used for analyzing sampled linear least squares problems, which are based on matrix tail inequalities, can be used to derive results that require \( \Omega(d \log d/\epsilon^2) \) samples at the very least; see Section 6.

4 Direct Methods

Direct methods attempt to compute the solutions of SILR problems using quasimatrix operations. This mostly involves FUNOPs (under the chebfun model), but in some cases the computation can be reduced to algorithms that operate in the standard model (without FUNOPs). For simplicity, we assume that the quasimatrix involved is either full rank or \( \lambda > 0 \).
4.1 Overdetermined SILR

Let $\mathbf{A}$ be a tall quasimatrix with $n$ columns. We can solve the SILR problem in Eq. (2) using the normal equations. The development is essentially the same as for the finite linear least squares case. Let $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{x}\|_2^2$ be the objective function. We have,

$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 + \lambda \|\mathbf{x}\|_2^2 = \mathbf{x}^T (\mathbf{A}^\star \mathbf{A} + \lambda \mathbf{I}_n) \mathbf{x} - 2 \text{Re} (\mathbf{x}^T \mathbf{A}^\star \mathbf{b}) + \|\mathbf{b}\|_2^2.$$

Thus the optimum value is obtained as the solution of the following linear system:

$$(\mathbf{A}^\star \mathbf{A} + \lambda \mathbf{I}_n) \mathbf{x} = \mathbf{A}^\star \mathbf{b}$$

(easily verified by computing the gradient of $f(\mathbf{x})$ and equating to zero). Note that since we assumed that either $\mathbf{A}$ is full rank or $\lambda > 0$, $\mathbf{A}^\star \mathbf{A} + \lambda \mathbf{I}_n$ is invertible.

Thus, we can find the optimal $\mathbf{x}^\star$ in the chebfun model by first computing $\mathbf{A}^\star \mathbf{A} + \lambda \mathbf{I}_n$ and $\mathbf{A}^\star \mathbf{b}$ $(n(n+3)/2$ FUNOPs), and then solving an $n \times n$ linear system $(O(n^3)$ FLOPs). However, using the Gram matrix $\mathbf{A}^\star \mathbf{A}$ entails a squaring of the condition number, so the use of a factorization is preferred numerically. It is simple algebra to show that if $\mathbf{A} = \mathbf{QR}$ is a reduced QR factorization of $\mathbf{A}$ then $\mathbf{x}^\star = (\mathbf{R} + \lambda \mathbf{R}^{-\star})^{-1} \mathbf{Q}^\star \mathbf{b}$, so $n$ FUNOPs and $O(n^3)$ FLOPs $(O(n^2)$ if $\lambda = 0$) are needed once we have a QR factorization. However, this entails explicitly inverting $\mathbf{R}^\star$, and that matrix might be ill-conditioned.

If $\mathbf{A}$ was a matrix, explicitly inverting $\mathbf{R}$ can be avoiding by factorizing the augmented matrix

$$\hat{\mathbf{A}} = \begin{bmatrix} \mathbf{A} \\ \sqrt{\lambda} \mathbf{I}_n \end{bmatrix}.$$ 

However, if $\mathbf{A}$ is a quasimatrix over $\mathbb{H}$ then $\hat{\mathbf{A}}$ is a quasimatrix over $\mathbb{H} \times \mathbb{C}^n$ (if column $j$ of $\mathbf{A}$ is $\mathbf{a}_j$, then column $j$ of the augmented quasimatrix is the tuple $(\mathbf{a}_j, \sqrt{\lambda} \mathbf{e}_j)$ where $\mathbf{e}_j$ is the $j$-th identity vector in $\mathbb{C}^n$), possibly making computations more cumbersome. We now show how it is possible to find $\mathbf{x}^\star$ using a QR factorization of $\mathbf{A}$ without explicitly inverting $\mathbf{R}$. This involves fairly standard linear algebra tricks. Suppose we have a QR factorization $\mathbf{A} = \mathbf{Q}_\mathbf{A} \mathbf{R}_\mathbf{A}$. Let $\mathbf{C}$ be the matrix obtained by augmenting $\mathbf{R}_\mathbf{A}$ with the matrix $\sqrt{\lambda} \mathbf{I}_n$, and form a QR factorization of it. That is,

$$\mathbf{C} = \begin{bmatrix} \mathbf{R}_\mathbf{A} \\ \sqrt{\lambda} \mathbf{I}_n \end{bmatrix} = \mathbf{Q}_\mathbf{C} \mathbf{R}_\mathbf{C}.$$ 

Let $\mathbf{Q}_{\mathbf{C},1}$ denote the top $n$ rows of $\mathbf{Q}_\mathbf{C}$, and $\mathbf{Q}_{\mathbf{C},2}$ the bottom. Now,

$$\begin{bmatrix} \mathbf{A} \\ \sqrt{\lambda} \mathbf{I}_n \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_\mathbf{A} & \mathbf{I}_n \end{bmatrix} \mathbf{C} = \begin{bmatrix} \mathbf{Q}_\mathbf{A} & \mathbf{I}_n \end{bmatrix} \begin{bmatrix} \mathbf{Q}_{\mathbf{C},1} \\ \mathbf{Q}_{\mathbf{C},2} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_\mathbf{A} \mathbf{Q}_{\mathbf{C},1} \\ \mathbf{Q}_\mathbf{A} \mathbf{Q}_{\mathbf{C},2} \end{bmatrix} \mathbf{R}_\mathbf{C}.$$

Also, since

$$\begin{bmatrix} \mathbf{Q}_{\mathbf{C},1} \\ \mathbf{Q}_{\mathbf{C},2} \end{bmatrix} \begin{bmatrix} \mathbf{Q}_\mathbf{A} \mathbf{Q}_{\mathbf{C},1} \\ \mathbf{Q}_\mathbf{A} \mathbf{Q}_{\mathbf{C},2} \end{bmatrix} = \mathbf{I}_n,$$

we have a QR factorization of $\hat{\mathbf{A}}$. This implies that $\mathbf{x}^\star$ is the solution of the triangular system

$$\mathbf{R}_\mathbf{C} \mathbf{x} = \mathbf{Q}_\mathbf{C} \mathbf{Q}_\mathbf{A} \mathbf{b}.$$ 

As is the case of finite linear least squares, a reduced SVD can be used to solve SILR problems as well. If $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^\star$ is a reduced SVD factorization, then simple algebra reveals that $\mathbf{x}^\star = \mathbf{V}(\Sigma^2 + \lambda \mathbf{I}_n)^{-1} \Sigma \mathbf{U}^\star \mathbf{b}$, so $n$ FUNOPs and $O(n^2)$ FLOPs are needed once we have an SVD factorization.

In certain cases it might be possible to compute $\mathbf{A}^\star \mathbf{A}$ and $\mathbf{A}^\star \mathbf{b}$ analytically, without resorting to FUNOPs. We give a concrete example later, when we discuss the underdetermined case.

---

We remark that the chebfun library does support hybrids of quasimatrices and a matrices (and calls such objects by the name “chebmatrix”).
4.2 Underdetermined SILR

Let \( A \) be a wide quasimatrix with \( n \) rows. Again, the following argument follows closely the one used for finite linear least squares. The space \( \text{range}(A^*) \) is a closed linear subspace of \( \mathcal{H} \), so we can write \( x^* = A^* y^* + z^* \) where \( y \in \mathbb{R}^n \) and \( z \perp \text{range}(A^*) \). Since \( A \), viewed as an operator, is bounded, \( \text{null}(A) = (\text{range}(A^*))^\perp \), so \( Az = 0 \). Thus, the objective at \( x^* \) is

\[
\|Ax^* - b\|_2^2 + \lambda\|x^*\|_2^2 = \|AA^* y^* - b\|_2^2 + \lambda\|A^* y^*\|_2^2 + \lambda\|z^*\|_2^2,
\]

where we used the fact that \( z^* \perp A^* y^* \). Obviously, \( z^* = 0 \), otherwise the objective can be reduced. Denoting \( K = AA^* \in \mathbb{R}^{n \times n} \), we find that \( y^* \) is the minimizer of

\[
f(y) = \|K y - b\|_2^2 + \lambda y^T Ky.
\]

This can be written as a determined (for \( \lambda = 0 \)) or overdetermined (\( \lambda > 0 \)) finite linear least squares problems, from which we find that \( y^* \) solves the equation

\[
(K^2 + \lambda K)y = Kb.
\]

Since we assumed that either \( A \) is full rank or \( \lambda > 0 \), \( K + \lambda I_n \) is invertible, and the vector \((K + \lambda I_n)^{-1}b\) solves the equation. The solution is unique, so \( y^* = (K + \lambda I_n)^{-1}b \). We find that

\[
x^* = A^* (K + \lambda I_n)^{-1}b.
\]

Thus, in the chebfun model we can find the optimal \( x^* \) by first computing \( K + \lambda I_n \) \((n(n + 1)/2\) FUNOPs), solving for \( y^* \) \((O(n^3)\) FLOPs), and finally computing \( A^* y^* \) \(n\) FUNOPs).

We can avoid forming the potentially ill-conditioned matrix \( K \) using a QR factorization of \( A^* \) in a way similar to the previous subsection, where now we have a QR factorization \( A^* = QA \). Similarly, we can factorize

\[
\begin{bmatrix}
A^* \\
\sqrt{\lambda} I_n
\end{bmatrix} =
\begin{bmatrix}
QA Q_{C,1} \\
Q_{C,2}
\end{bmatrix} R_C.
\]

This implies that

\[
\begin{bmatrix}
A \\
\sqrt{\lambda} I_n
\end{bmatrix} =
\begin{bmatrix}
Q_{C,1} Q_A^* \\
Q_{C,2}
\end{bmatrix} R_C
\]

is an LQ factorization of the augmented matrix. Hence, \( x^* \) is equal to

\[
x^* = QA Q_{C,1} (R_C)^{-1} b.
\]

An SVD factorization can be used as well: if \( A^* = U \Sigma V^* \) is an SVD factorization, then \( x^* = U(\Sigma^2 + \lambda I_n)^{-1} \Sigma V^* b \).

