RIDGE LEVERAGE SCORES FOR LOW-RANK MATRIX APPROXIMATION

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“Ridge Leverage Scores for Low-Approximation” = ”Dimensionality Reduction for k-Means Clustering and Low-Rank Approximation” + “Uniform Sampling for Matrix Approximation”
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Papers and slides available at chrismusco.com.
HOW TO DEAL WITH HUGE DATA SETS?

- Computing power (MapReduce, Hadoop, Apache Spark, etc.)
- Limited data access (iterative methods, stochastic methods)
- Dimensionality reduction ("sketch-and-solve")
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- dimensionality reduction ("sketch-and-solve")
Replace high dimensional data with low dimensional sketch.
Solution on sketch $\hat{A}$ should approximate original solution.
Replace dimensional of data points, not their number.
Reduce the number of data points, not their dimension.

\[ \text{n data points} \rightarrow \tilde{A} \rightarrow \tilde{\text{n' datapoints}} \]

\( \tilde{A} \) is often called a coreset.
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- **Johnson-Lindenstrauss projections** = super fast to apply, naturally adapts to streaming/distributed environments.
- **Deterministic methods (SVD, Frequent Directions)** = best data compression.
- **Data Selection/Sampling** = preserves structure and sparsity.
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WHAT’S THIS PAPER ABOUT?

1. **Leverage Scores** are used ubiquitously as importance sampling probabilities for matrix sketching.

2. These scores have been extended to sketches for low-rank approximation problems, but not in a satisfying way.

3. We give a more natural extension, via **Ridge Leverage Scores**. These scores lead to simple proofs and have a bunch of desirable properties and new applications.
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A sketch $\tilde{A}$ such that, for all vectors $x$, $\|x^T\tilde{A}\| = (1 \pm \epsilon)\|x^TA\|$.
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Applications:

- Approximate (constrained) linear regression.
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- Approximate (constrained) linear regression.
- Constructing preconditioners for iterative system solvers.
- Spectral sparsifiers for fast approximate graph algorithms.
Equivalent formulation of subspace embeddings:

$$\|x^T A\|_2^2 = (1 \pm \epsilon) \|x^T \tilde{A}\|_2^2$$
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$$x^T A A^T x = (1 \pm \epsilon) x^T \tilde{A} \tilde{A}^T x$$
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Let’s think about subspace embeddings as approximating the quadratic form \( A A^T \).
A \cdot A^T = A^T \cdot A
\[ A \mathbf{a}_1 \mathbf{a}_1^T = \mathbf{a}_1 \mathbf{a}_1^T = \mathbf{A} \mathbf{A}^T \]
\[ A \mathsf{a}_1 \mathsf{a}_2 \]

\[ A = A^T \]

\[ = \mathsf{a}_1^T \mathsf{a}_2 + \mathsf{a}_2^T \mathsf{a}_2 \]

\[ = A A^T \]
A^T A = \sum_{i=1}^{d} a_i a_i^T = AA^T
\[ \begin{align*}
\mathbf{A} \mathbf{A}^T &= \sum_{i=1}^{d} \mathbf{a}_i \mathbf{a}_i^T \\
&= \mathbf{A} \mathbf{A}^T
\end{align*} \]
**Sampling Scheme:** For any set of sampling probabilities $p_1, p_2, \ldots, p_d$ include column $a_i$ in $\tilde{A}$ with probability $p_i$ and reweight the column by $\frac{1}{p_i}$. 
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Then:

$$\mathbb{E} [\tilde{A}\tilde{A}^T] = \sum_{i=1}^{d} p_i \cdot \left( \frac{1}{p_i} a_i a_i^T \right)$$
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How to get good concentration?
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Need to select more “unique” columns with higher probability.

If we don’t select $a_i$ then $x^T A^T x = 0$, while $x^T A A^T x$ is positive. $x^T A^T x$ cannot equal $(1 - \epsilon)x^T A A^T x$. 

