SUBLINEAR TIME LOW-RANK APPROXIMATION OF POSITIVE SEMIDEFINITE MATRICES

Cameron Musco (MIT) and David P. Woodruff (CMU)

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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.





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Low-rank approximation is one of the most widely used methods for general matrix and data compression.



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Important Special Case: A is positive semidefinite (PSD). I.e.

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• Includes graph Laplacians, Gram matrices and kernel matrices, covariance matrices, Hessians for convex functions.







$$\mathbf{A}_k = \arg\min_{\mathbf{B}: \operatorname{rank}(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_F$$



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• Unfortunately, computing the SVD takes $O(nd^2)$ time.

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

$$\|\mathbf{A} - \mathbf{N}\mathbf{M}^{\mathsf{T}}\|_{\mathsf{F}} \leq (1+\epsilon)\|\mathbf{A} - \mathbf{A}_k\|_{\mathsf{F}}.$$

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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.

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

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- Compare to CW'13 which takes $O(nnz(\mathbf{A})) + n \cdot poly(k, 1/\epsilon)$.
- If k, 1/e are not too large compared to nnz(A), our runtime is significantly sublinear in the size of A.

LOWER BOUND FOR GENERAL MATRICES

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||A - NM^T||_F < ||A - A_k||_F + ε||A||_F.

WHAT ABOUT FOR PSD MATRICES?

Observation: For PSD **A**, we have for any entry \mathbf{a}_{ij} :

 $\mathbf{a}_{ij} \leq \max(\mathbf{a}_{ii}, \mathbf{a}_{jj})$

since otherwise $(\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{A} (\mathbf{e}_i - \mathbf{e}_j) < 0$.



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Question: How can we exploit additional structure arising from positive semidefiniteness to achieve sublinear runtime?

Very Simple Fact: Every PSD matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ can be written as $\mathbf{B}^T \mathbf{B}$ for some $\mathbf{B} \in \mathbb{R}^{n \times n}$.

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- **B** can be any matrix square root of **A**, e.g. if we let $V\Sigma V^{T}$ be the eigendecomposition of **A**, we can set $\mathbf{B} = \Sigma^{1/2} \mathbf{V}^{T}$.
- Letting b₁, ..., b_n be the columns of B, the entries of A contain every pairwise dot product a_{ij} = b_i^Tb_j.



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• The heavy diagonal observation is just one example. By Cauchy-Schwarz:

$$\mathbf{a}_{ij} = \mathbf{b}_i^{\mathsf{T}} \mathbf{b}_j \leq \sqrt{(\mathbf{b}_i^{\mathsf{T}} \mathbf{b}_i) \cdot (\mathbf{b}_j^{\mathsf{T}} \mathbf{b}_j)} = \sqrt{\mathbf{a}_{ii} \cdot \mathbf{a}_{jj}} \leq \max(\mathbf{a}_{ii}, \mathbf{a}_{jj}).$$

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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 \mathbf{a}_{ij} .

Why? **B** has the same (right) singular vectors as **A**, and its singular values are closely related: $\sigma_i(\mathbf{B}) = \sqrt{\sigma_i(\mathbf{A})}$.

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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, but this simple idea will lead to a sublinear time algorithm for **A**.

LOW-RANK APPROXIMATION VIA ADAPTIVE SAMPLING

Theorem (Deshpande, Vempala '06)

For any $\mathbf{B} \in \mathbb{R}^{n \times n}$, there exists a subset of $\tilde{O}(k^2/\epsilon)$ columns whose span contains $\mathbf{Z} \in \mathbb{R}^{n \times k}$ satisfying:

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Adaptive Sampling



Initially, start with an empty column subset $S := \{\}$. For $t = 1, ..., \tilde{O}(k^2/\epsilon)$ Let \mathbf{P}_S be the projection onto the columns in S. Add \mathbf{b}_i to S with probability $\frac{\|\mathbf{b}_i - \mathbf{P}_S \mathbf{b}_i\|^2}{\sum_{i=1}^n \|\mathbf{b}_i - \mathbf{P}_S \mathbf{b}_i\|^2} = \frac{\|\mathbf{b}_i\|^2}{\sum_{i=1}^n \|\mathbf{b}_i\|^2} = \frac{\mathbf{a}_{ii}}{\operatorname{tr}(\mathbf{A})}$.



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Theorem (Factor Matrix Low-Rank Approximation) There is an algorithm using $\tilde{O}(nk^2/\epsilon)$ accesses to $\mathbf{A} = \mathbf{B}^T \mathbf{B}$ which computes $\mathbf{Z} \in \mathbb{R}^{n \times k}$ satisfying with probability 99/100: $\|\mathbf{B} - \mathbf{Z}\mathbf{Z}^T\mathbf{B}\|_F \leq (1 + \epsilon)\|\mathbf{B} - \mathbf{B}_k\|_F.$ Theorem (Factor Matrix Low-Rank Approximation) There is an algorithm using $\tilde{O}(nk^2/\epsilon)$ accesses to $\mathbf{A} = \mathbf{B}^T \mathbf{B}$ which computes $\mathbf{Z} \in \mathbb{R}^{n \times k}$ satisfying with probability 99/100: $\|\mathbf{B} - \mathbf{Z}\mathbf{Z}^T\mathbf{B}\|_F \le (1 + \epsilon)\|\mathbf{B} - \mathbf{B}_k\|_F.$

• How does this translate to low-rank approximation of A itself?

Lemma If $\|\mathbf{B} - \mathbf{Z}\mathbf{Z}^T\mathbf{B}\|_F^2 \le \left(1 + \frac{\epsilon^{3/2}}{\sqrt{n}}\right) \|\mathbf{B} - \mathbf{B}_k\|_F^2$, then for $\mathbf{A} = \mathbf{B}^T\mathbf{B}$: $\|\mathbf{A} - \mathbf{B}^T\mathbf{Z}\mathbf{Z}^T\mathbf{B}\|_F^2 \le (1 + \epsilon)\|\mathbf{A} - \mathbf{A}_k\|_F^2$.

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- Our best algorithm accesses just $\tilde{O}\left(\frac{nk}{\epsilon^{2.5}}\right)$ entries of **A** and runs in $\tilde{O}\left(\frac{nk^2}{\epsilon^4}\right)$ time.

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• 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.

Solution: Sample both rows and columns of A.
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- Sample **AS** is a projection-cost-preserving sketch for **A** [Cohen et al '15,'17]. For any rank-*k* projection **P**,

$$\|\mathbf{AS} - \mathbf{PAS}\|_{F}^{2} = (1 \pm \epsilon) \|\mathbf{A} - \mathbf{PA}\|_{F}^{2}.$$

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- Since **B** has the same singular vectors as **A** and $\sigma_i(\mathbf{B}) = \sqrt{\sigma_i(\mathbf{A})}$, a low-rank approximation of **B** can used to find one for **A**, albiet with a \sqrt{n} factor loss in quality.
- Obtain near-optimal complexity using ridge leverage scores to sample both rows and columns of **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?

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• What can we do when we have PSD matrices with additional structure? E.g. kernel matrices.

Thanks! Questions?