A Practical Guide to Randomized Matrix Computations with MATLAB Implementations

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Abstract

Matrix operations such as matrix inversion, eigenvalue decomposition, singular value decomposition are ubiquitous in real-world applications. Unfortunately, many of these matrix operations so time and memory expensive that they are prohibitive when the scale of data is large. In real-world applications, since the data themselves are noisy, machine-precision matrix operations are not necessary at all, and one can sacrifice a reasonable amount of accuracy for computational efficiency.

In recent years, a bunch of randomized algorithms have been devised to make matrix computations more scalable. Mahoney [16] and Woodruff [31] have written excellent but very technical reviews of the randomized algorithms. Differently, the focus of this manuscript is on intuition, algorithm derivation, and implementation. This manuscript should be accessible to people with knowledge in elementary matrix algebra but unfamiliar with randomized matrix computations. The algorithms introduced in this manuscript are all summarized in a user-friendly way, and they can be implemented in lines of MATLAB code. The readers can easily follow the implementations even if they do not understand the maths and algorithms.

Keywords: matrix computation, randomized algorithms, matrix sketching, random projection, random selection, least square regression, randomized SVD, matrix inversion, eigenvalue decomposition, kernel approximation, the Nyström method.

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1 Introduction

Matrix computation plays a key role in modern data science. However, matrix computations such as matrix inversion, eigenvalue decomposition, SVD, etc, are very time and memory expensive, which limits their scalability and applications. To make large-scale matrix computation possible, randomized matrix approximation techniques have been proposed and widely applied. Especially in the past decade, remarkable progresses in randomized numerical linear algebra has been made, and now large-scale matrix computations are no longer impossible tasks.

This manuscript reviews the most recent progresses of randomized matrix computation. The papers written by Mahoney [16] and Woodruff [31] provide comprehensive and rigorous reviews of the randomized matrix computation algorithms. However, their focus are on the theoretical properties and error analysis techniques, and readers unfamiliar with randomized numerical linear algebra can have difficulty when implementing their algorithms.

Differently, the focus of this manuscript is on intuitions and implementations, and the target readers are those who are familiar with basic matrix algebra but has little knowledge in randomized matrix computations. All the algorithms in this manuscript are described in a user-friend way. This manuscript also provides MATLAB implementations of the important algorithms. MATLAB code is easy to understand\(^1\), easy to debug, and easy to translate to other languages. The users can even directly use the provided MATLAB code without understanding it. The package of the MATLAB code in this paper is available at https://sites.google.com/site/zjuwss/randmatrix.

This manuscript covers the following topics:

- Section 2 briefly reviews some matrix algebra preliminaries. This section can be skipped if the reader is familiar with matrix algebra.
- Section 3 introduces the techniques for generating a sketch of a large-scale matrix.
- Section 4 studies the least square regression (LSR) problem where \( n \gg d \).
- Section 5 studies efficient algorithms for computing the \( k \)-SVD of arbitrary matrices.
- Section 6 introduces techniques for sketching symmetric positive semi-definite (SPSD) matrices. The applications includes spectral clustering, kernel methods (e.g. Gaussian process regression and kernel PCA), and second-order optimization (e.g. Newton’s method).

\(^1\)If your are unfamiliar with a MATLAB function, you can simply type “help + functionname” in MATLAB and read the documentation.
2 Elementary Matrix Algebra

This section defines the matrix notation and goes through the very basics of matrix decompositions. Particularly, the singular value decomposition (SVD), the QR decomposition, and the Moore-Penrose inverse are used throughout this manuscript.

2.1 Notation

Let $A = [a_{ij}]$ be a matrix, $a = [a_i]$ be a column vector, and $a$ be a scalar. The $i$-th row and $j$-th column of $A$ are denoted by $a_i$; and $a_j$, respectively. When there is no ambiguity, either column or row can be written as $a_l$. Let $I_n$ be the $n \times n$ identity matrix, that is, the diagonal entries are ones and off-diagonal entries are zeros. The column space (the space spanned by the columns) of $A$ is set of all possible linear combinations of its column vectors. Let $\{1, 2, \cdots, n\}$.

Let $\text{nnz}(A)$ be the number of nonzero entries of $A$.

The vector $\ell_2$ norm is defined by

$$\|a\|_2 = \sqrt{\sum_i a_i^2}.$$ 

The matrix Frobenius norm is defined by

$$\|A\|_F = \sqrt{\sum_{ij} a_{ij}^2},$$

and the matrix spectral norm is defined by

$$\|A\|_2 = \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}.$$

2.2 Matrix Decompositions

**QR decomposition.** Let $A$ be an $m \times n$ matrix with $m \geq n$. The QR decomposition of $A$ is

$$A = Q_A R_A.$$

The matrix $Q_A$ has orthonormal columns, that is, $Q_A^T Q_A = I_n$. The matrix $R_A$ is upper triangular, that is, for all $i < j$, the $(i, j)$-th entry of $R_A$ is zero.

**SVD.** Let $A$ be an $m \times n$ matrix and $\rho = \text{rank}(A)$. The condensed singular value decomposition (SVD) of $A$ is

$$A = U_{mA} \Sigma_A V_{nA}^T = \sum_{i=1}^{\rho} \sigma_{A,i} u_{A,i} v_{A,i}^T.$$

Here $\sigma_{A,1} \geq \cdots \geq \sigma_{A,\rho} > 0$ are the singular values, $u_{A,1}, \cdots, u_{A,\rho} \in \mathbb{R}^m$ are the left singular vectors, and $v_{A,1}, \cdots, v_{A,\rho} \in \mathbb{R}^n$ are the right singular vectors.
In applications such as the principal component analysis (PCA), latent semantic indexing (LSI), word2vec, spectral clustering, we are only interested in the top $k (\ll m, n)$ singular values and singular vectors. The rank $k$ truncated SVD ($k$-SVD) is denoted by

$$A_k := \sum_{i=1}^{k} \sigma_{A,i} u_{A,i} v_{A,i}^T = U_{A,k} \Sigma_{A,k} V_{A,k}^T.$$ 

Here $U_{A,k}$ consists of the first $k$ singular vectors of $U_A$, and $\Sigma_{A,k}$ and $V_{A,k}$ are analogously defined. Among all the $m \times n$ rank $k$ matrices, $A_k$ is the closest approximation to $A$ in that

$$A_k = \arg\min_{X} \| A - X \|_F^2 = \arg\min_{X} \| A - X \|_2^2, \quad \text{s.t. rank}(X) \leq k.$$ 

Eigenvalue decomposition. The eigenvalue decomposition of an $n \times n$ symmetric matrix $A$ is defined by

$$A = U_A \Lambda_A U_A^T = \sum_{i=1}^{n} \lambda_{A,i} u_{A,i} u_{A,i}^T.$$ 

Here $\lambda_{A,1} \geq \cdots \geq \lambda_{A,n}$ are the eigenvalues of $A$, and $u_{A,1}, \ldots, u_{A,n} \in \mathbb{R}^n$ are the corresponding eigenvectors. $A$ is called symmetric positive semidefinite (SPSD) if and only if all the eigenvalues are greater than or equal to zero. If $A$ is SPSD, the SVD and eigenvalue decomposition of $A$ are identical.

2.3 Matrix (Pseudo) Inverse and Orthogonal Projector

For an $n \times n$ square matrix $A$, the matrix inverse exists if $A$ is non-singular (rank($A$) = $n$). Let $A^{-1}$ be the inverse of $A$. Then $AA^{-1} = A^{-1}A = I_n$.

Only square and nonsingular (aka. full rank) matrices have inverse. For the general rectangular matrices or rank deficient matrices, matrix pseudo-inverse is used as a generalization of matrix inverse. The book [1] offers a comprehensive study of the pseudo-inverses.

The Moore-Penrose inverse is the most widely used pseudo-inverse, which is defined by

$$A^\dagger := V_A \Sigma_A^{-1} U_A^T.$$ 

Let $A$ be any $m \times n$ and rank $\rho$ matrix. Then

$$AA^\dagger = U_A \Sigma_A V_A^T V_A \Sigma_A^{-1} U_A^T = U_A U_A^T = I_{\rho}.$$ 

which is a orthogonal projector. It is because for any matrix $B$, the matrix $AA^\dagger B = U_A U_A^T B$ is the projection of $B$ onto the column space of $A$.

2.4 Time and Memory Costs

The time complexities of the matrix operations are listed in the following.

- Multiplying an $m \times n$ matrix $A$ by an $n \times p$ matrix $B$: $O(mnp)$ float point operations (flops) in general, and $O(p \cdot \text{nnz}(A))$ if $A$ is sparse. Here \text{nnz}(A) is the number of nonzero entries of $A$. 


• QR decomposition, SVD, or Moore-Penrose inverse of an $m \times n$ matrix ($m \geq n$): $O(mn^2)$ flops.

• $k$-SVD of an $m \times n$ matrix: $O(nmk)$ flops (assuming that the spectral gap and the logarithm of error tolerance are constant)

• Matrix inversion or full eigenvalue decomposition of an $n \times n$ matrix: $O(n^3)$ flops

• $k$-eigenvalue decomposition of an $n \times n$ matrix: $O(n^2k)$ flops.

**Pass-efficient** means that the algorithm goes constant passes through the data. For example, the Frobenius norm of a matrix can be computed pass-efficiently, because each entry is visited only once. In comparison, the spectral norm cannot be computed pass-efficiently, because the algorithm goes at least $\log \frac{1}{\epsilon}$ passes through the matrix, which is not constant. Here $\epsilon$ indicates the desired precision.

**Memory cost.** If an algorithm goes through a matrix for constant passes, the matrix can be placed in large volume disks and barely costs RAM space. However, if an algorithm goes through a matrix for many passes (not constant passes), the matrix should be placed in RAM, otherwise the swaps between RAM and disk would be highly expensive. In this manuscript, memory cost means the size of the matrices frequently visited by the algorithm.
3 Matrix Sketching

Let \( A \in \mathbb{R}^{m \times n} \) be the given matrix, \( S \in \mathbb{R}^{n \times s} \) be a sketching matrix, e.g. random projection or column selection matrix, and \( C = AS \in \mathbb{R}^{m \times s} \) be a sketch of \( A \). The size of \( C \) is much smaller than \( A \), but \( C \) preserves some important properties of \( A \).

3.1 Theoretical Properties

The sketching matrix is useful if it has either or both of the following properties. The two properties are important, and the readers should try to understand them.

Property 1 (Subspace Embedding) For a \( m \times n \) \((m \ll n)\) matrix \( A \) and all \( m \)-dimension vector \( y \), the inequality
\[
\frac{1}{\gamma} \leq \frac{\|y^T AS\|_2^2}{\|y^T A\|_2^2} \leq \gamma
\]
holds with high probability. Here \( S \) is some \( n \times s \) \((s \ll n)\) sketching matrix.

