RANDOMIZED BLOCK KRYLOV METHODS FOR STRONGER AND FASTER APPROXIMATE SVD

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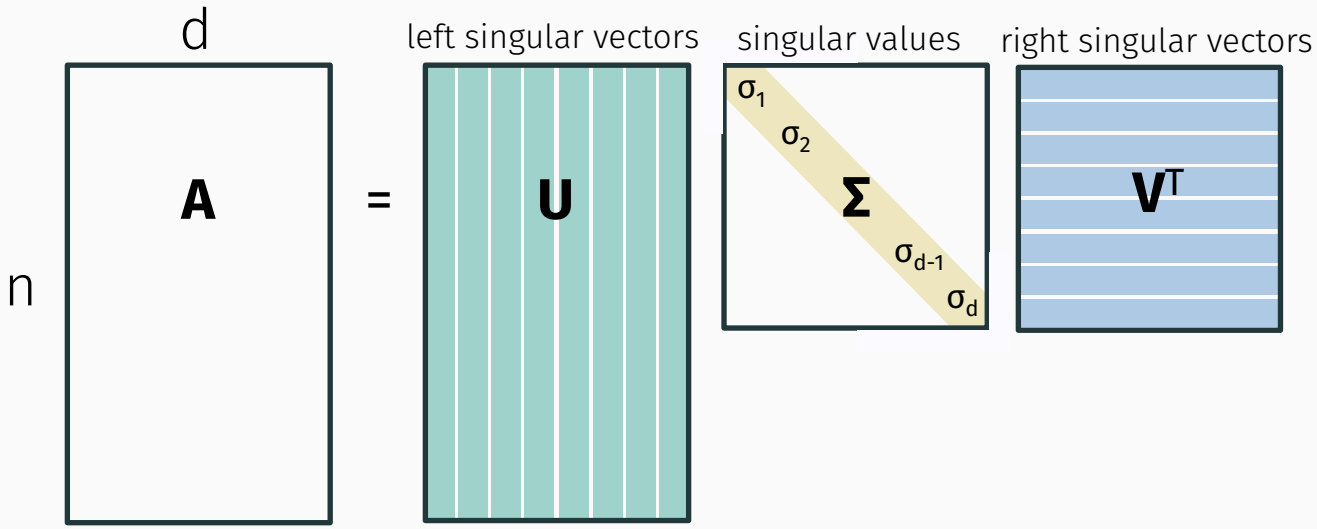
SINGULAR VALUE DECOMPOSITION



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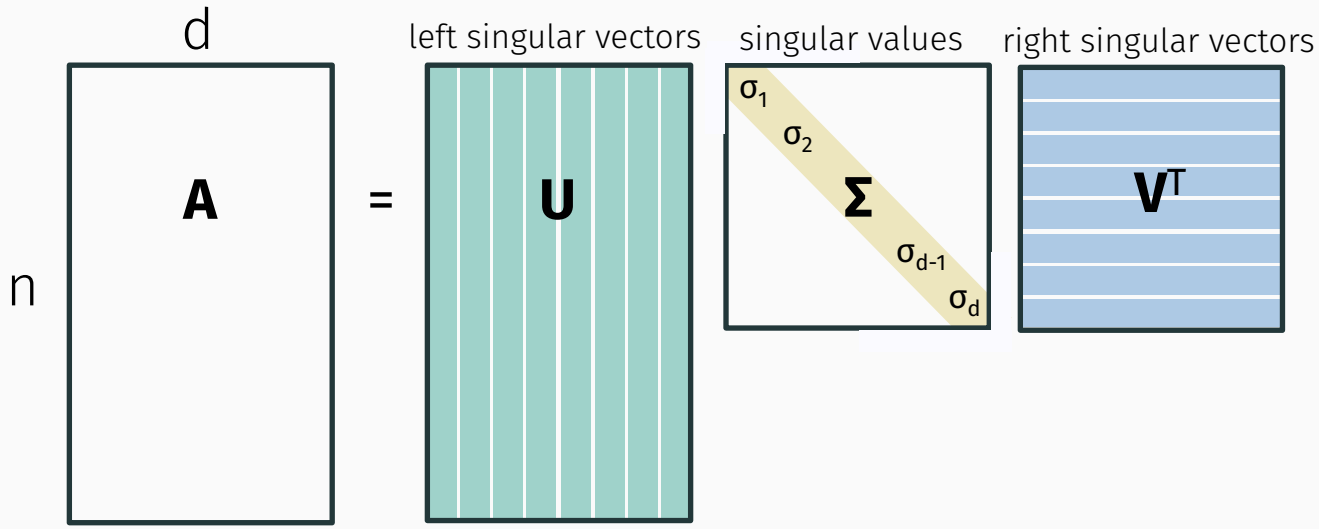

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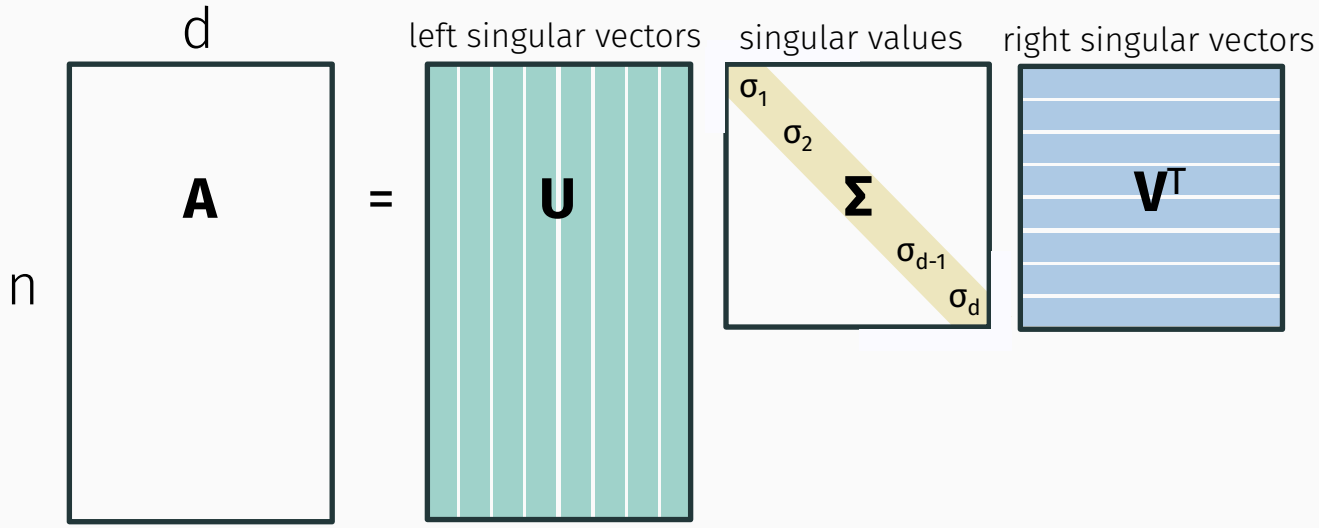

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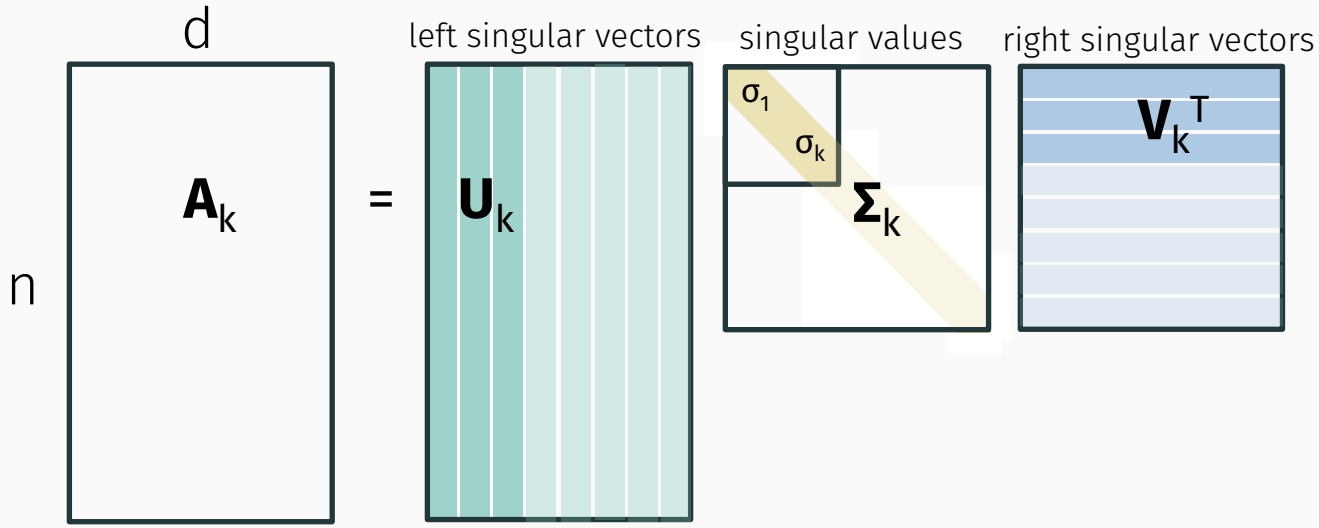

