FAR-FIELD COMPRESSION FOR FAST KERNEL SUMMATION METHODS IN HIGH DIMENSIONS
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Abstract. We consider fast kernel summations in high dimensions: given a large set of points in \(d\) dimensions \((d \gg 3)\) and a pair-potential function (the kernel function), we compute a weighted sum of all pairwise kernel interactions for each point in the set. Direct summation is equivalent to a (dense) matrix-vector multiplication and scales quadratically with the number of points. Fast kernel summation algorithms reduce this cost to log-linear or linear complexity.

Treecodes and Fast Multipole Methods (FMMs) deliver tremendous speedups by constructing approximate representations of interactions of points that are far from each other. In algebraic terms, these representations correspond to low-rank approximations of blocks of the overall interaction matrix. Existing approaches require an excessive number of kernel evaluations with increasing \(d\) and number of points in the dataset.

To address this issue, we use a randomized algebraic approach in which we first sample the rows of a block and then construct its approximate, low-rank interpolative decomposition. We examine the feasibility of this approach theoretically and experimentally. We provide a new theoretical result showing a tighter bound on the reconstruction error from uniformly sampling rows than the existing state-of-the-art. We demonstrate that our sampling approach is competitive with existing (but prohibitively expensive) methods from the literature. We also construct kernel matrices for the Laplacian, Gaussian, and polynomial kernels – all commonly used in physics and data analysis. We explore the numerical properties of blocks of these matrices, and show that they are amenable to our approach. Depending on the data set, our randomized algorithm can successfully compute low rank approximations in high dimensions. We report results for data sets from four dimensions up to 1000 dimensions.

Key words. kernel independent fast multipole methods, fast summation, randomized matrix approximation, interpolative decomposition, matrix sampling

1. Introduction. Given \(n\) source points \(x_j\) with densities \(q_j\), \(m\) target points \(y_i\), and a kernel function \(K\), we seek to evaluate the kernel sum

\[
 u_i = \sum_{j=1}^{n} K(y_i, x_j)q_j = \sum_{j=1}^{n} K_{ij}q_j
\]

for each target \(y_i\), with \(K_{ij} = K(y_i, x_j)\). Computing \(u \in \mathbb{R}^m\) is equivalent to a matrix-vector multiplication, \(u = Kq\), \(K \in \mathbb{R}^{m \times n}\), and it requires \(O(nm)\) work. It is prohibitively expensive for large \(m\) and \(n\). Fast kernel summation algorithms (also known as generalized N-body problems) aim to provide an approximate solution with guaranteed error in \(O(n + m)\) time. They do so by identifying and approximating blocks of \(K\) that have low-rank structure.

Fast kernel summations are a fundamental operation in computational physics. They are related to the solution of partial differential equations in which \(K\) is the corresponding Green’s function. Examples include the 3D Laplace potential (reciprocal distance kernel) and the heat potential (Gaussian kernel).

Kernel summations are also fundamental to non-parametric statistics and machine learning tasks such as density estimation, regression, and classification. Linear inference methods such as support vector machines [65] and dimension reduction methods such as principal components analysis [58] can be efficiently generalized to non-linear methods by replacing inner products with kernel evaluations [8]. Problems in statistics and machine learning are often characterized by very high-dimensional inputs.

Existing fast algorithms for the kernel summation problem hinge on the construction of efficient approximations of interactions\(^1\) between groups of sources and targets when these groups are far apart or

\(^1\)We use the term interaction between two points to refer to the value of the kernel \(K\).
well separated (see section 2). In physics/PDE community they are known as far-field approximations. From a linear algebraic point of view they correspond to low-rank decompositions of blocks of the matrix $K$. These approximations can be roughly grouped in three categories: analytic, semi-analytic, and algebraic.

In analytic methods, Taylor or kernel-dependent special function expansions are used to approximate the far-field. The classical Fast Multipole Method (FMM) \cite{38} is one of these. Semi-analytic methods rely only on kernel evaluations, but the low-rank constructions do use the analytical properties of the underlying kernels. For example, the kernel-independent fast multipole method \cite{74} requires that the underlying kernel is the Green’s function of a PDE. Finally, algebraic methods (e.g. \cite{55}) also only require kernel evaluations, but the only necessary condition is the existence a low-rank block structure for $K$.

In high dimensions, most existing methods fail. There are two main reasons for the lack of scalability of analytic and semi-analytic methods. The first reason is that all existing schemes require too many terms for the kernel approximation. Analytic and semi-analytic schemes can deliver approximations to arbitrary accuracy (in practice all the way to machine precision) in $O(n + m)$ time, but the constant can be very large. For $p$ terms in the series expansion, they require $p = c^d$ or $p = c^{d-1}$ terms to deliver error that decays exponentially in $c > 1$. Variants that can scale reasonably well beyond three dimensions scale as $p = d^c$ and deliver error that decays algebraically in $c$. For sufficiently large $d$ and $c > 1$, either of these methods become too expensive \cite{40}.

The second reason for lack of scalability of existing schemes is that they do not take advantage of any lower-dimensional structures that may be present in the data. For example, the data may be embedded in a low-dimensional manifold. This is mostly relevant in data analysis applications in which often the important dimension is not the ambient one but instead an intrinsic dimension that depends on the distribution of the source and target points.

A promising direction for scalable methods in high dimensions is to use algebraic approximations \cite{55}. These approximations are based on the observation that (1.1) is a matrix-vector multiplication and certain blocks of the matrix have low-rank structure. Algebraic methods are useful only if the approximation can be computed efficiently. Efficient methods for low dimensions do exist, but in high-dimensions they fail because the number of kernel evaluations required exceeds the cost of the direct summation.

Beyond scalability requirements, let us also mention the need to support several different kernels in a block-box fashion. Analytic or semi-analytic methods depend significantly on the type or class of kernel. Although there has been extensive work on these methods for classical kernels like the Gaussian, new kernel functions have been developed for a wide variety of data types, such as graphs \cite{48} and strings \cite{52}. Also, adaptive density estimation methods use kernels with variable bandwidth \cite{63}. This observation further motivates the use of entirely algebraic acceleration techniques for (1.1).

1.1. Contributions. In this paper, we make precise the ideas discussed above. First, we explore the low-rank structure of the far-field of several widely-used kernels in high-dimensions, and then we propose a new scheme that uses randomized sampling to construct interpolative decompositions \cite{56} of the far-field. Our goal is to design far-field approximations that do not scale exponentially with the ambient dimension of the input, do not require analytic information about the kernel function, and require a number of kernel evaluations that is smaller than the cost of the direct summation (in the case that the kernel is compressible).

In particular, our contributions are the following

- We examine the approximability of the far-field for Gaussian, Laplacian, and polynomial kernels in high dimensions. In particular we look at the structure of blocks of the matrix $K$
obtained from these kernels. For the Gaussian, we carefully study the effects of dimensionality and bandwidth.

- We propose a new sampling scheme, summarized in Figure 2.3, which can combined with the interpolative decomposition scheme [55] to construct approximations of the far field. The sampling scheme requires nearest neighbor information.

- We provide empirical results that show the effectiveness of our method for compressing general kernels for higher-dimensional data without prior knowledge of the structure of the kernel or any low-dimensional structures in the data. We show results for data sets with high ambient but low intrinsic dimension. Also, we explore kernel matrices for several data sets from the UCI ML repository [5].

- We show a new theoretical analysis of the reconstruction error of sampling columns of a matrix uniformly at random. We show a factor of $\sqrt{m/s}$ improvement over the existing best result [35] for $m$ columns and $s$ samples.

- We explore the use of heuristic approximations to theoretically optimal but prohibitively expensive sampling distributions. We show that in many cases of interest, a computationally inexpensive distribution based on nearest-neighbor information is as effective as one based on statistical leverage scores [54].

1.2. Limitations. First, here we only explore the feasibility of our far-field compression method. We do not integrate our work with a fast summation algorithm, such as a treecode or FMM. This integration will be reported elsewhere.

Second, our experiments cover a range of kernel functions, parameters, and input distributions. However, these are not comprehensive. Further experimentation, particularly on data from real application domains, would be informative.

Finally, our theoretical analysis still leaves a gap between the bounds we can prove and the most effective methods in practice. In particular, our results (along with those in the literature) sample from matrices with replacement (so that samples are independent). However, our experimental results only address the case of sampling without replacement. Further work is required to bridge this gap.

1.3. Related work. This paper builds on two largely distinct bodies of existing work: fast kernel summation methods and randomized algorithms for linear algebra. We briefly survey existing results here.

1.3.1. Kernel summation Methods. Broadly, fast kernel summation methods group the points using a space-partitioning tree, then approximate the interactions between distant groups of points. These methods can be categorized based on the method used to approximate groups of interactions. We group our survey of related work into analytic, semi-analytic, and algebraic methods. We describe several of these methods in greater detail in section 2.

Analytic. The most effective methods use analytic series expansions to approximate these interactions. This approach has its roots in the work of Barnes and Hut [6], Appel [4], and Greengard and Rokhlin [38]. These algorithms have been applied to the Laplace kernel up to three dimensions. The Fast Gauss Transform [39, 71, 49, 40] is a variant of the FMM for the Gaussian kernel. Similar approaches have been applied to solving the kernel summation problem for the Helmholtz [16, 17] and Maxwell equations [15].

Semi-analytic. This approach avoids the explicit use of series expansions. The contribution of a group of points can be approximated as the contribution of a carefully chosen, smaller, group of equivalent source points along with corresponding densities [3, 7]. These ideas have been extended to the kernel independent fast multipole method (KIFMM) [74] and the black-box fast multipole
Another kernel independent method that works well in high dimensions is discussed in [60] in the case where the kernel is diagonalizable in Fourier space. We also mention kernel-independent methods that only require the existence of bounds on the kernel as a function of distance [37, 51].

**Algebraic.** Given a tree data structure that can be used to define the near and far field of groups of points, numerical linear algebra methods can be used to approximate the far field. One set of algorithms uses the truncated singular value decomposition (SVD) to directly compute an approximation to the kernel sum [46, 47]. Several methods compute an approximate singular value decomposition of the kernel operator [72, 73, 34], and employ this approximation in the context of an FMM scheme. An alternative to the SVD is the interpolative decomposition [56], which uses columns of the matrix as basis vectors.

**1.3.2. Randomized linear algebra.** There is a rich literature on randomized algorithms for linear algebra that attempt to construct low-rank approximations of matrices. We briefly highlight some of the results with the most bearing on our work. For a more comprehensive review of randomized low rank approximations, see [42, 53].

**Random projections.** One approach employs the Johnson-Lindenstrauss lemma and the observation that a randomly chosen subspace of $\mathbb{R}^d$ will capture most of the action the kernel interactions [45, 19]. These random projection methods, first introduced by Sarlos [62], have been successfully applied to the construction of low-rank decompositions [56, 70]. However, these methods require the application of a projection operator to the matrix. This scheme ends up being at least as expensive as a matrix-vector multiply, making it inappropriate for our problem.