The subspace embedding property can be intuitively understood in the following way. For all \( n \)-dimensional vectors \( x \) in the row space of \( A \) (a rank \( m \) subspace within \( \mathbb{R}^n \)), the length of vector \( x \) does not change much after sketching: \( \|x\|_2 \approx \|xS\|_2 \). This property can be applied to speedup solving the \( \ell_2 \) regression problems.

Property 2 (Low-Rank Approximation) Let \( A \) be any \( m \times n \) matrix and \( k \) be any positive integer far smaller than \( m \) and \( n \). Let \( C = AS \in \mathbb{R}^{m \times s} \) where \( s \geq k \). The Frobenius norm error bound
\[
\|A - CC^\dagger A\|_F^2 \leq \eta\|A - A_k\|_F^2
\]
hold with high probability for some \( \eta \geq 1 \).

The following error bound is stronger and more interesting:
\[
\min_{\text{rank}(X) \leq k} \|A - CX\|_F^2 \leq \eta\|A - A_k\|_F^2
\]
because \( \|A - CC^\dagger A\|_F^2 \leq \min_{\text{rank}(X) \leq k} \|A - CX\|_F^2 \).

Intuitively speaking, the low-rank approximation property means that the columns of \( A_k \) are almost in the column space of \( C \). The low-rank approximation property enables us to solve \( k \)-SVD more efficiently (for \( k \leq s \)). Later on we will see that computing the \( k \)-SVD of \( CC^\dagger A \) is much less expensive than the \( k \)-SVD of \( A \).

The two properties can be verified by a few lines of MATLAB code. The readers are encouraged to have a try. With a proper sketching method and a relatively large \( s \), both \( \gamma \) and \( \eta \) should be near one.

\(^2\)Thus there always exists an \( m \) dimensional vector \( y \) such that \( x \) can be expressed as \( x = y^T A \).

\(^3\)Spectral norm bounds should be more interesting. However, spectral norm error is difficult to analyze, and existing spectral norm bounds are “weak” for their \( \eta \) are far greater than 1.
3.2 Random Projection

The subsection presents three matrix sketching techniques: Gaussian projection, subsampled randomized Hadamard transform (SRHT), and the count sketch. Gaussian projection and SRHT can be combined with the count sketch.

3.2.1 Gaussian Random Projection

The $n \times s$ Gaussian random projection matrix $S$ is a matrix formed by $S = \frac{1}{\sqrt{s}}G$, where each entry of $G$ is sampled i.i.d. from $\mathcal{N}(0,1)$. The Gaussian projection is also well known as the Johnson-Lindenstrauss transform due to the seminal work [15]. Gaussian projection can be implemented in four lines of MATLAB code.

```matlab
function [C] = GaussianProjection (A, s)
    n = size (A, 2);
    S = randn (n, s) / sqrt (s);
    C = A * S;
end
```

Gaussian projection has the following properties:

- Time cost: $O(mns)$
- Theoretical guarantees
  1. When $s = O(\epsilon^{-2}(m + \log \frac{1}{\delta}))$, the subspace embedding property with $\gamma = 1 + \epsilon$ holds with probability $\delta$.
  2. When $s = \frac{k}{\epsilon^2} + 1$, the low-rank approximation property with $\eta = 1 + \epsilon$ holds in expectation [2].
- Advantages
  1. Easy to implement: four lines of MATLAB code
  2. $C$ is a very high quality sketch of $A$
- Disadvantages:
  1. High time complexity to perform matrix multiplication
  2. Sparsity is destroyed: $C$ is dense even if $A$ is sparse

3.2.2 Subsampled Randomized Hadamard Transform (SRHT)

The Subsampled Randomized Hadamard Transform (SRHT) matrix is defined by $S = \frac{1}{\sqrt{sn}}DHnP$, where

- $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix with diagonal entries sampled uniformly from $\{+1, -1\}$;
**Algorithm 1** The Count Sketch.

1: input: $A \in \mathbb{R}^{m \times n}$
2: Initialize $C$ to be an $m \times s$ all-zero matrix;
3: for $i = 1$ to $n$ do
4:     sample $l$ from the set $[s]$ uniformly at random;
5:     sample $g$ from the set $\{+1, -1\}$ uniformly at random;
6:     update the $l$-th column of $C$ by $c_l \leftarrow c_l + ga_i$;
7: end for
8: return $C \in \mathbb{R}^{m \times s}$.

- $H_n \in \mathbb{R}^{n \times n}$ is defined recursively by
  $H_n = \begin{bmatrix} H_{n/2} & H_{n/2} \\ H_{n/2} & -H_{n/2} \end{bmatrix}$ and $H_2 = \begin{bmatrix} +1 & +1 \\ +1 & -1 \end{bmatrix}$.

For all $y \in \mathbb{R}^n$, the matrix vector product $y^T H_n$ can be performed in $O(n \log n)$ time by the fast Walsh–Hadamard transform algorithm in a divide-and-conquer fashion;

- $P \in \mathbb{R}^{n \times s}$ is a uniform sampling matrix.

SRHT can be implemented in nine lines of MATLAB code below. Notice that this implementation of SRHT is has $O(mN \log N)$ ($N \geq n$ is a power of two) time complexity, which is not efficient.

```matlab
function [C] = srht(A, s)
    n = size(A, 2);
    sgn = randi(2, [1, n]) * 2 - 3; % one half are +1 and the rest are -1
    A = bsxfun(@times, A, sgn); % flip the signs of each column w.p. 50%
    n = 2^ceil(log2(n));
    C = (fwht(A', n))'; % fast Walsh–Hadamard transform
    idx = sort(randsample(n, s));
    C = C(:, idx); % subsampling
    C = C * (n / sqrt(s));
end
```

The SRHT matrix has the following properties:

- Time complexity: the matrix product $AS$ can be performed in $O(mn \log s)$ time, which makes SRHT more efficient than Gaussian projection. (Unfortunately, the MATLAB code above does not have such low time complexity.)

- Theoretical property: when $s = O(\epsilon^{-2}(m + \log n) \log m)$, SRHT satisfies the subspace embedding property with $\gamma = 1 + \epsilon$ holds with probability 0.99 [31, Theorem 7].

### 3.2.3 The Count Sketch

The count sketch has similar properties as the Gaussian projection, and the count sketch can be applied very efficiently. The theoretical properties of the count sketch for matrix computation are established by Clarkson and Woodruff [6] and improved by some follow-up work.
The count sketch is described in Algorithm 1 and illustrated in Figure 1. The readers may have noticed that the count sketch does not explicitly form the sketching matrix $S$. In fact, $S$ is such a matrix that each row has only one nonzero entry, which is also illustrated. The count sketch can be implemented in 9 lines of MATLAB code.

```matlab
function [C] = CountSketch(A, s)
[m, n] = size(A);
sgn = randi(2, [1, n]) * 2 - 3;  % one half are +1 and the rest are -1
A = bsxfun(@times, A, sgn);  % flip the signs of each column w. p. 50%
l1 = randsample(s, n, true);  % sample n items from [s] with replacement
C = zeros(m, s);  % initialize C
for j = 1:n
    C(:, l1(j)) = C(:, l1(j)) + A(:, j);
end
```

The count sketch has the following properties:

- Time cost: $O(nnz(A))$
- Memory cost: $O(ms)$. When $A$ does not fit in memory, the algorithm keeps only $C$ in memory and goes one pass through the columns of $A$.
- Theoretical guarantees
  1. When $s = \tilde{O}\left(\frac{m^2}{\epsilon^2 \delta}\right)$, the subspace embedding property holds with $\gamma = 1 + \epsilon$ and probability $\delta$.
  2. When $s = \frac{2k}{\epsilon^2 \delta}$, the low-rank approximation property holds with $\eta = 1 + \epsilon$ relative error and probability $\delta$.
- Advantage: the count sketch is very efficient, especially when $A$ is sparse.
- Disadvantage: compared with Gaussian projection, the count sketch requires larger $s$ to attain the same accuracy. One simple improvement is to combine the count sketch with Gaussian projection or SRHT.
3.2.4 SRHT + CountSketch

Let $S_{cs}$ be $n \times s_{cs}$ count sketch matrix, $S_{srht}$ be $s_{cs} \times s$ SRHT matrix, and $S = S_{cs}S_{srht} \in \mathbb{R}^{n \times s}$. Let $s_{cs} = \tilde{O}(m^2 \epsilon^{-2})$ and $s = O(\epsilon^{-2}(\log m)(m + \log s_{cs})) = O(\epsilon^{-2}(\log m)(m + \log m/\epsilon))$. Then $S$ satisfies the following properties.

- **Time complexity:** the matrix product $AS$ can be computed in
  \[
  O\left(\frac{\text{nnz}(A)}{\text{count sketch}} + ms_{cs}\frac{\log s}{\text{SRHT}}\right) = \tilde{O}\left(\text{nnz}(A) + m^3 \epsilon^{-2} \log \frac{m}{\epsilon}\right)
  \]
  time.

- **Theoretical property:** the SRHT+CountSketch matrix $S$ satisfy the subspace embedding property with $\gamma = 1 + \epsilon$ holds with probability 0.99.

- **Advantages:**
  1. SRHT+CountSketch can be computed nearly as efficiently as the count sketch
  2. the size of SRHT+CountSketch is as small as SRHT

The theoretical property can be easily proved in the following way.

\[
\begin{align*}
(1 - \epsilon)^2\|y^T A\|_2^2 &\leq (1 - \epsilon)\|y^T AS_{cs}\|_2^2 \\
&\leq \|y^T (AS_{cs})_{srht}\|_2^2 \leq (1 + \epsilon)\|y^T AS_{cs}\|_2^2 \leq (1 + \epsilon)^2\|y^T A\|_2^2.
\end{align*}
\]

Here the inequalities all follows from the subspace embedding property of SRHT and the count sketch.

3.2.5 GaussianProjection + CountSketch

Let $S_{sc}$ be $n \times s_{cs}$ count sketch matrix, $S_{gp}$ be $s_{cs} \times s$ Gaussian projection matrix, and $S = S_{cs}S_{gp} \in \mathbb{R}^{n \times s}$. Then $S$ satisfies the following properties.

- **Time complexity:** the matrix product $AS$ can be computed in
  \[
  O\left(\frac{\text{nnz}(A)}{\text{count sketch}} + \frac{ms_{cs}s}{\text{Gaussian projection}}\right)
  \]
  time.

- **Theoretical properties:**
  1. When $s_{cs} = \tilde{O}(m^2 \epsilon^{-2})$ and $s = O(m \epsilon^{-2})$, the GaussianProjection+CountSketch matrix $S$ satisfy the subspace embedding property with $\gamma = 1 + \epsilon$ holds with probability 0.99.
  2. When $s_{cs} = O(k^2 + k/\epsilon)$ and $s = O(k/\epsilon)$, the GaussianProjection+CountSketch matrix $S$ satisfies the low-rank approximation property with $\eta = 1 + \epsilon$ [3, Lemma 12].