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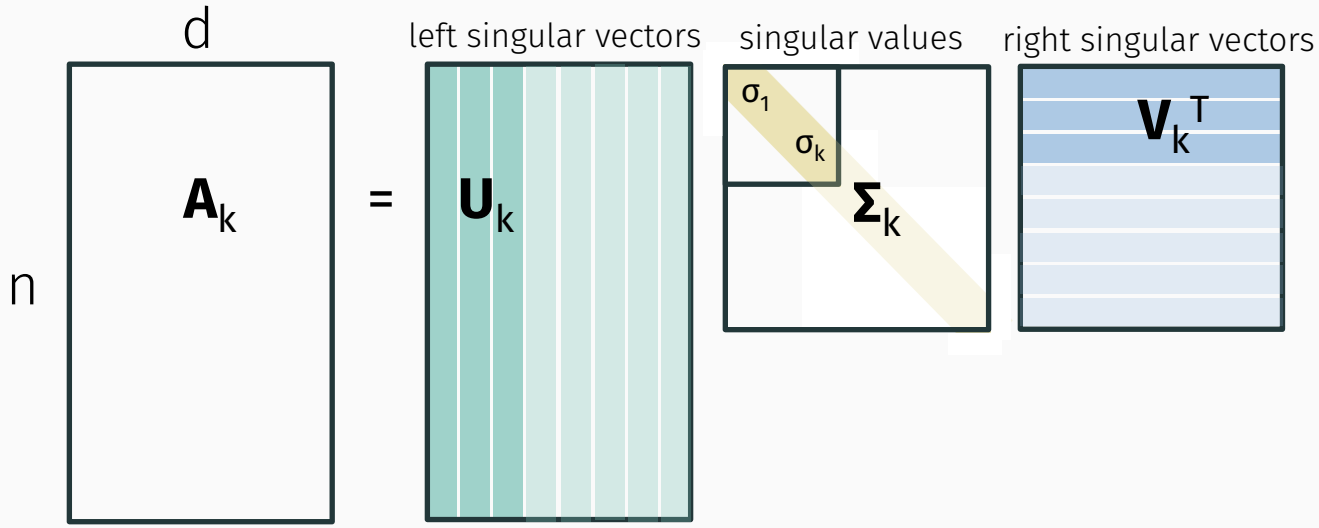

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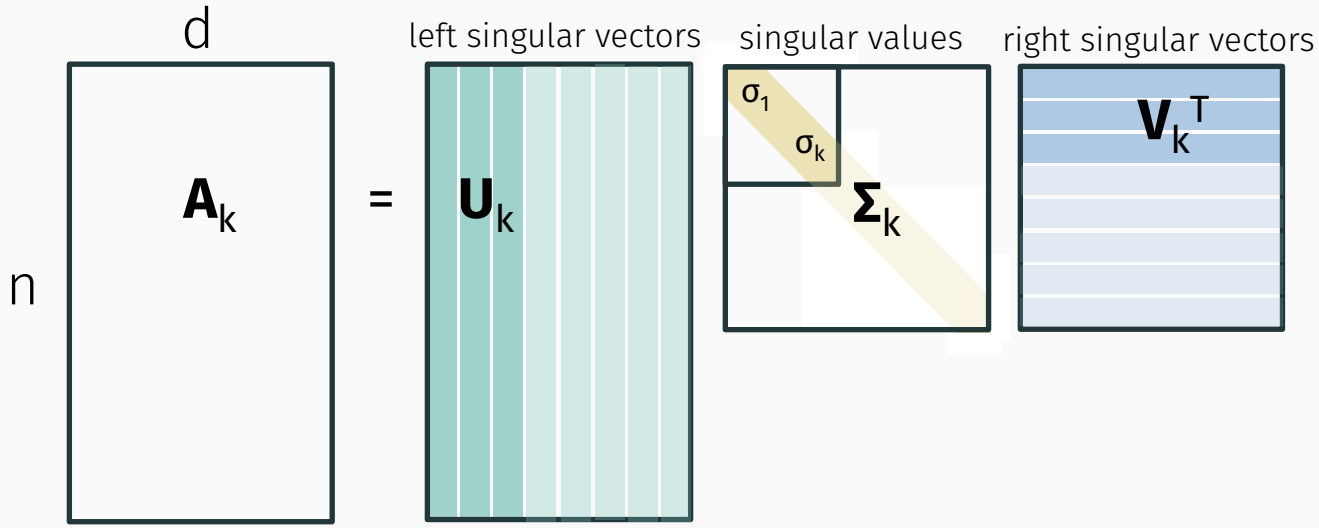

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STANDARD SVD APPROXIMATION METRICS

- Frobenius Norm Low-Rank Approximation:

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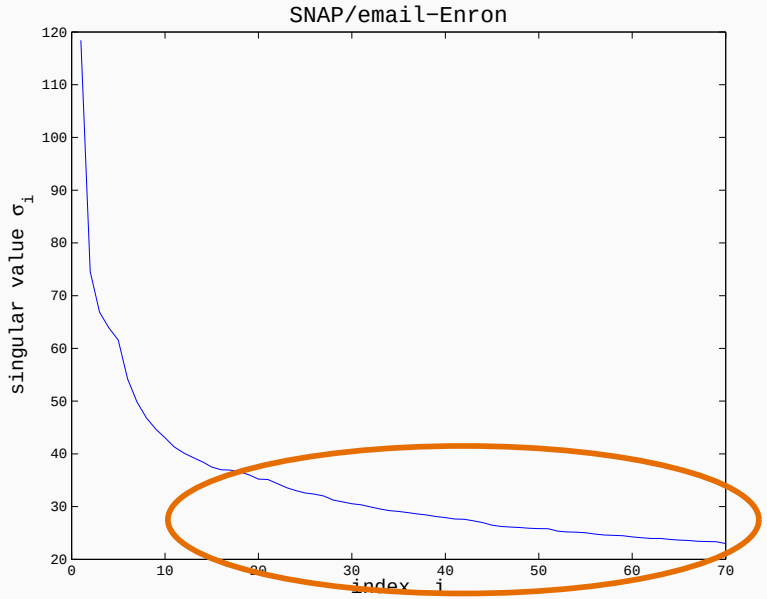
$$\|\mathbf{A}\|_F^2 = \sum_{i=1}^{d} \sigma_i^2 \text{ and } \|\mathbf{A} - \mathbf{U}_k \mathbf{U}_k^T \mathbf{A}\|_F^2 = \|\mathbf{A} - \mathbf{A}_k\|_F^2 = \sum_{i=k+1}^{d} \sigma_i^2.$$



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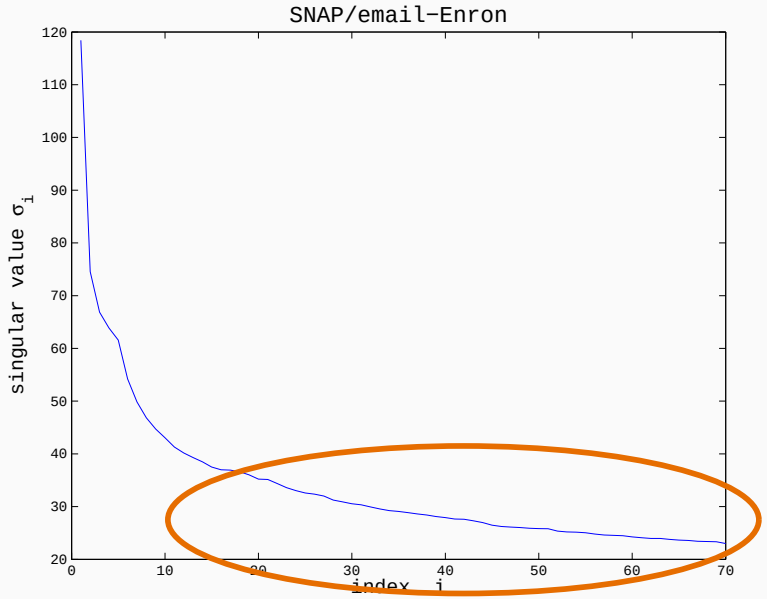

For many datasets literally any $\tilde{\mathbf{U}}_k$ would work!

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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).