In certain cases, it is possible to compute \( K \) analytically. As an example, consider again kernel ridge regression (Section 3.2) in the RKHS formulation (Eq. (9)). Due to the definition of \( \mathcal{H}_k \), the \( ij \) entry of \( K \) is

\[
K_{ij} = \langle k(x_i, \cdot), k(x_j, \cdot) \rangle_{\mathcal{H}_k} = k(x_i, x_j),
\]

thus we can form \( K + \lambda I_n \) and compute \( \alpha = (K + \lambda I_n)^{-1} y \) using \( O(n^2 d + n^3) \) FLOPs. The solution to Eq. (9) is then

\[
f^*(x) = \sum_{i=1}^n \alpha_i k(x_i, x).
\]

and all computations are done in the standard model.
5 Iterative Methods

In this section we discuss solving SILR problems using iterative methods. First, we consider using the classical approach of Krylov subspace methods. We show how methods such as LSMR or LSQR can be rather naturally generalized to quasimatrices. Next, we propose a novel method based on stochastic optimization which requires considerably less function operations, but depends on the ability to sample the quasimatrix. We also show that this algorithm can, in certain cases, be applied in the standard model (without FUNOPs).

5.1 Krylov Subspace Methods

Krylov subspace methods are one of the most important classes of iterative methods in numerical linear algebra. Many of the most widely used iterative linear solvers are Krylov subspace methods. One important benefit of Krylov subspace methods is that they only use matrix-vector operations. For SILR, when working in the chebfun model, this implies that each iteration does only $O(n)$ FUNOPs.

It was already observed by several authors that it is possible to generalize Krylov subspace methods to operator equations. For example, Olver suggested the use of GMRES with the differentiation operator $\frac{d}{dx}$, and the chebfun library implements GMRES for operator equations. Continuous analogues of CG, GMRES and MINRES appear in [19] in the context of differential operators. In the same vein, we can adapt Krylov subspace algorithms for finite linear least squares, such as LSQR [34] and LSMR [18], to solve SILR problems. Here we describe the LSMR algorithm for quasimatrices. The development is a rather straightforward generalization of the matrix case, but we show it for concreteness.

5.1.1 Golub-Kahan Bidiagonalization Process for Quasimatrices

LSMR and LSQR are based on Golub-Kahan bidiagonalization [20]. The goal of Golub-Kahan bidiagonalization is to iteratively find a decomposition $U^*AV = B$ where $U$ and $V$ have orthogonal columns, and $B$ is a bidiagonal matrix. When $A$ is a quasimatrix over $\mathcal{H}$, one of $U$ and $V$ is a quasimatrix over $\mathcal{H}$ and the other one is a matrix. The algorithm remains essentially unchanged, and is given in Algorithm ?? for a tall quasimatrix (for a wide quasimatrix the algorithm remains the same under the corresponding changes of norms).

After $k$ steps of the algorithm, we have $AV_k = U_{k+1}B_k$ and $A^*U_{k+1} = V_{k+1}L_{k+1}^*$. Note that, in the underdetermined case, where $A$ is a $\infty \times n$ quasimatrix, $V_k$ is an $n \times k$ matrix and $U_k$ is a $\infty \times k$ tall quasimatrix over $\mathcal{H}$. In the underdetermined case, $U_k$ is a $n \times k$ matrix and $V_k$ is a $\infty \times k$ tall quasimatrix over $\mathcal{H}$ such that $V_k^*V_k = U_k^*U_k = I_k$. The algorithm also defines a $(k + 1) \times k$ lower bidiagonal matrix $B_k$.

5.1.2 LSMR for Overdetermined SILR

Recall that the solution $x^*$ of an overdetermined SILR problem solves the normal equations $(A^*A + \lambda I_n)x^* = A^*b$. LSMR is equivalent to applying MINRES to the normal equations, i.e. in each iteration the minimizer of $A^*b - (A^*A + \lambda I_n)x$ is found under the constraint that $x$ belongs to the Krylov subspace. Thus, defining $r_k = b - Ax_k$ at iteration $k$, LSMR minimizes $\|A^*r_k - \lambda x_k\|_2$ subject to $x_k \in \mathcal{K}_k(A^*A, b)$, where $\mathcal{K}_k(A^*A, b) := \text{span} \{b, A^*A b, \ldots, (A^*A)^{k-1} b\}$ is the order $k$-th order Krylov subspace generated by $A^*A$ and $b$.

To find $x_k$, LSMR uses the Golub-Kahan bidiagonalization. After $k$ iterations we have $AV_k = U_{k+1}B_k$ and $A^*U_{k+1} = V_{k+1}L_{k+1}^*$, where $V_k$ is an $n \times k$ matrix and $U_k$ is a $\infty \times k$ tall quasimatrix over $\mathcal{H}$. Thus,

\[
A^*(AV_k) = (A^*U_{k+1})B_k = V_{k+1}L_{k+1}^*B_k = V_{k+1} \begin{bmatrix} B_k^T \alpha_{k+1} \beta_{k+1} e_{k+1}^T \end{bmatrix} \]

\[
A^*b = \beta_1 A^T u_1 = \alpha_1 \beta_1 V_{k+1} e_1 .
\]
Algorithm 1 (Tall) Quasimatrix Golub-Kahan Bidiagonalization.

1: Inputs:
Tall $\mathit{H} \times n$ quasimatrix $A$ over $H$, and $\mathit{H} \times 1$ quasimatrix $b$.

2: set:
$\beta_1 = \|b\|_H$, $u_1 = b/\beta_1$, $\alpha_1 = \|A^T u_1\|_2$, $v_1 = A^T u_1/\alpha_1$.

3: for $k = 1, 2, \ldots$,

*$\beta_{k+1} = \|Av_k - \alpha_k u_k\|_H, u_{k+1} = (Av_k - \alpha_k u_k)/\beta_{k+1}$

$\alpha_{k+1} = \|A^* u_{k+1} - \beta_{k+1} v_k\|_2, v_{k+1} = (A^* u_{k+1} - \beta_{k+1} v_k)/\alpha_{k+1}$.

4: Denote:
$V_k = \begin{bmatrix} v_1 & v_2 & \cdots & v_k \end{bmatrix}, U_k = \begin{bmatrix} u_1 & u_2 & \cdots & u_k \end{bmatrix}$

$B_k = \begin{bmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_k \\ \beta_{k+1} \\ \beta_k \end{bmatrix}$, $L_K = [B_k \alpha_{k+1} e_{k+1}]$.

(These equations are the same as in the matrix case: the quasimatrix algebra defined in Section 2 allows us to write essentially the same derivations). Since $x_k$ is in the Krylov subspace, we can write $x_k = V_k y_k$ for some $y_k \in \mathbb{C}^k$. Thus, we can write

$$\|A^*(Ax_k - b)\|_2^2 + \lambda \|x_k\|_2^2 = \|A^*(AV_k y_k - b)\|_2^2 + \lambda \|V_k y_k\|_2^2$$

$$= \left\| V_{k+1} \left( \begin{bmatrix} B_k^T \alpha_{k+1} e_{k+1}^T \end{bmatrix} y_k - \alpha_1 \beta_1 e_1 \right) \right\|^2_2 + \lambda \|y_k\|_2^2.$$

So, finding $y_k$ and $x_k$ has been reduced to the solution of a finite linear least squares problem. An algorithm for finding these vectors efficiently and iteratively is described in [18].

Stopping criteria: the Golub-Kahan process terminates whenever $\alpha_{k+1} = 0$ or $\beta_{k+1} = 0$, which implies that the last equation is zero. However, we can use one of the stopping criteria originally presented for the LSQR algorithm, involving the predetermined parameters ATOL, BTOL and CONLIM:

$S_1$: Stop if $\sqrt{||r_k||_H^2 + \lambda \|x_k\|_2^2} \leq ATOL ||b||_H + ATOL \sqrt{\sigma_{\text{max}}(B_k)^2 + \lambda} \|x_k\|_2$

$S_2$: Stop if $\|A^* r_k - \lambda x_k\|_2 \leq ATOL \sqrt{\sigma_{\text{max}}(B_k)^2 + \lambda} \|Ax_k - b\|_H^2 + \lambda$

$S_3$: Stop if $\sqrt{\sigma_{\text{max}}(B_k)^2 + \lambda} \leq \sigma_{\text{min}}(B_k)^2 + \lambda \geq \text{CONLIM}$.

The motivation for these stopping rules is the fact that $\sigma_{\text{max}}(B_k)$ and $\sigma_{\text{min}}(B_k)$ provide estimates for $\sigma_{\text{max}}(A)$ and $\sigma_{\text{min}}(A)$. This follows from the fact that $B_k^T B_k = V_k^* A^* A V_k$. See [18] for more details.

Complexity: when compared to the matrix version of LSQR, the quasimatrix version trades each matrix-vector product with $n$ FUNOPs. Thus, in terms of FUNOPs, $2n$ FUNOPs are required per iteration. Since
the number of iterations is $O(\sqrt{\kappa (A^*A + \lambda I_n)})$, overall complexity is $O(n\sqrt{\kappa (A^*A + \lambda I_n)})$ FUNOPs.

