SUBLINEAR TIME LOW-RANK APPROXIMATION OF POSITIVE SEMIDEFINITE MATRICES

Cameron Musco (MIT) and David P. Woodruff (CMU)
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- A near optimal low-rank approximation for any positive semidefinite (PSD) matrix can be computed in sublinear time (i.e. without reading the full matrix).
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- **Concrete**: Significantly improves on previous, roughly linear time approaches for general matrices, and bypasses a trivial linear time lower bound for general matrices.

- **High Level**: Demonstrates that PSD structure can be exploited in a much stronger way than previously known for low-rank approximation. Opens the possibility of further advances in algorithms for PSD matrices.
Low-rank approximation is one of the most widely used methods for general matrix and data compression.
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\[ A \rightarrow N \rightarrow M^T \]

1024 x 1024  rank-100 approximation
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Applications to clustering, topic modeling and latent semantic analysis, recommendation systems, distribution learning, and countless other problems.
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- In the multi-dimensional scaling literature, PSD low-rank approximation is known as ‘strain minimization’.
- Completion of (nearly) low-rank PSD matrices is applied in quantum state tomography and for global positioning using local distances (i.e. triangulation).
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Unfortunately, computing the SVD takes $O(nd^2)$ time.
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• Traditionally, the power method of iterative Krylov subspace methods which compute just the top $k$ singular vectors of $A$ are used in lieu of a full SVD.

Theorem (Clarkson, Woodruff '13)

There is an algorithm which in $O(nnz(A) + n \cdot \text{poly}(k, 1/\epsilon))$ time outputs $N \in \mathbb{R}^{n \times k}, M \in \mathbb{R}^{d \times k}$ satisfying with prob. $99/100$:

$$\|A - NM^T\|_F \leq (1 + \epsilon)\|A - A_k\|_F.$$
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• When $k, 1/\epsilon$ are not too large, runtime is linear in input size.
• Best known runtime for both general and PSD matrices.
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Similar runtimes possible via leverage score based sampling techniques.
Theorem (Main Result – Musco, Woodruff ‘17)

There is an algorithm running in $\tilde{O}\left(\frac{n k^2}{\epsilon^4}\right)$ time which, given PSD $A$, outputs $N, M \in \mathbb{R}^{n \times k}$ satisfying with probability $99/100$:

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- If $k, 1/\epsilon$ are not too large compared to $\text{nnz}(A)$, our runtime is significantly sublinear in the size of $A$. 
Theorem (Main Result – Musco, Woodruff ‘17)

There is an algorithm running in $O\left(\frac{nk^2}{\epsilon^4}\right)O\left(n^{3/2}\cdot\text{poly}(k/\epsilon)\right)$ time which, given PSD $A$, outputs $N, M \in \mathbb{R}^{n \times k}$ satisfying:

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- Compare to CW‘13 which takes $O(\text{nnz}(A)) + n \text{ poly}(k, 1/\epsilon)$.
- If $k, 1/\epsilon$ are not too large compared to nnz($A$), our runtime is significantly sublinear in the size of $A$. 
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\[ \|A - NM^T\|_F \leq \|A - A_k\|_F + \epsilon\|A\|_F. \]
**Observation:** For PSD $\mathbf{A}$, we have for any entry $a_{ij}$:

$$a_{ij} \leq \max(a_{ii}, a_{jj})$$

since otherwise $(\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{A} (\mathbf{e}_i - \mathbf{e}_j) < 0$, contradicting the positive semidefinite requirement.
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- So we can find any ‘hidden’ heavy entry by looking at its corresponding diagonal entries.
WHAT ABOUT FOR PSD MATRICES?

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**Question:** How can we exploit additional structure arising from positive semidefiniteness to achieve sublinear runtime?
Every PSD matrix is a Gram matrix

**Very Simple Fact:** Every PSD matrix $A \in \mathbb{R}^{n \times n}$ can be written as $B^T B$ for some $B \in \mathbb{R}^{n \times n}$. 
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- $B$ can be any matrix square root of $A$, e.g. if we let $V\Sigma V^T$ be the SVD of $A$, we can set $B = \Sigma^{1/2} V^T$.
- Letting $b_1, \ldots, b_n$ be the columns of $B$, the entries of $A$ contain every pairwise dot product $a_{ij} = b_i^T b_j$. 

