RANDOMIZED BLOCK KRYLOV METHODS FOR STRONGER AND FASTER APPROXIMATE SVD

Cameron Musco and Christopher Musco

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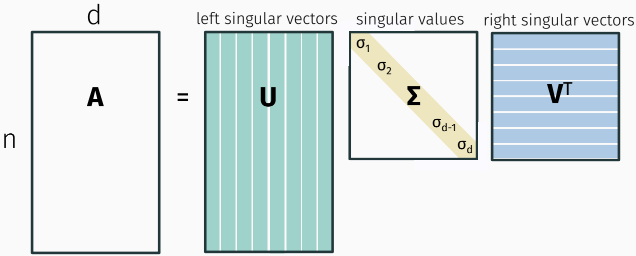
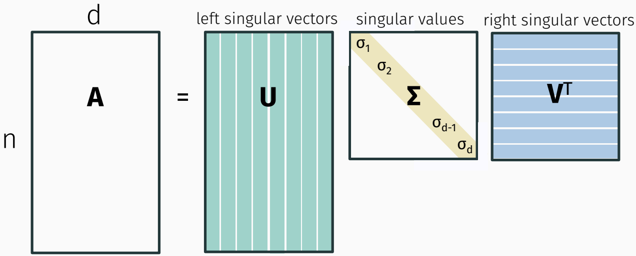
Massachusetts Institute of Technology, EECS

SINGULAR VALUE DECOMPOSITION





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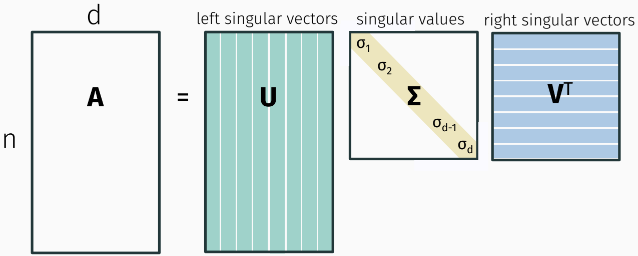

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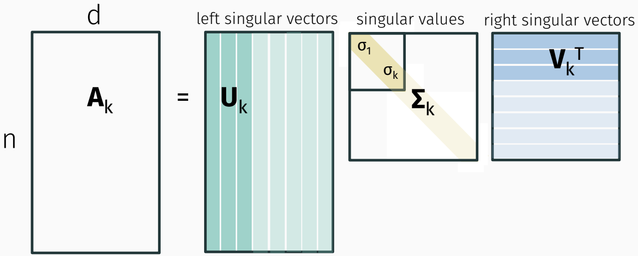

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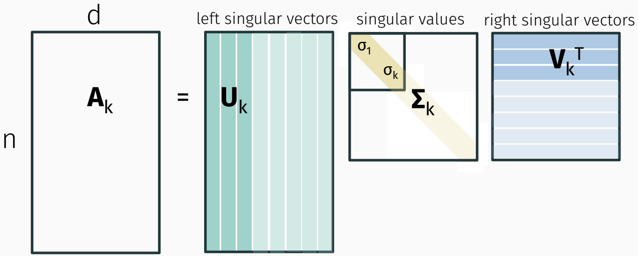

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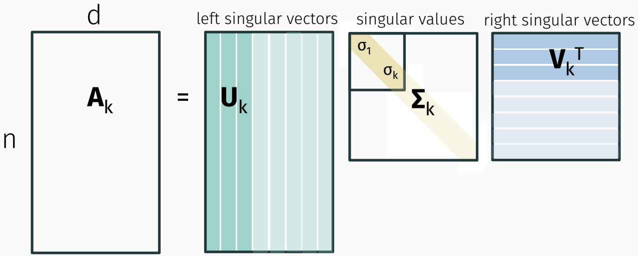