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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 SVD ALGORITHMS

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

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

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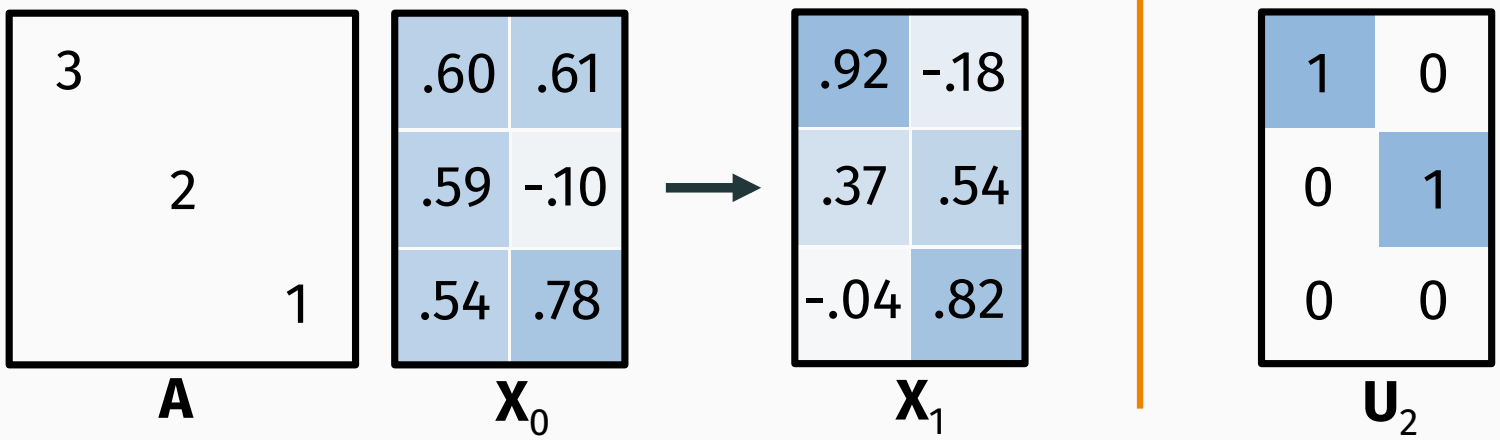

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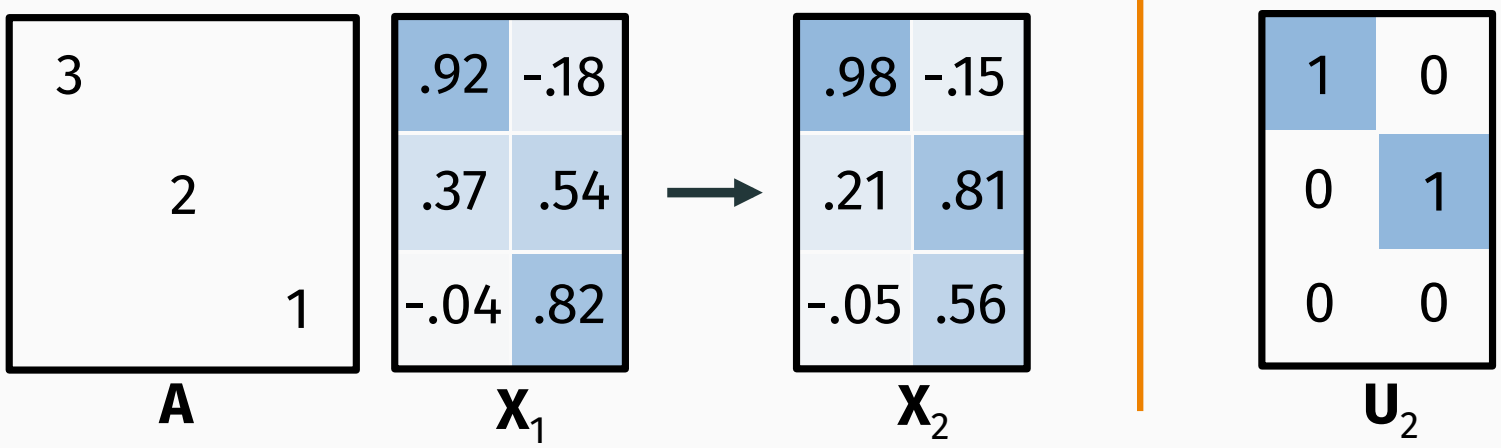

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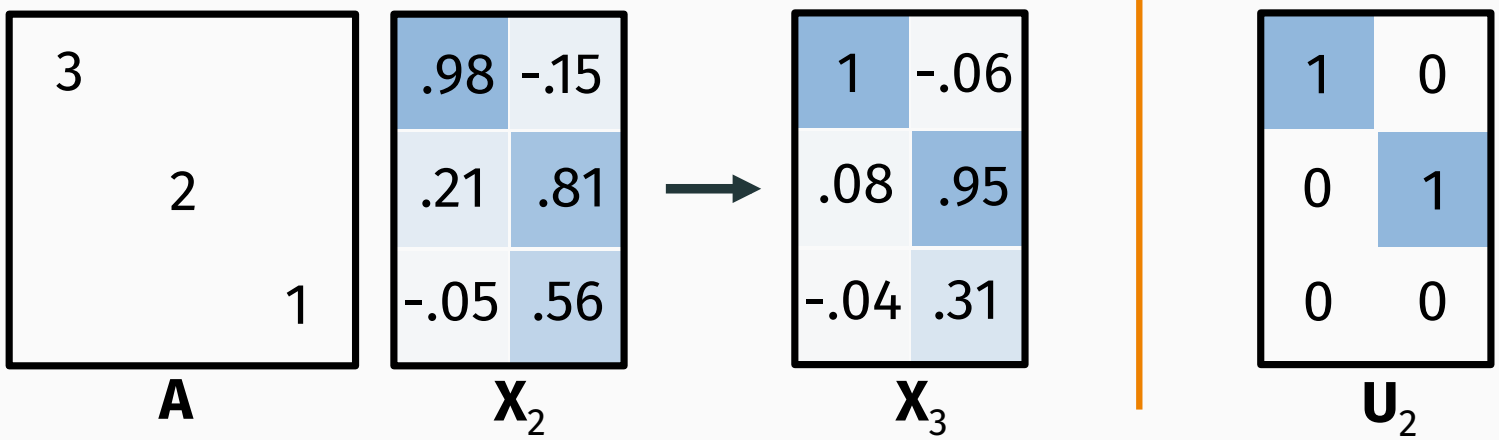

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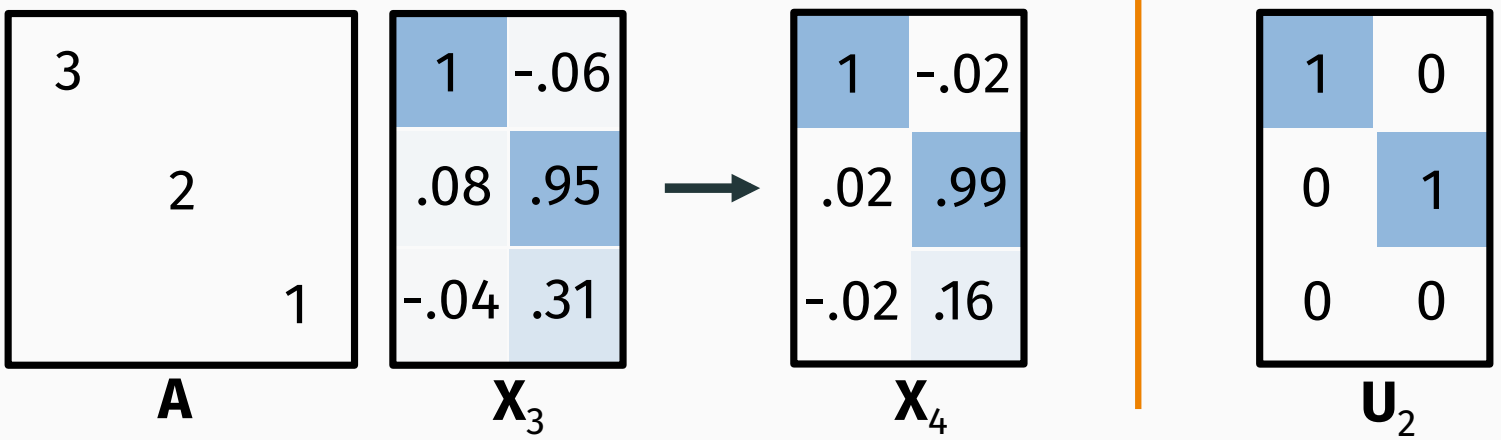