$$
\begin{align*}
\begin{array}{c}
\text{b}_i^T \\
B^T
\end{array} & \quad \begin{array}{c}
B \\
b_j
\end{array} & = & \begin{array}{c}
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The fact that \( \mathbf{A} \) is a Gram matrix places a variety of geometric constraints on its entries.
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- The heavy diagonal observation is just one example. By Cauchy-Schwarz:

$$a_{ij} = b_i^T b_j \leq \|b_i\| \|b_j\| = \sqrt{a_{ii} \cdot a_{jj}} \leq \max(a_{ii}, a_{jj}).$$
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**Another View:** $A$ contains a lot of information about the column span of $B$ in a very compressed form – with every pairwise dot product stored as $a_{ij}$. 
**Question:** Can we compute a low-rank approximation of $B$ using $o(n^2)$ column dot products? I.e. $o(n^2)$ accesses to $A$?
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**Why?** $B$ has the same (right) singular vectors as $A$, and its singular values are closely related: $\sigma_i(B) = \sqrt{\sigma_i(A)}$. 
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Why? $B$ has the same (right) singular vectors as $A$, and its singular values are closely related: $\sigma_i(B) = \sqrt{\sigma_i(A)}$.

- So the top $k$ singular vectors are the same for the two matrices. An optimal low-rank approximation for $B$ thus gives an optimal low-rank approximation for $A$. 

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- So the top $k$ singular vectors are the same for the two matrices. An optimal low-rank approximation for $B$ thus gives an optimal low-rank approximation for $A$.
- Things will be messier once we introduce approximation.
More concretely, we want to compute some orthogonal span $Z \in \mathbb{R}^{n \times k}$ (i.e. with $Z^T Z = I$) satisfying:

$$\|B - ZZ^T B\|_F \leq (1 + \epsilon)\|B - B_k\|_F$$

using a sublinear number of column dot products (i.e. accesses to $A = B^T B$).

Aside: Computing a low-rank approximation of $B$ is interesting in its own right. When $A$ is a kernel matrix, this is essentially the problem of kernel PCA.

- Can also be used to accelerate kernel ridge regression, $k$-means clustering, and CCA (Musco, Musco '17).
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Theorem (Deshpande, Vempala ‘06)

For any \( B \in \mathbb{R}^{n \times n} \), there exists a subset of \( 4k/\epsilon + 2k \log(k + 1) \) columns whose span contains \( Z \in \mathbb{R}^{n \times k} \) satisfying:

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$$\|\mathbf{B} - \mathbf{Z}\mathbf{Z}^T\mathbf{B}\|_F \leq (1 + \epsilon)\|\mathbf{B} - \mathbf{B}_k\|_F$$

**Observation:** Given column subset, $\mathbf{C}$ can be computed using just $\tilde{O}(n \cdot k/\epsilon)$ column dot products (i.e. must compute $(\mathbf{BS})^T\mathbf{B}$).
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**Adaptive Sampling Column Subset Selection**

Initially, start with an empty column subset $S := \emptyset$.

For $t = 1, \ldots, \tilde{O}(k^2/\epsilon)$

Let $P_S$ be the projection onto the columns in $S$.

Add $b_i$ to $S$ with probability $\frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|_F^2}$.
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Identifying the Column Subset

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\[
\begin{array}{c}
\text{b}_{S_1} \\
B
\end{array}
\quad
\begin{array}{c}
A
\end{array}
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Add \( b_i \) to \( S \) with probability \( \frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|_F^2} \).
Adaptive Sampling Column Subset Selection

Initially, start with an empty column subset $S := \emptyset$.

For $t = 1, \ldots, \tilde{O}(k^2/\epsilon)$

Let $P_S = \frac{b_{s_1} b_{s_1}^T}{\|b_{s_1}\|^2}$ be the projection onto the columns in $S$.

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Adaptive Sampling Column Subset Selection

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For $t = 1, \ldots, \tilde{O}(k^2 / \epsilon)$

Let $P_S = \frac{b_{s_1} b_{s_1}^T}{\|b_{s_1}\|^2}$ be the projection onto the columns in $S$.

Add $b_i$ to $S$ with probability $\frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|_F^2}$.
Adaptive Sampling Column Subset Selection

Initially, start with an empty column subset \( S := \{\} \).

For \( t = 1, \ldots, \tilde{O}(k^2/\epsilon) \)

Let \( P_S = \frac{b_{s_1} b_{s_2}^T}{\|b_{s_1}\|^2} \) be the projection onto the columns in \( S \).

Add \( b_i \) to \( S \) with probability \( \frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|_F^2} \).
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Initially, start with an empty column subset $S := \emptyset$.