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$$\mathbf{U}_k \mathbf{U}_k^T \mathbf{A} = \underset{\mathbf{B}: rank(\mathbf{B})=k}{\arg\min} \|\mathbf{A} - \mathbf{B}\|_2$$

- Frobenius Norm Low-Rank Approximation:

$$\|\mathbf{A} - \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T \mathbf{A}\|_F \leq (1+\epsilon) \|\mathbf{A} - \mathbf{U}_k \mathbf{U}_k^T \mathbf{A}\|_F$$

- Frobenius Norm Low-Rank Approximation (weak):

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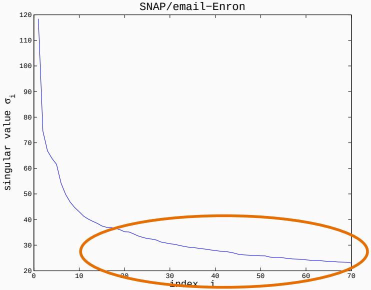

STANDARD SVD APPROXIMATION METRICS

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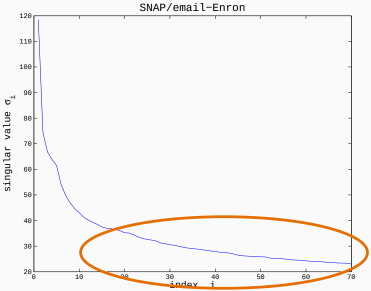

For many datasets literally any $\tilde{\mathbf{U}}_k$ would work!

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- Per Vector Principal Component Error (strongest):

$$\tilde{u}_i^T \mathbf{A}\mathbf{A}^T \tilde{u}_i \geq (1-\epsilon) u_i^T \mathbf{A}\mathbf{A}^T u_i \qquad \text{for all } i \leq k.$$

Classic Full SVD Algorithms (e.g. QR Algorithm):

All of these goals in roughly $O(nd^2)$ time (error dependence is $\log\log 1/\epsilon$ on lower order terms).

Unfortunately, this is much too slow for many data sets.

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How fast can we approximately compute just $u_1, \ldots, u_k$?

‘Weak’ Approximation Algorithms:

- Strong Rank Revealing QR (Gu, Eisenstat 1996):

$$\|\mathbf{A} - \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T \mathbf{A}\|_F \leq \text{poly}(n, k)\|\mathbf{A} - \mathbf{A}_k\|_F \text{ in time } O(ndk)$$

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- Sparse Subspace Embeddings (Clarkson, Woodruff 2013):

$$\|\mathbf{A} - \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T \mathbf{A}\|_F \leq (1+\epsilon)\|\mathbf{A} - \mathbf{A}_k\|_F \text{ in time } O(\text{nnz}(\mathbf{A})) + \tilde{O}\left(\frac{nk^2}{\epsilon^4}\right)$$

Iterative methods are the only game in town for stronger guarantees. Runtime is approximately:

$$O(\mathrm{nnz}(\mathbf{A})k \cdot \#iterations)$$

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- Stochastic Methods?

Traditional Power Method:

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$$\mathbf{X}_0 \in \mathbb{R}^{d \times k}, \qquad \mathbf{X}_{i+1} \leftarrow \textit{orthonormalize}(\mathbf{A}\mathbf{X}_i)$$

$$\underset{\mathbf{A}}{\begin{bmatrix} 3 & & \\ & 2 & \\ & & 1 \end{bmatrix}} \underset{\mathbf{X}_0}{\begin{bmatrix} .60 & .61 \\ .59 & -.10 \\ .54 & .78 \end{bmatrix}} \rightarrow \underset{\mathbf{X}_1}{\begin{bmatrix} .92 & -.18 \\ .37 & .54 \\ -.04 & .82 \end{bmatrix}} \quad \Big| \quad \underset{\mathbf{U}_2}{\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}}$$