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\( x^T\tilde{A}\tilde{A}^T x \) cannot equal \( (1 \pm \epsilon)x^T A A^T x \).
How to measure “unique-ness”: 

$$\text{Definition (Leverage Score, } a_i) = \min \|y\|^2 \text{ such that } a_i = Ay$$

Since we can choose $y$ to be the $i$th basis vector.
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$\tau(a_i) \leq 1$ since we can choose $y$ to be the $i^{th}$ basis vector.
How to measure “unique-ness”:

Definition (Leverage Score, $\tau$)

$$\tau(a_i) = \min \|y\|_2^2 \text{ such that } a_i = Ay$$

If more columns align with $a_i$, $\tau(a_i)$ decreases.
Problem: Find $\tau(a_i) = \min \|y\|_2^2$ such that $a_i = Ay$.

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$$\sum_i \tau(a_i) = \text{tr}(A^T (A^T A)^{-1} A) = \text{rank}(A) \leq n.$$
More specifically, to get a subspace embedding, we sample each column \( a_i \) with probability \( \tau(a_i) \cdot \frac{\log n}{\epsilon^2} \).
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We’re approximating $A$ with a sum of (binary) random matrices:

$$X_i = \begin{cases} \frac{1}{p_i} a_i a_i^T & \text{with probability } p_i \\ 0 & \text{with probability } (1 - p_i) \end{cases}$$

$$\tilde{A}\tilde{A}^T = \sum_{i=1}^d X_i.$$
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$\tau(a_i) \frac{\log n}{\epsilon^2}$ is the lowest $p_i$ which ensures $\frac{1}{p_i} a_i a_i^T \preceq \frac{\epsilon^2}{\log n} A A^T$. 

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“User-friendly tail bounds for sums of random matrices”, Joel Tropp
Theorem (Subspace Embedding via Sampling)

Sampling $O\left(\frac{n \log n}{\epsilon^2}\right)$ columns from $A$ by leverage score gives an $\epsilon$ factor subspace embedding with high probability.
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$$\sum_i \tau(a_i) \frac{\log n}{\epsilon^2}$$
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Fortunately, leverage scores are very robust – they can be estimated using very weak approximations to \(\mathbf{A}\).
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There are many generalizations and modifications of leverage scores.
Extensions to low-rank problems have been especially popular.
For subspace embeddings we approximate $A A^T = U U^T$. For $x^T A A^T x$ for all $x$ we need to preserve information about every singular direction/value. Specifically, it can be shown that $\epsilon_i(A) = (1 + \epsilon) \epsilon_i(A)$.
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For $x^T\tilde{A}\tilde{A}^Tx \approx x^TAA^Tx$ for all $x$ we need to preserve information about every singular direction/value. Specifically, it can be shown that $\sigma_i(\tilde{A}) = (1 \pm \epsilon)\sigma_i(A)$.
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For many sketching applications, we only need $\mathbf{\tilde{A}}$ to capture information about $\mathbf{A}$’s top singular directions/values.

In these cases, we should be able to obtain smaller sketches – i.e. $O(k)$ instead of $O(n)$. 

$\mathbf{A}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T$
Find low-rank matrix close to $A$. 

\[
\|A - A_k\|_F^2 = \text{sum of squared distances to hyperplane spanned by } Q.
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$$\|A QQ^T A\|_F^2 = \text{sum of squared distances to hyperplane spanned by } Q.$$
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$\|A - QQ^TA\|_F^2 = \text{sum of squared distances to hyperplane spanned by } Q.$
Without any constraints, finding the optimal rank $k \mathbf{Q}$ is equivalent to singular value decomposition: 

\[
\mathbf{A}_k = \Sigma_k \sigma_1 \sigma_2 \cdots \sigma_{d-1} \sigma_d \mathbf{U}_k \mathbf{V}_k^T
\]

where $\Sigma_k$ are the first $k$ singular values, $\mathbf{U}_k$ are the left singular vectors, and $\mathbf{V}_k$ are the right singular vectors.
Without any constraints, finding the optimal rank $k$ $Q$ is equivalent to singular value decomposition:

$$A_k = U_k \Sigma_k V_k^T$$

<table>
<thead>
<tr>
<th>left singular vectors</th>
<th>singular values</th>
<th>right singular vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_k$</td>
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\mathbf{A}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T
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where $\mathbf{A}_k$ is the low-rank approximation of $\mathbf{A}$, $\mathbf{U}_k$ are the left singular vectors, $\mathbf{\Sigma}_k$ are the singular values, and $\mathbf{V}_k$ are the right singular vectors.