**Subsampling.** Alternatively, one can use sampling to build an approximation. These methods vary the sampling distribution and which parts of the matrix to sample. The question what kind of sampling to use and whether we sample columns, rows or both. One approach samples individual entries of the matrix to obtain a sparse representation [1, 2]. Other methods construct a distribution over rows or columns. Frieze et al. [33] sample entire rows of the original matrix using a probability proportional to the row Euclidean norm. Extensions of this work use probabilities proportional to the volumes spanned by sets of vectors [20, 61].

**Statistical leverage scores.** Other papers utilize the concept of statistical leverage scores to form an importance sampling distribution [22, 29, 28, 27, 24, 25, 26, 66]. Importance sampling distributions based on the magnitudes of rows of the matrix of right or left singular vectors provide excellent theoretical guarantees for matrix approximations, and are also effective in practice. Broadly, these algorithms show that we can achieve high accuracy from a small ($O(r \log r)$ for a rank $r$ matrix) number of samples. Related algorithms have been developed for the column-subset selection problem [9], fast matrix-matrix multiplication [23], and least-squares solutions to over-determined systems [30].

**Nystrom methods.** Another line of work in the machine learning community is Nystrom methods [69]. Broadly, these methods attempt to approximate a positive semi-definite matrix by sampling a subset of its columns. These approaches use uniform distributions [66, 44, 35], and more complex distributions [26, 75, 36]. However, these methods apply to a more limited class of matrices than our approach and typically require more work than a matrix-vector multiplication.

**Compressed sensing.** Another line of research relevant to our problem is compressed sensing [12, 10, 11]. While not directly relevant to low-rank approximations, the theoretical machinery developed in this context is used in our work. In our case, since we want to approximate the matrix-vector product, we cannot use a method that touches all the entries the matrix. Also, we cannot compute sampling probabilities, they are too expensive. As we will see, the cost is too high even if we just sample some full rows (or columns).

We also mention one other randomized method for the evaluation of kernel summations [50]. This
Table 1.1

Notation used throughout the paper.

| Data Parameters | Kernel Functions and Matrices | Experiment Parameters |
|-----------------|-------------------------------|-----------------------|
| $d$ Dimension of input | $\tilde{K}$ approximate kernel function | $N$ total number of points sampled in experiments |
| $S$ set of $m$ source points | $\tilde{K}$ low-rank approximation of the kernel matrix | $\xi$ separation parameter between sources and targets |
| $T$ set of $n$ target points | $K'$ subsampled kernel matrix (in $\mathbb{R}^{s \times n}$ for $s \leq m$) | $h$ kernel bandwidth |
| $x_j$ source point | $\tilde{K}'$ low rank approximation of $K'$ | $p$ order of series approximation |
| $\tilde{x}_j$ equivalent source point or skeleton point | $\Pi$ orthogonal projection matrix | $s$ number of samples / interpolation points / sampling parameter in experiments section |
| $y_i$ target point | $\ell_i$ statistical leverage score of row / column $i$ | $r$ rank of a matrix approximation / number of skeleton points |
| $\tilde{y}_i$ check point or equivalent or subsampled target point | $\mu(K)$ concentration of matrix $K$ | $\kappa$ rank tolerance in experimental setup |
| $q_j$ charge or density on a source point | $\sigma_i(A)$ $i^{th}$ singular value of matrix $A$ | $K_S, K_N, K_F$ self, nearest neighbor, and far-field interactions |
| $u_i = u(y_i)$ potential at target point $i$ | $\epsilon$ rank tolerance parameter used in experiments |
| $n$ number of source points / number of matrix columns | | |
| $m$ number of target points / number of matrix rows | | |

method directly samples the far-field interactions, which can lead to large error and does not exploit the low-rank structure of the matrix.

In conclusion, all existing methods that are general enough for high-dimensions require an excessive number of kernel evaluations. A new scheme is required.

1.4. Organization. In section 2, we give a brief outline of existing methods for constructing low-rank approximations for kernel summation and we highlight where these methods break down for high-dimensional data. We then describe our approach. We prove basic results in section 3 and provide numerical experiments illustrating the feasibility of our approach in section 4.
2. Overview of outgoing representations. Let \( S = \{x_j\}_{j=1}^n \) be a set of \( n \) sources with charges \( \{q_j\}_{j=1}^n \) and \( T = \{y_i\}_{i=1}^m \) be a set of \( m \) targets. Computing the potential \( u_i = u(y_i) \) for all \( i \) is equivalent to a dense matrix-vector multiplication \( u = Kq \) and requires \( \mathcal{O}(nm) \) work to compute exactly. Many fast summation schemes construct an approximate kernel function \( \tilde{K}_S(y_i) \) such that

\[
\tilde{K}_S(y_i) \approx \sum_{j=1}^n K(y_i, x_j)q_j, \quad \forall y_i \in T.
\]

For methods based on analytic expansions, a low-rank approximation of \( K \) is constructed by finding functions \( \phi_k, \psi_k \) such that

\[
\tilde{K}_S(y_i) = \sum_{k=1}^p \psi_k(y_i)\phi_k(x_j)q_j
\]

with an error that depends on \( p \) and \( \|y - x\| \). Once such representation is found, the quantity \( z_k = \sum_j \phi_k(x_j)q_j \) can be precomputed and used in \( \tilde{K}_S(y_i) = \sum_k \psi_k(y_i)z_k \). When \( p \ll n \), a substantial speedup can be observed by replacing \( K \) with \( \tilde{K} \). Finding such low rank approximations (in the example we just discussed, computing \( z_k \) and \( \psi_k \)) is also referred to as constructing the outgoing representations of the source points \( S = \{x_j\} \).

For many kernels, this approach also requires that the sets of sources and targets be well separated. We require that

\[
\min_{y_i \in T} \min_{x_j \in S} \|y_i - x_j\|_2 > \delta,
\]

where \( \delta \) is a tolerance that depends on the type of the treecode used, the kernel, and the set of approximation functions used. In cases where the sets are not required to be well separated (such as the Gaussian kernel), we let \( \delta = 0 \).

For general source and target inputs and \( \delta > 0 \), this condition will not hold. A fast kernel summation scheme can overcome this problem by using hierarchical groupings of sources and targets (see Figure 2.1(b)). Once such groups have been identified, for each target point, we split interactions into near-field (those points which are not well separated) and the far-field (which are well separated from the target). We can then compute the near-field interactions directly, and efficiently approximate the far-field using an outgoing representation.

These hierarchical groupings are typically done using a spatial data structure, such as a \( d \)-dimensional octree or a \( kd \)-tree. Given such a tree, we perform two traversals. First, we construct an outgoing representation for each leaf. Then, we perform a preorder traversal, constructing an outgoing representation of each node by combining the representations of its children. Then, to evaluate the potential for each target point, we perform a postorder traversal, starting at the root (Algorithm 1). At a node, we bound the error due to applying our outgoing representation to approximate the potential at the target. If the error is small enough to satisfy some user-specified tolerance, we apply the approximation. Otherwise, we recurse, and evaluate the potential at leaves directly if necessary.

As described, the algorithm results in \( \mathcal{O}((n + m) \log n) \) complexity and is commonly referred to as a treecode. The Fast Multipole Method [38] extends this idea by also constructing an incoming representation which approximates the potentials due to a group of distant sources at a target point; it results in \( \mathcal{O}(n + m) \) complexity.

For the remainder of the paper, we strictly focus our attention on the construction of outgoing representations. Exactly the same process can be used to build incoming representations. Our method’s integration with a treecode and an FMM will be presented elsewhere.

Next, we discuss the main techniques for constructing the low-rank outgoing representations and their shortcomings when applied to high dimensional data. In this discussion, we fix a set \( S \) of \( n \) sources and a set \( T \) of \( m \) targets. The sources and targets will be assumed to be well-separated, where the precise value of \( \delta \) will depend on the context and will be made explicit if needed.
(a) **Well-separated sources and targets.**  (b) **Identifying well-separated sets with a tree.**

*Fig. 2.1.* We illustrate the concept of well-separatedness used in fast kernel summation algorithms. We show the set $S$ of sources in red and set $T$ of targets in blue. In *Figure 2.1(a)*, we show the sets with the separation parameter $\delta$. In *Figure 2.1(b)*, we show the use of a space-partitioning tree to identify well-separated sets. The sources in the tree node highlighted in red are well separated from all of the target points in the nodes highlighted in blue. The fast kernel summation literature typically refers to the well-separated targets in blue as the *far-field* and the remaining points (black and red) as the *near-field*.

**Algorithm 1 Treecode**(Target point $y$, Source tree node $S$)

```
if $y$ and $S$ are well-separated [Equation (2.2)] then
  return $u(y) = \tilde{K}_S(y)$
else if $T$ is a leaf then
  return $\sum_{x_j \in S} K(y,x_j)q_j$
else
  return $u(y) = \sum_{S'}$ Treecode$(y,S')$ for all children $S'$ of $S$
end if
```

2.1. **Types of outgoing representations.** We have outlined the basic structure of fast summation schemes, but we have left out the central detail – the method for constructing the outgoing representation of a group of sources. To facilitate the discussion, we classify these methods into three groups:

- **analytic** – based on kernel-dependent series expansions;
- **semi-analytic** – based on equivalent densities and on approximating the kernel at analysis-based target points;
- **algebraic** – based on approximating blocks of the kernel matrix directly.

We now review each of these methods in turn and highlight how each one scales poorly with the dimensionality of the problem. These methods are illustrated in *Figure 2.2*.

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2This is by no means a widely accepted classification. We use it here to facilitate the discussion.
Fig. 2.2. We illustrate three methods for computing an outgoing representation of the red source points. In Figure 2.2(a), we illustrate an analytic, single term expansion: the points are represented by their centroid. Higher order approximations can be viewed as Taylor expansions around this point and require a number of terms that grows significantly with the dimension $d$. In Figure 2.2(b), we show a method based on placing equivalent sources and finding equivalent densities that can approximate the far field (2.4). An outgoing representation is constructed so that the far field due to the true sources (red points) is reproduced by equivalent sources (magenta “X”). The charges on the equivalent sources are determined from interactions with fictitious check points (blue squares). As the dimension of the input increases, the number of equivalent sources and check points required grows quickly, since they must cover the surface of a bounding sphere or cube in $d$ dimensions. In Figure 2.2(c), we illustrate the skeletonization-based approach. We compute the interactions between the sources and carefully chosen targets (blue squares). Using these interactions, we compute an interpolative decomposition, and choose some skeleton sources (magenta points) to represent the far field. The number of skeleton points needed depends on the local intrinsic dimensionality and the kernel. However, with existing techniques, the number of targets needed can grow with the ambient dimension.

2.1.1. Analytic methods. The potential at a target point $y$ sufficiently distant from a set of sources is expanded around a point $x_c$ (generally the centroid of the sources) as:

\[
\tilde{K}(y) = \sum_{k=0}^{\infty} \psi_k (\|y - x_c\|) z_k
\]

for some coefficients $z_k$ and expansion basis $\psi_k$. (The simplest basis for a differentiable kernel can be obtained from its Taylor series.) The approximation is constructed by truncating the expansion after $p$ terms. In general, the better the basis, the faster the convergence.

Bases that deliver exponential convergence have been constructed for the Laplace [38], Helmholtz [16, 17], Maxwell [15], and Gaussian [39, 71, 49, 59, 40] kernels. Efficient approximations have also been carried out using the SVD of the kernel function [43, 34] and in a basis of Chebyshev polynomials [31, 32].