For $t = 1, \ldots, \tilde{O}(k^2/\epsilon)$

Let $P_S$ be the projection onto the columns in $S$.

Add $b_i$ to $S$ with probability $\frac{\|b_i - P_Sb_i\|^2}{\|B - P_SB\|_F^2}$.
Adaptive Sampling Column Subset Selection

Initially, start with an empty column subset $S := \emptyset$.

For $t = 1, ..., \tilde{O}(k^2/\epsilon)$

Let $P_S$ be the projection onto the columns in $S$.

Add $b_i$ to $S$ with probability $\frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|_F^2}$. 

\[ b_{s_1}, b_{s_2} \quad B \quad A \]
Adaptive Sampling Column Subset Selection
Initially, start with an empty column subset $S := \{\}$. For $t = 1, ..., \tilde{O}(k^2/\epsilon)$

Let $P_S$ be the projection onto the columns in $S$.

Add $b_i$ to $S$ with probability $\frac{||b_i - P_S b_i||^2}{||B - P_S B||^2_F}$. 
Adaptive Sampling Column Subset Selection

Initially, start with an empty column subset $S := \emptyset$.

For $t = 1, \ldots, \tilde{O}(k^2/\epsilon)$

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Initially, start with an empty column subset $S := \emptyset$. For $t = 1, \ldots, \tilde{O}(k^2/\epsilon)$

Let $P_S$ be the projection onto the columns in $S$.

Add $b_i$ to $S$ with probability $\frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|^2_F}$.
Adaptive Sampling Column Subset Selection

Initially, start with an empty column subset $S := \emptyset$.

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Adaptive Sampling Column Subset Selection
Initially, start with an empty column subset $S := \emptyset$.
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Let $P_S$ be the projection onto the columns in $S$.
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Adaptive Sampling Column Subset Selection
Initially, start with an empty column subset \( S := \{ \} \).
For \( t = 1, ..., \tilde{O}(k^2/\epsilon) \)
Let \( P_S \) be the projection onto the columns in \( S \).
Add \( b_i \) to \( S \) with probability
\[
\frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|^2_F}.
\]
Adaptive Sampling Column Subset Selection
Initially, start with an empty column subset \( S := \emptyset \).
For \( t = 1, \ldots, \tilde{O}(k^2/\epsilon) \)

Let \( P_S \) be the projection onto the columns in \( S \).
Add \( b_i \) to \( S \) with probability
\[
\frac{\|b_i - P_S b_i\|^2}{\|B - P_S B\|^2_F}.
\]
Theorem

There is an algorithm using $\tilde{O}(n \cdot k^2 / \epsilon)$ column dot products (i.e. accesses to $A = B^T B$) which computes sampling matrix $S \in \mathbb{R}^{n \times \tilde{O}(k^2 / \epsilon)}$ and $C \in \mathbb{R}^{\tilde{O}(k^2 / \epsilon) \times k}$ such that $Z = BSC$ satisfies with probability $99/100:

$$\|B - ZZ^T B\|_F \leq (1 + \epsilon)\|B - B_k\|_F.$$
Sublinear Dot Product Algorithm

**Theorem**

There is an algorithm using $\tilde{O}(n \cdot k^2 / \epsilon)$ column dot products (i.e. accesses to $A = B^T B$) which computes sampling matrix $S \in \mathbb{R}^{n \times \tilde{O}(k^2 / \epsilon)}$ and $C \in \mathbb{R}^{\tilde{O}(k^2 / \epsilon) \times k}$ such that $Z = BSC$ satisfies with probability $99/100$:

$$\|B - ZZ^T B\|_F \leq (1 + \epsilon)\|B - B_k\|_F.$$  

- I.e., a near optimal low-rank approximation can be found using much less information about $B$’s column span than a full SVD.
Theorem

There is an algorithm using $\tilde{O}(n \cdot k^2 / \epsilon)$ column dot products (i.e. accesses to $A = B^T B$) which computes sampling matrix $S \in \mathbb{R}^{n \times \tilde{O}(k^2 / \epsilon)}$ and $C \in \mathbb{R}^{\tilde{O}(k^2 / \epsilon) \times k}$ such that $Z = BSC$ satisfies with probability $99/100$:

$$\|B - ZZ^T B\|_F \leq (1 + \epsilon)\|B - B_k\|_F.$$ 

- I.e., a near optimal low-rank approximation can be found using much less information about $B$’s column span than a full SVD.
- But what can we do with this result?
As mentioned, if $Z$ gave an \textbf{optimal low-rank approximation} $\|B - ZZ^TB\|_F = \|B - B_k\|_F$ then it would immediately give an optimal approximation for $A = B^T B$. 