\[
\|\mathbf{A} - \mathbf{A}_k\|_F^2 = \|\mathbf{A} - \mathbf{U}_k \mathbf{U}_k^T \mathbf{A}\|_F^2 = \min \|\mathbf{A} - \mathbf{QQ}^T \mathbf{A}\|_F^2.
\]

Set $\mathbf{Q} = \mathbf{U}_k$, i.e. to the top $k$ singular vectors of $\mathbf{A}$.
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- nonnegative PCA
- sparse PCA
- $k$-means clustering (see slides on my website)
In either case, we need to capture information about A’s top singular vectors only.
Two well studied guarantees for low-rank sketching.
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Column Subset Selection:
Find an $\tilde{A}$ such that $\|A - proj_{\tilde{A}}(A)\|_F^2 \leq (1 + \epsilon)\|A - A_k\|_F^2$. 

SPECIFIC SKETCHING GUARANTEES
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**Projection Cost Preserving Sample:**
Find an \( \tilde{A} \) such that \( \|\tilde{A} - QQ^T\tilde{A}\|_F^2 = (1 \pm \epsilon)\|A - QQ^T\tilde{A}\|_F^2 \) for all rank \( k \) orthonormal matrices \( Q \).
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\[ \|\tilde{A} - QQ^\top A\|_F^2 = (1 \pm \epsilon)\|A - QQ^\top A\|_F^2 \]
Subspace Embedding implies Column Subset Selection and Projection Cost Preservation.
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But we would get a sketch with too many samples: $\tilde{O}(n)$ columns vs. ideally $\tilde{O}(k)$ columns.
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[Drineas, Mahoney, Muthukrishnan ‘08, and Sarlós ‘06]
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\tilde{\tau}(a_i) = a_i^T \left( (A_{2k}^T A_k)^{-1} + \frac{k}{\|A - A_{2k}\|_F^2} (I - U_{2k} U_{2k}^T) \right) a_i
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[Cohen, Elder, Musco, Musco, Persu ‘15]
Great, we can solve both low-rank sampling problems.
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2. The scores cannot be computed in a data stream.
Single Underlying Issue:
Existing low-rank scores are not **monotonic**.
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Single Underlying Issue:
Existing low-rank scores are not monotonic.

For standard leverage scores, adding a column to $A$ can only decrease the importance of existing columns.
Streaming setup:

Receive columns of $A$ one-by-one. Reject each with probability depending on its (low-rank) leverage score with respect to the columns seen so far [Kelner, Levin ‘11].
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![Diagram showing the streaming setup with columns and rejection probability]

Rejection probability only decreases, so we never delete a column with too high of probability.
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![Diagram showing the streaming setup and rejection probability](image)
Streaming setup:

Receive columns of $A$ one-by-one. Reject each with probability depending on it’s (low-rank) leverage score with respect to the columns seen so far [Kelner, Levin ‘11].

Rejection probability only decreases, so we never delete a column with too high of probability.
Iterative Leverage Score Sampling: Monotonicity is essential because it ensures that a uniform subsample of columns can at least be used to find upper bounds for leverage scores. [Cohen, Lee, Musco, Musco, Peng, Sidford ‘15]
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Why aren’t prior low-rank leverage scores monotonic?
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![Matrix Diagram]

<table>
<thead>
<tr>
<th>A</th>
<th>u_1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1 1 1 1 1 1</td>
<td>0</td>
</tr>
<tr>
<td>0 0 0 0 0 0 0</td>
<td>1</td>
</tr>
<tr>
<td>0 0 0 0 0 0 0</td>
<td>0</td>
</tr>
<tr>
<td>0 0 0 0 0 0 0</td>
<td>0</td>
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<tr>
<td>0 0 0 0 0 0 0</td>
<td>0</td>
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<td>0 0 0 0 0 0 0</td>
<td>0</td>
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<td>0</td>
</tr>
</tbody>
</table>

Adding a column could cause $a_i$ to drop significantly.