POWER METHOD REVIEW

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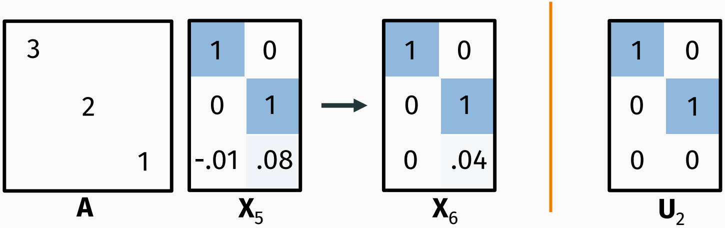

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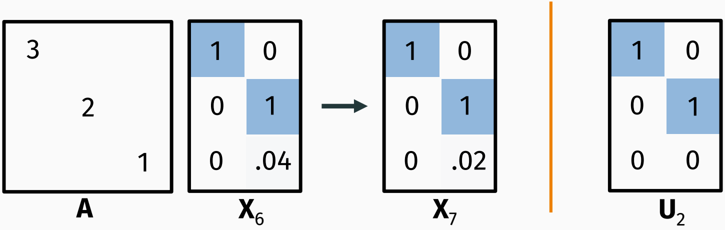

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Runtime for Block Power method is roughly:

$$O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log(d/\epsilon)}{(\sigma_k - \sigma_{k+1})/\sigma_k}\right)$$

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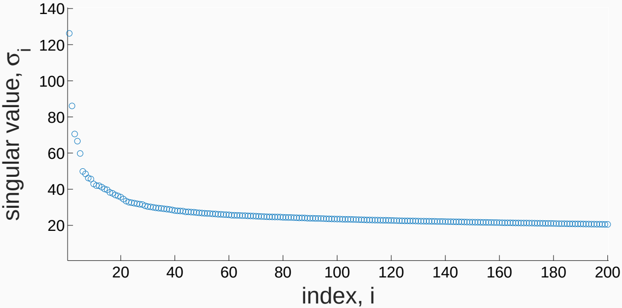
- While this gap is traditionally assumed to be constant, it is the dominant factor in the iteration count for many datasets.

TYPICAL GAP VALUES

Stanford Network Analysis Project – Slashdot Social Network



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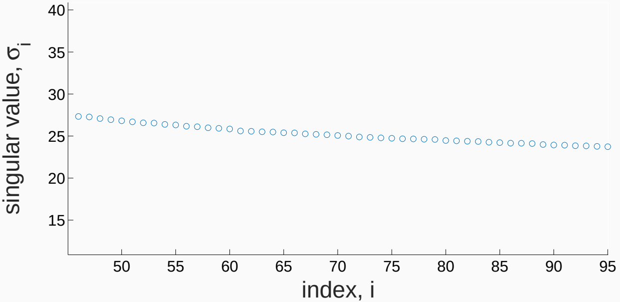

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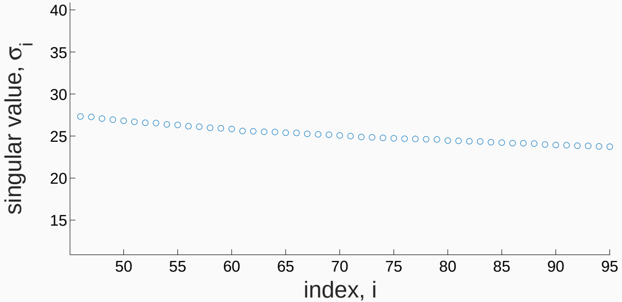
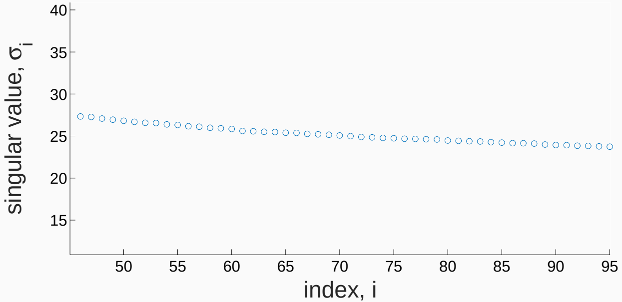