5.1.3 Numerical Example

We illustrate the use of LSMR for the problem of approximating the Runge function $f(x) = 1/(1 + 25x^2)$ on $[-1, 1]$ using a polynomial of degree 300. We can write the approximation as the solution of an overdetermined SILR problem where $A$ is any quasimatrix whose columns span the space of degree 300 polynomials. However, we want $A$ to be reasonably well conditioned so that LSMR will converge quickly, so we use Chebyshev polynomials as the columns of $A$ (we empirically observed that when the columns are the Chebyshev polynomials, $A$ is well-conditioned, though we are unaware of any analytical result showing this; note that taking the normalized Legendre polynomials instead would have resulted in an orthogonal $A$, which would have made for an uninteresting numerical example). Thus, we solve the SILR problem where

$$A = \begin{bmatrix} T_0 & T_1 & \ldots & T_{299} \end{bmatrix}, \quad b = \begin{bmatrix} 1/(1 + 25x^2) \end{bmatrix}.$$

In the above, $T_j$ is the $j$-th Chebyshev polynomial. We use $\lambda = 0$ (no regularization) and parameters $\text{ATOL} = \text{BTOL} = 10^{-7}$. Convergence plots are shown in Figure 1.

![Convergence plots](image)

Figure 1: Numerical illustration: using LSMR to solve a SILR related to approximating the Runge function using a polynomial.

5.2 Stochastic Variance Reduced Gradient (SVRG)

Recent literature on convex optimization advocated the use of stochastic methods. Even for the specialized cases of solving linear equations or linear least squares, such methods have been shown to be beneficial [27, 21]. In this section, we propose a method for solving SILR problems using Stochastic Variance Reduced Gradient (SVRG) [23, 48]. SVRG is a stochastic optimization method for minimizing objective functions that have finite sum structure, i.e. of the form

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x).$$

For such objective functions, we can compute stochastic gradients by sampling an index of the sum. SVRG’s main benefit comes from the fact that it combines such stochastic gradients with a small amount of full gradients (i.e. exact gradients of $f$). For strongly convex functions, the number of such full gradients we
need to compute is independent of the condition number (however, the number of stochastic gradients does depend on the average condition number).

For SILR, full gradients correspond to products of a quasimatrix $A$ with a vector or function, but this is the only operation that assumes the chebfun model and requires FUNOPs. Thus, by using SVRG we remove the condition number dependence for the number of FUNOPs required for convergence, which is a major improvement over Krylov methods. However, stochastic gradients in SVRG correspond to sampling objective functions, and for SILR this translates to sampling a row from a tall quasimatrix or a column from a wide quasimatrix. Thus, the quasimatrix must be a quasimatrix over a $L_2$ space, and must have a coordinate representation.

One obstacle in applying SVRG to SILR problems is that such problems cannot be written as a finite sum, but rather can be written as an integral of simpler functions, i.e.

$$f(x) = \int_{\Omega} f_\eta(x) d\mu(\eta).$$

We generalize SVRG and its analysis to handle such functions. The generalization might be of independent interest, and appears in Appendix A.

5.2.1 Overdetermined SILR

Consider the overdetermined SILR problem (Eq. (2)) where the quasimatrix $A$ is over $\mathcal{H} = L_2(\Omega, d\mu)$ for some index set $\Omega$. We further assume we have a coordinate representation $z_A : \Omega \to \mathbb{R}^n$ for $A$ and $z_b : \Omega \to \mathbb{R}$ for $b$. We further assume there exists a $M$ such that for every $\eta \in \Omega$ we have $\|z_A(\eta)\|_2^2 \leq M$. We can write the objective function in Eq. (2) as an integral:

$$\frac{1}{2} \|Ax - b\|_{L_2(\Omega, d\mu)}^2 + \frac{\lambda}{2} \|x\|_2^2 = \frac{1}{2} \sum_{i=1}^n x_i z_A(\cdot)_i - b\|_{L_2(\Omega, d\mu)}^2 + \frac{\lambda}{2} \|x\|_2^2$$

$$= \frac{1}{2} \|z_A(\cdot)^* x - b\|_{L_2(\Omega, d\mu)}^2 + \frac{\lambda}{2} \|x\|_2^2$$

$$= \frac{1}{2} \int_{\Omega} (z_A(\eta)^* x - z_b(\eta))^2 + \lambda \|x\|_2^2 \ d\mu(\eta)$$

$$= \int_{\Omega} f_\eta(x) d\mu(\eta)$$

where

$$f_\eta(x) := \frac{1}{2} (z_A(\eta)^* x - z_b(\eta))^2 + \frac{\lambda}{2} \|x\|_2^2.$$

We can now apply the aforementioned variant of SVRG [23] (see Appendix A), which is adapted for objective integrable functions. To do so, the following assumptions need to be verified:

**Assumption 4.** For all $\eta \in \Omega$, $\nabla f_\eta(x)$ is Lipschitz continuous, i.e., there exists $L_\eta > 0$ such that for all $x, y \in \mathbb{R}^n$

$$\|\nabla f_\eta(x) - \nabla f_\eta(y)\| \leq L_\eta \|x - y\|.$$

**Assumption 5.** Suppose that $f(x)$ is strongly convex, i.e., there exist $\gamma > 0$ such that for all $x, y \in \mathbb{R}^n$

$$f(x) - f(y) \geq \frac{\gamma}{2} \|x - y\|_2^2 + \nabla f(y)^T (x - y).$$

**Assumption 6.** The equality $\nabla f(x) = \int_{\Omega} \nabla f_\eta(x) d\mu(\eta)$ hold.

**Assumption 7.** $L_{sup} := \sup_{\eta \in \Omega} L_\eta < \infty$. 

17
We begin by writing
\[ f(x) := \frac{1}{2} \|Ax - b\|_{L_2(\Omega, d\mu)}^2 + \lambda \|x\|^2 = \frac{1}{2} x^T (K + \lambda I_n) x - x^T A^* b + \frac{1}{2} \|b\|_{L_2(\Omega, d\mu)}^2 \]
where \( K = AA^* \in \mathbb{R}^{n \times n} \). Thus,
\[ \nabla f(x) = A^*(Ax - b) + \lambda x. \]
It can be seen that Assumption 5 holds with \( \gamma = \lambda + \lambda_{\min}(K) \). We also have
\[ \nabla f_\eta(x) = z_A(\eta) (z_A(\eta)^* x - z_b(\eta)) + \lambda x \]
with
\[ \int_\Omega \nabla f_\eta(x) d\mu(\eta) = \int_\Omega z_A(\eta) (z_A(\eta)^* x - z_b(\eta)) + \lambda x d\mu(\eta) \]
\[ = \left( \int_\Omega z_A(\eta) z_A(\eta)^* d\mu(\eta) \right) x - \int_\Omega z_A(\eta) z_b(\eta) d\mu(\eta) + \lambda x \]
\[ = Kx - A^* b + \lambda x = \nabla f(x). \]
so Assumption 6 holds as well. Note that for every \( \eta \in \mathcal{X} \)
\[ \| \nabla f_\eta(x) - \nabla f_\eta(y) \|_2 = \| (z_A(\eta) z_A(\eta)^* + \lambda I_n) (x - y) \|_2 \]
\[ \leq (\| z_A(\eta) \|_2^2 + \lambda) \| x - y \|_2 \]
so each \( \nabla f_\eta \) is Lipschitz continuous with Lipschitz constant \( L_\eta = \| z_A(\eta) \|_2^2 + \lambda \). Thus, Assumptions 4 and 7 hold with \( L_{sup} = M + \lambda \).

Therefore, according to Theorem 22 (in Appendix A), if we set
\[ m = 50 \cdot \kappa, \quad \kappa = \frac{M + \lambda}{\lambda^2 + \lambda}, \quad \alpha = \frac{\theta}{M + \lambda}, \quad 0 < \theta < \frac{1}{4} \]
where \( \gamma \) is any lower bound on \( \sigma_{\min}(A) \) (if \( \lambda > 0 \) we can take \( \gamma = 0 \)), then taking \( \theta = 1/5 \) and assuming we start with \( x = 0 \) yields
\[ \mathbb{E} [f(\hat{x}_n)] - f(x^*) \leq \left( \frac{5}{6} \right)^n \left( \frac{1}{2} \| b \|_{L_2(\Omega, d\mu)}^2 - f(x^*) \right). \]

Overall, to reduce (in expectation) by a factor of \( \epsilon \) we need to do \( O(\log(1/\epsilon)) \) outer iterations, each requiring \( 2n \) FUNOPs. Each outer iteration requires \( O(\kappa) \) inner iterations, each requiring \( O(n + T) \) FLOPS where \( T \) is the cost of computing \( z_A(\eta) \) and \( z_b(\eta) \) for a given \( \eta \), so in total we need \( O((n + T) \cdot \kappa \cdot \log(1/\epsilon)) \) FLOPs. We see that in contrast with Krylov subspace methods, the number of FUNOPs does not depend on the condition number. The proposed algorithm is summarized in Algorithm 2.

### 5.2.2 Underdetermined SILR

We now consider the case that \( A \) is wide \( n \times \infty \) quasimatrix over \( L_2(\Omega, d\mu) \) of full rank, and \( b \in \mathbb{C}^n \). As explained in subsection 4.2, the optimal solution \( x^* \) has the form \( x^* = A^* y^* \) for \( y^* \in \mathbb{C}^n \). In addition, we have \( y^* = (K + \lambda I_n)^{-1} b \) where \( K = AA^* \). Hence,
\[ y^* = \arg \min_{y \in \mathbb{C}^n} \frac{1}{2} y^* (K + \lambda I_n) y - y^* b. \]
Thus, we can find approximate solutions to the regression problem by optimizing
\[ f(y) := \frac{1}{2} y^* (K + \lambda I_n) y - y^* b. \]
and returning \( \hat{x} = A^* \hat{y} \) for the \( \hat{y} \) found by the optimization process. Note that if we find a \( \hat{y} \) such that 
\[
 f(\hat{y}) \leq f(y^*) + \epsilon
\]
then for \( \hat{x} = A^* \hat{y} \) we have
\[
\|\hat{x} - x^*\|_2^2 \leq \frac{2\lambda_{\max}(K)}{\lambda_{\min}(K) + \lambda} \cdot \epsilon.
\]

We can again use SVRG (with the specific variant described in Appendix A) to minimize \( f(y) \). Since the assumptions are the same as in the previous section, and the developments are almost identical, we do not repeat them. The algorithm is almost identical to Algorithm 2 with two small differences: the equation for \( s_{\max} \) is replaced by \( (\log(6/5))^{-1} \cdot \log(\|b\|_2^2/(2\epsilon)) \), and \( \tilde{g} \) is \( A(A^* \hat{y} + \lambda \hat{y} - b) \).