Here $a_1^T({A_1}^T{A_1})^{-1}a_1 = 0$. 
Why aren’t prior low-rank leverage scores monotonic?
They depend on \((A_k A_k)^{-1}\), which is inherently unstable.

Adding a column could cause \(a_i^T (A_k A_k)^{-1} a_i\) to drop significantly.

Here \(a_1^T (A_1 A_1)^{-1} a_1 \implies 0\).
How to avoid instability?

- **Ridge Leverage Scores** of [Alaoui, Mahoney '15].

\[ i \left( A^T A + I \right)_{i,i} = \begin{cases} 8 & \text{for } i = k, \\ 2 & \text{for } i < k. \end{cases} \]
How to avoid instability?

“Soften” the existing definition of rank $k$ leverage scores.
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“Soften” the existing definition of rank \( k \) leverage scores.

\[
\tilde{\tau}(a_i) = a_i^T (A_{\mathbf{R}}^T A_{\mathbf{R}})^{-1} a_i
\]
How to avoid instability?

“Soften” the existing definition of rank $k$ leverage scores.

$$\tilde{\tau}(a_i) = a_i^T(A^TA + \lambda I)^{-1}a_i$$
How to avoid instability?

“Soften” the existing definition of rank $k$ leverage scores.

\[ \tilde{\tau}(a_i) = a_i^T (A^T A + \lambda I)^{-1} a_i \]

The $\lambda$-Ridge Leverage Scores of [Alaoui, Mahoney ‘15].
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$$\tilde{\tau}(a_i) = a_i^T(A^TA + \lambda I)^{-1}a_i$$

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$$\sigma_i \left( A^T A (A_k^T A_k)^{-1} \right) = \begin{cases} 1 & \text{for } i \geq k, \\ 0 & \text{for } i < k. \end{cases}$$
How to avoid instability?

“Soften” the existing definition of rank $k$ leverage scores.

$$\tilde{\tau}(a_i) = a_i^T(A^T A + \lambda I)^{-1} a_i$$

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$$\sigma_i \left( A^T A (A_k^T A_k)^{-1} \right) = \begin{cases} 1 & \text{for } i \geq k, \\ 0 & \text{for } i < k. \end{cases}$$

$$\sigma_i \left( A^T A (A^T A + \lambda I)^{-1} \right) = \frac{\sigma_i^2}{\sigma_i^2 + \lambda}$$
Relatively “gentle” soft step:

\[ \sigma_i \left( A^T A (B^T B)^{-1} \right) \]
We can “wash out” the importance of columns by computing leverage scores over \( A \) with an identity appended:
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$$y = a_i$$
We can “wash out” the importance of columns by computing leverage scores over $\mathbf{A}$ with an identity appended:
We can “wash out” the importance of columns by computing leverage scores over $A$ with an identity appended:

$$y = a_i \sqrt{\lambda}$$

Effect is weaker when $a_i$ aligns with large singular vectors of $A$. 
Theorem (Ridge Leverage Score Sampling)

With $\lambda$ set to $\|A - A_k\|_F^2/k$, sampling $O(k \log k/\epsilon^2)$ columns by ridge leverage score produces an $\epsilon$ error projection cost preserving sketch with high probability.
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With $\lambda$ set to $\|A - A_k\|_F^2/k$, sampling $O(k \log k/\epsilon^2)$ columns by ridge leverage score produces an $\epsilon$ error projection cost preserving sketch with high probability. Sampling $O(k \log k/\epsilon)$ columns produces an $\epsilon$ error column subset.