Median value of $\mathrm{gap}_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_k}$ for $k \leq 200$:

.0019

Stanford Network Analysis Project – Slashdot Social Network



Minimum value of $\text{gap}_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_k}$ for $k \leq 200$:

.00004

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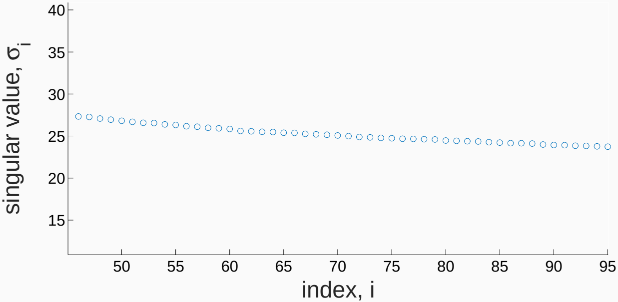

Minimum value of $\text{gap}_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_k}$ for $k \leq 200$:

Runtime = $O(25{,}000 \cdot \text{nnz}(\mathbf{A}) k \log(d/\epsilon))$

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GAP INDEPENDENT BOUNDS

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Improves on classical bounds when $\epsilon > (\sigma_k - \sigma_{k+1})/\sigma_k$.

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Long series of refinements and improvements:

- Rokhlin, Szlam, Tygert 2009
- Halko, Martinsson, Tropp 2011
- Boutsidis, Drineas, Magdon-Ismail 2011
- Witten, Candès 2014
- Woodruff 2014

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redSVD

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IBM

libSkylark

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Power Method

Krylov Methods

$$O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log(d/\epsilon)}{(\sigma_k - \sigma_{k+1})/\sigma_k}\right) \rightarrow O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log(d/\epsilon)}{\sqrt{(\sigma_k - \sigma_{k+1})/\sigma_k}}\right)$$

Power Method | **Krylov Methods**

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$$O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log d}{\epsilon}\right) \to \quad ?$$

No gap independent analysis of Krylov methods!

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$$O\left(\mathrm{nnz}(\mathbf{A})k \cdot \frac{\log d}{\epsilon}\right) \to \underbrace{O\left(\mathrm{nnz}(\mathbf{A})k \cdot \frac{\log d}{\sqrt{\epsilon}}\right)}_{\text{Our Contribution}}$$

A simple randomized Block Krylov Iteration gives all three of our target error bounds in time:

$$O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log d}{\sqrt{\epsilon}}\right)$$

$$\|\mathbf{A} - \mathbf{U}_k\mathbf{U}_k^T\mathbf{A}\|_2 \leq (1+\epsilon)\sigma_{k+1} \quad \text{and} \quad \tilde{u}_i^T\mathbf{A}\mathbf{A}^T\tilde{u}_i \geq \sigma_i^2 - \epsilon\sigma_{k+1}^2$$

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- Gives a runtime bound that is independent of **A**.
- Beats runtime of Block Power Method: $.0001 \rightarrow .01$.

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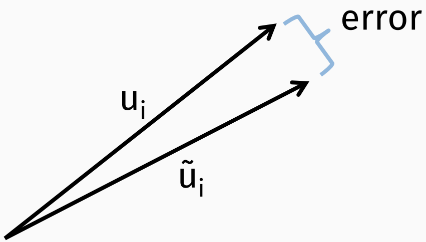
- Improves classic Lanczos bounds when $(\sigma_k - \sigma_{k+1})/\sigma_k < \epsilon$.

First Step: Where does gap dependence actually comes from?

To prove guarantees like: $\tilde{u}_i^T \mathbf{A}\mathbf{A}^T \tilde{u}_i \geq (1-\epsilon)\sigma_i^2$, classical analysis argues about convergence to $\mathbf{A}$'s true singular vectors.