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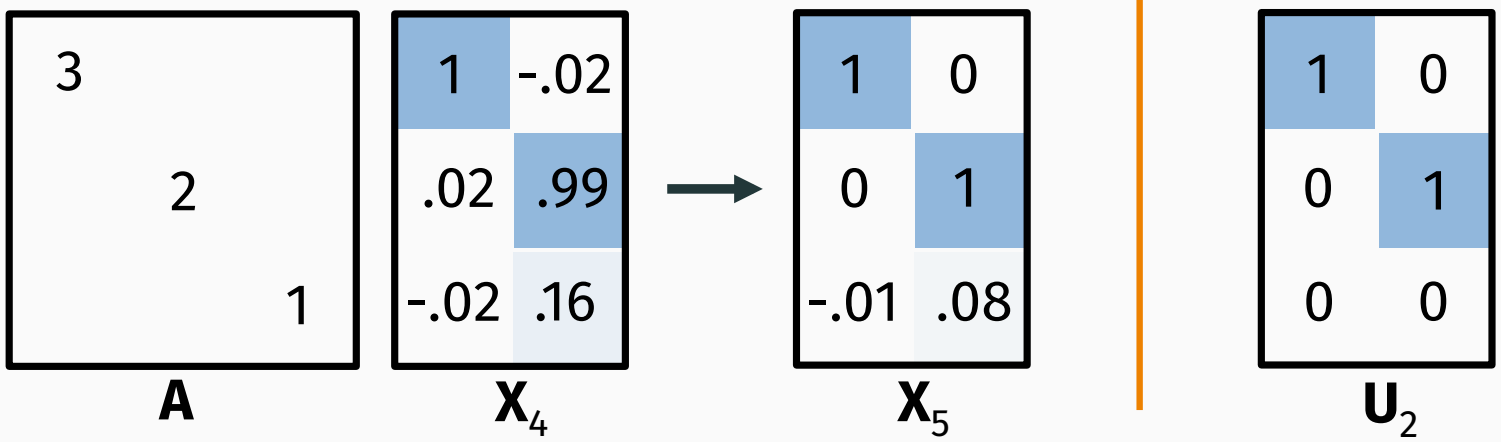

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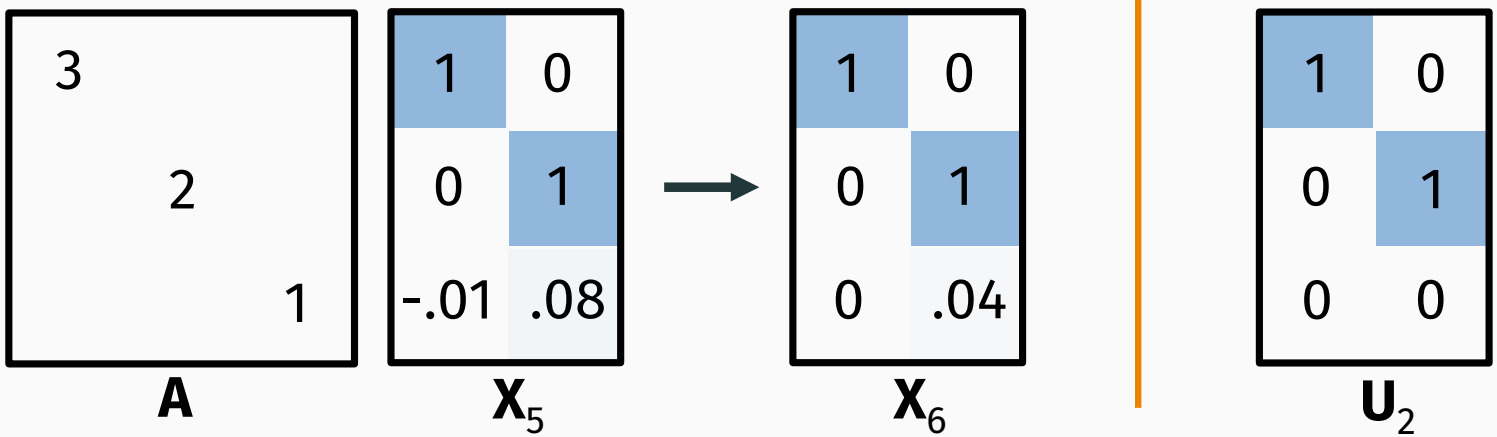

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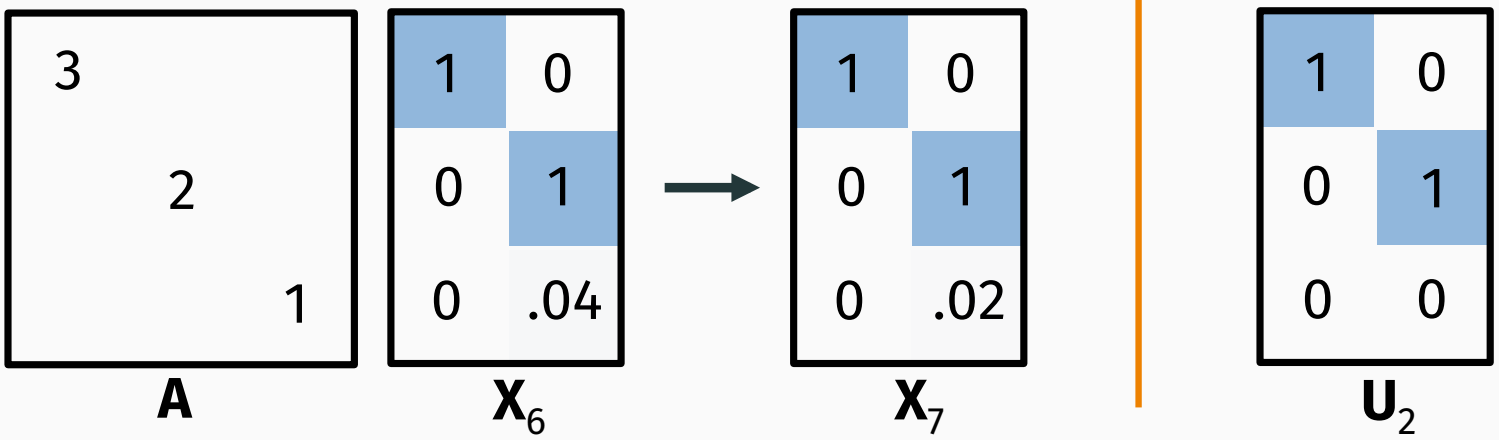

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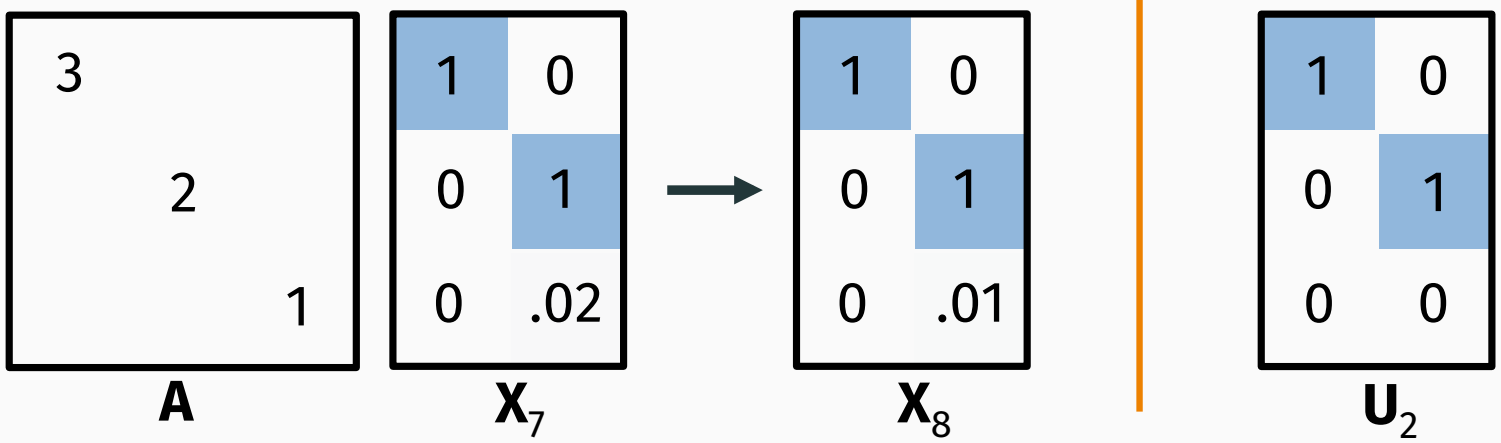

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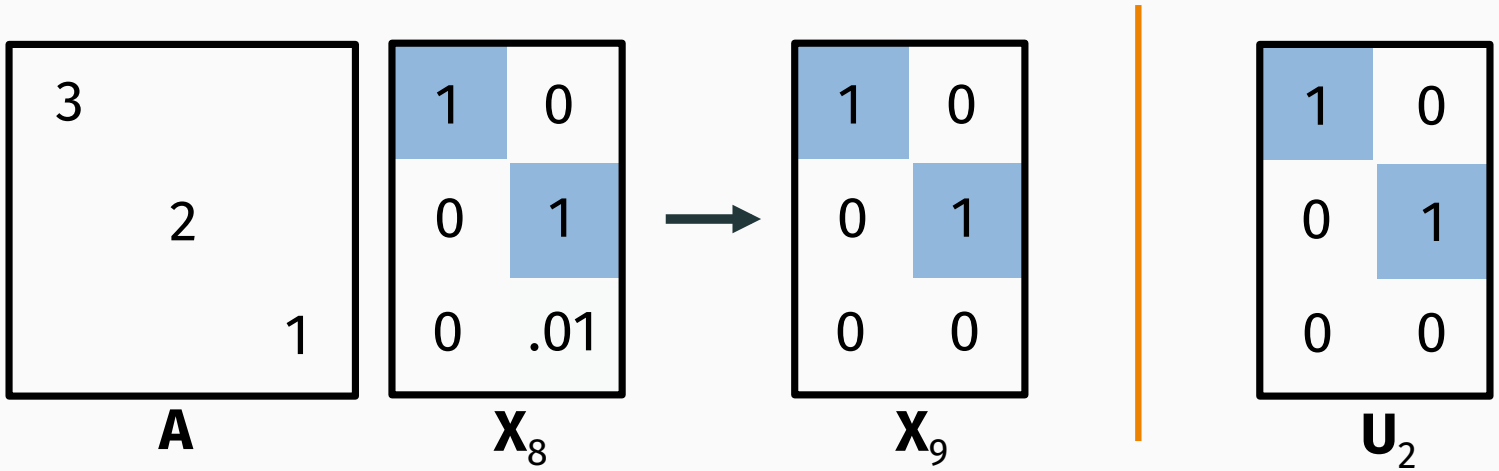