• Gives $n \cdot \text{poly}(k)$ time low-rank PSD matrix completion (i.e. when $\|A - A_k\|_F = 0$).
As mentioned, if $Z$ gave an optimal low-rank approximation

$$\| B - ZZ^T B \|_F = \| B - B_k \|_F$$

then it would immediately give an optimal approximation for $A = B^T B$.

$$B^T ZZ^T B$$
As mentioned, if \( Z \) gave an optimal low-rank approximation

\[
\| B - ZZ^T B \|_F = \| B - B_k \|_F
\]

then it would immediately give an optimal approximation for \( A = B^T B \).

\[
B^T ZZ^T B = (B^T ZZ^T)(ZZ^T B)
\]
As mentioned, if $Z$ gave an optimal low-rank approximation

$$\|B - ZZ^T B\|_F = \|B - B_k\|_F$$

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$$B^T ZZ^T B = (B^T ZZ^T)(ZZ^T B) = B_k^T B_k$$
As mentioned, if $Z$ gave an optimal low-rank approximation

$$\|B - ZZ^T B\|_F = \|B - B_k\|_F$$

then it would immediately give an optimal approximation for $A = B^T B$.

$$B^T ZZ^T B = (B^T ZZ^T)(ZZ^T B)$$

$$= B_k^T B_k$$

$$= V\Sigma_k^{1/2} \Sigma_k^{1/2} V^T$$
As mentioned, if \( Z \) gave an optimal low-rank approximation 
\[ \| B - ZZ^T B \|_F = \| B - B_k \|_F \]
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\[
B^T ZZ^T B = (B^T ZZ^T)(ZZ^T B) \\
= B_k^T B_k \\
= V \Sigma_k^{1/2} \Sigma_k^{1/2} V^T \\
= A_k.
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As mentioned, if $Z$ gave an optimal low-rank approximation

$$\|B - ZZ^T B\|_F = \|B - B_k\|_F$$

then it would immediately give an optimal approximation for $A = B^T B$.

$$B^T ZZ^T B = (B^T ZZ^T)(ZZ^T B)$$
$$= B_k^T B_k$$
$$= V \Sigma_k^{1/2} \Sigma_k^{1/2} V^T$$
$$= A_k.$$

- Gives $n \cdot \text{poly}(k)$ time low-rank PSD matrix completion (i.e. when $\|A - A_k\|_F = 0$).
Given $ZZ^T B$ we approximate $A$ with $B^T ZZ^T B$. 
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$B^T Z$ can be computed efficiently without explicitly forming $B$. 
Given $ZZ^T B$ we approximate $A$ with $B^T ZZ^T B$.

$B^T Z$ can be computed efficiently without explicitly forming $B$.

- $B^T Z = B^T (BSC) = ASC$. 
Given $Z Z^T B$ we approximate $A$ with $B^T Z Z^T B$.

$B^T Z$ can be computed efficiently without explicitly forming $B$.

- $B^T Z = B^T (B S C) = ASC$. 

$B^T Z = A S C$
Given \( ZZ^T B \) we approximate \( A \) with \( B^T ZZ^T B \).

\[ B^T Z \text{ can be computed efficiently without explicitly forming } B. \]

- \( B^T Z = B^T (BSC) = ASC. \)
Given $ZZ^T B$ we approximate $A$ with $B^T ZZ^T B$.

$B^T Z$ can be computed efficiently without explicitly forming $B$.

- $B^T Z = B^T (BSC) = ASC$.

- $n \cdot \text{poly}(k, 1/\epsilon)$ accesses to $A$ and run time.
What about when $Z$ just gives a near-optimal approximation?
What about when $Z$ just gives a near-optimal approximation?

**Lemma**

If $\|B - ZZ^TB\|_F^2 \leq \left(1 + \frac{\epsilon^{3/2}}{\sqrt{n}}\right) \|B - B_k\|_F^2$ where $Z = BSC$, then for $A = B^TB$:

$$\|A - B^TZZ^TB\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2.$$
What about when $Z$ just gives a near-optimal approximation?

Lemma

If $\|B - ZZ^T B\|_F^2 \leq \left(1 + \frac{\epsilon^{3/2}}{\sqrt{n}}\right) \|B - B_k\|_F^2$ where $Z = BSC$, then for $A = B^T B$:

$$\|A - (ASC)(ASC)^T\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2.$$
What about when $Z$ just gives a near-optimal approximation?