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- Can be used to prove strong per-vector error or spectral norm guarantees for $\|\mathbf{A} - \tilde{\mathbf{U}}_k \tilde{\mathbf{U}}_k^T \mathbf{A}\|_2$.
- Inherently requires an iteration count that depends on singular value gaps.

Traditional objective function: $\|u_i - \tilde{u}_i\|_2$

$$\underbrace{\begin{bmatrix} 3 & & \\ & 1.1 & \\ & & 1 \end{bmatrix}}_{\mathbf{A}} \quad \underbrace{\begin{bmatrix} .93 & .26 \\ -.35 & .51 \\ -.08 & .81 \end{bmatrix}}_{\mathbf{X}_0} \longrightarrow \underbrace{\begin{bmatrix} 1 & .01 \\ -.07 & .62 \\ .04 & .78 \end{bmatrix}}_{\mathbf{X}_1} \quad \Bigg| \quad \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}}_{\mathbf{U}_2}$$

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UNDERSTANDING GAP DEPENDENCE

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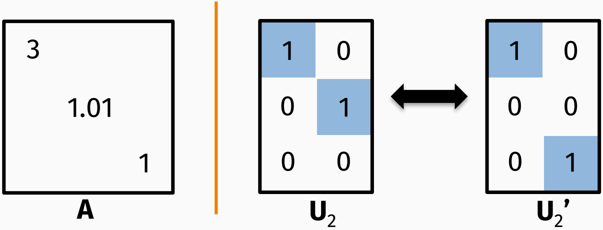

Minimizing $\|u_i - \tilde{u}_i\|_2$ is sufficient, but far from necessary.

Iterative methods viewed as denoising procedures for Random Sketching methods.

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- Gives an error bound for a single power method iteration.
- Meaningless unless $\|\mathbf{A} - \mathbf{A}_k\|_F$ (the ‘tail noise’) is very small.

How to avoid tail noise? Apply sketching method to $\mathbf{A}^q$ instead.

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This is exactly what Block Power Method does:

$$\mathbf{G} \to \mathbf{A}\mathbf{G} \to \mathbf{A}^2\mathbf{G} \to \ldots \to \mathbf{A}^q\mathbf{G}, \qquad \tilde{\mathbf{U}}_k = span(\mathbf{A}^q\mathbf{G})$$

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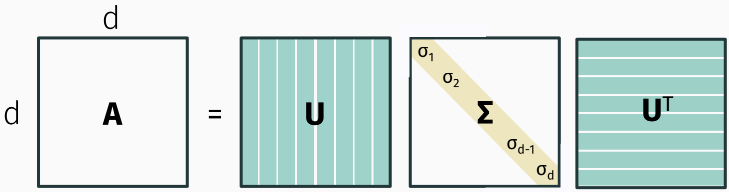

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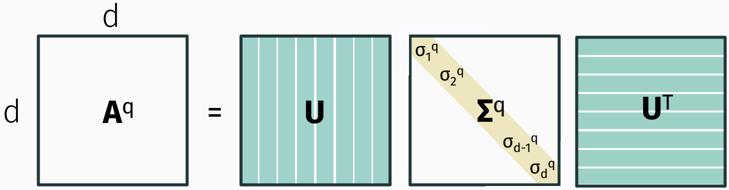

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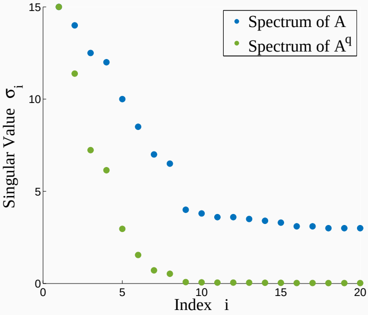

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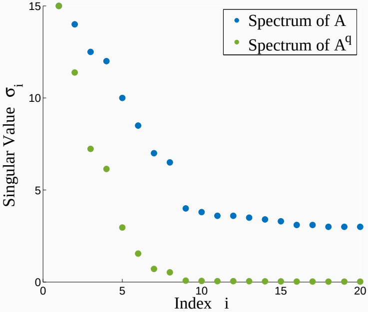

$\|\mathbf{A}^q - \mathbf{A}_k^q\|_F^2 = \sum_{i=k+1}^d \sigma_i^{2q}$ is extremely small.