In low dimensions, these expansions are optimal in terms of accuracy and cost. But the number of basis functions required generally scales unfavorably with the dimension $d$. For instance, the fast Gauss transform [39] requires $O(c^d)$ terms for a tensor product expansion, for a value $c > 1$ which is related to the convergence order of the series expansion to the exact solution. This result has been improved to $d^2$ (using so-called sparse grid expansions), but it is still expensive [71, 40] in high dimensions. Furthermore, analytic expansions cannot take advantage of the presence of nonlinear, lower dimensional structures in the distribution of points. Finally, they are kernel specific and their stability and optimal performance can be difficult to achieve.
2.1.2. Semi-analytic methods. This class of methods approximates the potential due to a collection of sources using additional fictitious source points, which, following [74], we term equivalent sources. We focus our discussion on the KIFMM [74], while noting that a similar method has been applied in other settings [3, 7, 57]. The idea is to find \( p \ll n \) equivalent sources \( \{\tilde{x}_j\}_{j=1}^p \) and equivalent densities \( \{\tilde{q}_j\}_{j=1}^p \) such that (2.1) becomes

\[
\tilde{K}_S(y) = \sum_{j=1}^{p} K(y, \tilde{x}_j) \tilde{q}_j
\]

In the KIFMM, the equivalent sources are placed on a convex surface (typically either a sphere or a cube) surrounding the true sources. The positions correspond to surface quadrature rules, and their number \( p \) scales as \( c^{d-1} \), where \( c > 1 \) depends on the target accuracy.

To obtain the equivalent densities \( \tilde{q}_j \), we solve a least-squares problem that minimizes the mismatch between the far field of the equivalent sources and the far field of the true sources at a set of target points. In the KIFMM, these are referred to as the check points and they are also fictitious. The check points are placed on a convex surface surrounding both true sources and equivalent sources. In the KIFMM, their positions correspond to surface quadrature rules and their number scales as \( O(p) \).

The advantage of semi-analytic methods is that they only require kernel evaluations and fairly general assumptions about the kernel function (e.g. that the far-field decays and that the kernel is a Green’s function). We call them semi-analytic, because the positions of equivalent sources and check points are chosen using arguments from analysis. Once these positions are chosen, we no longer require any information about the kernel other than how to evaluate it. While semi-analytic methods are effective in low dimensions, they share the same scalability issues with analytic methods: the number of equivalent sources scales poorly with increasing dimension. By sacrificing accuracy, sparse grids that scale as \( p = O(d^{c-1}) \) could be used to push these techniques to higher \( d \), but for large \( d \) and \( c > 1 \), this approach also becomes too costly.

2.1.3. Algebraic approximations. Both analytic and semi-analytic approximations make use of analytical properties of the kernel function. On the other hand, algebraic approximations work directly with the kernel matrix-vector product. They use methods from linear algebra to construct the outgoing representation.

Recall that Eqn. 1.1 can be viewed as the product of an \( m \times n \) matrix \( K \) with an \( n \)-vector \( q \). We (conceptually) construct an approximate matrix \( \tilde{K} \) such that the product \( \tilde{K} q \) can be efficiently computed. One common construction uses the truncated singular value decomposition [64]:

**Definition 2.1. Truncated Singular Value Decomposition.** For any matrix \( K \in \mathbb{R}^{m \times n} \), there exist matrices \( U \in \mathbb{R}^{m \times m} \) and \( V \in \mathbb{R}^{n \times n} \) and non-negative real numbers \( \sigma_1, \ldots, \sigma_n \) such that \( U \) and \( V \) have orthonormal columns and \( K = U \Sigma V^T \), where, \( \Sigma \) is the diagonal matrix with entries \( \sigma_i \). This is the singular value decomposition (SVD). The columns of \( U \) (\( V \)) are referred to as the left (right) singular vectors, and \( \sigma_i \) are the singular values.

For a given rank \( r \), the truncated SVD consists of the first \( r \) columns of \( U \) (denoted \( U_r \)) and \( V \) (\( V_r \)) along with the first \( r \) singular values (\( \Sigma_r \)). Furthermore, it provides the following error guarantees, which are optimal among any rank \( r \) approximation:

\[
\| K - U_r \Sigma_r V_r^T \|_2 = \sigma_{r+1}, \quad \| K - U_r \Sigma_r V_r^T \|_F = \sum_{k=r+1}^{n} \sigma_k
\]

If \( K \) has rank \( r \ll (m + n) \), then we can compute \( U_r \Sigma_r V_r^T q \) in \( O(r(m + n)) \) time, while incurring error bounded by \( \sigma_{r+1} \).
Another possible decomposition is the Interpolative Decomposition (ID), utilized in the context of the FMM by Martinsson and Rokhlin [55].

**Definition 2.2.** Interpolative Decomposition. Given a $m \times n$ matrix $K$, the rank $r$ interpolative decomposition consists of matrices $C \in \mathbb{R}^{m \times r}$ and $P \in \mathbb{R}^{r \times n}$ such that

(2.6) \[ K \approx CP \]

and

1. The columns of $C$ are a subset of the columns of $K$.
2. $P$ has the $r \times r$ identity matrix as a submatrix.

We refer to the column indices of $K$ chosen to make up $C$ as the skeleton and $P$ as the projection matrix. Note that some definitions differ slightly in the literature.

The ID can be computed by a rank-revealing QR factorization [41] (see Appendix, section 6).

**Theorem 2.3.** ([14].) We can form a rank $r$ interpolative decomposition $CP$ of an $m \times n$ matrix $K$ such that

(2.7) \[ \|K - CP\|_2 \leq \sqrt{1 + nr(n - r)\sigma_{r+1}(K)}. \]

The ID can be used to form an outgoing representation [55]. Since $C$ is a subset of the columns of $K$, $C_{ij} = K(y_i, \hat{x}_j)$ where $\hat{x}_j$ is one of the $r$ skeleton points. Given the original source charges $q_j$, we compute equivalent skeleton charges by

(2.8) \[ \hat{q} = Pq, \quad \hat{q} \in \mathbb{R}^r. \]

Then the potential $u(y_i)$ at any source $y_i$ in $T$ due to the charges in $S$ can be recovered as

(2.9) \[ u_i = Kq \approx C\hat{q} = \sum_{j=1}^{r} K(y_i, \hat{x}_j) \hat{q}_j. \]

The representation takes $O(nr)$ work to compute the equivalent charges and $O(r)$ kernel computations between the target and skeleton points. The approximation error satisfies

(2.10) \[ |u_i - \hat{u}_i| < O \left( \sqrt{1 + nr(n - r)\sigma_{r+1}(K)} \right). \]

If $K$ is numerically rank $r$, then this error term will be negligible.

The method sketched here has the advantage that it does not require any prior knowledge of the analytic structure of the kernel. As long as we are able to partition sources and targets so that the matrix $K$ is numerically low rank, this scheme will work.

However, any method based on the SVD or ID will have to overcome the high cost of computing the decomposition. A direct SVD or QR factorization of $K$ will require $O(mn^2)$ work, which is greater than the direct evaluation of the kernel summation. Although more efficient algorithms can compute the factorization in $O(mn^2)$ time, this is still too expensive for use as the basis for an outgoing representation. Therefore, algebraic methods require a smaller matrix that does not depend on $m$.

Note that (2.9) resembles (2.4). In some sense, the skeleton points correspond to the equivalent sources of the KIFMM and $Pq = \hat{q}$ corresponds to the equivalent densities. These methods differ in the way the equivalent source positions are chosen and the way the equivalent densities are computed.
Fig. 2.3. Two approaches for computing an algebraic outgoing representation. In both cases, we are interested in computing an outgoing representation of the red source points. One method \[55\] (Figure 2.3(a)), places a set of fictitious targets covering a ball or box surrounding the sources. It computes the matrix of interactions between targets and sources, and computes its ID. Our approach (Figure 2.3(b)) subsamples a set of the well-separated target points (shown in green). We then compute the ID of the resulting \( s \times n \) matrix \( K' \). The remaining question is how to choose the samples.

Rather than constructing an ID of the entire matrix \( K \), ID-based approaches construct a smaller matrix \( K' \) using some carefully chosen fictitious targets, similar to the check points used in the KIFMM \[55\]. That is, we place \( s \ll m \) fictitious targets on a surface that encloses the source region. Then we form the dense \( s \times n \) interaction matrix \( K' \) with these fictitious targets and compute its ID, from which we extract \( r \) skeleton points and, using \( P \), compute their equivalent densities. Existing ID-based outgoing representations successfully use this method \[55\].

SVD and ID algebraic decompositions have been successfully demonstrated in one \[73, 55\] and two \[34\] dimensions for a variety of kernel functions. As we mentioned, existing approaches suffer from the same problem in higher dimensions as the KIFMM: the number of interpolation points needed scales exponentially with \( d \).

2.2. Our approach. We propose an alternative approach to the formation of interpolative decompositions for outgoing representations. Rather than choosing fictitious target points according to quadratures chosen via an analytic approach, we choose a sub-sample of the target points themselves. We pick \( s \) points, either randomly or deterministically, from the entire set of targets \( T \). We use these target points to construct the subsampled matrix \( K' \in \mathbb{R}^{s \times n} \). We then construct an ID of this matrix and use it to obtain skeleton points and compute effective charges.

This approach has several possible advantages over existing methods. Methods using interpolation are not able to take the intrinsic dimensionality of the points into account when choosing interpolation points. This leads to their poor scaling with dimension, even if the data set occupies a (probably unknown) low-dimensional manifold. Since our method chooses points from the data set, this potentially allows our scheme to achieve accuracy with a number of samples that does not depend on \( d \), but only on the intrinsic dimension of the set.

Since the data points encode any local intrinsic dimension information, this potentially allows our method to achieve accuracy with a number of samples that does not depend on \( d \).

Furthermore, there are situations where creating new points is not straightforward. For instance,
Kernel-based learning methods are frequently applied to non-metric data such as strings, graphs, or documents. It is not always clear how to create a new string or graph for the purposes of interpolation.

We now explore the possibility of using a sample of the target points in order to compute interpolative decompositions for outgoing representations. We examine the error due to using a subsample of targets both theoretically and experimentally.

3. Theoretical results. Given an \( m \times n \) matrix \( K \), we will sample \( s \) of its rows to form \( K' \). Then, we compute a low-rank decomposition (such as the ID) of \( K' \) and use it to approximate the original matrix. This leaves several outstanding questions. We need to determine a sampling distribution over rows that is efficiently computable. Given this, we must understand the approximation error due to the sampling and the number of samples needed to achieve a given error.

A problem case. Clearly, the most straightforward approach is to sample rows uniformly at random. However, for arbitrary matrices, this will not work. Consider a rank two matrix \( K \) in which the first row of \( K \) is \( v_1^T \) and the other \( m - 1 \) rows are copies of \( v_2^T \) for some orthogonal vectors \( v_1 \) and \( v_2 \). The row space will be spanned by \( v_1 \) and \( v_2 \). However, if we sample less than \( m \) rows of \( K \), we will likely capture only the part of the row space spanned by \( v_2 \). This example shows that in general, it is not possible to succeed by uniformly sampling a small number of rows. Instead, we will either require a more sophisticated method of choosing rows or some restriction on the input rows to eliminate difficult cases like the one above.