Lemma

If $\|B - ZZ^T B\|_F^2 \leq \left(1 + \frac{\epsilon^{3/2}}{\sqrt{n}}\right) \|B - B_k\|_F^2$ where $Z = BSC$, then for $A = B^T B$:

$$\|A - (ASC)(ASC)^T\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2.$$
What about when $Z$ just gives a near-optimal approximation?

**Lemma**

If $\|B - ZZ^T B\|_F^2 \leq \left(1 + \frac{\epsilon^{3/2}}{\sqrt{n}}\right) \|B - B_k\|_F^2$ where $Z = BSC$, then for $A = B^T B$:

$$\|A - (ASC)(ASC)^T\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2.$$ 

This will give an low-rank approximation algorithm which accesses just $\tilde{O}\left(\frac{nk^2}{\epsilon^{3/2}/\sqrt{n}}\right) = n^{3/2} \cdot \text{poly}(k, 1/\epsilon)$ entries of $A$. 

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**Boosting to a PSD Matrix Approximation**

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\[ \| A - B^T ZZ^T B \|_F^2 = \| B^T (I - ZZ^T) B \|_F^2 \]
PROOF OF BOOSTING LEMMA

\[ \| A - B^T Z Z^T B \|_F^2 = \| B^T (I - ZZ^T) B \|_F^2 = \sum_{i=1}^{n-k} \sigma_i^2 (B^T (I - ZZ^T) B) \]
\[ \|A - B^T ZZ^T B\|_F^2 = \|B^T (I - ZZ^T) B\|_F^2 \]

\[ = \sum_{i=1}^{n-k} \sigma_i^2 (B^T (I - ZZ^T) B) \]

\[ = \sum_{i=1}^{n-k} \sigma_i^4 ((I - ZZ^T) B). \]
PROOF OF BOOSTING LEMMA

\[ \|A - B^T ZZ^T B\|_F^2 = \|B^T (I - ZZ^T) B\|_F^2 \]

\[ = \sum_{i=1}^{n-k} \sigma_i^2 (B^T (I - ZZ^T) B) \]

\[ = \sum_{i=1}^{n-k} \sigma_i^4 (I - ZZ^T) B. \]

• Write \((I - ZZ^T) B = U \Sigma V^T\) using the SVD and note that
  \(B^T (I - ZZ^T) B = B^T (I - ZZ^T) (I - ZZ^T) B = V \Sigma U^T U \Sigma V^T = V^T \Sigma^2 V.\)
\textbf{PROOF OF BOOSTING LEMMA}

\begin{align*}
\|A - B^T ZZ^T B\|_F^2 &= \|B^T (I - ZZ^T) B\|_F^2 \\
&= \sum_{i=1}^{n-k} \sigma_i^2(B^T(I - ZZ^T)B) \\
&= \sum_{i=1}^{n-k} \sigma_i^4((I - ZZ^T)B).
\end{align*}

- Write \((I - ZZ^T)B = U\Sigma V^T\) using the SVD and note that
  \(B^T(I - ZZ^T)B = B^T(I - ZZ^T)(I - ZZ^T)B = V\Sigma U^T U\Sigma V^T = V^T \Sigma^2 V.\)
- So the error on \(A\) is just a \textbf{higher moment} of the error on \(B\):
  \[\|B - ZZ^T B\|_F^2 = \sum_{i=1}^{n-k} \sigma_i^2(B - ZZ^T B).\]
\begin{equation}
\|A - BZZ^T B\|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4 (B - ZZ^T B)
\end{equation}
\[ \| A - B Z Z^T B \|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4 (B - ZZ^T B) \]

Have: \[ \| B - ZZ^T B \|_F^2 - \| B - B_k \|_F^2 \leq \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \]
PROOF OF BOOSTING LEMMA

\[ \| A - B ZZ^T B \|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4 (B \ - \ ZZ^T B) \]

Have: \[ \left[ \sum \sigma_i^2 (B \ - \ ZZ^T B) \right] - \left[ \sum \sigma_i^2 (B \ - \ B_k) \right] \leq \frac{e^{3/2}}{\sqrt{n}} \| B \ - \ B_k \|_F^2 \]
PROOF OF BOOSTING LEMMA

\[ \|A - BZZ^T B\|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4 (B - ZZ^T B) \]