- $q = \tilde{O}(1/\epsilon)$ ensures that any singular value below σ_{k+1} becomes extremely small in comparison to any singular value above $(1+\epsilon)\sigma_{k+1}$.

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- $\mathbf{A}$ and $\mathbf{A}^q$ have the same singular vectors so $\tilde{\mathbf{U}}_k$ is good for $\mathbf{A}$.

We use new tools for converting **very small** Frobenius norm low-rank approximation error to spectral norm and per vector error, without arguing about convergence of $\tilde{u}_i$ and u_i.

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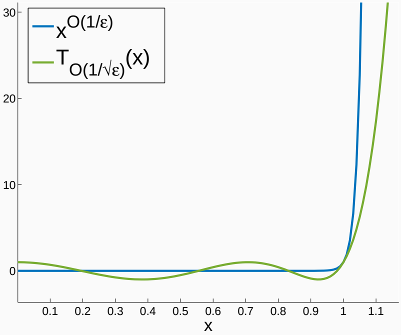

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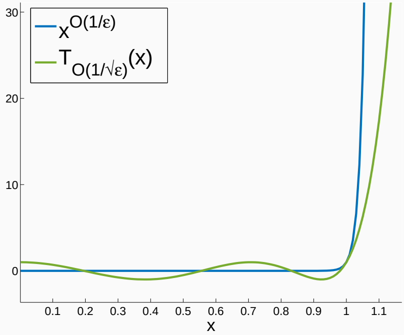

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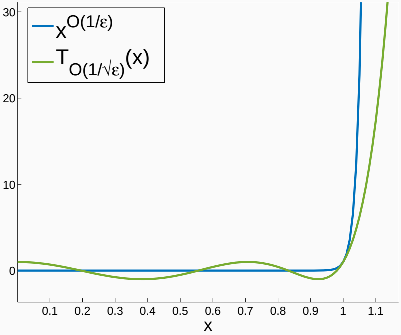

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Block Krylov Iteration:

$$\mathcal{K} = \underbrace{\left[\mathbf{G}, \mathbf{A}\mathbf{G}, \mathbf{A}^2\mathbf{G}, \ldots, \mathbf{A}^q\mathbf{G}\right]}_{\text{Krylov subspace}}$$

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Solution: Returning the best $\tilde{\mathbf{U}}_k$ in the span of $\mathcal{K}$ is only better then returning $span(T_q(\mathbf{A})\mathbf{G})$.

What is the best $\tilde{\mathrm{U}}_k$?

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- For Block Power Method, did not need to consider this – $\tilde{\mathbf{U}}_k = span(\mathbf{A}^q\mathbf{G})$ was the only option.
- In classical Lanczos/Krylov analysis, convergence to the true singular vectors also lets us avoid this issue. Use Rayleigh Ritz procedure.

- Project $\mathbf{A}$ to $\mathcal{K}$ and take the top k singular vectors (using an accurate classical method):

$$\tilde{\mathbf{U}}_k = span\left((\mathbf{P}_{\mathcal{K}}\mathbf{A})_k\right)$$

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- Equivalent to the classic Block Lanczos algorithm in exact arithmetic.

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Take away: Modern denoising analysis gives new insight into the practical effectiveness of Rayleigh-Ritz projection.

Similar to randomized Block Power Method – extremely simple (pseudocode in paper).