Furthermore, $(\|A - A_k\|_F^2/k)$-ridge leverage scores are monotonic with respect to column additions.
Since $\lambda = \|A - A_k\|_F^2$ can only increase as columns are added to $A$, this perspective immediately implies that ridge leverage score are monotonic.
With $\lambda$ set to $\|A - A_k\|_F^2/k$, sampling by ridge leverage score produces a sketch $\tilde{A}$ such that:

$$(1 - \epsilon)\tilde{A}\tilde{A}^T - \epsilon \frac{\|A - A_k\|_F^2}{k} I \preceq AA^T \preceq (1 + \epsilon)\tilde{A}\tilde{A}^T + \epsilon \frac{\|A - A_k\|_F^2}{k} I$$
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Multiplicative error of a \textit{subspace embedding}.

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\[
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Multiplicative error of a subspace embedding.

Additive error of a Frequent Directions sketch [Ghashami, Liberty, Phillips, Woodruff].

Both are known to give projection cost preserving sketches. Handling both errors simultaneously is tedious, but not hard.
\[
(1 - \epsilon)\tilde{A}\tilde{A}^T - \epsilon \frac{\|A - A_k\|_F^2}{k} I \preceq AA^T \preceq (1 + \epsilon)\tilde{A}\tilde{A}^T + \epsilon \frac{\|A - A_k\|_F^2}{k} I
\]
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\[\|\tilde{A} - QQ^T\tilde{A}\|^2_F = (1 \pm \epsilon)\|A - QQ^TA\|^2_F\]
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\| (I - QQ^T)\tilde{A} \|_F^2 = (1 \pm \epsilon)\| (I - QQ^T)A \|_F^2
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\[\|(I - QQ^T)\tilde{A}\|^2_F = (1 \pm \epsilon)\|(I - QQ^T)A\|^2_F\]

Sum of vector products with \(\tilde{A}\). Each preserved to within a 
\((1 \pm \epsilon)\) factor, so the entire sum is as well.
\[
(1 - \epsilon)\hat{A}\hat{A}^T - \epsilon \frac{\|A - A_k\|_F^2}{k} \preceq AA^T \preceq (1 + \epsilon)\hat{A}\hat{A}^T + \epsilon \frac{\|A - A_k\|_F^2}{k}
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**Intuition:**

Dealing with rank \(k\) operators (\(Q\) is rank \(k\)), so we only pay the additive error \(k\) times.
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\]

\[=
\epsilon \|A - A_k\|_F^2
\]

\[\leq \epsilon \|A - QQ^T A\|_F^2
\]

Since \(A_k\) is a better low-rank approximation than any \(QQ^T A\).
Proof follows directly from our “appending an identity” view!
Proof:

1. Leverage score sampling clearly works if we set $p_i > \log \frac{n}{\epsilon}$.
2. Take identity columns with probability one, everything else with leverage score probabilities.
3. Obtain a sketch $B = [\tilde{A}; p I]$ satisfying:
   \[
   (1 + \epsilon)BB^T \preceq AA^T + I \preceq (1 + \epsilon)BB^T 
   \]
4. \[
   (1 + \epsilon)(\tilde{A}\tilde{A}^T + I) \preceq AA^T + I \preceq (1 + \epsilon)(\tilde{A}\tilde{A}^T + I) 
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   \]

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   (1 - \epsilon)(\tilde{A}\tilde{A}^T + \lambda I) \preceq AA^T + \lambda I \preceq (1 + \epsilon)(\tilde{A}\tilde{A}^T + \lambda I)
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$$
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$$

$$
= \sum_{i=1}^{d} \frac{\sigma_i(A)}{\sigma_i(A) + \frac{||A - A_k||_F^2}{k}}
$$

$$
\leq k + \sum_{i=k+1}^{d} \frac{\sigma_i(A)}{\sigma_i(A) + \frac{||A - A_k||_F^2}{k}}
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$$= k + \frac{k}{k}$$
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$$\leq k + \sum_{i=k+1}^{d} \frac{\sigma_i(A)}{\|A - A_k\|_F^2} \frac{\|A - A_k\|_F^2}{k}$$

$$= k + k = O(k).$$
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