- **Advantages:**
  1. the size of GaussianProjection+CountSketch is as small as Gaussian projection
  2. the time complexity is much lower than Gaussian projection when $n \gg m$
  3. the implementation is easier than SRHT+CountSketch
3.3 Column Selection

This subsection presents three column selection techniques: uniform sampling, leverage score sampling, and local landmark selection. Different from random projection, column selection do not have to visit every entry of $A$, and column selection preserves the sparsity/non-negativity properties of $A$.

3.3.1 Uniform Sampling

Uniform sampling is the most efficient way to form a sketch. The most important advantage is that uniform sampling forms a sketch without seeing the whole data matrix. When applied to kernel methods, uniform sampling avoids computing every entry of the kernel matrix.

The performance of uniform sampling is data-dependent. When the leverage scores (defined in Section 3.3.2) are uniform, or equivalently, the matrix coherence (namely the greatest leverage score) is small, uniform sampling has good performance. The analysis of uniform sampling can be found in [12, 13].

3.3.2 Leverage Score Sampling

Before studying leverage score sampling, let’s first define leverage scores. Let $A$ be an $m \times n$ matrix, with $\rho = \text{rank}(A) < n$, and $V \in \mathbb{R}^{n \times \rho}$ be the right singular vectors. The (column) leverage scores of $A$ are defined by

$$l_i := \|v_i\|_2^2, \quad \text{for } i = 1, \cdots, n.$$

Leverage score sampling is to select each columns of $A$ with probability proportional to its leverage scores. (Sometimes each selected column should be scaled by $\sqrt{\frac{\rho}{s_i}}$.)

It can be roughly implemented in 8 lines MATLAB code.

```matlab
function [C, idx] = LeverageScoreSampling(A, s)
    n = size(A, 2);
    [~, ~, V] = svd(A, 'econ');
    leveragescores = sum(V.^2, 2);
    prob = leveragescores / sum(leveragescores);
    idx = randsample(n, s, true, prob);
    idx = unique(idx); % eliminate duplicates
    C = A(:, idx);
end
```

There are a few things to remark:

- To sample columns according to the leverage scores of $A_k$ where $k \ll m, n$, Line 3 can be replaced by

```matlab
[~, ~, V] = svds(A, k);
```

- Theoretical properties

1. When $s = O(m \log m + m \epsilon^{-1})$, the leverage score sampling satisfies the subspace embedding property with $\gamma = 1 + \epsilon$ holds with high probability [6].
2. When $s = k\epsilon^{-2} \log k$, the leverage score sampling (according to the leverage scores of $A_k$) satisfies the low-rank approximation property with $\eta = 1 + \epsilon$ [9].

- Computing the leverage scores is as expensive as computing SVD, so leverage score sampling is not a practical way to sketch the matrix $A$ itself.

- When the leverage scores are near uniform, there is little difference between uniform sampling and leverage score sampling.

### 3.3.3 Local Landmark Selection

Local landmark selection is a very effective heuristic for finding representative columns. Zhang & Kwok [33] proposed to let $k = s$ and run $k$-means or $k$-centroids clustering algorithm to cluster the columns of $A$ to $s$ class, and use the $s$ centroids as the sketch of $A$. This heuristic works very well in practice, though it has little theoretical guarantee.

There are several tricks to make the local landmark selection more efficient.

- One can simply solve $k$-centroids clustering approximately rather than accurately. For example, it is unnecessary to wait for $k$-centroids clustering to converge; run $k$-centroids for a few iterations suffices.

- When $n$ is large, one can uniformly sample a subset of the data, e.g. $\max\{0.2n, 20s\}$ data points, and perform local landmark selection on this smaller dataset.

- In supervised learning problems, each datum $a_i$ is associated with a label $y_i$. We can partition the data to $g$ groups according to the labels and run $k$-centroids clustering for each group. In this way, $s = gk$ data points are selected as a sketch of $A$. 

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4 Least Square Regression

Let $A$ be an $n \times d$ ($n \geq d$) matrix whose rows correspond to data and rows corresponds to features, and let $b \in \mathbb{R}^{n}$ contain the response/label of each datum. The least square regression (LSR)

$$\min_{x} \|Ax - b\|_{2}^{2}$$

is a ubiquitous problem in statistics, computer science, economics, etc. When $n \gg d$, LSR can be solved efficiently using randomized algorithms.

4.1 Standard Solutions

The least square regression (LSR) problem (1) has closed form solution

$$x^{\ast} = A^{\dagger}b.$$ 

The Moore-Penrose inverse can be computed by SVD which costs $O(nd^{2})$ time.

LSR can also be solved by numerical algorithms such as the conjugate gradient (CG) algorithm, and machine-precision can be attained in a reasonable number of iterations. Let $\kappa(A) := \sigma_{1}(A)/\sigma_{d}(A)$ be the condition number of $A$. The convergence of CG depends on $\kappa(A)$:

$$\frac{\|A(x^{(t)} - x^{\ast})\|_{2}^{2}}{\|A(x^{(0)} - x^{\ast})\|_{2}^{2}} \leq 2 \left( \frac{\kappa(A) - 1}{\kappa(A) + 1} \right)^{t},$$

where $x^{(t)}$ is the model in the $t$-th iteration of CG. The per-iteration time cost of CG is $O(nnz(A))$. To attain $\|A(x^{(t)} - x^{\ast})\|_{2}^{2} \leq \epsilon$, the number of iteration is roughly

$$\left( \log \frac{1}{\epsilon} + \log(\text{InitialError}) \right) \frac{\kappa(A) - 1}{2}.$$ 

Since the time cost of CG heavily depends on the unknown condition number $\kappa(A)$, CG can be very slow if $A$ is ill-conditioned.

4.2 Inexact Solution

Any sketching matrix $S \in \mathbb{R}^{n \times s}$ can be used to solve LSR approximately as long as it satisfies the subspace embedding property. We consider the following LSR problem:

$$\tilde{x} = \min_{x} \| (S^{T}A)x - S^{T}b \|_{2}^{2},$$

which can be solved in $O(sd^{2})$ time.

If $S$ is a Gaussian projection matrix, SRHT matrix, count sketch, or leverage score sampling matrix, and $s = \text{poly}(d/\epsilon)$ for any error parameter $\epsilon \in (0, 1)$, then

$$\|A\tilde{x} - b\|_{2}^{2} \leq (1 + \epsilon)^{2} \min_{x} \|Ax - b\|_{2}^{2}$$

is guaranteed.
4.2.1 Implementation

If \( S \) is the count sketch matrix, the inexact LSR algorithm can be implemented in 5 lines of MATLAB code. Here CountSketch is a MATLAB function described in Section 3.2.3. The total time cost is \( O(\text{nnz}(A) + \text{poly}(d/\epsilon)) \) and memory cost is \( O(\text{poly}(d/\epsilon)) \), which are lower than the cost of exact LSR when \( d \ll n \).

```matlab
function [xtilde] = InexactLSR(A, b, s)
    d = size(A, 2);
    sketch = (CountSketch([A; b], s))';
    Asketch = sketch(:, 1:d); % Asketch = S' \cdot A
    bsketch = sketch(:, end); % bsketch = S' \cdot b
    xtilde = Asketch \ bsketch;
end
```

There are a few things to remark:
- The inexact LSR is useful only when \( n > \text{poly}(d/\epsilon) \).
- The size of sketch \( s \) is a polynomial function of \( 1/\epsilon \) rather than logarithm of \( 1/\epsilon \), thus the algorithm cannot attain high precision.

4.2.2 Theoretical Explanation

By the subspace embedding property, it can be easily shown that \( \tilde{x} \) is a good solution. Let \( D = [A, b] \in \mathbb{R}^{n \times (d+1)} \) and \( z = [x; -1] \in \mathbb{R}^{n+1} \). Then

\[
A \tilde{x} - b = Dz \quad \text{and} \quad S^T A \tilde{x} - S^T b = S^T Dz,
\]

and the subspace embedding property indicates \( \frac{1}{\eta} \|Dz\|_2^2 \leq \|S^T Dz\|_2^2 \leq \eta \|Dz\|_2^2 \) for all \( z \). Thus

\[
\frac{1}{\eta} \|\tilde{x} - b\|_2^2 \leq \|S^T (\tilde{x} - b)\|_2^2 \quad \text{and} \quad \|S^T (Ax^* - b)\|_2^2 \leq \eta \|Ax^* - b\|_2^2.
\]

The optimality of \( \tilde{x} \) indicates \( \|S^T (\tilde{x} - b)\|_2^2 \leq \|S^T (Ax^* - b)\|_2^2 \), and thus

\[
\frac{1}{\eta} \|\tilde{x} - b\|_2^2 \leq \|S^T (\tilde{x} - b)\|_2^2 \leq \|S^T (Ax^* - b)\|_2^2 \leq \eta \|Ax^* - b\|_2^2.
\]

\[\Rightarrow \|\tilde{x} - b\|_2^2 \leq \eta^2 \|Ax^* - b\|_2^2.\]

If \( S \) is a Gaussian projection matrix, SRHT matrix, count sketch, or leverage score sampling matrix, and \( s = \text{poly}(d/\epsilon) \) for any error parameter \( \epsilon \in (0, 1] \), then \( \eta = 1 + \epsilon \) is guaranteed. Hence

\[\|\tilde{x} - b\|_2^2 \leq (1 + \epsilon)^2 \min_x \|Ax - b\|_2^2.\]

4.3 Machine-Precision Solution

Randomized algorithms can also be applied to find machine-precision solution to LSR, and the time complexity is lower than the standard solutions.
4.3.1 Basic Idea: Preconditioning

We have discussed previously that the time cost of the conjugate gradient (CG) algorithm is roughly
\[ \frac{\kappa(A) - 1}{2} \left( \log \frac{1}{\epsilon} + \log(\text{InitialError}) \right) \text{nnz}(A), \]
which depends on the condition number of \( A \). To make CG efficient, one can find a \( d \times d \) preconditioning matrix \( T \) such that \( \kappa(AT) \) is small, solve
\[ z^* = \arg\min_z \| (AT)z - b \|_2^2 \]
by CG, and let \( x^* = Tz^* \). In this way, the time cost of CG is roughly
\[ \frac{\kappa(AT) - 1}{2} \left( \log \frac{1}{\epsilon} + \log(\text{InitialError}) \right) \text{nnz}(A). \]
If \( \kappa(AT) \) is a small constant, e.g. \( \kappa(AT) = 2 \), then (3) can be very efficiently solved by CG.

Now let’s consider how to find the preconditioning matrix \( T \). Suppose (unreasonably) that the upper triangular matrix of the QR decomposition \( A = QA_R \) is known to us. Then \( T = R_A^{-1} \) is a perfect preconditioning matrix because \( \kappa(A R_A^{-1}) = \kappa(Q_A) = 1 \). Unfortunately, the preconditioning matrix \( T = R_A^{-1} \) is not a practical choice because computing the QR decomposition is as expensive as solving LSR.