### 5.2.3 SVRG for Kernel Ridge Regression

Recall that KRR can be recasted as an underdetermined SILR problem (subsection 3.2). We can use the algorithm from the previous subsection to solve this SILR problem. However, since we can compute \( K \) via the kernel function without assuming the chebfun model, we can avoid performing FUNOPs when computing \( \tilde{g} \). That is, we can apply SVRG under the standard model. For this case, the assumptions hold with \( M = d \).

We illustrate the performance of this algorithm on a small scale experiment. The goal is to learn a one dimensional dataset generated by noisily sampling the function \( f^*(x) = \sin(6x) + \sin(60e^x) \), i.e. \( y_i = f^*(x_i) + \epsilon_i \) with \( \epsilon_i \sim N(0, 0.3^2) \). The training set consists of 400 equispaced examples on \([-1, 1]\), and we use the Gaussian kernel. The goal was to reach error \( \epsilon = 10^{-2} \). The experiment was run with fixed step size of \( \alpha = 10^{-4} < 1/2L_{\sup} \). We varied both the value of \( m \) and \( s \). Results are reported in Figure 2.
Figure 2: Experiment with SVRG for KRR. The target function and the samples are shown in the top left graph. The top right and bottom left graph show the test error when varying $s$ or $m$ (respectively). In the bottom right we show the test error as a function of the number of operations.

6 Converting SILR to Finite Linear Least Squares via Sampling

All the previous algorithms we presented for solving SILR problems either assumed the chebfun model, or relied on the ability to compute the Gram matrix using an analytic formula (e.g. kernel ridge regression). In practice, such formulas are not always available, and the chebfun model is implemented only in software, and even then only when the columns/rows of the quasimatrix are univariate functions$^4$. Thus, a different technique is needed in order to solve SILR problems that violate these constraints. One natural approach for approximately solving a SILR problem is to discretize the infinite dimension via sampling.

For brevity, let us focus on overdetermined SILR (Eq. (2)). In order to discuss sampling, we need a coordinate representation of $A$. Thus, we assume that $\mathcal{H} = L_2(\Omega, d\mu)$ for some measurable index set $\Omega \subseteq \mathbb{R}^d$ and that we have a coordinate representation $z_A : \Omega \rightarrow \mathbb{C}^n$ for $A$ and $z_b : \Omega \rightarrow \mathbb{C}$ for $b$. A generic approach is as follows. We first select $s$ coordinates $\eta_1, \ldots, \eta_s \in \Omega$, and associated weights $w_1, \ldots, w_s \in \mathbb{R}$. We then form the row sampled matrix $A_\eta$ and row sampled vector $b_\eta$ as follows:

\[
A_\eta = \begin{bmatrix}
w_1z_A(\eta_1)^* \\
w_2z_A(\eta_2)^* \\
\vdots \\
w_sz_A(\eta_s)^*
\end{bmatrix}, \quad b_\eta = \begin{bmatrix}
w_1z_b(\eta_1) \\
w_2z_b(\eta_2) \\
\vdots \\
w_sz_b(\eta_s)
\end{bmatrix}.
\]

$^4$While chebfun does support bivariate functions, it does not seem to support quasimatrices of bivariate functions.
We now solve the sampled problem (which is a finite linear least squares problem):

\[ \hat{x} = \arg \min_{x \in \mathbb{C}^n} \| A \eta x - b \eta \|_2^2 + \lambda \| x \|_2^2. \]

Solving this sampled problem can be considered as an approximation to the SILR problem, and as explained in Section 3, it is the scheme used in least squares approximation of functions [11, 12] and random Fourier features [37].

To make the method concrete we need to address a couple of related questions. Given \( \eta_1, \ldots, \eta_s \), can we relate \( \hat{x} \) to \( x^* \)? How can we select \( \eta_1, \ldots, \eta_s \) and \( w_1, \ldots, w_s \in \mathbb{R} \) so that \( \hat{x} \) is a good enough approximate solution? Similar questions have been asked, and answered, for finite linear least squares [47, 1, 2], and various structural conditions have been suggested. The following result is similar to ones that appear in the literature on sampling finite linear least squares problems.

**Proposition 8.** Consider the overdetermined SILR

\[ \min_{x \in \mathbb{C}^n} \| A x - b \|_2^2 + \lambda \| x \|_2^2 \]

along with a full rank tall quasimatrix \( A \) over \( \mathbb{H} \) with \( n \) columns and \( \lambda \geq 0 \). Assume that \( (\| A x^* - b \|_2^2 + \lambda \| x^* \|_2^2) / 2 \geq \lambda \). Also assume that we are given a matrix \( A \eta \in \mathbb{R}^{s \times n} \) and a vector \( b \eta \in \mathbb{R}^s \) such that

\[ (1 - \epsilon) (\| A x - b \|_2^2 + \lambda \| x \|_2^2) \leq \| A \eta x - b \eta \|_2^2 + \lambda \| x \|_2^2 \leq (1 + \epsilon) (\| A x - b \|_2^2 + \lambda \| x \|_2^2) \] \hspace{1cm} (13)

for all \( x \in \mathbb{C}^n \). Then,

\[ \| A \hat{x} - b \|_2^2 + \lambda \| x \|_2^2 \leq \frac{1 + 2\epsilon}{1 - \epsilon} (\| A x^* - b \|_2^2 + \lambda \| x^* \|_2^2). \]

**Proof.** We have

\[
\begin{align*}
\| A \hat{x} - b \|_2^2 + \lambda \| x \|_2^2 & \leq \frac{1}{1 - \epsilon} (\| A \eta \hat{x} - b \eta \|_2^2 + \lambda \| \hat{x} \|_2^2 + \lambda) - \lambda \\
& \leq \frac{1}{1 - \epsilon} (\| A \eta x^* - b \eta \|_2^2 + \lambda \| x^* \|_2^2 + \lambda) - \lambda \\
& \leq \frac{1 + \epsilon}{1 - \epsilon} (\| A x^* - b \|_2^2 + \lambda \| x^* \|_2^2 + \lambda) - \lambda \\
& \leq \frac{1 + 2\epsilon}{1 - \epsilon} (\| A x^* - b \|_2^2 + \lambda \| x^* \|_2^2)
\end{align*}
\]

where the first and third inequalities use Eq. (13), the second inequality follows from \( \hat{x} \) being the minimizer of the sampled SILR, and the last inequality uses the first assumption. \( \square \)

Note that Proposition 8 does not require \( A \eta \) and \( b \eta \) to actually be row samples of \( A \) and \( b \).

### 6.1 Randomized Sampling

One approach for selecting \( \eta_1, \ldots, \eta_s \) and \( w_1, \ldots, w_s \) is to sample \( \eta_1, \ldots, \eta_s \) randomly from \( \Omega \) and set the weights accordingly. The question is what distribution on \( \Omega \) to use, and how to set the weights? To answer these questions, we show a general result on the number of samples \( s \) required to ensure Eq. (13) holds given some distribution on \( \Omega \) and a specific way to set the weights. The result is based on the concept of ridge leverage scores [17] [13], which we generalize to quasimatrices (the generalization is similar to the one used in [3, 4]).
Definition 9. Let $A$ be a quasimatrix over $L_2(\Omega, d\mu)$ equipped with a coordinate representation $z$, and $\lambda \geq 0$. Further assume that $\mu$ is a probability measure for which a corresponding density $p$ exists. The $\lambda$-leverage function of $A$ is

$$\tau_\lambda : \Omega \to \mathbb{R}, \quad \tau_\lambda(\eta) := p(\eta)z(\eta)^*(K + \lambda I_n)^{-1}z(\eta)$$

where $K = A^*A$ if $A$ is a tall quasimatrix, or $K = AA^*$ if $A$ is a wide quasimatrix.

Proposition 10 (Similar to Proposition 5 in [3]). Under the same conditions in Definition 9,

$$\int_\Omega \tau_\lambda(\eta)d\eta = \text{Tr} \left( (K + \lambda I_n)^{-1}K \right) =: s_\lambda(A).$$

($s_\lambda(A)$ is called the statistical dimension of $A$).

Lemma 11 (Similar to Lemma 8 in [3]). Consider the overdetermined SILR

$$\min \|Ax - b\|_{L^2(\Omega, d\mu)}^2 + \lambda \|x\|_2^2$$

where $A$ is tall quasimatrix $A$ with $n$ columns, and $\lambda \geq 0$. If $\lambda = 0$, further assume that $A$ is full rank. Assume we have coordinate representation $z_A : \Omega \to \mathbb{C}^n$ for $A$ and $z_b : \Omega \to \mathbb{C}$ for $b$. Assume that

$$\left\| \begin{bmatrix} A^* & b^* \end{bmatrix} \right\|_2 \geq \lambda.$$

Let $\tau_\lambda(\eta)$ be the $\lambda$-leverage function of $[A \ b]$. Let $\hat{\tau} : \Omega \to \mathbb{R}$ be a measurable function such that $\hat{\tau}(\eta) \geq \tau_\lambda(\eta)$ for all $\eta \in \Omega$, and assume that $s_{\hat{\tau}} = \int_\Omega \hat{\tau}(\eta)d\eta < \infty$. Also, denote $p_{\hat{\tau}}(\eta) = \hat{\tau}(\eta)/s_{\hat{\tau}}$.