We begin by discussing a way to formalize the “difficulty” of a matrix, like in our example. We require a measure of the contribution of each row to the total action of the matrix. In the example above, the first row \( v_1^T \) is more significant to the row space of the matrix than any other single row. There are several ways to measure how “concentrated” the row space of a matrix is along a few of its rows or columns. Following previous work, we use the concepts of statistical leverage scores and concentration.

Definition 3.1. Statistical Leverage [21]. Let \( K \in \mathbb{R}^{m \times n} \) and let \( U \in \mathbb{R}^{m \times n} \) be the left singular vectors of \( K \). Let \( U_i \) be the \( i^{th} \) row of \( U \). Then, the statistical leverage scores \( \ell_i \) of the rows of \( K \) are defined by

\[
\ell_i = \| U_i \|_2^2.
\]

Note that if we are sampling columns, then the leverage scores of columns can be defined with respect to the right singular vectors. Intuitively, the leverage scores give us a measure of the contribution of each row to the total row space of the matrix. The maximum leverage score is sometimes referred to as the coherence of \( K \).

We also require a related definition, the concentration, which applies to any matrix with orthogonal columns, and is related to the coherence. Note that some definitions differ in the details. We give the one used in the remainder of the paper here.

Definition 3.2. Concentration. [10] Let \( Q \in \mathbb{R}^{n \times n} \) have orthogonal columns such that \( Q^T Q = nI \). Then, the concentration \( \mu \) is:

\[
\mu(Q) = \max_{i,j} |Q_{i,j}|.
\]

For an interpretation, see [10]. Note that \( 1 \leq \mu(Q) \leq \sqrt{n} \). If \( \mu \approx 1 \) (e.g., for a scaled Fourier matrix), then the matrix is not concentrated. In this case, the row space cannot depend heavily on any single column. If \( \mu \) is large (\( \approx \sqrt{n} \)) (e.g., for a scaled identity matrix) then there is at least column which makes a very significant contribution to the row space of the matrix.
These definitions attempt to formalize the concern raised in our example above: a small number of rows may have a disproportionate effect on the action of the matrix. This in turn can increase the number of samples required to achieve a given accuracy. Existing methods center around two main approaches to overcome this obstacle. One approach uses some pre-processing of the matrix to make the leverage scores more uniform or reduce the concentration before constructing the smaller matrix $K'$. The other approach constructs an importance sampling distribution which samples rows with probability proportional to their norm or leverage score. This will preferentially select “difficult” rows like $v_1$ in our example. Next, we briefly review some of the main results regarding these two approaches.

3.1. Sampling strategies and main results. We examine two successful strategies for constructing submatrices: random projections and importance sampling distributions.

Most results in the literature on subsampling from matrices deal with sampling columns instead of rows. Clearly, sampling rows of $K$ is equivalent to sampling columns from $K^T$. In order to follow the results from the literature more closely, we switch to the consideration of columns for this discussion. We discuss a general matrix $A \in \mathbb{R}^{n \times m}$ with $m \geq n$ and discuss the construction of a subsampled or projected matrix $A' \in \mathbb{R}^{n \times s}$. This can be thought of as the transpose of the matrix $K$ from the remainder of the paper.

Random projections. Rather than directly sampling columns of $A$, these methods project the matrix $A$ onto some smaller space. A typical result for random projections is from [42] (pp 226).

**Theorem 3.3.** Let $r$ be the target rank, and choose an oversampling parameter $s = r + \ell$ for some $\ell \geq 4$. Let $\Omega$ be an $m \times (r + \ell)$ matrix with iid Gaussian entries and let $C = A\Omega$. Then, with probability at least $1 - 3\ell^{-\ell}$:

$$\| (I - \Pi)A \|_2 \leq (1 + 9\sqrt{(r+\ell)m})\sigma_{r+1}$$

where $\Pi$ projects onto the span of $C$. The problem with this approach is that computing $C$ costs $O(mnr)$ work. The complexity can be improved to $O(mn \log r)$ using a more sophisticated $\Omega$ [67]. In either case, the cost exceeds the cost of applying $A$ to a vector, so it cannot be used in our context.

Importance sampling. The other major approach considers a more sophisticated way to choose rows. We begin with the gold standard for sampling rows or columns directly from a matrix: using an importance distribution based on leverage scores. The following result is from [54].

**Theorem 3.4.** Let $\epsilon > 0$ and $s = O(r \log r/\epsilon^2)$. Draw $s$ columns from an importance sampling distribution where the probability of choosing a column is proportional to its leverage score. Then, with high probability,

$$\| A - \Pi A \|_F \leq (1 + \epsilon/2) \sum_{j=r+1}^{m} \sigma_j(A)$$

where $\Pi$ is the projection of $A$ onto the space spanned by the selected columns. This is only a factor of $(1 + \epsilon)$ worse than the optimal rank $r$ approximation obtained from the SVD. A similar result exists for the spectral norm [9]. Unfortunately, computing the leverage scores requires a basis for the left singular vectors of $A$. Computing this will in turn require $O(n^2m)$ work and requires access to the entire matrix $A$.

---

3Randomized methods can approximate these scores, but they still require $O(r^2m)$ work and the ability to compute the product of $A$ with a vector.
Other sampling-based approaches utilize simpler importance distributions. For instance, a result due to Frieze et al. [33] samples columns with a probability proportional to their Euclidean norm.

**Theorem 3.5.** Sample $s$ columns of $A$ with probability proportional to their Euclidean norms with replacement. Let $\Pi$ be the projection onto the best rank-$r$ subspace of the sampled columns. Then, with high probability:

\[
\|A - \Pi A\|_F^2 \leq \sum_{k=r+1}^{n} \sigma_k^2(A) + \frac{10r}{s} \|A\|_F^2.
\]

An importance sampling distribution based on row norms is easier to compute than one based on leverage scores. Later work improves this result with a more sophisticated sampling distribution [20]. Either approach still requires access to the entire matrix and is thus not practical in our context.

So in a nutshell, the two basic approaches for approximating $A$ do not work in our context because they are too expensive. We require a scheme that is cheaper than a matrix vector multiplication – i.e. cheaper than $O(mn)$.

**Uniform sampling.** One solution is to sample from a predetermined distribution, such as the uniform distribution. These results follow the intuition discussed above: if $A$ has low concentration and low rank, then all columns make a roughly equal contribution to its range. In this case, we intuitively expect that uniform sampling will work quite well.

Uniform sampling approaches utilize a number of samples that grows with the concentration of the matrix $A$. Previous results have focussed on Nystrom extensions – sampling columns to approximate a positive semi-definite matrix. For instance, in [35], the authors show that uniform sampling of $s = \mathcal{O}(\mu r \log r)$ columns of a positive semi-definite matrix $A$ can provide spectral norm error bounded by $\sigma_{r+1}(1 + 2m/s)$. Compressed sensing approaches also consider uniform sampling. In [66], the authors show that in the case of a matrix of exactly rank $r$, uniform sampling of a matrix with low coherence results in exact reconstruction with high probability.

We extend these results in several ways. First, we show a spectral norm error bound for uniform sampling from a general, rectangular matrix $A$, rather than a PSD matrix. Second, our result holds for matrices which are not exactly of rank $r$. Third, we improve on the result in [35] by a factor of $\sqrt{m/s}$.

**Theorem 3.6.** Let $A \in \mathbb{R}^{n \times m}$ be any matrix with $m > n$. Let $A' \in \mathbb{R}^{n \times s}$ be the submatrix of $A$ obtained by randomly sampling $s$ columns of $A$ uniformly and independently. Let $\Pi$ be an orthogonal projector onto the space spanned by the columns of $A'$. Let $r$ be a targeted approximation rank.

Then, for any $\delta > 0$, if $V$ is the matrix of the right singular vectors of $A$ and

\[
s \geq r \mu^2(\sqrt{mV}) \max \{C_1 \log(r), C_2 \log(3/\delta)\}
\]

we have that with probability at least $(1 - \delta)$,

\[
\| (I - \Pi) A \|_2 \leq (\sqrt{1 + 6m/s}) \sigma_{r+1}(A)
\]

for some fixed positive constants $C_1$ and $C_2$ and where $\sigma_{r+1}$ is the $(r + 1)^{th}$ singular value of $A$.

We include the full proof in the appendix, but briefly sketch it here. A useful approach in the randomized matrix approximation literature is to decompose the approximation into two stages: the construction of a randomized “sketching” matrix to perform the sampling and a deterministic bound that connects the properties of any sketching matrix to the error. We view the random subsampling as a matrix projection. We then apply a result from the compressed sensing literature to show that
the projection matrix corresponding to our random sampling has a well-behaved spectrum with high probability.

Theorem 3.6 tells us that given a well-behaved matrix (in the sense of low concentration) then with high probability our sampled matrix captures the action of the original matrix.

The theorem does not directly tell us how effective an approximation built from a subsampled matrix will be. The following theorem from Halko et al. [42] gives us some handle on how a rank $r$ approximation of the subsampled matrix behaves.

**Theorem 3.7.** Let $A \in \mathbb{R}^{n \times m}$, $A' \in \mathbb{R}^{n \times s}$, and $\Pi$ be a projection onto the columns of $A'$. Let $\tilde{A}$ be the best rank $r$ approximation to $\Pi A$. Then,

$$\|A - \tilde{A}\| \leq \sigma_{r+1}(A) + \|(I - \Pi)A\|$$

In other words, we only incur at most another factor of $\sigma_{r+1}(A)$ error if we do the SVD or ID on the projection of $A$ onto the columns we sampled.

Therefore, we have shown that in the case where the matrix has numerical rank $r$ and low concentration $\mu$, we can compute an accurate decomposition by uniformly sampling $O(r \log r)$ columns.

The sampling step does not require us to touch (or even evaluate) the full matrix $A$.

We now show how the above error guarantees fit into the overall framework of this paper. We bound the total error in our final quantity of interest, the matrix-vector product $Kq$.