Woodruff [31] proposed to use sketching to find \( R_A \) approximately in \( O(\text{nnz}(A) + \text{poly}(d)) \) time. Let \( S \) be a sketching matrix and let \( S^T A = \tilde{Q}_A \tilde{R}_A \) be the QR decomposition of \( S^T A \). Using the subspace embedding property, one can easily show that \( \kappa(\tilde{A} \tilde{R}_A^{-1}) \) is close to one, and thus \( \tilde{R}_A^{-1} \) is a good preconditioning matrix.

4.3.2 Algorithm Description

The algorithm is described in Algorithm 2. If \( S_1 \) and \( S_2 \) are both count sketch matrices, the LSR problem can be solved up to an \( 1 + \epsilon \) factor with probability 0.9 in
\[ O \left( \text{nnz}(A) \log \frac{n}{\epsilon} + d^3 \log^2 d + d^2 \log \frac{1}{\epsilon} \right) \]
time [31, Theorem 24]. The analysis of the algorithm exploits the subspace embedding property.

Line 10 in the algorithm should be cautiously implemented. Do not compute the matrix product \( AT \) because it would take \( O(\text{nnz}(A) d) \) time! For example, Line 10 can be implemented by the following gradient descent iteration or its variants.
\[
\begin{align*}
  r & \leftarrow b - A T z^{(t)}; \quad /\!/ \text{the residual} \\
  z^{(t+1)} & \leftarrow z^{(t)} + T^T A^T r. \quad /\!/ \text{gradient descent}
\end{align*}
\]
In this way, the matrix product \( AT \) is never performed.

\[ ^4 \text{Since } AT \text{ is well conditioned, the vanilla gradient descent and CG has little difference.} \]
Algorithm 2 Machine-Precision Solution to LSR.

1: \textbf{input:} $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^n$.
2: // Find an initial solution with constant factor bound
3: Draw a sketching matrix $S_1 \in \mathbb{R}^{n \times \text{poly}(d)}$;
4: $x^{(0)} = \arg\min_x \| (S_1^T A) x - (S_1^T b) \|_2^2$;
5: // Find a preconditioning matrix
6: Draw a sketching matrix $S_2 \in \mathbb{R}^{n \times \text{poly}(d)}$;
7: $QR$ decomposition $[\tilde{Q}_A, \tilde{R}_A] = \text{qr}(S_2^T A)$;
8: Let the preconditioning matrix be $T = \tilde{R}_A^{-1} A \in \mathbb{R}^{d \times d}$;
9: // CG algorithm with preconditioning
10: Solve $z^* = \arg\min_z \| A T z - b \|_2^2$ by the CG algorithm, which takes $x^{(0)}$ as the initial solution;
11: \textbf{return} $x^* = T z^* \in \mathbb{R}^d$.

4.4 Extensions

This subsection considers two extensions of the standard LSR problem\cite{1}. The first extension will be used to make randomized $k$-SVD more efficient. The second extension will be applied to the SPSD matrix sketching problem.

4.4.1 Extension 1

The LSR problem described previously is a special case of

$$X^* = \arg\min_X \| A \bar{X} - B \|_F^2,$$

where $m = 1$. This problem can be solved by the algorithms described in Section 4.2 and 4.3. Particularly, we can draw a sketching matrix $S \in \mathbb{R}^{n \times s}$ and solve the smaller-scale problem

$$\tilde{X} = \arg\min_X \| S^T A \tilde{X} - S^T B \|_F^2,$$

to obtain an inexact solution. Clarkson & Woodruff \cite[Theorem 46]{6} showed that using the SRHT+CountSketch matrix (see Section 3.2.4) $S$ with $s_{cs} = O(d^2 \log^6 d + \frac{d^2}{\epsilon})$ and $s = O(\frac{d^2 \log d}{\epsilon})$ ensures $1 + \epsilon$ relative error.

4.4.2 Extension 2

A more complicated problem has also been considered in the literature \cite{23, 27, 22}:

$$X^* = \arg\min_X \| A \bar{X} \bar{C} - B \|_F^2,$$

where $n, m \geq d_1, d_2$. The solution is:

$$X^* = A^\dagger B C^\dagger,$$

which cost $O(mn \cdot \min\{d_1, d_2\})$ time. Wang et al. \cite{28} proposed an algorithm to solve (4) up to $1 + \epsilon$ relative error in

$$O(d_1 d_2 \epsilon^{-1} \min\{m, n\} \min\{d_1, d_2\}).$$
time, which is useful when $\max\{m, n\} \gg d_1, d_2$. The basic idea is to solve

$$\hat{X} = \arg\min_X \| S_1^T (AXC - B) S_2 \|_F^2$$

where $S_1$ and $S_2$ are column sampling matrices. The algorithm can be implemented in 4 lines of MATLAB code:

```matlab
function [Xtilde] = InexactGeneralizedLSR(A, C, B, s1, s2)
    [~, idxA] = LeverageScoreSampling(A', s1);
    [~, idxC] = LeverageScoreSampling(C, s2);
    Xtilde = pinv(A(idxA, :)) * B(idxA, idxC) * pinv(C(:, idxC));
end
```

Here $s_1 = \sqrt{q d_1 \epsilon^{-1/2}}$, $s_2 = \sqrt{q d_2 \epsilon^{-1/2}}$, $q = \min\{m, n\}$, and the function “LeverageScoreSampling” is described in Section 3.3.2. Empirically, setting $s_1 = s_2 = \mathcal{O}(d_1 + d_2)$ suffices for high precision. The experiments in [28] also indicates that uniform sampling has nearly the same performance as leverage score sampling.
5  Rank $k$ Singular Value Decomposition

This section considers the $k$-SVD of a large scale matrix $A \in \mathbb{R}^{m \times n}$, which may not fit in memory.

5.1  Standard Solutions

The standard solutions to $k$-SVD include the power iteration algorithm and the Krylov subspace methods. Their time complexities are considered to be $\tilde{O}(mnk)$, where the $\tilde{O}$ notation hides parameters such as the spectral gap and logarithm of error tolerance. Here we introduce a simplified version of the block Lanczos method \cite{18} which costs time $O(mnkq)$, where $q = \log \frac{n}{\epsilon}$ is the number of iterations, and the inherent constant depends weakly on the spectral gap. The block Lanczos algorithm is described in Algorithm 3 can be implemented in 17 lines of MATLAB code.

```matlab
function [U, S, V] = BlockLanczos(A, k, q)
    s = 2 * k;  \% can be tuned
    [m, n] = size(A);
    C = A * randn(n, s);
    Krylov = zeros(m, s * q);
    Krylov(:, 1:s) = C;
    for i = 2:q
        C = A' * C;
        C = A * C;
        Krylov(:, (i-1)*s+1: i*s) = C;
    end
    [Q, ~] = qr(Krylov, 0);
    [Ubar, S, V] = svd(Q' * A, 'econ');
    Ubar = Ubar(:, 1:k);
    S = S(1:k, 1:k);
    V = V(:, 1:k);
    U = Q * Ubar;
end
```

Although the block Lanczos algorithm can attain machine precision, it inevitably goes many passes through $A$, and it is thus slow when $A$ does not fit in memory.

Facing large-scale data, we must trade off between precision and computational costs. We are particularly interested in approximate algorithm that satisfies:

1. The algorithm goes constant passes through $A$. Then $A$ can be stored in large volume disks, and there are only constant swaps between disk and RAM.

2. The algorithm only keeps a small-scale sketch of $A$ in memory.

3. The time cost is $O(mnk)$ or lower.

5.2  A Prototype Randomized $k$-SVD Algorithm

This subsection describes a randomized algorithm that computes the $k$-SVD of $A$ up to $1 + \epsilon$ Frobenius norm relative error. The algorithm is proposed by \cite{14}, and it is described in Algorithm 4.

\footnote{We introduce this algorithm because it is easy to understand. However, as $q$ grows, columns of the Krylov matrix gets increasingly linearly dependent. Thus there are many numerical treatments to strengthen stability (see the numerical stable algorithms in \cite{21}).}
Here the second equality is a well known fact. The matrix $A_k$ is well approximated by $\hat{A}_k := Q_C X^*,$ so we need only to find the $k$-SVD of $\hat{A}_k$:

$$\hat{A}_k := Q_C X^* = Q_C (Q_C^T A)_k = Q_C U \Sigma V^T = \tilde{U} \tilde{\Sigma} \tilde{V}^T.$$
It is easy to check that \( \tilde{U} \) and \( \tilde{V} \) have orthonormal columns and \( \tilde{\Sigma} \) is a diagonal matrix. Notice that the accuracy of the randomized \( k \)-SVD depends only on the quality of the sketch matrix \( C \).

### 5.2.3 Implementation

The algorithm is described in Algorithm 4 and can be implemented in 5 lines of MATLAB code. Here \( s = O(\frac{k}{\epsilon}) \) is the size of the sketch.

```matlab
function [Utilde, Stilde, Vtilde] = ksvdPrototype(A, k, s)
C = CountSketch(A, s);
[Q, R] = qr(C, 0);
[Ubar, Stilde, Vtilde] = svds(Q’*A, k);
Utilde = Q*Ubar;
```

Empirically, using “svd(Q’*A, ‘econ’)” followed by discarding the \( k+1 \) to \( s \) components should be faster than the “svds” function in Line 4.

The algorithm has the following properties:

1. The algorithm goes 2 passes through \( A \);
2. The algorithm only keeps an \( m \times O(\frac{k}{\epsilon}) \) sketch \( C \) in memory;
3. The time cost is \( O(\text{nnz}(A)k/\epsilon) \).

### 5.3 Faster Randomized \( k \)-SVD

The prototype algorithm spends most of its time on solving (6); if (6) can be solved more efficiently, the randomized \( k \)-SVD can be even faster. The readers may have noticed that (6) is the least square regression (LSR) problem discussed in Section 4.4.1. Yes, we can solve (6) efficiently by the inexact LSR algorithm presented in the previous section.

#### 5.3.1 Theoretical Explanation

Now we draw a \( m \times p \) RSHT+CountSketch (or GaussianProjection+CountSketch) matrix \( P \) and solve this problem:

\[
\tilde{X} = \arg\min_{\text{rank}(X) \leq k} \left\| P^T Q C X - P^T A \right\|_F^2. \tag{7}
\]

To understand this trick, the readers can retrospect the extension of LSR in Section 4.4.1. Let

\[
P = \underbrace{P_{cs}}_{m \times p_{cs}} \underbrace{P_{srht}}_{p_{srht} \times p},
\]

where \( p_{cs} = s^2 \log^6 \frac{s}{\epsilon} + \frac{s}{\epsilon} \) and \( p = \frac{s}{\epsilon} \log \frac{s}{\epsilon} \). The subspace embedding property of RSHT+CountSketch [6, Theorem 46] implies that

\[
(1 + \epsilon)^{-1} \| Q C \tilde{X} - A \|_F^2 \leq \| P^T (Q C \tilde{X} - A) \|_F^2 \leq \| P^T (Q C X^* - A) \|_F^2 \leq (1 + \epsilon) \| Q C X^* - A \|_F^2,
\]

\[
\Rightarrow \| Q C \tilde{X} - A \|_F^2 \leq (1 + \epsilon)^2 \| Q C X^* - A \|_F^2 \leq (1 + \epsilon)^3 \| A - A_k \|_F^2.
\]
Algorithm 5 Faster Randomized k-SVD Algorithm.