Suppose we sample $\eta_1, \ldots, \eta_s$ using $p_{\hat{\tau}}$ and set $w_j = \sqrt{\frac{p(\eta_j)}{s_{\hat{\tau}}(\eta_j)}}$. Given $\epsilon \leq 1/2$ and $0 < \delta < 1$, if $s \geq \frac{8}{3} s_{\hat{\tau}}e^{-2 \ln(16s_\lambda)}$, then

$$(1 - \epsilon) \left( \|Ax - b\|_{L^2(\Omega, d\mu)}^2 + \lambda \|x\|_2^2 + \lambda \right) \leq \|A_{\eta_1}x - b_{\eta_1}\|_2^2 + \lambda \|x\|_2^2 + \lambda \leq (1 + \epsilon) \left( \|Ax - b\|_{L^2(\Omega, d\mu)}^2 + \lambda \|x\|_2^2 + \lambda \right)$$

holds with probability of at least $1 - \delta$.

Proof Sketch. The proof is very similar to the proof of [3] Lemma 8, so we give only a sketch of the proof. Denote

$$\hat{A} = \begin{bmatrix} A & b \\ \sqrt{\lambda} I_{n+1} \end{bmatrix}, \quad \hat{A}_\eta = \begin{bmatrix} A_\eta & b_\eta \\ \sqrt{\lambda} I_{n+1} \end{bmatrix}, \quad \hat{x} = \frac{1}{\sqrt{1 + \|x\|_2^2}} \begin{bmatrix} x \\ -1 \end{bmatrix}.$$

Then, the inequality (14) is equivalent to

$$(1 - \epsilon)\|\hat{A}\hat{x}\|_{L^2(\chi, d\mu)}^2 \leq \|\hat{A}_\eta\hat{x}\|_{L^2(\chi, d\mu)}^2 \leq (1 + \epsilon)\|\hat{A}\hat{x}\|_{L^2(\chi, d\mu)}^2$$

i.e.,

$$-\epsilon \hat{A}^* \hat{A} \leq \hat{A}_\eta \hat{\eta} \hat{A}_\eta - \hat{A}^* \hat{A} \leq \epsilon \hat{A}^* \hat{A}.$$

We write $\hat{A}^* \hat{A} = V^* \Sigma^2 V$. The claim is now equivalent to

$$-\epsilon I_d \leq \Sigma^{-1} V^* \hat{A}_\eta \hat{A}_\eta V \Sigma^{-1} - I_d \leq \epsilon I_d.$$

Notice that

$$A_\eta^* A_\eta = \sum_{j=1}^n w_j^2 z_A(\eta_j)z_A(\eta_j)^*, \quad b_\eta^* b_\eta = \sum_{j=1}^n w_j^2 z_b(\eta_j)z_b(\eta_j)^*. $$
It can be seen that \( \mathbf{z}(\eta) = \begin{bmatrix} \mathbf{z}_A(\eta) \\ \mathbf{z}_b(\eta) \end{bmatrix} \) is a coordinate representation for the quasimatrix part of \( \hat{\mathbf{A}} \). Let

\[
\mathbf{S}_j = \frac{p(\eta_j)}{p(\hat{\eta}_j)} \Sigma^{-1} \mathbf{V}^* \mathbf{z}(\eta_j) \mathbf{z}(\eta_j)^* \mathbf{V} \Sigma^{-1}.
\]

It is possible to show that \( \mathbb{E}[\mathbf{S}_j^2] \leq s_\tau \mathbb{E}[\mathbf{S}_j] \) and \( \mathbf{Tr}(\mathbb{E}[\mathbf{S}_j]) = s_\tau \cdot s_\lambda(\hat{\mathbf{K}}) \). The claim follows from [10] Corollary 7.3.3.

A similar result appears in [12] for truncated and conditioned least squares approximations of functions, however without any ridge term. The ridge leverage function can be viewed as a variant of the Christoffel function [11] in the context of function approximation using sampling. When using natural sampling, where individual coordinates are sampled using either rejection sampling or inversion transform sampling, the number of samples required for Eq. (14) to hold with high probability depends on the coherence quantity appears in [11] in the context of function approximation using sampling.

One natural strategy for selecting the \( \eta_1, \ldots, \eta_s \) is to sample them using the distribution \( \mu \). We call this strategy "natural sampling". Using Lemma 11 we can give a bound on the number of samples needed when sampling \( \eta_1, \ldots, \eta_s \) using this strategy and setting all the weights to \( 1/s \).

**Proposition 12.** Let \( \tau_\lambda(\eta) \) be the \( \lambda \)-leverage function of \( \begin{bmatrix} \mathbf{A} & \mathbf{b} \end{bmatrix} \). Suppose that \( M_\lambda = M_\lambda(\begin{bmatrix} \mathbf{A} & \mathbf{b} \end{bmatrix}) := \sup_{\eta \in \Omega} \tau_\lambda(\eta)/p(\eta) \) is finite. Suppose we sample \( \eta_1, \ldots, \eta_s \) using \( \mu \), and set \( w_j = 1/s \) for \( j = 1, \ldots, s \). If

\[
s \geq \frac{8}{3} M_\lambda \epsilon^{-2} \ln(16 s \lambda(\begin{bmatrix} \mathbf{A} & \mathbf{b} \end{bmatrix})/\delta)
\]

then Eq. (14) holds with probability of at least \( 1 - \delta \).

**Proof.** Let us define \( \hat{\tau}(\eta) = M_\lambda p(\eta) \). Notice that \( s_\tau = M_\lambda \) and that \( p_\lambda(\eta) = p(\eta) \). Thus, the conditions of Proposition 11 hold if we sample using \( p(\cdot) \) and set the weights to \( 1/s \), and the claim follows.

The quantity \( M_\lambda \) is a generalization of the concept of matrix coherence [5] to quasimatrices. A similar quantity appears in [11] in the context of function approximation using sampling. When using natural sampling, the number of samples required for Eq. (14) to hold with high probability depends on the coherence of the quasimatrix, which can be large. Sampling using the ridge leverage scores, often referred to as leverage score sampling, yields a better bound since \( s_\lambda(\begin{bmatrix} \mathbf{A} & \mathbf{b} \end{bmatrix}) \leq M_\lambda(\begin{bmatrix} \mathbf{A} & \mathbf{b} \end{bmatrix}) \).

Of course, it is not simple to sample using the ridge leverage function. Cohen and Migliorati suggested a method from leverage score sampling when \( \lambda = 0 \) [12]. Their method is based on sequential conditional sampling, where individual coordinates are sampled using either rejection sampling or inversion transform sampling. An alternative approach is to find some simple and easy way to sample upper bound on \( \tau_\lambda \). For this to be worthwhile, the bound has to be tighter than the bound \( \tau_\lambda(\eta) \leq M_\lambda p(\eta) \) used in Proposition 12.

This approach is used in [3, 4].

### 6.2 Quadrature Sampling

In this section, we discuss deterministic sampling using quadrature formulas. For simplicity, we assume that \( \Omega = [-1, 1] \) and that \( \mu \) is the Lebesgue measure on \([-1, 1]\). Accordingly, the sampling scheme is based on the Gauss-Legendre quadrature. Higher dimensional domains can be handled via tensoring the quadrature. We also assume that \( \lambda > 0 \). Let \( \mathbf{z}_A : \mathbb{R} \rightarrow \mathbb{C}^n \) be a coordinate representation of \( \mathbf{A} \). We can write

\[
\mathbf{A}^* \mathbf{A} = \int_{-1}^{1} \mathbf{z}_A(\eta) \mathbf{z}_A(\eta)^* d\eta.
\]

Furthermore, for every \( \mathbf{x} \in \mathbb{R}^n \)

\[
\|\mathbf{A} \mathbf{x}\|^2_{L_2([-1,1], d\mu)} = \int_{-1}^{1} \mathbf{x}^T \mathbf{z}_A(\eta) \mathbf{z}_A(\eta)^* d\eta = \int_{-1}^{1} |\mathbf{z}_A(\eta)^* \mathbf{x}|^2 d\eta.
\]

23
Let $z_b : \mathbb{R} \to \mathbb{C}$ be a coordinate representation of $b$. Then,

$$A^*b = \int_{-1}^{1} z_A(\eta)\overline{z_b(\eta)}d\eta, \quad \|b\|^2_{L_2([-1,1],d\mu)} = \int_{-1}^{1} |z_b(\eta)|^2 d\eta.$$ 

We conclude that the overdetermined SILR can be written as an integral form

$$\int_{-1}^{1} f_x(\eta)d\eta = \|Ax - b\|^2_{L_2([-1,1],d\mu)} + \lambda\|x\|^2_2$$

where

$$f_x(\eta) = |z_A(\eta)^* x - z_b(\eta)|^2 + \frac{\lambda}{2}\|x\|^2_2.$$ 

The underlying idea is to approximate the integral in Eq. (15) using the Gauss-Legendre quadrature. For a given $\epsilon \in (0,1)$, our algorithm sets the nodes $\eta_1, \ldots, \eta_s \in [-1,1]$ to be the Gauss-Legendre quadrature nodes, and sets the weights $w_1, \ldots, w_s > 0$ so that their square are the Gauss-Legendre quadrature weights. We set $s$ to be large enough so that

$$\left| \int_{-1}^{1} f_x(\eta)d\eta - \sum_{j=1}^{s} w_j^2 f_x(\eta_j) \right| \leq \epsilon.$$ 

Once $\eta_1, \ldots, \eta_s$ and the weights $w_1, \ldots, w_s$ are computed, we can define $A_\eta$ and $b_\eta$ as before. We have

$$\sum_{j=1}^{s} w_j^2 f_x(\eta_j) = \|A_\eta x - b_\eta\|^2_2 + \lambda\|x\|^2_2$$

so if Eq. (16) holds then Eq. (13) holds (with $\mathcal{H} = L_2([-1,1],d\mu)$), and we can apply Proposition 8.

To determine how many quadrature nodes $s$ are needed so that Eq. (16) holds, we can apply the following theorem, which is a modified version of [40, Theorem 11] for the function $g_x(\eta) := f_x(\eta)/(\int_{-1}^{1} f_x(\eta)d\eta + \lambda)$. Since the proof is a simple modification of the proof [40, Theorem 11], we omit it.