**Theorem 3.8.** Let $K$ be the $m \times n$ matrix of interactions between sources and targets. Sample $s$ columns of $K^T$ under the conditions of Theorem 3.6, and construct a rank $r$ ID $\tilde{K}'$ of the subsampled matrix $K'$. Then, the total error incurred is bounded by:

$$\|Kq - \tilde{K}'q\| \leq \|q\| \left[ \sigma_{r+1}(K) + \left(1 + 6 \frac{m}{s}\right)^\frac{1}{2} \sigma_{r+1}(K') + (1 + nr(n - r)) \frac{1}{2} \sigma_{r+1}(K') \right].$$

**Proof.** We factor out the term $\|q\|$. Let $K'_{(r)}$ be the best rank $r$ approximation of $K'$. We insert this matrix using the triangle inequality to obtain

$$\|Kq - \tilde{K}'q\| \leq \|q\| \left(\|K - K'_{(r)}\| + \|K'_{(r)} - \tilde{K}'\|\right)$$

We now bound the two terms on the right side of Equation 3.10 separately. The first term can be bounded using theorem 3.7.

$$\|K - K'_{(r)}\| \leq \sigma_{r+1}(K) + \|K (I - \Pi)\|$$

where $\Pi$ is the projection onto the span of the subsampled rows. Since we assume that the number of samples is chosen to satisfy theorem 3.6, we apply it to $K^T$ obtain

$$\|K (I - \Pi)\| \leq \left(1 + 6 \frac{m}{s}\right)^\frac{1}{2} \sigma_{r+1}(K)$$

The second term is just the error between using the SVD and ID to form rank $r$ approximations to the matrix $K'$. Once again employing the triangle inequality and Theorem 2.3, we have that

$$\|K'_{(r)} - \tilde{K}'\| \leq \|K'_{(r)} - K'\| + \|K' - \tilde{K}'\| \leq \sigma_{r+1}(K') + (1 + nr(n - r)) \frac{1}{2} \sigma_{r+1}(K')$$
Combining these bounds completes the proof. □

Note that the same proof structure can be applied to any sub-sampling method for which we have a bound on the quantity \( \| (I - \Pi) K \| \) as in Equation 3.12. Also note that, while this result depends on the singular values of the subsampled matrix \( K' \), these are only scaled by \( n \). Since we are interested in the case where \( m \gg n \), this will not dominate the error.

3.2. Heuristic improvement using geometric information. The results we have discussed so far hold for any matrix. However, our goal is to construct outgoing representations for treecodes. This restriction provides additional structure which our sampling method can use. For instance, the data points are typically points in a metric space, and the kernel function commonly decays with increasing distance between its arguments.

In this case, the rows with the largest norm will correspond to the targets closest to the set \( S \). This suggests a heuristic to approximate the Euclidean norm sampling distribution of Frieze et al. [33] (Theorem 3.5). We can sample targets (i.e. rows) with probability inversely proportional to their distance from the source set. Note that these distances can be efficiently approximated, for instance with the tree structure used in the treecode. We also expect the largest entries of the matrix to approximate the leverage scores. Additionally, we can use nearest-neighbor information to construct an approximate importance sampling distribution. We can choose the nearest targets to the source set deterministically.

We consider both of these sampling distributions in the remainder of the paper: sampling from probabilities inversely proportional to the distance from the sources, and choosing nearest neighbors deterministically. While we leave a theoretical analysis of these heuristics to future work, in the next section, we explore their performance empirically.

4. Experimental results. In this section, we conduct numerical experiments to demonstrate the effectiveness of our scheme for several different kernels.

We focus on constructing an outgoing representation for \( n \) source points. In order for our sampling-based approach to computing outgoing representations to work, we require two things: first, the \( m \times n \) kernel submatrix \( K \) representing the interactions between the sources and all distant target points needs to be numerically low rank. If this is not the case, then we will not be able to construct a cost-effective outgoing representation. Second, we require that we can compute an approximation from a few subsampled rows of \( K \).

We wish to investigate the following questions with our experiments:

- First, how well can we compress the interactions due to distant targets in high dimensions? We explore the numerical rank of \( K \) for a range of kernel parameters and properties of the input points (i.e. dimensionality, spatial distribution). These experiments are used to determine the feasibility of using a low-rank approximation of the far field.
- Second, how well do different sampling schemes do in capturing this low-rank far-field approximation when compared to the SVD of the entire matrix? We find that the nearest-neighbor sampling works almost as well as leverage score sampling for kernels which are functions of distances and, when combined with the ID, results in a compression nearly as good as that obtained using an SVD of the full matrix \( K \).

Unlike existing approaches, the effectiveness of the compression of our method depends only on the intrinsic dimensionality of the dataset and not the ambient dimension. We provide some examples that demonstrate this property of our scheme.

Next, we detail the experimental setup. In our results, we devote a section to each of the Gaussian, Laplace, and polynomial kernels. For each kernel, we first discuss the kernel function and our choices of
parameters. We then explore the numerical rank of kernel submatrices and test our ability to compute outgoing representations using row sampling.

4.1. Experimental Setup. Throughout, we consider the interactions between a compact set of sources and a set of distant targets. We examine the construction of an outgoing representation to compactly capture the potential due to these sources at a distant target. We now describe our basic experimental setup and illustrate it in Figure 4.1.

1. Sample $N$ points from a $d$-dimensional distribution.
2. Choose a center point $x_c$ (typically the origin). Let the source set $S$ be the $n$ points closest to $x_c$. Define $\rho$ to be the maximum distance between $x_c$ and any source point.
3. Define the target set $T = \{y : \|y - x_c\| \geq \xi \rho\}$. The parameter $\xi$ controls the separation between sources and targets. Call the number of targets $m$.
4. Compute the $m \times n$ matrix $K$ of all interactions between sources and targets.

For each set of experiments (per kernel), the main parameters are:
- The choice of input distribution, especially its dimensionality $d$.
- The total number of points $N$ drawn from the distribution, along with the center of the sources $x_c$ and the number of source points $n$.
- The "well-separatedness" parameter $\xi$.
- Any parameters for the kernel function, such as a bandwidth $h$.

Choice of $d$. For small values of $d$ (1, 2, 3), existing kernel summation algorithms are efficient and accurate. We are primarily interested in higher dimensions where these methods fail. We show results
from four to 64 dimensions for normally distributed data and construct low-intrinsic dimensional data sets with ambient dimension as large as 1,000. We also use real data sets with tens of dimensions.

**Choice of** $n$. We fix $n$ at 500 throughout our experiments. Intuitively, we expect that the interaction between sources and targets has some “true” rank, for given locations of points. If this is the case, as we increase $n$, we should see better and better compression. However, this is not a viable strategy in the context of fast kernel summation methods, since we will still need to compute direct interactions between sources and themselves. Therefore, we choose $n = 500$ as an intermediate value, i.e. one that is large enough for us to see some compression, but small enough so that the direct interactions between $n$ points are efficiently computable.

**Choice of** $\xi$. We fix $\xi = 1$ unless otherwise noted. If $\xi < 1$, then some of the sources are included in the target set. These self-interactions would be computed directly in a treecode or FMM, so we are not interested in a compact representation of them. On the other hand, for large values of $\xi$, most of the $N$ points will no longer be included in the target set, particularly in high dimensions. Therefore, we choose $\xi = 1$ as a compromise value for the Gaussian and polynomial kernels. For the Laplace kernel, we explore $\xi = 2$ and $\xi = 4$, which corresponds to the separation required for the series-based approximations in the original FMM.

### 4.1.1. Data sets

We use the following data sets in our experiments:

- **Normal.** These data are drawn independently from the standard multivariate normal distribution in $d$ dimensions. These experiments represent a worst-case example where the data truly fill out the ambient space. The optimal bandwidth for the kernel density estimation task can also be computed exactly for this data set [63], giving us a starting point for bandwidth selection in our experiments.

- **Low intrinsic dimension.** We draw data from the standard multivariate normal distribution in $d_i$ dimensions. We pad these data with zeros so that they live in $d_e$ dimensions, with $d_e \gg d_i$. We then apply a random rotation and add small uniform noise. This artificial example allows us to directly examine if our approach can successfully capture a low dimensional structure in the data.

- **Real data.** We use the following real data distributions from the UCI ML repository [5]: the Color Histogram, Color Moments, and Co-occurrence Texture feature sets from the Corel Images data set. The properties of these sets are given in Table 4.1. We translate and scale each set so that it is contained in the unit hypercube.

### 4.1.2. Distances in high dimensions

Before we proceed, we take a moment to discuss the consequences of increasing the dimension of the data set. For data in high dimensions, the pairwise distances between points will tend to converge around a single distance – this is an example of the concentration of measure effect [68]. We plot histograms of the pairwise distances between points in the source and target sets for the $d$-dimensional standard normal distribution in Figure 4.2. These plots illustrate that the pairwise distance distributions become increasingly peaked as $d$ increases.

| Set               | $d$ | $N$  |
|-------------------|-----|------|
| Color Hist.       | 32  | 68040|
| Color Mom.        | 9   | 68040|
| Cooc. Text.       | 16  | 68040|

Table 4.1

Real data sets from the UCI ML repository [5] used in our experiments.
This effect is significant for our choice of the parameter $\xi$ in the experiments. Recall that we identify the $n$ points closest to $x_c$ as the sources, and call $\rho$ the largest distance from $x_c$ to a source. The target set then consists of all points at a distance of at least $\xi\rho$ from $x_c$. As $d$ increases and the distribution of pairwise distances becomes more peaked, a small increase in $\xi$ can lead to a very large fraction of the points being excluded from the target set. This observation informs our choices of $\xi$ in the experiments.

4.1.3. Subsampling methods. To quantify the compressibility and performance of subsampling methods, we perform the following experiments.

1. We fix an error tolerance $\epsilon$ and compute the $\epsilon$-rank $r$ of the kernel matrix $K$ – i.e. the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$.
2. We sample $m_s$ rows of $K$ (according to one of the distributions below) to form an $m_s \times n$ submatrix $K'$.
3. We compute a rank $r$ interpolative decomposition of of $K'$.
4. We reconstruct the entire matrix $K$ from this ID, and report its relative error.

For these experiments, we consider the following sampling distributions, each characterized by a parameter $s \in (0, 1]$.

- **Uniform sampling**: Choose a number of rows $m_s = \lceil s m \rceil$. Then, choose a subset of $m_s$ rows uniformly at random, without replacement.
• **Distance sampling**: Choose a number of rows \( m_s = \lceil sm \rceil \). Then, construct an importance sampling distribution where the probability of choosing row \( i \) is proportional to the distance between target point \( i \) and the source center \( x_c \). We sample from this distribution without replacement.

• **Leverage sampling**: Choose a number of rows \( m_s = \lceil sm \rceil \). Then, construct an importance sampling distribution where the probability of choosing row \( i \) is proportional to its leverage score (See section 3). We sample from this distribution without replacement.

• **Nearest neighbors**: Deterministically select the \( m_s = \lceil sm \rceil \) target points that are closest to the source points. Then, choose the rows of \( K \) corresponding to these targets.

As we have seen, leverage-score sampling should give the best results, but it is too expensive to be used in our context. We use it as the gold-standard for comparison with the other sampling methods. On the other hand, the uniform distribution requires no previous knowledge and is cheap and easy to implement. The results in section 3 suggest that it will be successful if the concentration of the matrix is small, but it is not clear *a priori* if this will be the case. The distance sampling distribution represents a compromise between these extremes. While we expect that closer points will have larger kernel interactions, and thus correspond to more significant rows of \( K \), the distances could be efficiently approximated using a space-partitioning tree or clustering. We also use the deterministic selection of nearest neighbors as a selection method and compare it to the randomized sampling methods.

It is possible that most of the interactions between sources and targets are captured by the nearest neighbors. Examining the results obtained from using these points deterministically, we can observe whether including farther points in our approximation is important for an accurate decomposition. Distance sampling and nearest neighbors require precomputations that in turn need to be accelerated using fast methods, since their direct calculation is \( O(mn) \). Nearest neighbors can be computed efficiently in low dimensions [37]. In high dimensions, methods on binary tree partitions or hashing methods can be used for exact or approximate schemes, for instance with random projection trees [18].