1: **Input:** an $m \times n$ matrix $A$ and the target rank $k$.
2: Set the parameters as $s = O(\frac{1}{\epsilon^2})$, $p_{cs} = s^2 \log^6 \frac{n}{\epsilon^2}$, and $p = \frac{s}{\epsilon^2} \log \frac{n}{\epsilon}$.
3: Draw a $n \times s$ count sketch matrix $S$ and perform sketching: $C = AS$.
4: Draw an $m \times p_{cs}$ count sketch matrix $P_{cs}$ and an $p_{cs} \times p$ matrix $P_{srht}$.
5: Perform Sketching: $D = P^T_{srht} P^T_{cs} C \in \mathbb{R}^{p \times s}$ and $L = P^T_{srht} P^T_{cs} A \in \mathbb{R}^{p \times n}$.
6: QR decomposition: $[Q_D, R_D] = qr(D)$.
7: k-SVD: $(\tilde{U}, \hat{\Sigma}, \tilde{V}) = svds(Q_D L, k)$.
8: SVD: $(\hat{U}, \hat{\Sigma}, \hat{V}) = svd(C R_D^T U \hat{\Sigma})$.
9: $\tilde{V} = \hat{V} \hat{V}_t$.
10: return $U \hat{\Sigma} \hat{V}^T \approx A_k$.

Here the second inequality follows from the optimality of $\tilde{X}$, and the last inequality follows from the low-rank approximation property of the sketch $C = AS$. Thus, by solving (7) we get k-SVD up to $1 + O(\epsilon)$ Frobenius norm relative error.

5.3.2 Algorithm Derivation

The faster randomized k-SVD is described in Algorithm 5 and derived in the following. The algorithm solves

$$\tilde{X} = \arg\min_{\text{rank}(X) \leq k} \left\| P^T C X - P^T A \right\|_F^2$$

(8)
to obtain the rank $k$ matrix $\tilde{X} \in \mathbb{R}^{c \times n}$, and approximates $A_k$ by

$$A_k \approx C \tilde{X}$$

Define $D = P^T C$, $L = P^T A$, and let $Q_D R_D = D$ be the QR decomposition. Then (8) becomes

$$\tilde{X} = \arg\min_{\text{rank}(X) \leq k} \left\| D_{p \times s} X - L_{s \times n} \right\|_F^2 = D^T Q_D (Q_D^T L)_k = R_D^T (Q_D^T L)_k$$

Based on the defined notation, we decompose $A_k \approx C \tilde{X}$ by

$$A_k \approx C \tilde{X} = CR_D^T (Q_D^T L)_k = CR_D^T U \hat{\Sigma} \tilde{V}^T = \hat{U} \hat{\Sigma} \tilde{V}^T = \hat{U} \hat{\Sigma} \hat{V}^T = \hat{U} \hat{\Sigma} \hat{V}_t^T \hat{V}_t^T.$$

\[\text{Instead, we can solve (7) to approximate } A_k \text{ by } Q_C \tilde{X}. \text{ However, this requires the QR decomposition of } C \text{ which is expensive in practice.}\]
5.3.3 Implementation

The faster randomized $k$-SVD is described in Algorithm 5 and implemented in 18 lines of MATLAB code. For simplicity of implementation, we use Gaussian projection in place of SRHT.

```matlab
function [Utilde, Stilde, Vtilde] = ksvdFaster(A, k, s, p1, p2)
    n = size(A, 2);
    C = CountSketch(A, s);
    A = [A, C];
    A = A';
    sketch = CountSketch(A, p1);
    clear A % A (m-by-n) will not be used
    sketch = GaussianProjection(sketch, p2);
    sketch = sketch';
    L = sketch(:, 1:n);
    D = sketch(:, n+1:end);
    clear sketch % sketch (p2-by-(n+c)) will not be used
    [QD, RD] = qr(D, 0);
    [Ubar, Sbar, Vbar] = svds(QD' * L, k);
    clear L % L (p2-by-n) will not be used
    C = C * (pinv(RD) * (Ubar * Sbar));
    [Utilde, Stilde, Vhat] = svd(C, 'econ');
    Vtilde = Vbar * Vhat;
```

There are a few things to remark:

1. The algorithm goes only two passes through $A$.
2. The algorithm costs time $O(\text{nnz}(A) + (m + n)\text{poly}(k/\epsilon))$.
3. The parameters should be set as $k < s < p2 < p1 \ll m, n$.
4. Line 8 can be removed or replaced by other sketching methods.
5. “$A$”, “sketch”, and “$L$” are the most memory expensive variables in the program, but fortunately, they are swept only one or two passes. If “$A$”, “sketch”, and “$L$” do not fit in RAM, they should be stored in disk and loaded to RAM block-by-block to perform computations.
6. Unless both $m$ and $n$ are large enough, this algorithm may be slower than the prototype algorithm.
6 SPSD Matrix Sketching

This section considers SPSD matrix \( K \in \mathbb{R}^{n \times n} \), which can be a kernel matrix, a social network graph, a Hessian matrix, or a Fisher information matrix. Our objective is to find a low-rank decomposition \( K \approx LL^T \). (Notice that \( LL^T \) is always SPSD, no matter what \( L \) is.) If \( K \) is symmetric but not SPSD, it can be approximated by \( K \approx CZC^T \) where \( Z \) is symmetric but not necessarily SPSD.

6.1 Motivations

This subsection provides three motivation examples to show why we seek to sketch \( K \) by \( K \approx LL^T \) or \( K \approx CZC^T \).

6.1.1 Forming a Kernel Matrix

In the kernel approximation problems, we are given

- an \( n \times d \) matrix \( X \), whose rows are data points \( x_1, \ldots, x_n \in \mathbb{R}^d \),
- a kernel function, e.g. the Gaussian RBF kernel function defined by

\[
\kappa(x_i, x_j) = \exp\left(-\frac{1}{2\sigma^2} \|x_i - x_j\|_2^2\right)
\]

where \( \sigma > 0 \) is the kernel width parameter.

The RBF kernel matrix can be computed by the following MATLAB code:

```matlab
function [K] = rbf(X1, X2, sigma)
K = X1 * X2';
X1_row_sq = sum(X1.^2, 2) / 2;
X2_row_sq = sum(X2.^2, 2) / 2;
K = bsxfun(@minus, K, X1_row_sq);
K = bsxfun(@minus, K, X2_row_sq');
K = K / (sigma^2);
K = exp(K);
end
```

If \( X_1 \) and \( X_2 \) are respectively \( n_1 \times d \) and \( n_2 \times d \) matrices, then the output of “rbf” is an \( n_1 \times n_2 \) matrix.

Kernel methods requires forming the \( n \times n \) kernel matrix \( K \) whose the \((i, j)\)-th entry is \( \kappa(x_i, x_j) \).

The RBF kernel matrix can be computed by the MATLAB function

```matlab
K = rbf(X, X, sigma)
```

in \( O(n^2d) \) time.

In presence of millions of data points, it is prohibitive to form such a kernel matrix. Fortunately, a sketch of \( K \) can be obtained very efficiently. Let \( S \in \mathbb{R}^{n \times s} \) be a uniform column selection matrix described in Section 3.3, then \( C = KS \) can be obtained in \( O(nsd) \) time by the following MATLAB code.

---

\(^7\)The local landmark selection is sometimes a better choice. Do not use random projections, because they inevitably visit every entry of \( K \).
function [C] = rbfSketch(X, sigma, s)
    n = size(X, 1);
    idx = sort(randsample(n, s));
    C = rbf(X, X(idx,:), sigma);

6.1.2 Matrix Inversion

Let $K$ be an $n \times n$ kernel matrix, $y$ be an $n$ dimensional vector, and $\alpha$ be a positive constant. Kernel methods such as the Gaussian process regression (or the equivalent the kernel ridge regression) and the least square SVM require solving

$$(K + \alpha I_n)w = y$$

to obtain $w \in \mathbb{R}^n$. The exact solution costs $O(n^3)$ time and $O(n^2)$ memory.

If we have a rank $l$ approximation $K \approx LL^T$, then $w$ can be approximately obtained in $O(nl^2)$ time and $O(nl)$ memory. Here we need to apply the Sherman-Morrison-Woodbury matrix identity

$$(A + BCD)^{-1} = A^{-1} - A^{-1}B(C^{-1} + DA^{-1}B)^{-1}DA^{-1}.$$  

We expand $(LL^T + \alpha I_n)^{-1}$ by the above identity and obtain

$$(LL^T + \alpha I_n)^{-1} = \alpha^{-1}I_n - \alpha^{-1}L(\alpha I_l + L^T L)^{-1}L^T,$$

and thus

$$w = (K + \alpha I_n)^{-1}y \approx \alpha^{-1}y - \alpha^{-1}L(\alpha I_l + L^T L)^{-1}L^T y.$$  

The matrix inversion problem not only appears in the kernel methods, but also in the second order optimization problems. Newton’s method and the so-called natural gradient method require computing $H^{-1}g$, where $g$ is the gradient and $H$ is the Hessian matrix or the Fisher information matrix. Since low-rank matrices are not invertible, the naive low-rank approximation $H \approx CZC^T$ does not work. To make matrix inversion possible, one can use the spectral shifting trick of [26]: fix a small constant $\alpha > 0$, form the low-rank approximation $H - \alpha I_n \approx CZC^T$, and compute $H^{-1}g \approx (CZC^T + \alpha I_n)^{-1}g$. Besides the low-rank approximation approach, one can approximate $H$ by a block diagonal matrix or even its diagonal, because it is easy to invert a diagonal matrix or a block diagonal matrix.