Have:

\[ \left[ \sum \sigma_i^2 (B - ZZ^T B) \right] - \left[ \sum \sigma_i^2 (B - B_k) \right] \leq \frac{e^{3/2}}{\sqrt{n}} \|B - B_k\|_F^2 \]

\[ \sigma_i^2 (B - ZZ^T B) \]

\[ \sigma_i^2 (B - B_k) = \sigma_{i+k}^2 (B) \]
\[ \| A - BZZ^T B \|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4 (B - ZZ^T B) \]

Have:

\[ \left[ \sum \sigma_i^2 (B - ZZ^T B) \right] - \left[ \sum \sigma_i^2 (B - B_k) \right] \leq \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \]
**Proof of Boosting Lemma**

\[ \| A - B ZZ^T B \|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4 (B - ZZ^T B) \]

Have:

\[ \left[ \sum \sigma_i^2 (B - ZZ^T B) \right] - \left[ \sum \sigma_i^2 (B - B_k) \right] \leq \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \]
**Proof of Boosting Lemma**

\[
\|A - BZZ^T B\|_F^2 = \sum_{i=1}^{n-k} \sigma_i^4(B - ZZ^T B)
\]

\[
\leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \|B - B_k\|_F \right]^2
\]

Have:
\[
\left[ \sum \sigma_i^2(B - ZZ^T B) \right] - \left[ \sum \sigma_i^2(B - B_k) \right] \leq \frac{\epsilon^{3/2}}{\sqrt{n}} \|B - B_k\|_F^2
\]
\[ \| A - B^T Z Z^T B \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \right]^2 \]
\[ \| A - B^T ZZ^T B \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \right]^2 \]

If \( \sigma_{k+1}^2(B) \geq \sqrt{\frac{\epsilon}{n}} \| B - B_k \|_F^2 \) then can bound as:
\[
\|A - B^T ZZ^T B\|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \|B - B_k\|_F^2 \right]^2
\]

If \( \sigma_{k+1}^2(B) \geq \sqrt{\frac{\epsilon}{n}} \|B - B_k\|_F^2 \) then can bound as:

\[
\|A - B^T ZZ^T B\|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + (1 + \epsilon)^2 \sigma_{k+1}^4(B)
\]
\[ \| A - B^T ZZ^T B \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \right]^2 \]

If \( \sigma_{k+1}^2(B) \geq \sqrt{\frac{\epsilon}{n}} \| B - B_k \|_F^2 \) then can bound as:

\[ \| A - B^T ZZ^T B \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + (1 + \epsilon)^2 \sigma_{k+1}^4(B) \]

\[ \leq (1 + \epsilon)^2 \sum_{i=k+1}^{n} \sigma_i^4(B) \]
\[
\|A - B^T ZZ^T B\|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \|B - B_k\|_F^2 \right]^2
\]

If \( \sigma_{k+1}^2(B) \geq \sqrt{\frac{\epsilon}{n}} \|B - B_k\|_F^2 \) then can bound as:

\[
\|A - B^T ZZ^T B\|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + (1 + \epsilon)^2 \sigma_{k+1}^4(B)
\]

\[
\leq (1 + \epsilon)^2 \sum_{i=k+1}^{n} \sigma_i^4(B)
\]

\[
= (1 + \epsilon)^2 \sum_{i=k+1}^{n} \sigma_i^2(A)
\]
\[ \| \mathbf{A} - \mathbf{B}^T \mathbf{Z} \mathbf{Z}^T \mathbf{B} \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(\mathbf{B}) + \left[ \sigma_{k+1}^2(\mathbf{B}) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| \mathbf{B} - \mathbf{B}_k \|_F^2 \right]^2 \]

If \( \sigma_{k+1}^2(\mathbf{B}) \geq \sqrt{\frac{\epsilon}{n}} \| \mathbf{B} - \mathbf{B}_k \|_F^2 \) then can bound as:

\[ \| \mathbf{A} - \mathbf{B}^T \mathbf{Z} \mathbf{Z}^T \mathbf{B} \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(\mathbf{B}) + (1 + \epsilon)^2 \sigma_{k+1}^4(\mathbf{B}) \]

\[ \leq (1 + \epsilon)^2 \sum_{i=k+1}^{n} \sigma_i^4(\mathbf{B}) \]

\[ = (1 + \epsilon)^2 \sum_{i=k+1}^{n} \sigma_i^2(\mathbf{A}) \]

\[ = (1 + 3\epsilon)\| \mathbf{A} - \mathbf{A}_k \|_F^2. \]
PROOF OF BOOSTING LEMMA

\[ \| A - B^T Z Z^T B \|_F^2 \leq \sum_{i=k+2}^n \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \right]^2 \]