4.2. **Gaussian kernel.** We begin with the Gaussian kernel.

\[
K(y, x) = \exp \left( -\frac{1}{2h^2} \| x - y \|^2 \right)
\]

The kernel is characterized by a *bandwidth* \( h \in (0, \infty) \).

4.2.1. **Choice of parameters.** Clearly, the choice of bandwidth is critical to the behavior of the Gaussian kernel. As \( h \) tends to zero, the kernel matrix \( K \) will become increasingly sparse. When the sources are not included in the target set, the rank of \( K \) will become zero. On the other hand, as \( h \) grows, all entries of \( K \) will tend toward 1, resulting in a rank 1 matrix. While both these cases will compress extremely effectively, neither is of much practical interest.

Furthermore, we expect the behavior of the kernel to depend on the simultaneous choice of \( h \) and \( d \). As we discussed in Figure 4.2, the distances between pairs of sources and targets become increasingly concentrated in high dimensions. Therefore, a single fixed value of \( h \) will demonstrate very different behavior as \( d \) increases.\(^4\)

In order to determine a scale of \( h \) that will account for this variation, we consider the choice of bandwidth made in solving kernel density estimation problems in non-parametric statistics. Silverman

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\(^4\)In the literature, when studying the performance of far-field compression, a fixed set of values of \( h \) is typically used, e.g. \( h \in \{10^{-3}, \ldots, 10^3\} \). However, we find that this approach is not very informative as the range of values of \( h \) for which the kernel exhibits interesting behavior becomes more narrow with increasing dimension.
Table 4.2
Values of $h_S$ (Equation 4.2) as a function of $d$ for $N = 10^5$ points drawn from a standard normal distribution.

| $d$ | $h_S$ |
|-----|-------|
| 4   | 0.2143|
| 8   | 0.3396|
| 16  | 0.5060|
| 32  | 0.6722|
| 64  | 0.8022|

Table 4.3
Values of $h$ determined experimentally for normally distributed data. The columns correspond to different rank budgets of $\kappa = 1\%$ and $\kappa = 20\%$ of the columns. The “+” and “−” correspond to the larger and smaller values of $h$ where this rank budget is achieved. All values are in units of $h_S$ computed for the given dimension (Table 4.2). The sample mean over 30 independent realizations of the data is given, with the sample standard deviation in parentheses. We use $N = 10^5$ for all experiments.

| $d$ | $\kappa = -1\%$ | $\kappa = -20\%$ | $\kappa = +20\%$ |
|-----|-----------------|-----------------|-----------------|
| 4   | 0.0587 (0.014)  | 0.1656 (0.008)  | 1.1719 (≈0)    |
| 8   | 0.1879 (0.05)   | 0.4082 (0.016)  | 2.6367 (≈0)    |
| 16  | 0.3708 (0.09)   | 0.6700 (0.035)  | 3.9062 (≈0)    |
| 32  | 0.5398 (0.17)   | 0.8999 (0.063)  | 3.955 (≈0)     |
| 64  | 0.6887 (0.24)   | 1.1989 (0.102)  | 4.2090 (0.016) |

[63] gives the asymptotically optimal (in terms of expected squared error) choice of $h$ for KDE when the true underlying distribution is the standard multivariate normal:

$$h_S = \left(\frac{4}{2d + 1}\right)^{\frac{1}{2d + 4}} N^{-\frac{1}{2d + 4}}.$$  

We use the value $h_S$ (which depends on $d$) as a reference scale in our experiments.

Let us emphasize that in practice, the value of $h$ depends on the algorithm and the application. Commonly, the value is chosen through cross-validation on some objective function of interest. This in turn requires a search over many values of $h$. We suggest $h_S$ as a starting point for this search, and we explore a range of values. In exploring this range an additional criterion is the magnitude of the far field. If the contribution of the far-field becomes too small, the kernel is too narrow and nearest neighbors can capture the interactions accurately. On the other hand if the far field becomes dominant, the kernel compresses quite well.

4.2.2. Singular values of $K$. Following our intuition above, we expect that for very small and very large values of $h$, the kernel will compress easily. For values in between, we expect the singular values to be flatter, thus implying a greater difficulty in approximating the kernel. We would like to know the width of this “difficult” region for different values of $d$. We empirically measure this range in the following way:

- We specify a rank tolerance $\epsilon$.
- We specify a rank budget $\kappa \in (0, 1]$ as a percentage of $n$, the largest possible rank of $K$.
- We search over bandwidths $h$ such that the $\epsilon$-rank of $K$ is close to $\kappa n$. Note that we expect there to be two ranges of $h$ where this occurs, one for small $h$ and one for larger $h$. 

For data drawn from the standard normal distribution and \( x_c \) at the origin, we approximately compute these values of \( h \) using binary search. Our results are given in Table 4.3 in units of \( h_S \).

We then plot the singular values of \( K \) for these values of \( h \) in Figure 4.3. These values suggest that for \( n = 500 \), we are not yet in the regime where \( K \) can be compressed with high accuracy. If computational resources are available, increasing \( n \) may be preferable. However, here we do not consider the dependence on \( n \) since this is a performance optimization in which one balances direct interactions and far-field interactions. Also, this amount of compression is sufficient for lower accuracy, such as is commonly required in machine learning applications.

These results show that the range of values of \( h \) for which the singular values decay quickly increases as \( d \) increases. As we demonstrated previously, for truly high-dimensional data, the pairwise distances between sources and targets will concentrate around a single value. Therefore, for more values of \( h \), the quantity \( \|x - y\|^2 / h^2 \) will be either very small or very large. This in turn makes the singular values decay quickly.

**Influence of nearest neighbors.** The Gaussian kernel decays quickly with increasing distance. Therefore, one possible approximation strategy is to compute the kernel interactions between nearby pairs of points and truncate the remaining interactions. In Table 4.4, we break down the total interactions for target points in order to demonstrate that the contribution of distant source points can be significant. In the case that more distant points make a significant contribution, an approximation scheme like ours is necessary to accurately compute the kernel sum.

We set \( \xi = 1 \) and \( n = 500 \) and draw \( N \) data points from the standard multivariate normal distribution. We fix the \( n \) points closest to the origin as the source points, and we consider all \( N \) points (including the sources) as targets. We also define the \( n \) next-closest points to the origin as the nearest neighbors of the sources. We refer to the remaining \( N - 2n \) points as the far-field.

We compute the \( N \times n \) matrix \( K \) of interactions between sources and targets. We partition \( K \) into three submatrices according to the sets identified above: self-interactions, nearest neighbor interactions, and far-field interactions. In other words, we have:

\[
K = \begin{bmatrix}
K_S \\
K_N \\
K_F
\end{bmatrix}
\]

where \( K_S \) is the \( n \times n \) matrix of interactions between the sources and themselves, \( K_N \) is the \( n \times n \) matrix of interactions between the \( n \) nearest neighbors and the sources, and \( K_F \) is the \( (N - 2n) \times n \) matrix of interactions between the far field and the sources.

We are interested in quantifying the contribution of each of the three sets to the total action of the matrix \( K \). We compute the following quantities:

\[
\text{Self} = \frac{\|K_S\|_2}{\|K\|_2}
\]

\[
\text{NN} = \frac{\|K_N\|_2}{\|K\|_2}
\]

\[
\text{Far} = \frac{\|K_F\|_2}{\|K\|_2}
\]

We compute these quantities for several values of \( d \) and \( h \) in Table 4.4. We see that for larger values of \( h \), an accurate approximation algorithm must take the distant targets into account.
Table 4.4

Fractions of interactions for given values of \( d \) and \( h \) for the Gaussian kernel and standard multivariate normal data. Reported values are \( \|K_s\|_2/\|K\|_2 \) as percentages for each matrix described in section 4.2.2. All experiments use \( N = 10^5 \), \( \xi = 1 \), and \( n = 500 \) with \( n \) nearest neighbors.

| \( d \) | \( h \) | Self (Eqn. 4.5) | NN (Eqn. 4.6) | Far (Eqn. 4.6) |
|---|---|---|---|---|
| 4 | −1% | 100.00 | 0.56 | 0.00 |
| 4 | −20% | 100.00 | 26.24 | 0.00 |
| 4 | \( h_S \) | 84.44 | 40.52 | 38.09 |
| 4 | +20% | 78.38 | 42.41 | 46.74 |
| 8 | −1% | 100.00 | 0.02 | 0.00 |
| 8 | −20% | 100.00 | 12.48 | 0.01 |
| 8 | \( h_S \) | 93.34 | 27.48 | 30.48 |
| 8 | +20% | 37.55 | 26.54 | 88.82 |
| 16 | −1% | 100.00 | 0.00 | 0.00 |
| 16 | −20% | 100.00 | 0.40 | 0.00 |
| 16 | \( h_S \) | 99.98 | 7.55 | 1.18 |
| 16 | +20% | 19.25 | 15.13 | 96.96 |
| 32 | −1% | 100.00 | 0.00 | 0.00 |
| 32 | −20% | 100.00 | 0.03 | 0.00 |
| 32 | \( h_S \) | 100.00 | 0.15 | 0.00 |
| 32 | +20% | 18.48 | 13.50 | 97.35 |
| 64 | −1% | 100.00 | 0.00 | 0.00 |
| 64 | −20% | 100.00 | 0.00 | 0.00 |
| 64 | \( h_S \) | 100.00 | 0.00 | 0.00 |
| 64 | +20% | 18.94 | 13.07 | 97.32 |

4.2.3. Subsampling. We have shown that the submatrix \( K \) can be meaningfully compressed for a range of values of \( d \) and \( h \) and that the far field is significant for some of these values. We now turn to our results on subsampling rows to build an outgoing representation. In Figures 4.4, 4.5, and 4.6, we show these results for 4, 16, and 64 dimensional data, respectively.

We select the data and partition them into sources and targets as before. We fix \( \epsilon = 10^{-2} \) and choose the approximation rank \( r \) as the smallest \( r \) such that

\[
\frac{\sigma_{r+1}(K)}{\sigma_1(K)} < \epsilon.
\]

With this choice of \( r \), the best possible reconstruction error is \( \sigma_{r+1}(K)/\sigma_1(K) \), even if we were to use the SVD. Therefore, we do not observe any reconstruction errors better than this ratio even when sampling all of the rows (i.e. when \( s = 1 \)).

For small bandwidths (corresponding to 1% and 20% of the possible rank), the leverage score and nearest neighbor sampling methods perform very well, obtaining the same approximation quality as the full-row decomposition with a very small fraction of the rows. The uniform and distance distributions obtain very poor accuracy for even 10% of the rows. This suggests that the nearest neighbors account for most of the interaction, and that the quality of the decomposition is very sensitive to having these neighbors in the sample. This fits with the results in Table 4.4 for smaller values of \( h \). For the larger
bandwidths, we see that at about 1% of the rows, all of our row selection methods perform nearly as well as the decomposition of the full matrix.

4.2.4. Low intrinsic dimensions. We show results on our artificial distribution with low intrinsic dimension in Figure 4.7. In our experiments, we see that despite the extremely high ambient dimension, we are still able to compute an accurate approximation using a subsample of the rows. We also see qualitatively the same behavior as the results in Figure 4.4. Note that in 1,000 dimensions, existing methods will be prohibitively expensive. Without any a priori information about the low dimensional structure in this data set, our method is able to efficiently compute an outgoing representation.