6.1.3 Eigenvalue Decomposition

With the low-rank decomposition $K \approx LL^T$ at hand, we first approximately decompose $K$ by

$$K \approx LL^T = (U_L \Sigma_L V_L^T)(U_L \Sigma_L V_L^T)^T = U_L \Sigma_L^2 U_L^T,$$

and then discard the $k + 1$ to $l$ components in $U_L$ and $\Sigma_L$. Here $L = U_L \Sigma_L V_L^T$ is the SVD of $L$, which can be obtained in $O(nl^2)$ time and $O(nl)$ memory. In this way, the rank $k$ ($k \leq \text{rank}(L)$) eigenvalue decomposition is approximately computed.
6.2 A Prototype Algorithm

From now on, we will consider how to find the low-rank approximation $K \approx LL^T$. As usual, the simplest approach is to form a sketch $C = KS \in \mathbb{R}^{n \times s}$ and solve

$$\mathbf{X}^* = \min_{\mathbf{X}} \|K - CXC^T\|_F^2 = C^T K (C^T)^T \quad \text{or} \quad \mathbf{Z}^* = \min_{\mathbf{Z}} \|K - QCZC\|_F^2 = Q^T C K Q C,$$

where $Q_C$ is the orthonormal bases of $C$ computed by SVD or QR decomposition. It is obvious that $CX^* = Q_C Z^* Q^T_C$. In this way, a rank $c$ approximation to $K$ is obtained. This approach is first studied by [14]. Wang et al. [26] showed that if $C$ contains $s = \mathcal{O}(k/\epsilon)$ columns of $K$ chosen by adaptive sampling, the error bound

$$\mathbb{E}\|K - Q_C Z^* Q^T_C\|_F^2 \leq (1 + \epsilon)\|K - K_k\|_F^2$$

is guaranteed. Other sketching methods can also be applied, although currently they do not have $1 + \epsilon$ error bound. In the following we implement the prototype algorithm (with the count sketch) in 5 lines of MATLAB code. Since the algorithm goes only two passes through $K$, when $K$ does not fit in memory, we can store $K$ in the disk and keep one block of $K$ in memory at a time. In this way, $\mathcal{O}(ns)$ memory is enough.

```matlab
function [QC, Z] = spsdPrototype(K, s)
n = size(K, 2);
C = CountSketch(K, s);
[QC, ~] = qr(C, 0);
Z = QC' * K * QC;
```

Despite its simplicity, the algorithm has several drawbacks.

- The time cost of this algorithm is $\mathcal{O}(ns^2 + \text{nnz}(K)s)$, which can be quadratic in $n$.
- The algorithm must visit every entry of $K$, which can be a serious drawback when applied to kernel methods. It is because computing the kernel matrix $K$ costs $\mathcal{O}(n^2 d)$ time, where $d$ is the dimension of the data points.

Therefore, we are interested in computing a low-rank approximation in linear time (w.r.t. $n$) and avoiding visiting every entry of $K$.

6.3 Faster SPSD Matrix Sketching

The readers may have noticed that (9) is the problem studied in Section 4.4.2. We can thus draw a column selection matrix $P \in \mathbb{R}^{n \times p}$ and approximately solve (9) by

$$\tilde{Z} = \min_{\tilde{Z}} \|P^T (K - Q_C Z Q_C) P\|_F^2 = \left(\mathbf{P}^T Q_C\right)^\dagger \mathbf{P}^T K \mathbf{P} \left(\mathbf{Q}_C^T \mathbf{P}\right)^\dagger.$$

Then we can approximate $K$ by $Q_C \tilde{Z} Q_C^T$. We describe the faster SPSD matrix sketching in Algorithm 6.

There are a few things to remark.
Algorithm 6 Faster SPSD Matrix Sketching.

1: **Input:** an \( n \times n \) matrix \( K \) and integers \( s \) and \( p \) \((s \leq p \ll n)\).
2: Perform column selection matrix \( S \in \mathbb{R}^{n \times s} \);
3: Perform sketching: \( C = AS \);
4: QR decomposition: \( [Q_C, R_C] = qr(C) \);
5: Draw a column selection matrix \( P \in \mathbb{R}^{n \times p} \);
6: Compute \( Z = (P^T Q_C)^\dagger (P^T K P) (Q_C P)^\dagger \);
7: **return** \( Q_C Z Q_C^T \approx A \).

- Since we are trying to avoid computing every entry of \( K \), we should use uniform sampling or local landmark selection to form \( C = KS \).
- Let \( P \in \mathbb{R}^{n \times p} \) be a leverage score sampling matrix according to the columns of \( C^T \). That is, it samples the \( i \)-th column with probability proportional to \( q_i \), where \( q_i \) is the squared \( \ell_2 \) norm of the \( i \)-th row of \( Q_C \) (for \( i = 1 \) to \( n \)). When \( p = \mathcal{O}(\sqrt{ns} \epsilon^{-1/2}) \), the following error bounds hold with high probability \cite{28}:

\[
\| K - Q_C Z Q_C^T \|_F^2 \leq (1 + \epsilon) \min_Z \| K - Q_C Z Q_C^T \|_F^2 .
\]

- Let \( S \) be a uniform sampling matrix and \( P \) be a leverage score sampling matrix. The algorithm visits only \( ns + p^2 = \mathcal{O}(n) \) entries of \( K \). The overall time and memory costs are linear in \( n \).

- Assume \( S \) is a column selection matrix. Let the sketch \( C = KS \) contains the columns of \( K \) indexed by \( S \subset [n] \), and the column selection matrix \( P \) are indexed by \( P \subset [n] \). Empirically, enforcing \( S \subset P \) significantly improves the approximation quality.

- Empirically, letting \( p \) be several times larger than \( s \), e.g. \( p = 4s \), is sufficient for a high quality.

The algorithm can be implemented in 12 lines of MATLAB code:

```matlab
function [QC, Z] = spsdFaster(K, s)
p = 4 * s; % can be tuned
n = size(K, 2);
S = sort(randSample(n, s)); % uniform sampling
C = K(:, S);
[QC, ~] = qr(C, 0);
quadraticSum = sum(QC.^2, 2); % the sampling probability
q = quadraticSum / sum(quadraticSum);
P = randSample(n, p, true, q); % leverage score sampling
P = unique([P; S]); % enforce P to contain S
PQCinv = pinv(QC(P, :));
Z = PQCinv * K(P, P) * PQCinv';
```

The above implementation assumes that \( K \) is a given matrix. In the kernel approximation problems, we are only given a \( n \times d \) matrix \( X \), whose rows are data points, and a kernel function, e.g. the RBF kernel with width parameter \( \sigma \). We should implement the faster SPSD sketching algorithm in the following way.
function [QC, Z] = spsdFaster(X, sigma, s)

p = 4 * s; % can be tuned
n = size(X, 1);
S = sort(randsample(n, s)); % uniform sampling
C = rbf(X, X(S, :), sigma);
[QC, ~] = qr(C, 0);
q = sum(QC.^2, 2); % the sampling probability
q = q / sum(q);
P = randsample(n, p, true, q);
P = unique([P; S]); % enforce P contains S
PQCinv = pinv(QC(P, :));
Ksub = rbf(X(P, :), X(P, :), sigma);
Z = PQCinv * Ksub * PQCinv';

The above implementation avoids computing the whole kernel matrix, and is thus highly efficient when applied to kernel methods.

6.4 The Nyström Method

Let $S$ be an $n \times s$ column selection matrix and $C = KS \in \mathbb{R}^{n \times s}$ be a sketch of $K$. Recall the model (10) proposed in the previous subsection. It is easy to verify that $Q_C Z Q_C^T = CXC^T$, where $\tilde{X}$ is defined by

$$\tilde{X} = \min_X \|P^T(K - CXC)P\|_F^2 = (P^T C)^\dagger (P^T K P)(C^T P)^\dagger.$$

One can simply set $P = S \in \mathbb{R}^{n \times s}$ and let $W = S^T C = S^T KS$. Then the solution $\tilde{X}$ becomes

$$\tilde{X} = (S^T C)^\dagger (S^T K S)(C^T S)^\dagger = W^\dagger W W^\dagger = W^\dagger.$$

The low-rank approximation

$$K \approx CW^\dagger C^T$$

is called the Nyström method [19, 29]. The Nyström method is perhaps the most extensively used kernel approximation approach in the literature. See Figure 2 for the illustration of the Nyström method.

There are a few things to remark:

- The Nyström is highly efficient. When applied to speedup kernel methods, the scalability can be as large as $n = 10^6$.

- The Nyström method is a rough approximation to $K$ and is well known to be of low accuracy. If a moderately high accuracy is required, one had better to use the method in the previous subsection.

- The $s \times s$ matrix $W$ is usually ill-conditioned, and thus the Moore-Penrose inverse can be numerically instable. (It is because the bottom singular values of $W$ blow up during the Moore-Penrose inverse.) A very effective heuristic is to drop the bottom singular values of $W$: set a parameter $k < s$, e.g. $k = \lceil 0.8s \rceil$, and approximate $K$ by $C(W_k)^\dagger C^T$.

- There are many choices of the sampling matrix $S$. See [13] for more discussions.
The Nyström method can be implemented in 11 lines of MATLAB code. The output of the algorithm is $L \in \mathbb{R}^{n \times k}$, where $LL^T$ is the Nyström approximation to $K$.

```matlab
function [L] = Nyström(X, sigma, s)
k = ceil(0.8 * s); % can be tuned
n = size(X, 1);
S = sort(randsample(n, s)); % uniform sampling
C = rbf(X, X(S, :), sigma); % C = K(:, S)
W = C(S, :);
[UW, SW, ~] = svd(W); % C = SWU'^T
SW = 1 ./ sqrt(SW(1:k));
L = C * UW; % K is approximated by L * L'
```

Here we use the RBF kernel function implemented in Section 6.1. Line 8 sets $k = \lceil 0.8c \rceil$, which can be better tuned to enhance numerical stability. Notice that $k$ should not be set too small, otherwise the accuracy would be affected.

### 6.5 More Efficient Extensions

Several SPSD matrix approximation methods have been proposed recently, and they are more scalable than the Nyström method in certain applications. This subsection briefly describes some of these methods.

#### 6.5.1 The Memory Efficient Kernel Approximation (MEKA)

MEKA [22] exploits the block structure of kernel matrices and is more memory efficient than the Nyström method. MEKA first partitions the data $x_1, \cdots, x_n$ into $b$ groups (e.g. by inexact kmeans

---

*aLet $W_k = U_{W,k}A_{W,k}U_{W,k}^T$ be the $k$-eigenvalue decomposition of $W$ and set $L = CU_{W,k}A_{W,k}^{-1} \in \mathbb{R}^{n \times k}$.**
clustering), accordingly, the kernel matrix $K$ has $b \times b$ blocks:

$$
K = \begin{bmatrix}
K_{[1,1]} & \cdots & K_{[1,b]} \\
\vdots & \ddots & \vdots \\
K_{[b,1]} & \cdots & K_{[b,b]}
\end{bmatrix} = 
\begin{bmatrix}
K_{[1]} \\
\vdots \\
K_{[b]}
\end{bmatrix}.
$$

Then MEKA approximately computes the top left singular vectors of $K_{[1:]}, \ldots, K_{[b:]},$ denote $U_{[1]}, \ldots, U_{[b]}$, respectively. For each $(i, j) \in [b] \times [b]$, MEKA finds a very small-scale matrix $Z_{[i,j]}$ by solving

$$
Z_{[i,j]} = \arg\min_Z \| K_{[i,j]} - U_{[i]} Z_{[i,j]} U_{[j]}^T \|_F^2.
$$

This can be done efficiently using the approach in Section 4.4.2. Finally, the low-rank approximation is

$$
K \approx 
\begin{bmatrix}
U_{[1]} & 0 \\
\vdots & \vdots \\
0 & U_{[b]}
\end{bmatrix}
\begin{bmatrix}
Z_{[1,1]} & \cdots & Z_{[1,b]} \\
\vdots & \ddots & \vdots \\
Z_{[b,1]} & \cdots & Z_{[b,b]}
\end{bmatrix}
\begin{bmatrix}
U_{[1]} & 0 \\
\vdots & \vdots \\
0 & U_{[b]}
\end{bmatrix}^T = U Z U^T.
$$

Since $Z$ and $U_{[1]}, \ldots, U_{[b]}$ are small-scale matrices, MEKA is thus very memory efficient. There are several things to remark:

- MEKA can be used to speedup Gaussian process regression and least square SVM. However, MEKA can be hardly applied to speedup $k$-eigenvalue decomposition, because it requires the $k$-SVD of $U Z^{1/2}$, which destroys the sparsity and significantly increases memory cost.