**Theorem 13.** Let $E$ be the (Bernstein) ellipse in the complex plane with foci $\pm 1$ that passes through $i$, and let $p = 1 + \sqrt{2}$. Assume that both real and imaginary parts of $z_A(\cdot), i = 1, \ldots, n$ and $z_b(\cdot)$ are analytic on $\mathbb{R}$, and denote their analytic continuations by $\tilde{z}_A(\cdot)$ and $\tilde{z}_b(\cdot)$ correspondingly. Denote

$$M_A := \sup_{\eta \in E} \|	ilde{z}_A(\eta)\|_\infty, \quad M_b := \sup_{\eta \in E} \|	ilde{z}_b(\eta)\|_\infty.$$ 

Then, given a small $\epsilon$, for

$$s \geq \frac{\ln \left(8(\lambda^{-1}(nM_A^2 + M_b^2) + 1)\right) - \ln \epsilon - \ln \sqrt{2}}{2\ln(1 + \sqrt{2})} + 1$$

we have

$$\left| \int_{-1}^{1} g_x(\eta)d\eta - \sum_{j=1}^{s} w_j g_x(\eta_j) \right| \leq \epsilon$$

where $\eta_1, \ldots, \eta_s$ are chosen to be the Gauss-Legendre quadrature nodes, and $w_1^2, \ldots, w_s^2$ are the Gauss-Legendre quadrature weights.
Remark 14. For $\eta \in E$, we denote $c_\times = \|A\mathbf{x} - \mathbf{b}\|^2_{L_2([-1,1], d\mu)} + \lambda \|\mathbf{x}\|^2_2$ and bound $g_\times(\eta)$ as follows

$$g_\times(\eta) = \frac{1}{c_\times} \left( |z_A(\eta) \mathbf{x} - z_b(\eta)|^2 + \frac{\lambda}{2} \|\mathbf{x}\|^2_2 \right)$$

$$= \frac{1}{c_\times} \left( |[z_A(\eta) \mathbf{x} - z_b(\eta)|^2 + \frac{\lambda}{2} \|\mathbf{x}\|^2_2 \right)$$

$$= \frac{1}{c_\times} \left( |[z_A(\eta) \mathbf{x} - z_b(\eta)|^2 + \frac{\lambda}{2} \|\mathbf{x}\|^2_2 \right)$$

$$\leq \frac{1}{c_\times} \left( |[z_A(\eta) \mathbf{x} - z_b(\eta)|^2 + \frac{\lambda}{2} \|\mathbf{x}\|^2_2 \right)$$

$$= \mathbf{K}^{-1} \left[ \frac{z_A(\eta) \mathbf{x} - z_b(\eta)|^2 + \frac{\lambda}{2} \|\mathbf{x}\|^2_2 \right]$$

$$\leq \lambda^{-1} (\|z_A(\eta)\|^2 + |z_b(\eta)|^2) + \frac{1}{2}$$

where $\mathbf{K} = \begin{bmatrix} A^* A & A^* \mathbf{b} \\ \mathbf{b}^* A & \mathbf{b}^* \mathbf{b} \end{bmatrix} + \lambda \mathbf{I}_{n+1}$ and in the first inequality we use the Cauchy-Schwarz inequality. Theorem 13 yields

$$\frac{\int_{-1}^{1} f_\times(\eta) d\eta - \sum_{j=1}^s w_j^2 f_\times(\eta_j)}{\int_{-1}^{1} f_\times(\eta) d\eta + \lambda} = \frac{\int_{-1}^{1} g_\times(\eta) d\eta - \sum_{j=1}^s w_j^2 g_\times(\eta_j)}{\int_{-1}^{1} g_\times(\eta) d\eta + \lambda} \leq \epsilon.$$  

We can generalize the above theorem, which is specific for $\Omega = [-1,1]$, to complex sets and/or high dimensional sets with a variety of probability measures on them, as done in [40].

6.3 Numerical Example

We illustrate both sampling approaches, randomized and quadrature, on a small numerical example. Consider trying to approximate on $[-1,1]$ the Runge function using polynomial of degree 39. We use the Chebyshev basis, i.e.

$$A = \begin{bmatrix} T_0 & T_1 & \ldots & T_{39} \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 1 + 25x^2 \end{bmatrix}$$

with $\lambda = 10^{-4}$.

The leftmost graph in Figure 3 shows the ridge leverage density of $[A \ b]$, and compares it to the uniform density. We also plot the density of the limiting distribution of Legendre nodes. We see very close alignment between the ridge leverage score density and the density of the Legendre nodes. We note that in this case $s_\lambda = 39.99$. In contrast $M_\times = 798.28$, and thus we will need about 95% less samples when using leverage score sampling compared to natural sampling. However, even for $s_\lambda = 0.01$, the number of samples required for randomized sampling is huge. In contrast, for $\epsilon = 0.01$ only $s = 73$ features are required using quadrature features. Nevertheless, in the experiments we use $s = 100$ for both randomized and quadrature sampling.

The middle and rightmost graph in Figure 3 shows the function approximation (on the left), and the error in approximating the function (on the right). We use both natural sampling and leverage score sampling, where we used inverse transform sampling for leverage score sampling. With $s = 100$, using quadrature sampling and leverage score sampling we get small errors: the maximum absolute error is $4.48 \times 10^{-4}$ for quadrature sampling, and $9.82 \times 10^{-4}$ for leverage score sampling. Natural sampling has large error near the boundary of $[-1,1]$ (as expected), and the maximum absolute error is 0.0581.
Figure 3: Numerical illustration: approximating the Runge function using various sampling methods.

7 Conclusions and Future Work

In this paper, we gave an algebraic framework for working with quasimatrices and explored the use of this framework to solve semi-infinite linear regression problems, i.e. regression problems where the system’s matrix has an infinite amount of rows or columns. We discussed various applications, such as function approximation and supervised learning (using kernel ridge regression). We offered several classes of algorithms for solving SILR problems: direct methods, iterative methods (generalizing known iterative methods such as LSMR as an example of a Krylov subspace method and SVRG as an example of a stochastic optimization method). Finally, motivated by recent research on randomized numerical linear algebra methods for solving finite linear least squares problems, we explored the use of sampling techniques to approximate the solution of a SILR, where sampling can be either randomized or deterministic. Possible future directions are to further leverage advanced randomized linear algebra methods, such as sketching, whereas the main challenge is in how to generate a random quasimatrix from the correct distribution. Another interesting idea is to generalize the Batson-Spielman-Srivastava (BSS) process for iteratively building a spectral approximation of a matrix using columns samples [6] to quasimatrices.

Acknowledgements

This research was supported by BSF grant 2017698.

References

[1] Haim Avron, Kenneth L Clarkson, and David P Woodruff. Faster kernel ridge regression using sketching and preconditioning. SIAM Journal on Matrix Analysis and Applications, 38(4):1116–1138, 2017.

[2] Haim Avron, Kenneth L. Clarkson, and David P. Woodruff. Sharper Bounds for Regularized Data Fitting. In Klaus Jansen, José D. P. Rolim, David Williamson, and Santosh S. Vempala, editors, Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques (APPROX/RANDOM 2017), volume 81 of Leibniz International Proceedings in Informatics (LIPIcs), pages 27:1–27:22, Dagstuhl, Germany, 2017. Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik.

[3] Haim Avron, Michael Kapralov, Cameron Musco, Christopher Musco, Ameya Velingker, and Amir Zandieh. Random Fourier features for kernel ridge regression: Approximation bounds and statistical guarantees. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 253–262. JMLR. org, 2017.

[4] Haim Avron, Michael Kapralov, Cameron Musco, Christopher Musco, Ameya Velingker, and Amir Zandieh. A universal sampling method for reconstructing signals with simple Fourier transforms. In
Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing, pages 1051–1063, 2019.

[5] Haim Avron, Petar Maymounkov, and Sivan Toledo. Blendenipik: Supercharging LAPACK’s least-squares solver. *SIAM Journal on Scientific Computing*, 32(3):1217–1236, 2010.

[6] Joshua Batson, Daniel A. Spielman, and Nikhil Srivastava. Twice-Ramanujan sparsifiers. *SIAM Review*, 56(2):315–334, 2014.

[7] Zachary Battles. *Numerical linear algebra for continuous functions*. PhD thesis, University of Oxford, 2005.

[8] Zachary Battles and Lloyd N Trefethen. An extension of matlab to continuous functions and operators. *SIAM Journal on Scientific Computing*, 25(5):1743–1770, 2004.

[9] Peter Borwein and Tamás Erdélyi. *Polynomials and polynomial inequalities*, volume 161. Springer Science & Business Media, 2012.

[10] Kenneth L. Clarkson, Petros Drineas, Malik Magdon-Ismail, Michael W. Mahoney, Xiangrui Meng, and David P. Woodruff. The fast Cauchy transform and faster robust linear regression. *SIAM Journal on Computing*, 45(3):763–810, 2016.

[11] Albert Cohen, Mark A Davenport, and Dany Leviatan. On the stability and accuracy of least squares approximations. *Foundations of computational mathematics*, 13(5):819–834, 2013.

[12] Albert Cohen and Giovanni Migliorati. Optimal weighted least-squares methods. *The SMAI journal of computational mathematics*, 3:181–203, 2017.

[13] Michael B Cohen, Cameron Musco, and Christopher Musco. Input sparsity time low-rank approximation via ridge leverage score sampling. In *Proceedings of the Twenty-Eighth Annual ACM-SIAM Symposium on Discrete Algorithms*, pages 1758–1777. SIAM, 2017.

[14] Felipe Cucker and Steve Smale. On the mathematical foundations of learning. *Bulletin of the American Mathematical Society*, 39:1–49, 2002.