POWER METHOD RUNTIME

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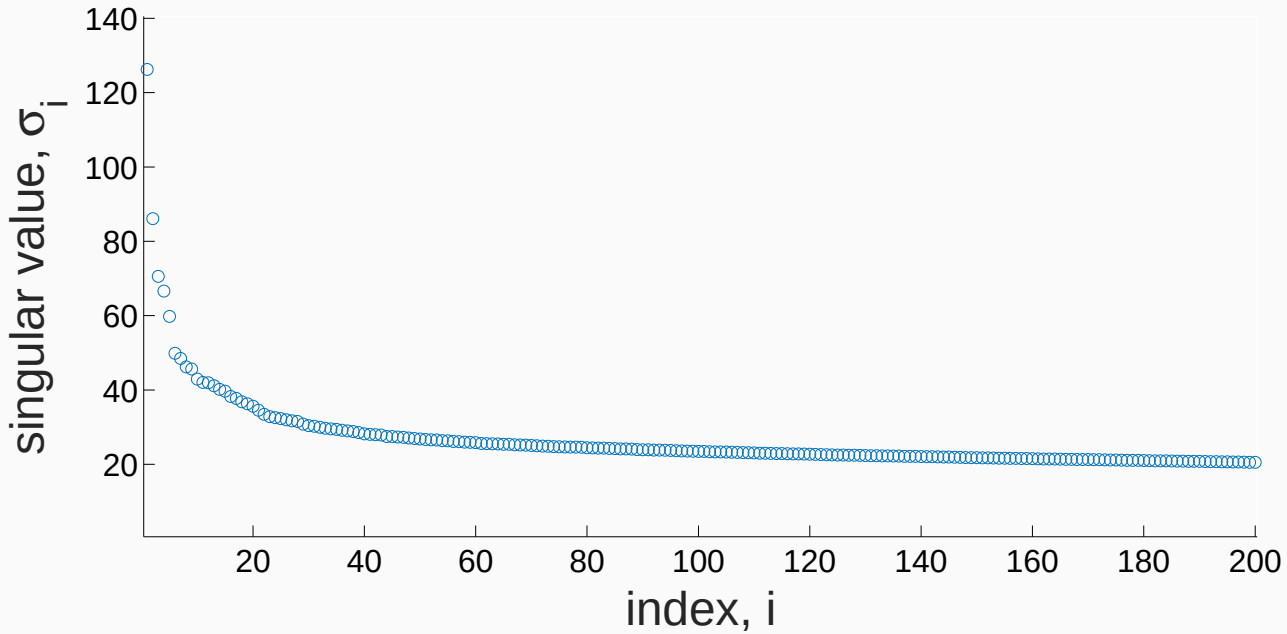
- While this gap is traditionally assumed to be constant, it is the dominant factor in the iteration count for many datasets.

TYPICAL GAP VALUES

Stanford Network Analysis Project – Slashdot Social Network



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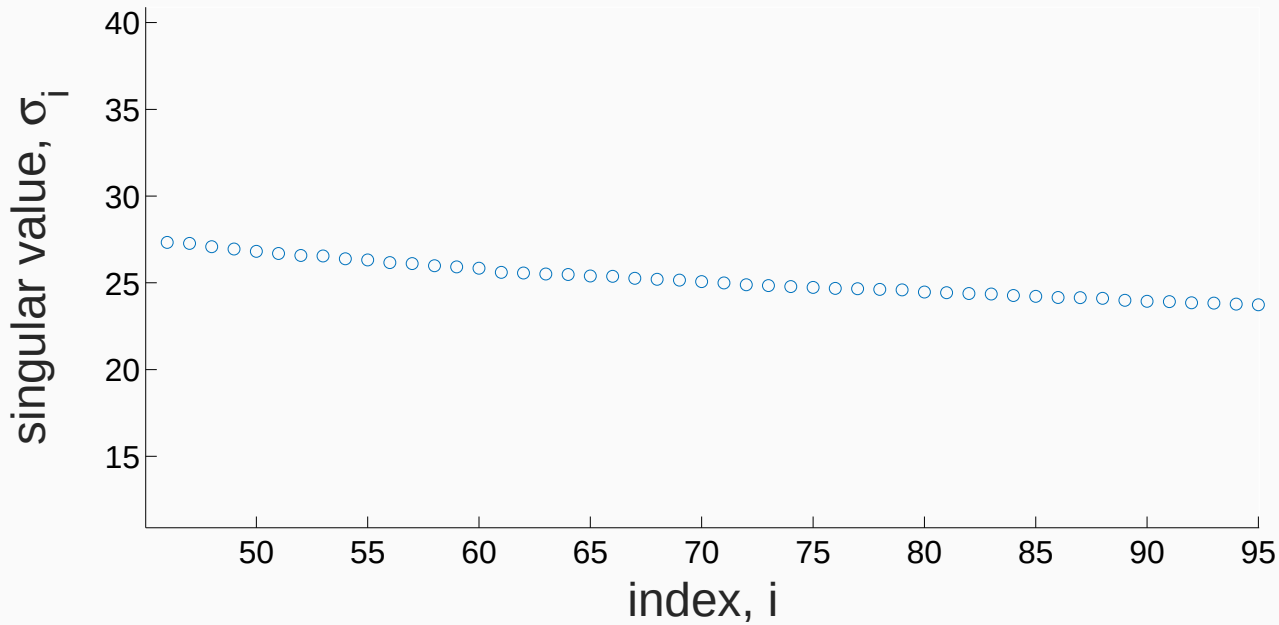

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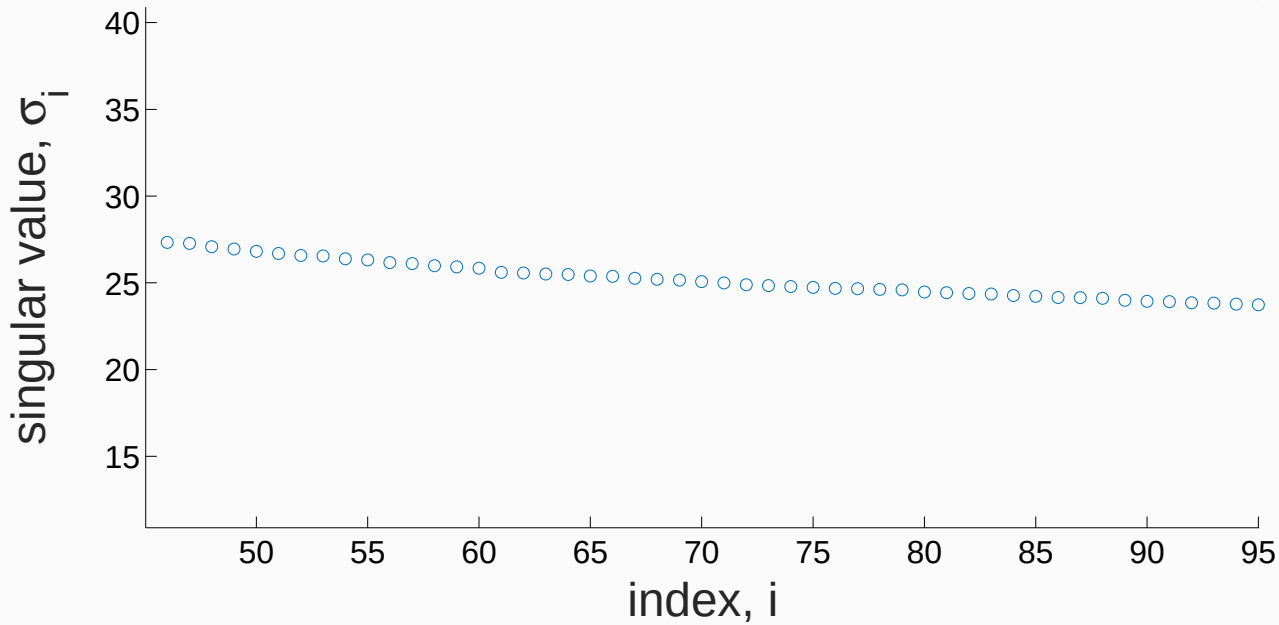

Median value of $\text{gap}_k = \frac{\sigma_k - \sigma_{k+1}}{\sigma_k}$ for $k \leq 200$:

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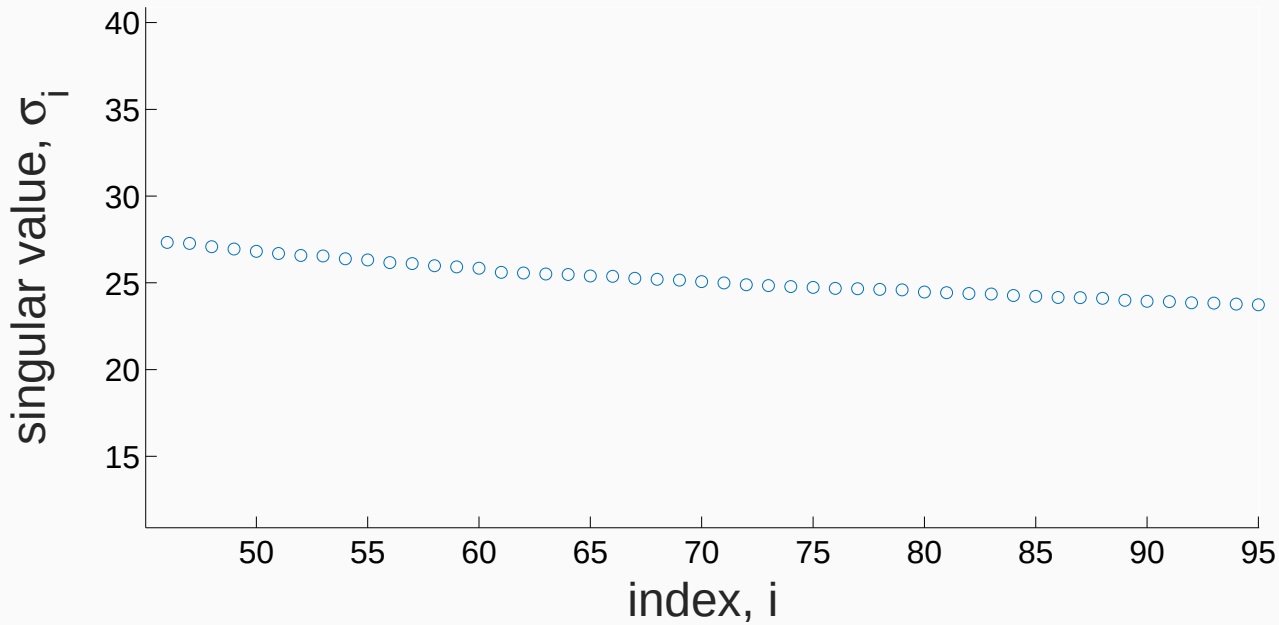

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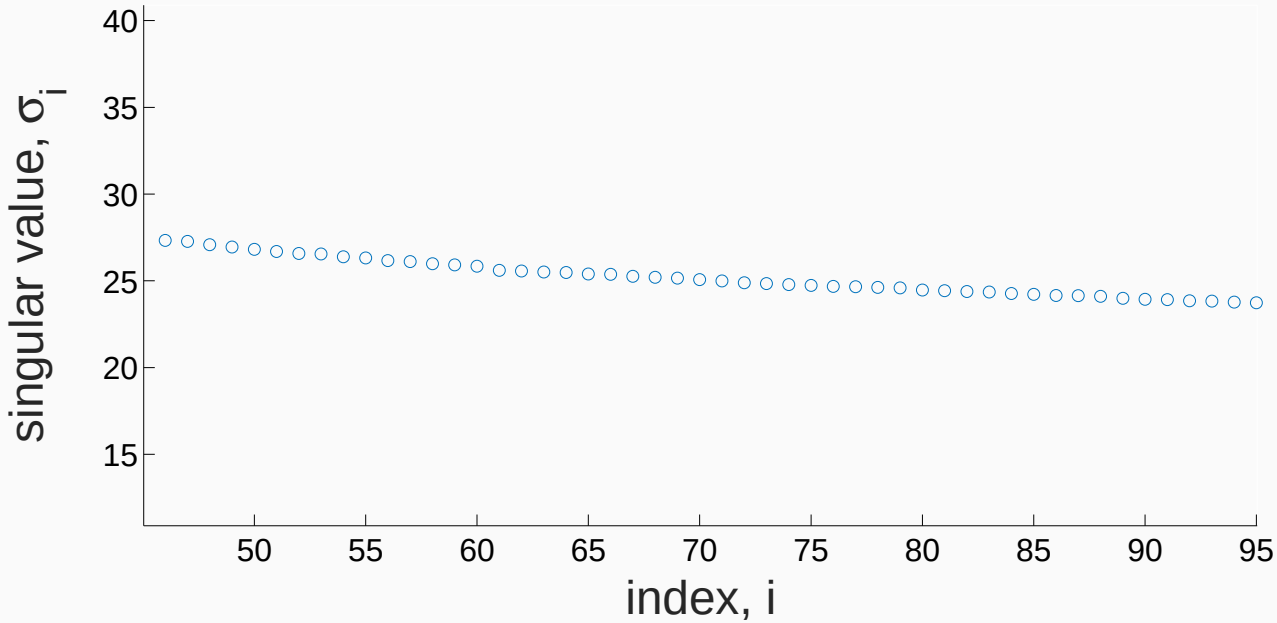

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$$\text{Runtime} = O(25{,}000 \cdot \text{nnz}(\mathbf{A})k \log(d/\epsilon))$$

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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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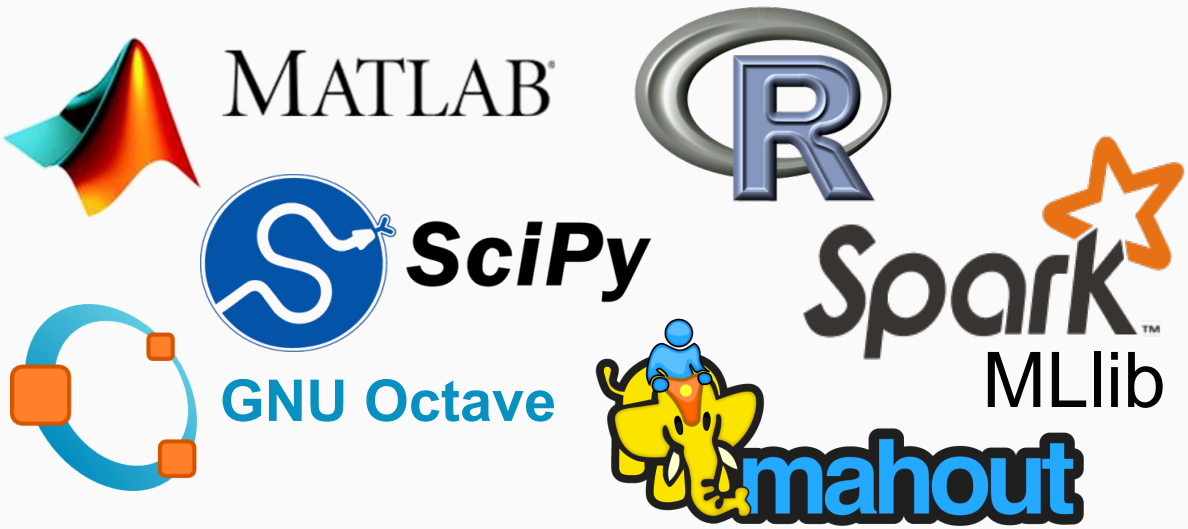

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Power Method

Krylov Methods

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

Power Method	Krylov Methods
$O\left(\mathrm{nnz}(\mathbf{A})k \cdot \frac{\log(d/\epsilon)}{(\sigma_k - \sigma_{k+1})/\sigma_k}\right) \rightarrow$	$O\left(\mathrm{nnz}(\mathbf{A})k \cdot \frac{\log(d/\epsilon)}{\sqrt{(\sigma_k - \sigma_{k+1})/\sigma_k}}\right)$
$O\left(\mathrm{nnz}(\mathbf{A})k \cdot \frac{\log d}{\epsilon}\right) \rightarrow$	?

No gap independent analysis of Krylov methods!

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

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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OUR MAIN RESULT

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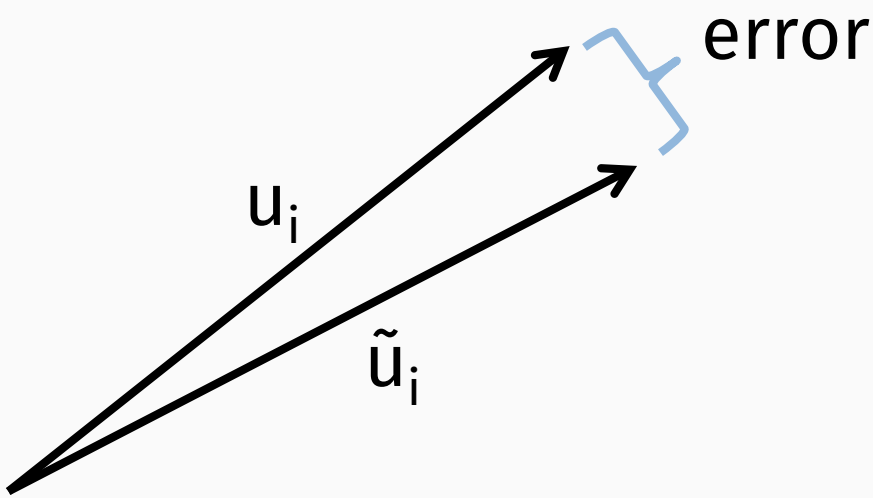
- Beats runtime of Block Power Method: 10,000 $\rightarrow$ 100.
- Improves classic Lanczos bounds when $(\sigma_k - \sigma_{k+1})/\sigma_k < \epsilon$.