If \( \sigma_{k+1}^2(B) \leq \sqrt{\frac{\epsilon}{n}} \| B - B_k \|_F^2 \) then can bound as:
\[ \| A - B^T ZZ^T B \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \right]^2 \]

If \( \sigma_{k+1}^2(B) \leq \sqrt{\frac{\epsilon}{n}} \| B - B_k \|_F^2 \) then can bound as:

\[ \| A - (B^T ZZ^T B) \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left( \sqrt{\frac{\epsilon}{n}} + \frac{\epsilon^{3/2}}{\sqrt{n}} \right)^2 \| B - B_k \|_F^4 \]
\begin{align*}
\|A - B^T Z Z^T B\|_F^2 &\leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \|B - B_k\|_F^2 \right]^2 \\
\text{If } \sigma_{k+1}^2(B) &\leq \sqrt{\frac{\epsilon}{n}} \|B - B_k\|_F^2 \text{ then can bound as:} \\
\|A - (B^T Z Z^T B)\|_F^2 &\leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left( \sqrt{\frac{\epsilon}{n}} + \frac{\epsilon^{3/2}}{\sqrt{n}} \right)^2 \|B - B_k\|_F^4 \\
&\leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \frac{4\epsilon}{n} \left( \sum_{i=k+1}^{n} \sigma_i^2(B) \right)^2
\end{align*}
PROOF OF BOOSTING LEMMA

\[ \| A - B^T ZZ^T B \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \| B - B_k \|_F^2 \right]^2 \]

If \( \sigma_{k+1}^2(B) \leq \sqrt{\frac{\epsilon}{n}} \| B - B_k \|_F^2 \) then can bound as:

\[ \| A - (B^T ZZ^T B) \|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left( \sqrt{\frac{\epsilon}{n}} + \frac{\epsilon^{3/2}}{2} \sqrt{n} \right)^2 \| B - B_k \|_F^4 \]

\[ \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + 4\epsilon \cdot \left( \sum_{i=k+1}^{n} \sigma_i^2(B) \right)^2 \]

\[ \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + 4\epsilon \cdot \sum_{i=k+1}^{n} \sigma_i^4(B) \]
\[
\|A - B^T ZZ^T B\|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left[ \sigma_{k+1}^2(B) + \frac{\epsilon^{3/2}}{\sqrt{n}} \|B - B_k\|_F^2 \right]^2
\]

If \( \sigma_{k+1}^2(B) \leq \sqrt{\frac{\epsilon}{n}} \|B - B_k\|_F^2 \) then can bound as:

\[
\|A - (B^T ZZ^T B)\|_F^2 \leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \left( \sqrt{\frac{\epsilon}{n}} + \frac{\epsilon^{3/2}}{\sqrt{n}} \right)^2 \|B - B_k\|_F^4
\]

\[
\leq \sum_{i=k+2}^{n} \sigma_i^4(B) + \frac{4\epsilon}{n} \cdot \left( \sum_{i=k+1}^{n} \sigma_i^2(B) \right)^2
\]

\[
\leq \sum_{i=k+2}^{n} \sigma_i^4(B) + 4\epsilon \cdot \sum_{i=k+1}^{n} \sigma_i^4(B)
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\[
\leq (1 + 4\epsilon) \sum_{i=k+1}^{n} \sigma_i^2(A)
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Theorem (‘Slow’ Sublinear Time Low-Rank Approximation)

There is an algorithm which given PSD $A \in \mathbb{R}^{n \times n}$ accesses $O\left(\frac{n^3}{2} \cdot \text{poly}(k, 1/\epsilon)\right)$ entries of the matrix and outputs $N, M \in \mathbb{R}^{n \times k}$ which satisfy with probability $99/100$:

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Recall that our algorithm is based off adaptive sampling - we iteratively select \( \tilde{O}(k^2/\epsilon) \) columns of \( B \) and project to them.
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- Requires accessing the diagonal and $\tilde{O}(\sqrt{nk^2})$ columns of $\mathbf{A}$. 

![Diagram of matrix A with diagonal highlighted]
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Recall that our algorithm is based off adaptive sampling - we iteratively select $\tilde{O}(k^2 \cdot \sqrt{n})$ columns of $B$ and project to them.

- Requires accessing the diagonal and $\tilde{O}(\sqrt{n}k^2)$ columns of $A$.