- Indiscreet implementation, e.g. the implementation provided by [22], can make MEKA numerically unstable, as was reported by [26, 25]. The readers had better to follow the stabler implementation in [25].

### 6.5.2 The Structured Kernel Interpolation (SKI)

SKI [30] is a memory efficient extension of the Nyström method. Let $S$ be a column selection matrix, $C = KS$, and $W = S^T C = S^T KS$. The Nyström method approximates $K$ by $C W^\dagger C^T$. SKI further approximates each row of $C$ by a convex combination of two rows of $W$ and obtain $C \approx X W$. Notice that each row of $X$ has only two nonzero entries, which makes $X$ extremely sparse. In this way, $K$ is approximated by

$$
K \approx C W^\dagger C \approx (X W)^\dagger (X W)^T = X W X^T.
$$

Much accuracy is lost in the second approximation, so SKI is much less accurate than the Nyström method. For the same reason as MEKA, there is no point in applying SKI to speedup $k$-eigenvalue decomposition of $K$.

### 6.6 Extension to Rectangular Matrices: The CUR Matrix Decomposition

This subsection considers the problem of sketching any rectangular matrix $A$ by the CUR matrix decomposition [16]. The CUR matrix decomposition is an extension of the previously discussed SPSD matrix sketching methods.
6.6.1 Motivation
Suppose we are given \( n \) training data \( x_1, \cdots, x_n \in \mathbb{R}^d \), \( m \) test data \( x'_1, \cdots, x'_m \in \mathbb{R}^d \), and a kernel function \( \kappa(\cdot, \cdot) \). In their generalization (test) stage, kernel methods such as GPR and KPCA form an \( m \times n \) matrix \( K_* \), where \( (K_*)_{ij} = \kappa(x'_i, x_j) \), and apply \( K_* \) to some vectors or matrices. Notice that it takes \( O(mnd) \) time to form \( K_* \) and \( O(mnp) \) time to multiply \( K_* \) by an \( n \times p \) matrix. If \( m \) is as large as \( n \), the generalization stage of such kernel methods can be very expensive. Fortunately, with the help of the CUR matrix decomposition, the generalization stage of GPR or KPCA merely costs time linear in \( m+n \).

6.6.2 The Prototype CUR Decomposition
Suppose we are given an arbitrary \( m \times n \) rectangular matrix \( A \), which can be the aforementioned \( K_* \). We sample \( c \) columns of \( A \) to form \( C = AS_C \in \mathbb{R}^{m \times c} \), sample \( r \) rows of \( A \) to form \( R = AS_R \in \mathbb{R}^{r \times n} \), and compute the intersection matrix \( U^\star \in \mathbb{R}^{c \times r} \) by solving
\[
U^\star = \arg\min_U \| A - \underbrace{C}_m \times \underbrace{U}_c \times \underbrace{R}_r \times \|_F^2 = C^\dagger A R^\dagger. \tag{11}
\]
The approximation \( A \approx CU^\star R \) is well known as the CUR decomposition \[16\]. This formulation bears a strong resemblance with the prototype SPSD matrix sketching method in \[9\].

The prototype CUR decomposition is not very useful because (1) its time cost is \( O(mn \cdot \min\{c,r\}) \) and (2) it visits every entry of \( A \).

6.6.3 Faster CUR Decomposition
Analogous to the SPSD matrix sketching, we can compute \( U^\star \) approximately and significantly more efficiently. Let \( P_C \in \mathbb{R}^{m \times p_c} \) and \( P_R \in \mathbb{R}^{n \times p_r} \) be some column selection matrices. Then we solve this problem in stead of (11):
\[
\tilde{U} = \arg\min_U \| \underbrace{P_C^T A P_R}_{p_c \times p_r} - \underbrace{P_C^T C U}_{m \times c} \times \underbrace{R P_R}_{r \times p_r} \|_F^2 = (P_C^T C)^\dagger (P_C^T A P_R)(R P_R)^\dagger. \tag{12}
\]
The faster CUR decomposition is very similar to the faster SPSD matrix sketching method in Section 6.3. The faster CUR decomposition has the following properties:

- It visits only \( mc + nr + p_c p_r \) entries of \( A \), which is linear in \( m+n \). This is particularly useful when applied to kernel methods, because it avoids forming the whole kernel matrix.
- The overall time and memory costs are linear in \( m+n \).
- If \( P_C \) is the leverage score sampling matrix corresponding to the columns of \( C^T \) and \( P_R \) is the leverage score sampling matrix corresponding to the columns of \( R \), then \( \tilde{U} \) is a very high quality approximation to \( U^\star \) \[28\]:
\[
\| A - C\tilde{U}R \|_F^2 \leq (1+\epsilon) \min_U \| A - CUR \|_F^2
\]
holds with high probability.
Empirically speaking, setting $P_C$ and $P_R$ be uniform sampling matrices works nearly as well as leverage score sampling matrices, and setting $p_c = p_r = O(c + r)$ suffices for a high approximation quality. If $A$ is a full-observed matrix, the CUR matrix decomposition can be computed by the following MATLAB code.

```matlab
function [C, U, R] = curFaster(A, c, r)
    pc = 2 * (r + c); % can be tuned
    pr = 2 * (r + c); % can be tuned
    [m, n] = size(A);
    SC = sort(randsample(n, c));
    SR = sort(randsample(m, r));
    C = A(:, SC);
    R = A(SR, :);
    PC = sort(randsample(m, pc));
    PR = sort(randsample(n, pr));
    PC = unique([PC; SR]); % enforce PC to contain SR
    PR = unique([PR; SC]); % enforce PR to contain SC
    Kblock = rbf(Xtest(PC, :), Xtrain(PR, :), sigma);
    U = pinv(C(PC, :)) * Kblock * pinv(R(:, PR));
end
```

Let’s consider the kernel approximation problem in Section 6.6.1. Let $X_{train} \in \mathbb{R}^{n \times d}$ be the training data and $X_{test} \in \mathbb{R}^{m \times d}$ be the test data. We use the RBF kernel with kernel width parameter $\sigma$. The $m \times n$ matrix $K_s$ can be approximated by $\tilde{K}_s = CUR$, which is the output of the following MATLAB procedure.

```matlab
function [C, U, R] = curFasterKernel(Xtest, Xtrain, sigma, c, r)
    pc = 2 * (r + c); % can be tuned
    pr = 2 * (r + c); % can be tuned
    m = size(Xtest, 1);
    n = size(Xtrain, 1);
    SC = sort(randsample(n, c));
    SR = sort(randsample(m, r));
    C = rbf(Xtest, Xtrain(SC, :), sigma);
    R = rbf(Xtest(SR, :), Xtrain, sigma);
    PC = sort(randsample(m, pc));
    PR = sort(randsample(n, pr));
    PC = unique([PC; SR]); % enforce PC to contain SR
    PR = unique([PR; SC]); % enforce PR to contain SC
    Kblock = rbf(Xtest(PC, :), Xtrain(PR, :), sigma);
    U = pinv(C(PC, :)) * Kblock * pinv(R(:, PR));
end
```

The time cost of this procedure is linear in $m + n$, and $\tilde{K}_s = CUR$ can be applied to $n$ dimensional vector in $O(nr + mc)$ time. In this way, the generalization of GPR and KPCA can be efficient.

### 6.7 Applications

This subsection provides the implementations of kernel PCA, spectral clustering, Gaussian process regression, all sped-up by randomized algorithms.

#### 6.7.1 Kernel Principal Component Analysis (KPCA)

Suppose we are given
• \(n\) training data \(\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d\),

• \(m\) test data \(\mathbf{x}_1', \cdots, \mathbf{x}_m' \in \mathbb{R}^d\), (\(\mathbf{x}_i'\) is not the transpose \(\mathbf{x}_i^T\)),

• a kernel function \(\kappa(\cdot, \cdot)\), e.g. the RBF kernel function,

• a target rank \(k\) \((\ll n, d)\).

The goal of KPCA is to extract \(k\) features of each training datum and each test datum, which may be used in clustering or classification. The standard KPCA consists of the following steps:

1. Training
   (a) Form the \(n \times n\) kernel matrix \(\mathbf{K}\) of the training data, whose the \((i, j)\)-th entry is \(\kappa(\mathbf{x}_i, \mathbf{x}_j)\);
   (b) Compute the \(k\)-eigenvalue decomposition \(\mathbf{K}_k = \mathbf{U}_k \Lambda_k \mathbf{U}_k^T\);
   (c) Form the \(n \times k\) matrix \(\mathbf{U}_k \Lambda_k^{1/2}\), whose the \(i\)-th row is the feature of \(\mathbf{x}_i\);

2. Generalization (test)
   (a) Form the \(m \times n\) kernel matrix \(\mathbf{K}_*\) whose the \((i, j)\)-th entry is \(\kappa(\mathbf{x}_i', \mathbf{x}_j)\);
   (b) Form the \(m \times k\) matrix \(\mathbf{K}_* \mathbf{U}_k \Lambda_k^{-1/2}\), whose the \(i\)-th row is the feature of \(\mathbf{x}_i'\).

The most time and memory expensive step in training is the \(k\)-eigenvalue decomposition of \(\mathbf{K}\), which can be sped-up by the sketching techniques discussed in this section. Empirically, the faster SPSD matrix sketching in Section 6.3 is much more accurate than the Nyström method in Section 6.4, and their time and memory costs are all linear in \(n\). Thus the faster SPSD matrix sketching can be better choice. KPCA can be approximately solved by several lines of MATLAB code.

```matlab
function [U, lambda, featuretrain] = kpcaTrain(Xtrain, sigma, k)
s = k * 10; % can be tuned
[QC, Z] = spsdFaster(Xtrain, sigma, s); % QC has orthogonal columns
clear Xtrain
[UZ, SZ, ~] = svd(Z); % UZ contains the top k eigenvectors
lambda = diag(SZ); % lambda is the vector containing the top k eigenvalues
featuretrain = bsxfun(@times, UZ(:, 1:k), (sqrt(lambda))')
end
```

```matlab
function [featuretest] = kpcaTest(Xtrain, Xtest, sigma, U, lambda)
Ktest = rbf(Xtest, Xtrain, sigma);
U = bsxfun(@times, U, (1 ./ sqrt(lambda))')
featuretest = Ktest * U;
end
```

In the function “kpcaTrain”, the input variable “Xtrain” has \(n\) rows, each of which corresponds to a training datum. The rows of the output “featuretrain” and “featuretest” are the features extracted by KPCA, and the features can be used to perform classification. For example, suppose each datum \(\mathbf{x}_i\) is associated with a label \(y_i\), and let \(\mathbf{y} = [y_1, \cdots, y_n]^T \in \mathbb{R}^n\). We can use \(k\)-nearest-neighbor
to predict the labels of the test data.