UNDERSTANDING GAP DEPENDENCE

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 **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.

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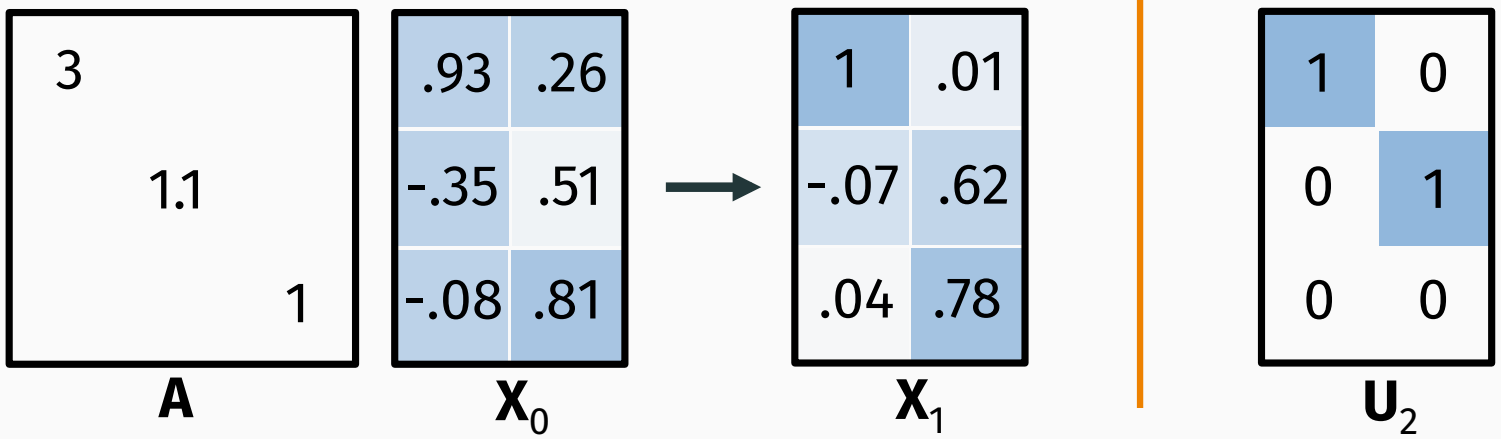

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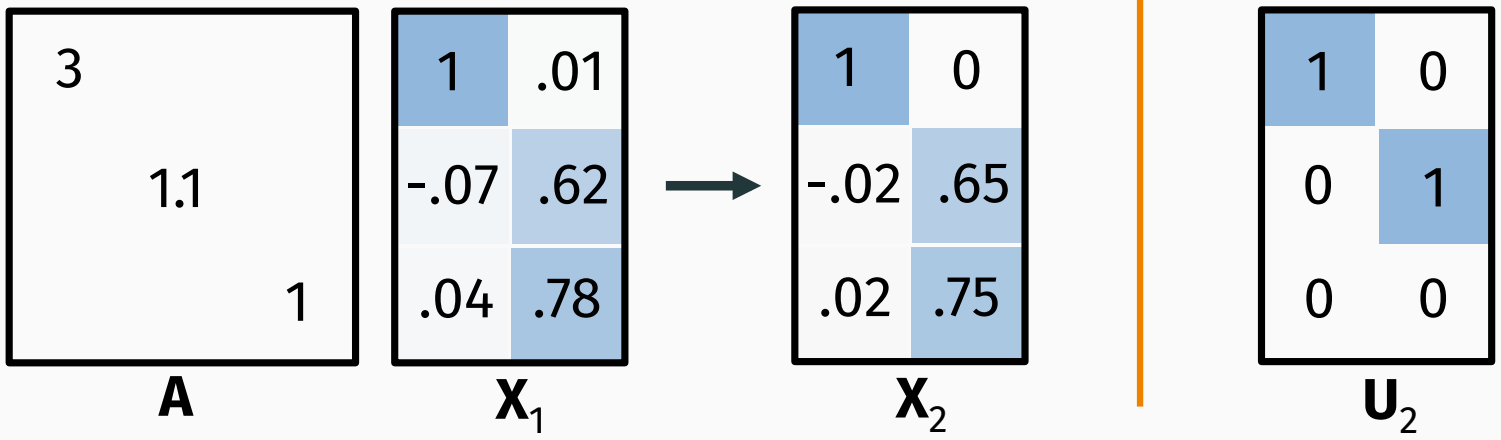

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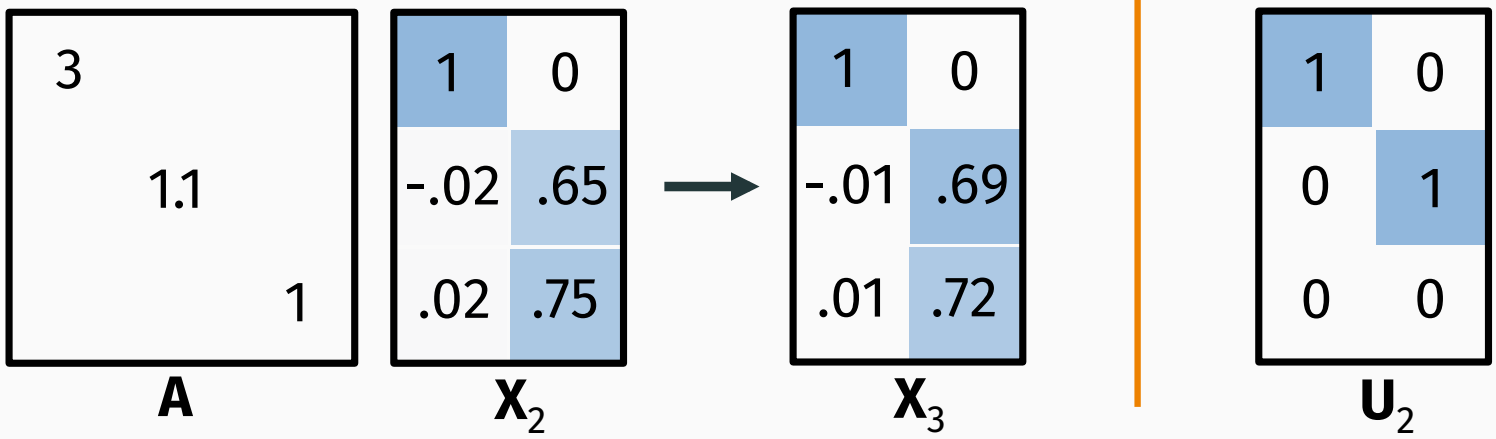

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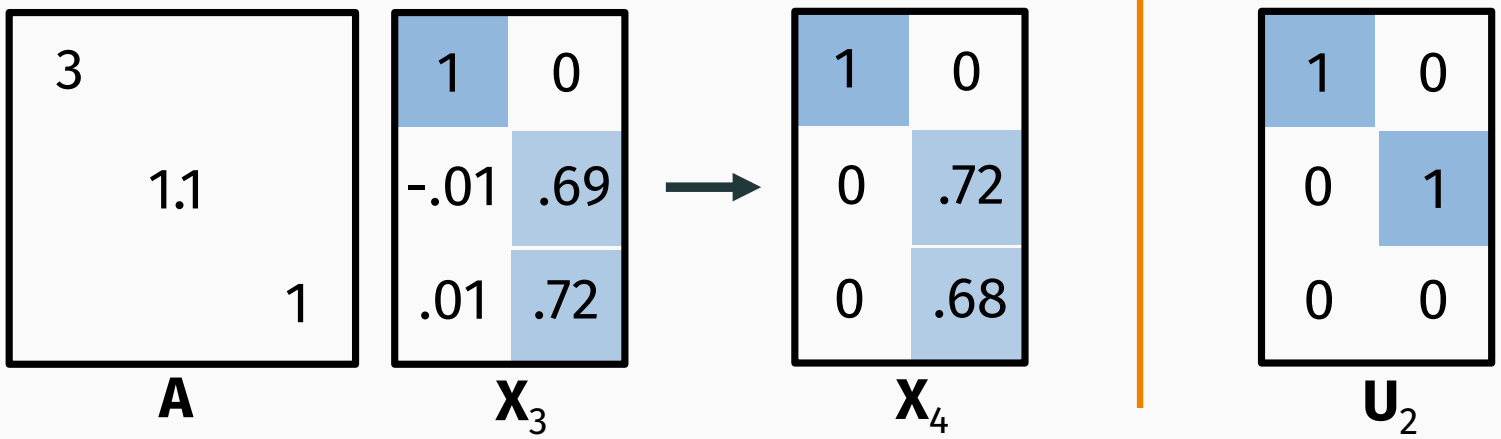