[15] Carl de Boor. An alternative approach to (the teaching of) rank, basis, and dimension. *Linear Algebra and its Applications*, 146:221–229, 1991.

[16] Petros Drineas, Michael W. Mahoney, S. Muthukrishnan, and Tamás Sarlós. Faster least squares approximation. *Numerische Mathematik*, 117(2):219–249, Feb 2011.

[17] Ahmed El Alaoui and Michael W Mahoney. Fast randomized kernel methods with statistical guarantees. *stat*, 1050:2, 2014.

[18] David Chin-Lung Fong and Michael Saunders. LSMR: An iterative algorithm for sparse least-squares problems. *SIAM Journal on Scientific Computing*, 33(5):2950–2971, 2011.

[19] Marc Auréle Gilles and Alex Townsend. Continuous analogues of Krylov subspace methods for differential operators. *SIAM Journal on Numerical Analysis*, 57(2):899–924, 2019.

[20] Gene Golub and William Kahan. Calculating the singular values and pseudo-inverse of a matrix. *Journal of the Society for Industrial and Applied Mathematics, Series B: Numerical Analysis*, 2(2):205–224, 1965.

[21] Alon Gonen, Francesco Orabona, and Shai Shalev-Shwartz. Solving ridge regression using sketched preconditioned SVRG. In Maria Florina Balcan and Kilian Q. Weinberger, editors, *Proceedings of The 33rd International Conference on Machine Learning*, volume 48 of *Proceedings of Machine Learning Research*, pages 1397–1405, New York, New York, USA, 20–22 Jun 2016. PMLR.
[22] Behnam Hashemi and Yuji Nakatsukasa. On the spectral problem for trivariate functions. *BIT Numerical Mathematics*, 58(4):981–1008, 2018.

[23] Rie Johnson and Tong Zhang. Accelerating stochastic gradient descent using predictive variance reduction. In *Advances in Neural Information Processing Systems*, pages 315–323, 2013.

[24] Nidal Kamel, Ibrahim Kajo, and Yassine Ruichek. On visual periodicity estimation using singular value decomposition. *Journal of Mathematical Imaging and Vision*, 61(8):1135–1153, 2019.

[25] Kirthevasan Kandasamy, Maruan Al-Shedivat, and Eric P Xing. Learning HMMs with nonparametric emissions via spectral decompositions of continuous matrices. In D. Lee, M. Sugiyama, U. Luxburg, I. Guyon, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 29. Curran Associates, Inc., 2016.

[26] Yuji Koyano, Kohei Yatabe, and Yasuhiro Oikawa. Infinite-dimensional SVD for analyzing microphone array. In *2017 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 176–180. IEEE, 2017.

[27] Yin Tat Lee and A. Sidford. Efficient accelerated coordinate descent methods and faster algorithms for solving linear systems. In *2013 IEEE 54th Annual Symposium on Foundations of Computer Science (FOCS)*, pages 147–156, Los Alamitos, CA, USA, oct 2013. IEEE Computer Society.

[28] Xiangrui Meng, Michael A. Saunders, and Michael W. Mahoney. LSRN: A parallel iterative solver for strongly over- or underdetermined systems. *SIAM Journal on Scientific Computing*, 36(2):C95–C118, 2014.

[29] Yurii Nesterov. *Introductory lectures on convex optimization: A basic course*, volume 87. Springer Science & Business Media, 2003.

[30] Paul Nevai. Géza Freud, orthogonal polynomials and Christoffel functions. A case study. *Journal of Approximation Theory*, 48(1):3–167, 1986.

[31] Sheehan Olver. Preconditioned GMRES for oscillatory integrals. 2008.

[32] Sheehan Olver. GMRES for the differentiation operator. *SIAM Journal on Numerical Analysis*, 47(5):3359–3373, 2009.

[33] Sheehan Olver. Shifted GMRES for oscillatory integrals. *Numerische Mathematik*, 114(4):607–628, 2010.

[34] Christopher C Paige and Michael A Saunders. LSQR: An algorithm for sparse linear equations and sparse least squares. *ACM Transactions on Mathematical Software (TOMS)*, 8(1):43–71, 1982.

[35] Edouard Pauwels, Francis Bach, and Jean-Philippe Vert. Relating leverage scores and density using regularized Christoffel functions. In *NIPS2018*, 2018.

[36] Mert Pilanci and Martin J. Wainwright. Iterative Hessian sketch: Fast and accurate solution approximation for constrained least-squares. *J. Mach. Learn. Res.*, 17(1):1842–1879, January 2016.

[37] Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In *Advances in neural information processing systems*, pages 1177–1184, 2008.

[38] Vladimir Rokhlin and Mark Tygert. A fast randomized algorithm for overdetermined linear least-squares regression. *Proceedings of the National Academy of Sciences*, 105(36):13212–13217, 2008.

[39] Bernhard Schölkopf, Ralf Herbrich, and Alex J. Smola. *A Generalized Representer Theorem*, pages 416–426. Springer Berlin Heidelberg, Berlin, Heidelberg, 2001.
The usual SVRG algorithm \cite{SVRG} is defined for objective functions that have finite sum structure, i.e.
\[ f(x) = \frac{1}{n} \sum_{i=1}^{n} f_i(x). \] (17)

Here we propose a variant of the algorithm designed for objective functions that can be written as an integral. Let \( \mu \) be some probability measure on a measurable index set, \( \Omega \). Our variant of SVRG is designed for functions that can be written as
\[ f(x) = \int_{\Omega} f_\eta(x) d\mu(\eta) \] (18)
where the integral should be interpreted as a Lebesgue integral. Notice that Eq. (17) is a special case of Eq. (18): \( \Omega = \{1, \ldots, n\} \) and \( \mu(A) = \frac{|A|}{n} \). The proposed algorithm is summarized in Algorithm 3.

Algorithm 3 SVRG for integrable objective functions.

1: Inputs: initial \( x_0 \), learning rate \( \alpha \), frequency \( m \)
2: Iterate: for \( s = 1, 2, \ldots \)
3: \hspace{1cm} \tilde{x} = x_{s-1}
4: \hspace{1cm} \tilde{\mu} = \nabla \int_{\Omega} f_\eta(\tilde{x}) d\mu(\eta) = \nabla f(\tilde{x})
5: \hspace{1cm} x_0 = \tilde{x}
6: Iterate: for \( k = 1, 2, \ldots, m \)
7: \hspace{1cm} \text{sample } \eta_k \text{ according to the probability of } \eta \text{ and update}
8: \hspace{1cm} x_k = x_{k-1} - \alpha (\nabla f_{\eta_k}(x_{k-1}) - \nabla f_{\eta_k}(\tilde{x}) + \tilde{\mu})
9: end
10: option I: set \( \bar{x}_s = x_m \)
11: option II: set \( \bar{x}_s = \frac{1}{m} \sum_{k=1}^{m} x_k \)
12: end

A Stochastic Variance Reduced Gradient with Integrable Sums
As in common convex optimization, certain assumptions must be made in order for the algorithm to converge. We prove that Algorithm 3 converges and analyze the convergence rate, when the following assumptions hold. We start with assumptions that are analogous to the assumptions in finite sum SVRG, which we already mentioned in Section 5.2.

**Assumption 15.** For all \( \eta \in \Omega \), \( \nabla f_\eta(x) \) is Lipschitz continuous, i.e., there exists \( L_\eta > 0 \) such that for all \( x, y \in \mathbb{R}^n \)
\[
\| \nabla f_\eta(x) - \nabla f_\eta(y) \| \leq L_\eta \| x - y \|.
\]

**Assumption 16.** Suppose that \( f(x) \) is strongly convex, i.e., there exist \( \gamma > 0 \) such that for all \( x, y \in \mathbb{R}^n \)
\[
f(x) - f(y) \geq \frac{\gamma}{2} \| x - y \|^2 + \nabla f(y)^T (x - y).
\]

Next, we list assumptions that trivially hold for the finite case but are required for the continuous case.

**Assumption 17.** The equality \( \nabla f(x) = \int_\Omega \nabla f_\eta(x) d\mu(\eta) \) hold.

Suppose \( \Omega = \mathbb{R}^d \) and \( f_\eta(x), \nabla f_\eta(x) \in L_1(\Omega) \) with respect to \( \eta \). Then, Assumption 17 holds from Leibniz integral rule.

**Assumption 18.** \( L_{\sup} := \sup_{\eta \in \Omega} L_\eta < \infty \).

Assumptions 17 and 18 imply that \( \nabla f(x) \) is Lipschitz continuous with Lipschitz constant \( L \leq L_{\sup} \). Note that for the finite sum case, Assumptions 17 and 18 hold trivially, but this is no longer the case in the integrable case.

**Corollary 19.** If Assumptions 17, 18 hold, then we can make Assumptions 15, 16 hold for the continuous case.

We now analyze Algorithm 17. The analysis follows the analysis in [23, 48] quite closely, making adjustments where necessary for integrals instead of sums, and using the additional assumptions when needed.