When the number of test data $m$ is large, the function “kpcaTest” is costly. The users should apply the CUR decomposition in Section [6.6.3] to speedup computation.

```matlab
function [featuretest] = kpcaTestCUR(Xtrain, Xtest, sigma, U, lambda)
c = max(100, ceil(size(Xtrain, 1) / 20)); % can be tuned
r = max(100, ceil(size(Xtest, 1) / 20)); % can be tuned
[C, Utilda, R] = curFasterKernel(Xtest, Xtrain, sigma, c, r);
U = bsxfun(@times, U, (1 ./ sqrt(lambda))');
featuretest = C * (Utilda * (R * U));
end
```

### 6.7.2 Spectral Clustering

Spectral clustering is one of the most popular clustering algorithms. Suppose we are given

- $n$ data points $x_1, \cdots, x_n \in \mathbb{R}^d$,
- a kernel function $\kappa(\cdot, \cdot)$,
- $k$: the number of classes.

Spectral clustering performs the following operations:

1. Form an $n \times n$ kernel matrix $K$, where big $k_{ij}$ indicates $x_i$ and $x_j$ are similar;
2. Form the degree matrix $D$ with $d_{ii} = \sum_j k_{ij}$ and $d_{ij} = 0$ for all $i \neq j$;
3. Compute the normalized graph Laplacian $G = D^{-1/2}KD^{-1/2} \in \mathbb{R}^{n \times n}$;
4. Compute the top $k$ eigenvectors of $G$, denote $U \in \mathbb{R}^{n \times k}$, and normalize the rows of $U$;
5. Apply $k$-means clustering on the rows of $V$ to obtain the class labels.

The first step costs $O(n^2d)$ time and the fourth step costs $O(n^2k)$ times, which limit the scalability of spectral clustering. Fowlkes et al. [11] proposed to apply the Nyström method to make spectral clustering more scalable by avoiding forming the whole kernel matrix and speeding-up the $k$-eigenvalue decomposition. Empirically, the algorithm in Section [6.3] is more accurate than the Nyström method in Section [6.4] and they both runs in linear time. Spectral clustering with the randomized algorithm in Section [6.3] can be implemented in 16 lines of MATLAB code.

```matlab
function [labels] = SpectralClusteringFaster(X, sigma, k)
s = k * 10; % can be tuned
n = size(X, 1);
[QC, Z] = spsdFaster(X, sigma, s); % K is approximated by QC * Z * QC'
[UZ, SZ, ~] = svd(Z);
SZ = sqrt(diag(SZ));
UZ = bsxfun(@times, UZ, SZ') % now Z = UZ * UZ'
```
When the scale of data is too large for the faster SPSD matrix sketching algorithm in Section 6.3, one can instead use the more efficient Nyström method in Section 6.4: simply replace Lines 4 to 8 by

$$L = \text{Nystrom}(X, \sigma, s);$$

### 6.7.3 Gaussian Process Regression (GPR)

The Gaussian process regression (GPR) is one of the most popular machine learning methods. GPR is the foundation of Bayesian optimization and has important applications such as automatically tuning the hyper-parameters of deep neural networks. Suppose we are given

- $n$ training data $x_1, \ldots, x_n \in \mathbb{R}^d$,
- labels $y = [y_1, \ldots, y_n]^T \in \mathbb{R}^n$ of the training data,
- $m$ test data $x'_1, \ldots, x'_m \in \mathbb{R}^d$, ($x'_i$ is not the transpose $x_i^T$),
- and a kernel function $\kappa(\cdot, \cdot)$, e.g. the RBF kernel with kernel width parameter $\sigma$.

**Training.** In the training stage, GPR requires forming the $n \times n$ kernel matrix $K$ where $k_{ij} = \kappa(x_i, x_j)$ and computing the model

$$w = (K + \alpha I_n)^{-1} y.$$ 

Here $\alpha$ is a tuning parameter that indicates the noise intensity in the labels $y$. It takes $O(n^2 d)$ time to form the kernel matrix and $O(n^3)$ time to compute the matrix inversion. To make the training efficient, we can first sketch the SPSD matrix $K$ to obtain $K \approx LL^T$ and then apply the technique in Section 6.1.2 to obtain $w$. Empirically, when applied to speedup GPR, the algorithms discussed in Section 6.3 and Section 6.4 has similar accuracy, thus we choose to use the Nyström method which is more efficient.

The training GPR with the Nyström approximation can be implemented in the following MATLAB code. The time cost is $O(nl^2 + nld)$ and the space cost is $O(nl + nd)$.

```matlab
function [w] = gprTrain(Xtrain, ytrain, sigma, alpha)
% Xtrain = [x1, x2, ..., xn] \in \mathbb{R}^{d \times n}
% ytrain = [y1, y2, ..., yn] \in \mathbb{R}^n
% sigma = kernel width
% alpha = noise parameter
l = 100; % can be tuned
L = Nystrom(Xtrain, sigma, l); % K is approximated by L * L'
l = size(L, 2); 
w = L' * ytrain;
```
The input “sigma” is the kernel width parameter and “alpha” indicates the noise intensity in the observation.

**Generalization (test).** After obtaining the trained model \( \mathbf{w} \in \mathbb{R}^n \), GPR can predict the unknown labels of the \( m \) test data \( \mathbf{x}'_1, \ldots, \mathbf{x}'_m \in \mathbb{R}^d \). GPR forms an \( m \times n \) kernel matrix \( \mathbf{K}_s \) whose the \((i,j)\)-th entry is \( \kappa(\mathbf{x}'_i, \mathbf{x}_j) \) and compute \( \mathbf{y}_* = \mathbf{K}_s \mathbf{w} \in \mathbb{R}^m \). The \( i \)-th entry in \( \mathbf{y}_* \) is the predictive label of \( \mathbf{x}'_i \). The generalization can be implemented in four lines of MATLAB code.

```matlab
function [ytest] = gprTest(Xtrain, Xtest, sigma, w)
Ktest = rbf(Xtest, Xtrain, sigma);
ytest = Ktest * w;
end
```

It costs \( O(mn) \) time to compute \( \mathbf{K}_s \) and \( O(mn) \) time to apply \( \mathbf{K}_s \) to \( \mathbf{w} \). If \( m \) is small, the generalization stage can be performed straightforwardly. However, if \( m \) is as large as \( n \), the time cost will be quadratic in \( n \), and the user should apply the CUR decomposition in Section 6.6.3 to speedup computation.

```matlab
function [ytest] = gprTestCUR(Xtrain, Xtest, sigma, w)
c = max(100, ceil(size(Xtrain, 1) / 20)); % can be tuned
r = max(100, ceil(size(Xtest, 1) / 20)); % can be tuned
[C, Utild, R] = curFasterKernel(Xtest, Xtrain, sigma, c, r);
ytest = C * (Utild * (R * w));
end
```
A Several Facts of Matrix Algebra

This section lists some facts that have been applied in this paper.

Fact 1 The matrices $Q_1 \in \mathbb{R}^{m \times n}$ and $Q_{n \times p}$ ($m \geq n \geq p$) have orthonormal columns. Then the matrix $Q = Q_1 Q_2$ has orthonormal columns.

Fact 2 Let $A$ be any $m \times n$ and rank $\rho$ matrix. Then $AA^\dagger B = U_A U_A^T B = A X^* = U_A Z^*$, where

$$X^* = \arg\min_X \|B - AX\|^2_F,$$

and

$$Z^* = \arg\min_Z \|B - U_A Z\|^2_F.$$

This is the reason why $AA^\dagger B$ and $U_A U_A^T B$ are called the projection of $B$ onto the column space of $A$.

Fact 3 [31, Lemma 44] The matrices $Q \in \mathbb{R}^{m \times s}$ ($m \geq s$) has orthonormal columns. The solution to

$$\arg\min_{\text{rank}(X) \leq k} \|A - QX\|^2_F$$

is $X^* = (Q^T A)_k$, where $(Q^T A)_k$ denotes the closest rank $k$ approximation to $Q^T A$.

Fact 4 Let $A^\dagger$ be the Moore-Penrose inverse of $A$. Then $AA^\dagger A = A$ and $A^\dagger AA^\dagger = A^\dagger$.

Fact 5 Let $A$ be an $m \times n$ ($m \geq n$) matrix and $A = Q_A R_A$ be the QR decomposition of $A$. Then

$$\begin{bmatrix} A^\dagger \\ \hline \\ n \times m \end{bmatrix} \begin{bmatrix} \hline \\ R_A^T \\ \hline \\ Q_A \end{bmatrix} = \begin{bmatrix} \hline \\ R_A^T \\ \hline \\ Q_A \end{bmatrix}.$$

Fact 6 Let $C$ be a full-rank matrix with more rows than columns. Let $C = Q_C R_C$ be the QR decomposition and $C = U_C \Sigma_C V_C$ be the condensed SVD. Then the leverage scores of $C$, $Q_C$, $U_C$ are the same.
B Notes and Further Reading

The $\ell_p$ Regression Problems. Section 4 has applied the sketching methods to solve the $\ell_2$ norm regression problem more efficiently. The more general $\ell_p$ regression problems have also been studied in the literature [4, 5, 17, 7]. Especially, the $\ell_1$ is of great interest because it demonstrate strong robustness to noise. Currently the strongest result is the $\ell_p$ row sampling by Lewis weights [7].

Distributed SVD. In the distributed model, each machine holds a subset of columns of $A$ and should output the top singular values and singular vectors. In this model, the communication cost should also be considered, as well as the time and memory costs. The seminal work [10] proposed to build a coreset to capture the properties of $A$, which facilitates low computation and communication costs. Later on, several algorithms with stronger error bound and lower communication and computation costs have been proposed. Currently, the state of the art is [3].

Random Feature for Kernel Methods. Section 6 has introduced the sketching methods for kernel methods. A parallel line of work is the random feature methods [20] which also form low-rank approximations to kernel matrices. Section 6.5.3 of [24] offers simple and elegant proof of a random feature method. Since the sketching methods usually works better than the random feature methods (see the examples in [32]), the users are advised to apply the sketching methods introduced in Section 6. Besides the two kinds of low-rank approximation approaches, the stochastic optimization approach [8] also demonstrates very high scalability.
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