4.2.5. UCI datasets. We show results for UCI data sets in Figures 4.8, 4.9, and 4.10. We determine the bandwidth by direct experimentation. As in our other experiments, we choose a targeted $\epsilon$-rank, then vary $h$ until we achieve this rank. We select a point at random to be $x_c$. Our results (averaged over independent choices of $x_c$) are shown in Table 4.5. Once again, the leverage sampling and nearest neighbor methods can accurately reconstruct the matrix from 1% of its rows. For the smaller bandwidth shown, the uniform and distance sampling distributions do not provide an accurate reconstruction, but they perform comparably to the other methods for larger $h$.

| Data             | $\kappa = -20\%$ | $\kappa = +20\%$ | $h_S$ |
|------------------|-------------------|-------------------|-------|
| Color hist.      | 0.0481 (0.0086)   | 0.2184 (0.0296)   | 0.6794|
| Color moments    | 0.0716 (0.0117)   | 0.3815 (0.0515)   | 0.3769|
| Cooc texture     | 0.0266 (0.0087)   | 0.1318 (0.0293)   | 0.5159|

We see similar behavior as in our synthetic data experiments. For larger values of $h$, all of our row selection methods are effective with roughly 1% of the rows. For small values of $h$, the nearest neighbor and leverage sampling methods achieve high accuracy, while the other sampling distributions do not.

4.3. Laplace kernel. The Laplace kernel is given by:

\[
K(y, x) = \begin{cases} 
\log \|x - y\| & d = 2 \\
\|x - y\|^{2-d} & d \neq 2.
\end{cases}
\]

(4.8)

The Laplace kernel lacks any parameters other than the dimension of the inputs. However, unlike the Gaussian kernel, it has a singularity at $x = y$.

4.3.1. Choice of parameters. The only parameter we need for our experiments is the well-separateness parameter $\xi$. In series-expansion based methods for this kernel, some separation between the sources and targets is required for the series to converge. This is due to the singularity in the kernel function as the distance between its arguments goes to zero. Therefore, we examine values of $\xi$ that are strictly greater than one.

We also examine smaller values of $d$ for our synthetic data experiments. This is because $r^{-d+2}$ will quickly go to zero for larger values of $d$. For this reason, we also omit experiments on the low intrinsic dimensional set and our real data sets.
4.3.2. Spectrum of $K$. We explore the compression of $K$ for $\xi = 2$ and 4 in Figure 4.11. The singular values decay more quickly for $\xi = 4$. However, for both values, the Laplace kernel submatrix compresses more effectively than for the Gaussian kernel. We see that the use of the ID as an outgoing representation is feasible for this kernel.

4.3.3. Subsampling. We show subsampling results for the Laplace kernel in Figure 4.12 for $\xi = 2$. We note that for all four values of $d$, the four methods for selecting rows perform very similarly. In all cases, 1% of the rows are sufficient to form an approximation that is as accurate as the decomposition of the full matrix.

4.4. Polynomial kernel. The polynomial kernel is defined as:

\[(4.9) \quad K(y, x) = \left(\frac{x^T y}{h} + c\right)^p\]

This kernel is characterized by three parameters: the degree $p$, bandwidth $h$, and a constant $c$. However, the constant $c$ can be set to 1 without loss of generality [13].

4.4.1. Choice of parameters. We examine quadratic and cubic polynomial kernels ($p = 2$ and 3), since these tend to be the most common in practice. As $p$ increases, the kernel matrix will be dominated by the inner products of the largest magnitude data vectors. We therefore restrict our attention to these two values.

Unlike in the Gaussian case, we do not have any a priori scale for the bandwidth. We therefore resort to direct experimentation to cover a wide range of values of $h$.

4.4.2. Compression of kernel submatrices. We begin by examining the singular values of the polynomial kernel submatrices. We show results for the quadratic kernel in Figure 4.13 and cubic kernel in Figure 4.14 for a range of values of $h$.

The most striking feature of these plots is the sharp drop-off in the spectrum for most values of $d$ and $h$, but especially for smaller values of $d$. We see that as $h$ increases, the spectrum decreases more sharply, since the value of the kernel approaches one for all arguments as $h$ grows. The spectra for the quadratic and cubic kernels are qualitatively similar.

4.4.3. Subsampling. We show subsampling results for a subset of bandwidths – $h = 0.01$ in Figure 4.15 and $h = 100$ in Figure 4.16. As we see in Figures 4.13 and 4.14, the kernel tends to compress better for larger bandwidths. We chose these bandwidths to represent a case with more compression and one with less. We provide a selection of values of $d$ and $p = 2$ and 3.

Once again, 1% of the rows is sufficient to capture the approximation accuracy of the decomposition of the whole matrix in this case. However, we note that in some experiments (Figures 4.15(a) and 4.17(a)), the nearest neighbors subsampling method performs substantially worse than the other methods. Note that the polynomial kernel is not a function of the distance between the points. Therefore, in this case, we do not expect the nearest neighbors to necessarily be a good approximation of either the leverage scores or the Euclidean norms of the rows.

4.4.4. Low intrinsic dimension. We show results for our low intrinsic dimension synthetic data in Figure 4.17. Once again, our sampling methods are effective in this case, despite the high ambient dimension. However, we see an interesting trend for $h = 0.01$. The deterministic selection of rows based on the nearest target points shows significantly larger error than any of the other methods, including the random selection of rows with probabilities based on distances. Note that this kernel does not decrease with increasing distance between its arguments. Therefore, it is not surprising that nearest neighbors do not necessarily capture the most important target points.
4.4.5. Real data sets. We show results on two of our real data sets in Figures 4.18 and 4.19. Once again, we see that subsampling rows is extremely effective for both these data sets.

5. Conclusion. We demonstrate that the method of randomly sampling rows to build an approximation of a kernel submatrix may be useful for the efficient construction of outgoing representations in fast kernel summation algorithms. This approach has two major advantages: first, it requires no prior knowledge about the kernel function, and second, it can work even for extremely high dimensional data. We show empirically that this approach is effective for several commonly used kernel functions and data sets. We also prove a new theorem about random sampling, showing that uniformly chosen rows can provide a very accurate approximation in many cases. Our next steps will include an exploration of this approach in the context of a treecode or FMM. To integrate this with a treecode, one needs to decide on the number of points per box and on the number of rows to subsample while maximizing accuracy and minimizing cost.

6. Appendix.

6.1. Computation of the interpolative decomposition. We compute the interpolative decomposition of a matrix $K \in \mathbb{R}^{m \times n}$ as follows:

1. Fix an approximation rank $r$.
2. Compute a rank-revealing QR factorization $K = QR\Pi^T$, where $Q \in \mathbb{R}^{m \times n}$ has orthonormal columns, $\Pi$ is a column permutation of $K$, and $R \in \mathbb{R}^{n \times n}$ is an upper triangular matrix which we partition as

   $R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}$

   where $R_{11} \in \mathbb{R}^{r \times r}$.
3. The projection matrix $P$ is the minimum-norm solution to the under-determined system

   $R_{11}P = R_{12}$

4. The skeleton is the first $r$ columns selected by $\Pi$.

6.2. Proof of Theorem 3.6. We require two preliminary results for the proof. First, a deterministic bound on matrix projections, proved by Halko et al. [42] (Theorem 9.1):

   **Theorem 6.1.** Let $A$ be an $n \times m$ matrix with singular value decomposition $U, \Sigma, V^T$ and let $r \geq 0$. Let $\Omega$ be any matrix in $\mathbb{R}^{m \times s}$ for $s \geq r$. Partition $\Sigma$ into $\Sigma_1$ and $\Sigma_2$, such that $\Sigma_1$ contains the first $r$ singular values, and $\Sigma_2$ the rest. Let $\Omega_1 = V_1^T \Omega$ and $\Omega_2 = V_2^T \Omega$, where $V_1$ is the first $r$ columns of $V$, and $V_2$ is the rest. Then, if $\Omega_1$ has full row rank,

   $\| (I - \Pi) A \|_2^2 \leq \| \Sigma_2 \|^2 + \| \Sigma_2 \Omega_2 \Omega_2^T \|$  

   where $\Pi$ is an orthogonal projection onto the range of $A\Omega$, and $\Omega_2^T$ is the Moore-Penrose pseudoinverse of $\Omega_1$.

   The second is a theorem of Candes and Romberg [10]:

   **Theorem 6.2.** Let $Q$ be an $n \times n$ matrix such that $Q^T Q = nI$. Let $T$ be a fixed index set of size $r$ and $W$ be an index set of size $s$ chosen uniformly at random. Let $Q_{W,T}$ be the submatrix of $Q$ with rows and columns indexed by $W$ and $T$, respectively. Then, for any $\delta > 0$ and for some fixed, positive constants $C_1$ and $C_2$, and number of samples $s$ such that

   $s \geq r \cdot \mu^2(Q) \cdot \max \{ C_1 \log r, C_2 \log(3/\delta) \}$

   where $\mu(Q)$ is the numerical condition number of $Q$.
the matrix $Q_{WT}$ is nearly orthogonal with high probability. More precisely:

\begin{equation}
Pr \left( \left\| \frac{1}{s} Q_{WT}^T Q_{WT} - I \right\|_2 \geq \frac{1}{2} \right) \leq \delta
\end{equation}

We will apply this result through the following corollary showing that the subsampled matrix has full rank with high probability.

**Corollary 6.3.** Under the conditions of Theorem 6.2, the matrix $Q_{WT}$ has rank $r$ with probability at least $1 - \delta$.

**Proof.** Let the conditions of the theorem hold. Then, with probability at least $1 - \delta$, we have that

\begin{equation}
\left\| \frac{1}{s} Q_{WT}^T Q_{WT} - I \right\|_2 < \frac{1}{2}
\end{equation}

For a contradiction, let $x$ be a unit vector in the null space of $Q_{WT}$, then

$$
\left\| \frac{1}{s} (Q_{WT}^T Q_{WT} - I) x \right\| = \left\| \frac{1}{s} Q_{WT}^T Q_{WT} x - I x \right\| = \|x\| = 1
$$

Therefore, in the event that Eqn. 6.6 holds, $Q_{WT}$ must have full rank. □

We now prove Theorem 3.6. We choose a matrix $\Omega$ corresponding to a random subset of columns and construct the matrices $\Omega_1$ and $\Omega_2$ from the statement of Theorem 6.1. We show that $\Omega_1$ satisfies the conditions of the theorem using Corollary 6.3. Using this fact, we apply the theorem to bound the 2-norm of the error incurred by the projection.

**Proof.** (of Theorem 3.6). Let $U \Sigma V^T$ be the SVD of $A$, and let $V_1 (\Sigma_1)$ be the first $r$ right singular vectors (values) and $V_2 (\Sigma_2)$ be the rest.