**Lemma 20.** Suppose Assumptions 15, 17, 18 hold. Let \( x^* = \arg \min_x f(x) \) and \( L_{\sup} = \sup_{\eta \in \Omega} L_\eta \). Then
\[
\int_\Omega \| \nabla f_\eta(x) - \nabla f_\eta(x^*) \|_2^2 d\mu(\eta) \leq 2 L_{\sup} (f(x) - f(x^*))
\]

**Proof.** Given any \( \eta \in \Omega \), let
\[
g_\eta(x) = f_\eta(x) - f_\eta(x^*) - \nabla f_\eta(x^*)^T(x - x^*)
\]

It can be seen that \( \nabla g_\eta(x^*) = 0 \), and hence \( x^* = \arg \min_x g_\eta(x) \). Moreover, from Assumption 15, \( \nabla g_\eta(x) = \nabla f_\eta(x) - \nabla f_\eta(x^*) \) is Lipschitz continuous with constant \( L_\eta \). This yields
\[
g_\eta(x) - g_\eta(y) \leq \frac{L_\eta}{2} \| x - y \|^2 + \nabla g_\eta(y)^T (x - y)
\]

for any \( x, y \in \mathbb{R}^n \) (see [29, Lemma 1.2.3]). Replacing \( x \) with \( x - \frac{1}{L_\eta} \nabla g_\eta(x) \) and \( y \) with \( x \), gives
\[
g_\eta \left( x - \frac{1}{L_\eta} \nabla g_\eta(x) \right) \leq g_\eta(x) - \frac{1}{2 L_\eta} \| \nabla g_\eta(x) \|^2.
\]

Since \( \min_x g_\eta(x) = g_\eta(x^*) = 0 \), we have \( 0 \leq g_\eta(x - \nabla g_\eta(x)/L_\eta) \), which implies
\[
\frac{1}{2 L_\eta} \| \nabla g_\eta(x) \|^2 \leq g_\eta(x).
\]
Substituting the definition of $g$ gives
\[ \|\nabla f_\eta(x) - \nabla f_\eta(x^*)\|^2 \leq 2L_\eta \left( f_\eta(x) - f_\eta(x^*) - \nabla f_\eta(x^*)^T (x - x^*) \right). \]

Now, by taking an integral over $\Omega$, we have
\[ \int_\Omega \|\nabla f_\eta(x) - \nabla f_\eta(x^*)\|^2 d\mu(\eta) \leq 2L_{\sup} \int_\Omega f_\eta(x) - f_\eta(x^*) - \nabla f_\eta(x^*)^T (x - x^*) d\mu(\eta) \]
\[ = 2L_{\sup} \left( f(x) - f(x^*) - \nabla f(x^*)^T (x - x^*) \right) = 2L_{\sup} (f(x) - f(x^*)) \]
where in the first inequality we use Assumption [18] in the second equality we use Assumption [17] and the last equality is due to the fact that $\nabla f(x^*) = 0$.

Corollary 21. Denote $v_k = \nabla f_{\eta_k}(x_{k-1}) - \nabla f_{\eta_k}(\bar{x}) + \hat{\mu}$. Then, conditioned on $x_{k-1}$ we have
\[ \mathbb{E}\|v_k\|^2 \leq 4L_{\sup} (f(x_{k-1}) - 2f(x^*) + f(\bar{x})). \]

Proof. Conditioned on $x_{k-1}$, taking expectation with respect to $\eta_k$ gives $\mathbb{E}[\nabla f_{\eta_k}(x_{k-1})] = \nabla f(x_{k-1})$. Similarly, $\mathbb{E}[\nabla f_{\eta_k}(\bar{x})] = \nabla f(\bar{x})$. Therefore
\[ \mathbb{E}\|v_k\|^2 = \mathbb{E}\left[ \nabla f_{\eta_k}(x_{k-1}) - \nabla f_{\eta_k}(\bar{x}) + \hat{\mu} + \nabla f_{\eta_k}(x^*) - \nabla f_{\eta_k}(x^*) \right]^2 \]
\[ \leq 2\mathbb{E}\|\nabla f_{\eta_k}(x_{k-1}) - \nabla f_{\eta_k}(x^*)\|^2 + 2\mathbb{E}\|\nabla f_{\eta_k}(x^*) - \nabla f_{\eta_k}(\bar{x}) + \hat{\mu}\|^2 \]
\[ = 2\mathbb{E}\|\nabla f_{\eta_k}(x_{k-1}) - \nabla f_{\eta_k}(x^*)\|^2 + 2\mathbb{E}\|\nabla f_{\eta_k}(\bar{x}) - \nabla f_{\eta_k}(x^*) - \mathbb{E}[\nabla f_{\eta_k}(\bar{x}) - \nabla f_{\eta_k}(x^*)]\|^2 \]
\[ \leq 2\mathbb{E}\|\nabla f_{\eta_k}(x_{k-1}) - \nabla f_{\eta_k}(x^*)\|^2 + 2\mathbb{E}\|\nabla f_{\eta_k}(\bar{x}) - \nabla f_{\eta_k}(x^*)\|^2 \]
\[ \leq 4L_{\sup} (f(x_{k-1}) - 2f(x^*) + f(\bar{x})) \]
where in the first inequality we use $\|a + b\|^2 \leq 2(\|a\|^2 + \|b\|^2)$. The second equality uses $\mathbb{E}[\nabla f_{\eta_k}(\bar{x})] = \hat{\mu}$, $\mathbb{E}[\nabla f_{\eta_k}(x^*)] = \nabla f(x^*) = 0$. The second inequality uses the fact that for any $\xi \in \mathbb{R}^d$: $\mathbb{E}\|\xi - \mathbb{E}\xi\|^2 = \mathbb{E}\|\xi\|^2 - \mathbb{E}\|\xi\|^2 \leq \mathbb{E}\|\xi\|^2$. In the last inequality we use Lemma [20].

Now we can proceed to prove the main theorem.

Theorem 22. Suppose Assumptions [16, 17, 18] hold, and let $x^* = \arg\min_x f(x)$ and $L_{\sup} = \sup_{\eta \in \Omega} L_\eta$. In addition, assume that there exists $0 < \alpha < \frac{1}{2L_{\sup}}$ a sufficiently large $m$ such that
\[ \rho = \frac{1}{\gamma\alpha(1 - 2L_{\sup}\alpha)m} + \frac{2L_{\sup}\alpha}{(1 - 2L_{\sup}\alpha)} < 1. \]
Then SVRG (Algorithm [3]) with option II has geometric convergence in expectation:
\[ \mathbb{E}[f(\bar{x}_s)] - f(x^*) \leq \rho^s (f(\bar{x}_0) - f(x^*)). \]

Proof. From Assumption [16] and using Eq. (20) we have
\[ f(x^*) - f(x_{k-1}) \geq -\nabla f(x_{k-1})^T (x_{k-1} - x^*) \]
\[ f(x_k) - f(x_{k-1}) \geq -\alpha \mathbb{E}[v_k]^T v_k. \]
Dividing both sides of the above inequality by 

\[-\nabla f(x_{k-1})^T (x_{k-1} - x^*) \leq f(x^*) - f(x_k) - \alpha E[\nu_k]^T v_k.\]

(22)

Thus, we have

\[
E\|x_k - x^*\|^2 = E\|x_{k-1} - \alpha v_k - x^*\|^2 = \|x_{k-1} - x^*\|^2 - 2\alpha \nabla f(x_{k-1})^T (x_{k-1} - x^*) + \alpha^2 E\|v_k\|^2 \\
\leq \|x_{k-1} - x^*\|^2 - 2\alpha (f(x_k) - f(x^*)) - 2\alpha^2 E\|v_k\|^2 \\
+ 4L_{sup} \alpha^2 (f(x_{k-1}) - 2f(x^*) + f(\hat{x}))
\]

where the equality uses Eq. (20) and the inequality uses Eq. (22) and Corollary 21.

Now, consider a fixed stage $s$, such that $x_0 = \hat{x} = \bar{x}_{s-1}$ and $\bar{x}_s = \frac{1}{m} \sum_{k=1}^m x_k$. By summing the previous inequality over $k = 1, \ldots, m$ and taking expectation with respect to the history of the random variables $\eta_1, \ldots, \eta_m$, we obtain

\[
E\|x_m - x^*\|^2 \leq \|x_0 - x^*\|^2 - 2\alpha \sum_{k=1}^m (E[f(x_k)] - f(x^*)) - 2\alpha^2 \sum_{k=1}^m E[\|v_k\|^2] \\
+ 4L_{sup} \alpha^2 \sum_{k=1}^m (E[f(x_{k-1})] - f(x^*)) + 4L_{sup} \alpha^2 m (f(\hat{x}) - f(x^*)) \\
\leq \|\bar{x} - x^*\|^2 - 2\alpha \sum_{k=1}^m (E[f(x_k)] - f(x^*)) - 2\alpha^2 \sum_{k=1}^m E[\|v_k\|^2] \\
+ 4L_{sup} \alpha^2 \sum_{k=1}^m (E[f(x_k)] - f(x^*)) + 4L_{sup} \alpha^2 \sum_{k=1}^m E[\|v_k\|^2] + 4L_{sup} \alpha^2 m (f(\hat{x}) - f(x^*)) \\
\leq \|\bar{x} - x^*\|^2 - 2\alpha (1 - 2L_{sup} \alpha) \sum_{k=1}^m (E[f(x_k)] - f(x^*)) + 4L_{sup} \alpha^2 m (f(\hat{x}) - f(x^*)) \\
\leq \left(\frac{2}{\gamma} + 4L_{sup} \alpha^2 m\right) (f(\bar{x}_{s-1}) - f(x^*)) - 2\alpha (1 - 2L_{sup} \alpha) \sum_{k=1}^m (E[f(x_k)] - f(x^*)).
\]

The second inequality is due to the strong convexity in Eq. (21), and the third inequality uses the assumption $2L_{sup} \alpha < 1$ such that $(4L_{sup} \alpha^3 - 2\alpha^2) \|v_k\|^2 \leq 0$. The last inequality uses Assumption 16, with $x$ replaced by $\hat{x}$ and $y$ replaced by $x^*$. In addition, $f(\bar{x}_s) \leq \frac{1}{m} \sum_{k=1}^m f(x_k)$ due to the convexity of $f$. Therefore, we obtain

\[
2\alpha (1 - 2L_{sup} \alpha) m (E[f(\bar{x}_s)] - f(x^*)) \leq \left(\frac{2}{\gamma} + 4L_{sup} \alpha^2 m\right) (f(\bar{x}_{s-1}) - f(x^*)).
\]

Dividing both sides of the above inequality by $2\alpha (1 - 2L_{sup} \alpha) m$ gives

\[
E[f(\bar{x}_s)] - f(x^*) \leq \rho^s (f(\bar{x}_0) - f(x^*)).
\]