- If we take fewer columns, we can miss a $\sqrt{n} \times \sqrt{n}$ block which contains a constant fraction of $A$’s Frobenius norm.
LIMITATIONS OF COLUMN SAMPLING

- Probability that a column sample hits a single off-diagonal entry is $O(1/\sqrt{n})$.
- So $\Omega(\sqrt{n})$ samples are required to find the block.
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Limitations of column sampling

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![Diagram showing a matrix with diagonal and off-diagonal entries.](image)
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\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{A matrix $A$ with $n^{1/3}$ columns and $n^{2/3}$ rows.}
\end{figure}
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Highlights the difference between low-rank approximation of $A$ and its square root $B$.

• $\sigma_1^2(A) = n$ and $\|A - A_1\|_F^2 \approx n$. Even obtaining a 2-approximation to the best rank-1 approximation requires finding the block.

• $\sigma_1^2(B) = \sqrt{n}$ and $\|B - B_1\|_F^2 \approx n$, so the block does not need to be recovered to obtain a $\left(1 + \frac{1}{\sqrt{n}}\right)$-optimal approximation.
**Solution:** Sample both rows and columns of $A$. 
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- Instead of adaptive sampling we use ridge leverage scores, which can also be computed using an iterative sampling scheme making $\tilde{O}(nk)$ accesses to $A$ (Musco, Musco ’17).
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- Same intuition – select a diverse set of columns which span a near-optimal low-rank approximation of the matrix. However come with much stronger guarantees.
- Sample $AS$ is a projection-cost-preserving sketch for $A$. For any rank-$k$ projection $P$,

$$\|AS - PAS\|_F^2 = (1 \pm \epsilon)\|A - PA\|_F^2.$$
Technological Challenge:
Proving that $S_2AS_1$ is a projection-cost preserving sketch of $AS_1$. 

\[
\begin{align*}
\text{A} & \quad \xrightarrow{\text{ridge leverage sample}} \quad AS_1 \\
& \quad \xrightarrow{\sqrt{nk}/\epsilon^2} \quad S_2AS_1
\end{align*}
\]
**Technical Challenge:** Proving that $S_2 AS_1$ is a projection-cost preserving sketch of $AS_1$. 
Recover low-rank approximation using projection-cost preserving sketches.
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• View each entry of $A$ as encoding a large amount of information about its square root $B$. In particular $a_{ij} = b_i^T b_j$. 
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• Use this view to find a low-rank approximation to $B$ using sublinear accesses to $A$. 

• Obtain near-optimal complexity using ridge leverage scores to sample both rows and columns of $A$. 
• View each entry of $\mathbf{A}$ as encoding a large amount of information about its square root $\mathbf{B}$. In particular $a_{ij} = b_i^T b_j$.

• Use this view to find a low-rank approximation to $\mathbf{B}$ using sublinear accesses to $\mathbf{A}$.

• Since $\mathbf{B}$ has the same singular vectors as $\mathbf{A}$ and $\sigma_i(\mathbf{B}) = \sqrt{\sigma_i(\mathbf{A})}$, a low-rank approximation of $\mathbf{B}$ can used to find one for $\mathbf{A}$, albeit with a $\sqrt{n}$ factor loss in quality.
SUMMARY OF MAIN IDEAS

- View each entry of $\mathbf{A}$ as encoding a large amount of information about its square root $\mathbf{B}$. In particular $a_{ij} = b_i^T b_j$.
- Use this view to find a low-rank approximation to $\mathbf{B}$ using sublinear accesses to $\mathbf{A}$.
- Since $\mathbf{B}$ has the same singular vectors as $\mathbf{A}$ and $\sigma_i(\mathbf{B}) = \sqrt{\sigma_i(\mathbf{A})}$, a low-rank approximation of $\mathbf{B}$ can used to find one for $\mathbf{A}$, albeit with a $\sqrt{n}$ factor loss in quality.
- Obtain near-optimal complexity using ridge leverage scores to sample both rows and columns of $\mathbf{A}$. 
**OPEN QUESTIONS**

• What else can be done for PSD matrices? We give applications to ridge regression, but what other linear algebraic problems require a second look?

• Are there other natural classes of matrices that admit sublinear time low-rank approximation?

• Starting points are matrices that break the $\Omega(n \text{nnz}(A))$ time lower bound: e.g. binary matrices, diagonally dominant matrices.
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• What can we do when we have PSD matrices with additional structure?

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- Can apply our algorithm – accessing an entry of \( A \) is equivalent to computing a single kernel dot product. But in some cases you may be able to do something smarter.
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- Low-rank approximation of the square root kernel matrix (the ‘kernelized dataset’) is also interesting here.
Thanks! Questions?