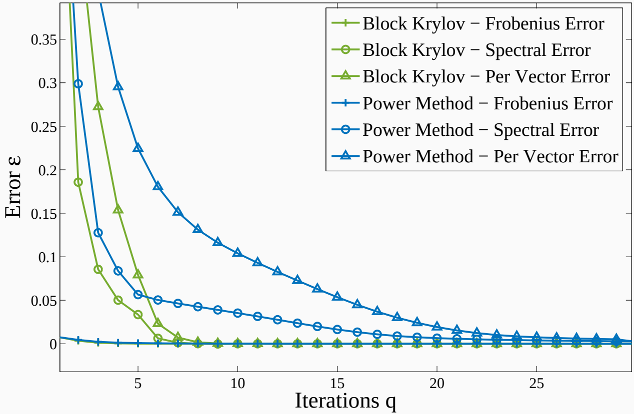
Block Power Method

```
X = randn(d,k);
for i=1:iter
    [X,R] = qr(A*X);
end
U = X;
```

Block Krylov Iteration

```
X = randn(d,k);
K = zeros(d,k*iter);
for i=1:iter
    [X,R] = qr(A*X);
    K(:,(i-1)*k+1:i*k) = X;
end
[Q,R] = qr(K);
[U,S] = svd(Q'*A,'econ');
U = Q*U(:,1:k);
```

Block Krylov beats Block Power Method definitively for small ϵ.



20 Newsgroups, $k = 20$

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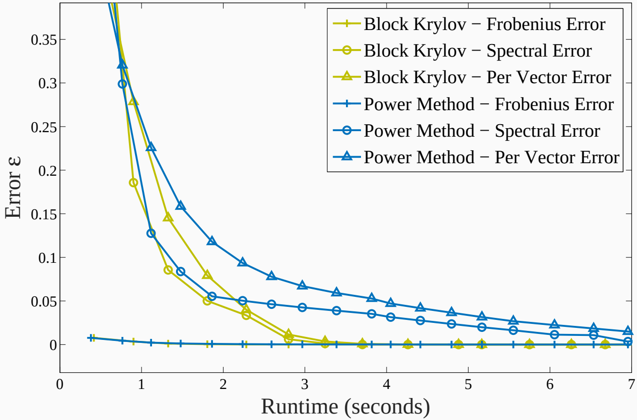


20 Newsgroups, $k = 20$

Main Takeaway: First gap independent bound for Krylov methods.

$$O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log d}{\sqrt{(\sigma_k - \sigma_{k+1}/\sigma_k}}\right) \rightarrow O\left(\text{nnz}(\mathbf{A})k \cdot \frac{\log d}{\sqrt{\epsilon}}\right)$$

Open Questions

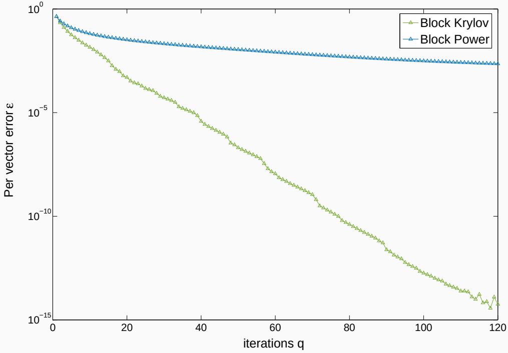
- Full stability analysis.
- 'Master' error metric for gap independent results.
- Gap independent bounds for other methods (e.g. online and stochastic PCA).
- Analysis for small space/restarted block Krylov methods?

Thank you!

Stability

- Lanczos algorithms are often considered to be unstable.
- Largely due to the fact that a recurrence is used to efficiently compute a basis for the Krylov subspace “on the fly”.
- Since our subspace is small, we do not use the recurrence. Computing the basis explicitly avoids serious stability issues.
- There is some loss of orthogonality between blocks. However it only occurs once the algorithm has converged and we can show that it is not an issue in practice.

On poorly conditioned matrices Randomized Block Krylov Iteration still significantly outperforms Block Power Method.



Per Vector Error for $k = 10$, $\kappa = 100{,}000$