Fix some small constant $\delta > 0$ and sample $s$ integers from $\{1, \ldots, m\}$ uniformly with replacement, where $s \geq \mu^2 (\sqrt{mV}) \{C_1 \log r, C_2 \log (3/\delta)\}$. Let $A'$ be the matrix whose columns are the corresponding $s$ columns of $A$, scaled by $\sqrt{\mu}$. Let $O \in \mathbb{R}^{m \times s}$ be the matrix whose columns consist of the standard basis vectors in $\mathbb{R}^m$ corresponding to the sampled columns. Let $\Omega = \sqrt{\mu} O$. Define the $r \times s$ matrix $\Omega_1 = V_1^T \Omega$ and the $(m - r) \times s$ matrix $\Omega_2 = V_2^T \Omega$.

The matrix $\sqrt{mV}$ satisfies the conditions of Theorem 6.2 with $W$ as our sampled column indices and the set $T$ as the first $r$ columns of $V$. The matrix $Q_{WT}$ from the theorem corresponds to the matrix $\sqrt{mO}^T V_1 = \sqrt{s} \Omega_1^2$ in this case. Then, we have that with probability at least $1 - \delta$,

\begin{equation}
\left\| \frac{1}{s} (\sqrt{s} \Omega_1) (\sqrt{s} \Omega_2^T) - I \right\| = \|\Omega_1 \Omega_1^T - I\| < \frac{1}{2}
\end{equation}

Also, from Corollary 6.3, we have that the matrix $\Omega_1$ has rank $r$ in this event. For the remainder of the proof, we restrict our attention to the case where Equation 6.7 holds. Since this occurs with probability at least $1 - \delta$, this is sufficient to prove the result.

Theorem 6.1 applies to any matrix $\Omega$, so we apply it to the $\Omega$ we constructed from our column samples. We obtain

\begin{equation}
\| (I - P) A \|^2 \leq \| \Sigma_2 \|^2 + \| \Sigma_2 \Omega_2 \Omega_1^T \|^2
\end{equation}

where $P$ is an orthogonal projection onto the span of the columns of $A'$. We can now use our construction to bound the terms on the right hand side.
Note that \( \| \Sigma_2 \|^2 = \sigma_{r+1}^2 \), since \( \Sigma_2 \) is the matrix diag(\( \sigma_{r+1}, \ldots, \sigma_n \)).

Furthermore, since the rows of \( \Omega_1 \) are linearly independent, we have that

\[
\Omega_1^T = \Omega_1^T (\Omega_1 \Omega_1^T)^{-1}
\]

We now bound the quantity on the right hand side of Equation 6.8 as:

\[
\Sigma_2 \Omega_2 \Omega_1^T = \Sigma_2 \Omega_2 \Omega_1^T (\Omega_1 \Omega_1^T)^{-1} \| \Sigma_2 \| \| \Omega_2 \Omega_1^T \| \| (\Omega_1 \Omega_1^T)^{-1} \| \leq \sigma_{r+1}^2 \| \Sigma_2 \| \| \Omega_2 \Omega_1^T \| \| (\Omega_1 \Omega_1^T)^{-1} \|
\]

We can complete the proof by bounding each of the three terms in Equation 6.11. The first term is clearly equal to \( \sigma_{r+1}^2 \).

From Equation 6.7 we have that \( \Omega_1 \Omega_1^T \) cannot be too far from the identity. We use this fact to show that

\[
\| (\Omega_1 \Omega_1^T)^{-1} \| \leq 2
\]

For a contradiction, let \( x \) be a unit vector such that \( \| (\Omega_1 \Omega_1^T)^{-1} x \| = \| y \| \geq 2 \). Then,

\[
\frac{\| ((\Omega_1 \Omega_1^T)^{-1} - I) y \|}{\| y \|} = \frac{\| x - y \|}{\| y \|} \geq \frac{\| x \| - \| y \|}{\| y \|} = 1 - \frac{1}{\| y \|} \geq \frac{1}{2}
\]

This contradicts the assumption that \( \| \Omega_1 \Omega_1^T - I \| < \frac{1}{2} \).

We now bound \( \| \Omega_2 \Omega_1^T \| \) by \( \| \Omega_2 \|^2 \| \Omega_1 \|^2 \). From Equation 6.7, we have that

\[
\| \Omega_1 \|^2 \leq \frac{3}{2}
\]

For the other term, we use

\[
\| V_2^T \Omega \|^2 \leq \| V_2 \|^2 \| \Omega \|^2 = \frac{m}{s}
\]

Tying this all together, we have that

\[
\| (I - P_{K_1 \Omega}) K \|^2 \leq \| \Sigma_2 \|^2 + \| \Sigma_2 \Omega_2 \Omega_1^T \|^2 \leq \sigma_{r+1}^2 + \| \Sigma_2 \|^2 \| \Omega_2 \Omega_1^T \|^2 (\Omega_1 \Omega_1^T)^{-1} \| \leq \sigma_{r+1}^2 + \sigma_{r+1}^2 \left( \frac{m}{s} \right) \left( 3 \frac{2}{2} \right)^2 \left( 1 + 6 \frac{m}{s} \right) \sigma_{r+1}^2
\]
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Fig. 4.3. **Singular values of the Gaussian kernel.** We report the compressibility of the far field by computing the singular values of $K$ for the Gaussian kernel. We draw $N = 10^5$ points from a standard normal distribution. We set $n = 500$ and $\xi = 1$. The specified values of $\kappa$ correspond to the bandwidths given in Table 4.3. The trend lines show $d = 4$ (blue), $d = 8$ (red), $d = 16$ (green), $d = 32$ (magenta), and $d = 64$ (black).
Fig. 4.4. **ID compression; Gaussian kernel; normal data, d = 4.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We draw $N = 10^5$ points from the 4-dimensional standard normal distribution and set $n = 500$. We use the bandwidth given in the subfigure captions and table 4.3. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.5. ID compression; Gaussian kernel; normal data, $d = 16$. We show the approximation error of the ID obtained from a subsampled matrix $K'$. We draw $N = 10^5$ points from the 16-dimensional standard normal distribution and set $n = 500$. We use the bandwidth given in the subfigure captions and table 4.3. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.6. ID compression; Gaussian kernel; normal data, $d = 64$. We show the approximation error of the ID obtained from a subsampled matrix $K'$. We draw $N = 10^5$ points from the 64-dimensional standard normal distribution and set $n = 500$. We use the bandwidth given in the subfigure captions and table 4.3. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.7. **ID compression; Gaussian kernel; low-dimensional data, \( d_i = 4, d_e = 1000 \).** We show the approximation error of the ID obtained from a subsampled matrix \( K' \). We draw \( N = 10^5 \) points from our low-dimensional data distribution with intrinsic dimension 4 and ambient dimension 1,000. We set \( n = 500 \). We use the bandwidth given in the subfigure captions and table 4.3. We set \( \epsilon = 10^{-2} \) and choose the rank \( r \) so that it is the smallest \( r \) such that \( \sigma_{r+1}(K)/\sigma_1(K) < \epsilon \). Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.8. **ID compression; Gaussian kernel; Color Histogram data.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We use the Color Histogram data set, with $N = 68,040$ and $d = 32$. We choose $x_c$ uniformly at random and set $n = 500$. We use the bandwidth given in the subfigure captions and table 4.5. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.

Fig. 4.9. **ID compression; Gaussian kernel; Color Moments data.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We use the Color Moments data set, with $N = 68,040$ and $d = 9$. We choose $x_c$ uniformly at random and set $n = 500$. We use the bandwidth given in the subfigure captions and table 4.5. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.10. **ID compression; Gaussian kernel; Cooc Texture data.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We use the Cooc Texture data set, with $N = 68,040$ and $d = 16$. We choose $x_c$ uniformly at random and set $n = 500$. We use the bandwidth given in the subfigure captions and table 4.5. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.

Fig. 4.11. **Singular values of the Laplace kernel.** We report the compressibility of the far field by computing the singular values of $K$ for the Laplace kernel. We draw $N = 10^5$ points from a standard normal distribution. We set $n = 500$ and $\xi$ in the subfigure captions. The trend lines show $d = 2$ (blue), $d = 3$ (red), $d = 4$ (green), and $d = 5$ (magenta).
Fig. 4.12. **ID compression; Laplace kernel; normal data.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We draw $N = 10^5$ points from the $d$-dimensional standard normal distribution ($d$ in subfigure captions) and set $n = 500$. We set $\xi = 2$. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.13. **Singular values of the polynomial kernel.** We report the compressibility of the far field by computing the singular values of $K$ for the polynomial kernel with $p = 2$. We draw $N = 10^5$ points from a standard normal distribution. We set $n = 500$ and $\xi = 1$. The specified values of $\kappa$ correspond to the bandwidths given in Table 4.3. The trend lines show $d = 4$ (blue), $d = 8$ (red), $d = 16$ (green), $d = 32$ (magenta), and $d = 64$ (black).
Fig. 4.14. **Singular values of the polynomial kernel.** We report the compressibility of the far field by computing the singular values of $K$ for the polynomial kernel with $p = 3$. We draw $N = 10^5$ points from a standard normal distribution. We set $n = 500$ and $\xi = 1$. The specified values of $\kappa$ correspond to the bandwidths given in Table 4.3. The trend lines show $d = 4$ (blue), $d = 8$ (red), $d = 16$ (green), $d = 32$ (magenta), and $d = 64$ (black).

Fig. 4.15. **ID compression; polynomial kernel; normal data, $h = 0.01$.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We draw $N = 10^5$ points from the $d$-dimensional standard normal distribution and set $n = 500$. We use $h = 0.01$. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.16. **ID compression; polynomial kernel; normal data, \( h = 100 \).** We show the approximation error of the ID obtained from a subsampled matrix \( K' \). We draw \( N = 10^5 \) points from the \( d \)-dimensional standard normal distribution and set \( n = 500 \). We use \( h = 100 \). We set \( \epsilon = 10^{-2} \) and choose the rank \( r \) so that it is the smallest \( r \) such that \( \sigma_r(K)/\sigma_1(K) < \epsilon \). Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.

Fig. 4.17. **ID compression; polynomial kernel; low-dimensional data, \( p = 2 \).** We show the approximation error of the ID obtained from a subsampled matrix \( K' \). We draw \( N = 10^5 \) points from our low-dimensional data distribution with intrinsic dimension \( 4 \) and ambient dimension \( 1,000 \). We set \( n = 500 \). We use the bandwidth given in the subfigure captions. We set \( \epsilon = 10^{-2} \) and choose the rank \( r \) so that it is the smallest \( r \) such that \( \sigma_r(K)/\sigma_1(K) < \epsilon \). Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.
Fig. 4.18. **ID compression; polynomial kernel; Color Histogram data.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We use the Color Histogram data set, with $N = 68,040$ and $d = 32$. We choose $x_c$ uniformly at random and set $n = 500$. We use the bandwidth given in the subfigure captions. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.

Fig. 4.19. **ID compression; polynomial kernel; Color Moments data.** We show the approximation error of the ID obtained from a subsampled matrix $K'$. We use the Color Moments data set, with $N = 68,040$ and $d = 32$. We choose $x_c$ uniformly at random and set $n = 500$. We use the bandwidth given in the subfigure captions. We set $\epsilon = 10^{-2}$ and choose the rank $r$ so that it is the smallest $r$ such that $\sigma_{r+1}(K)/\sigma_1(K) < \epsilon$. Each trend line represents a different subsampling method, with blue for the uniform distribution, red for distances, black for leverage, and green for the deterministic selection of nearest neighbors.