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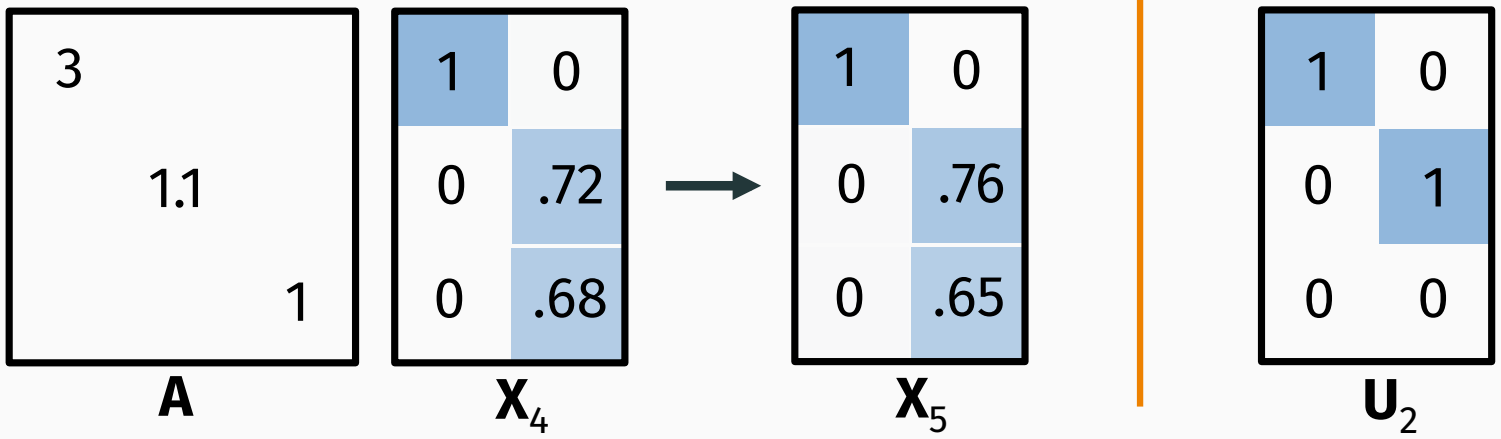

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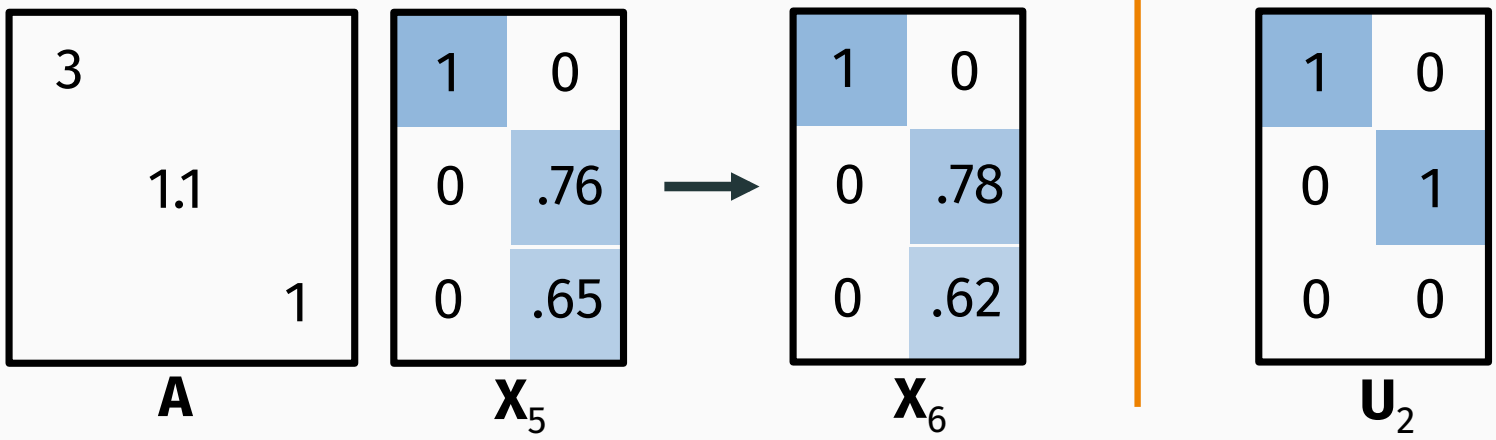

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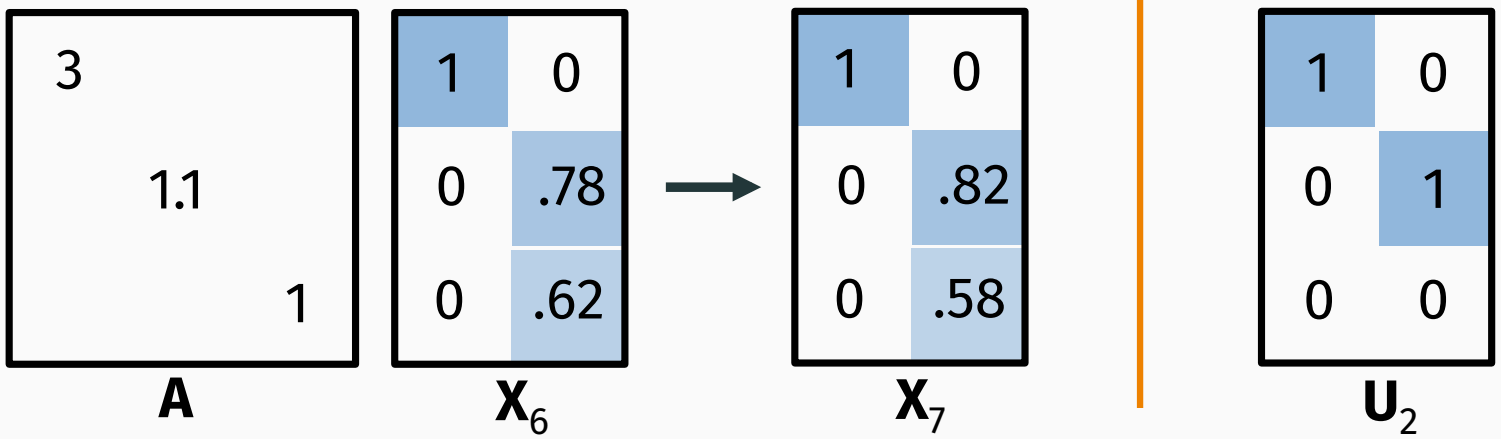

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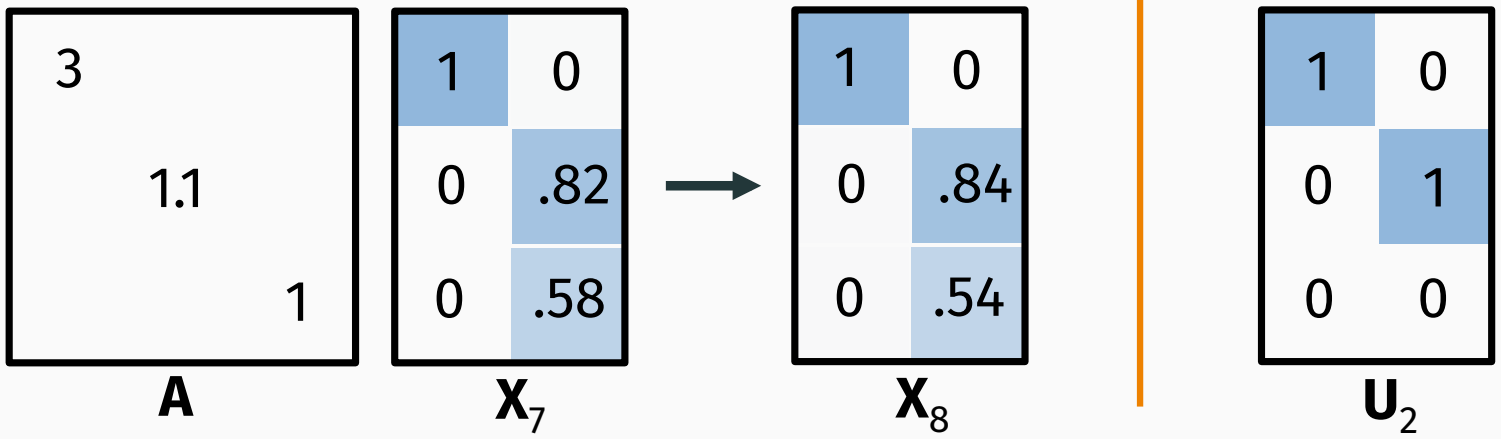

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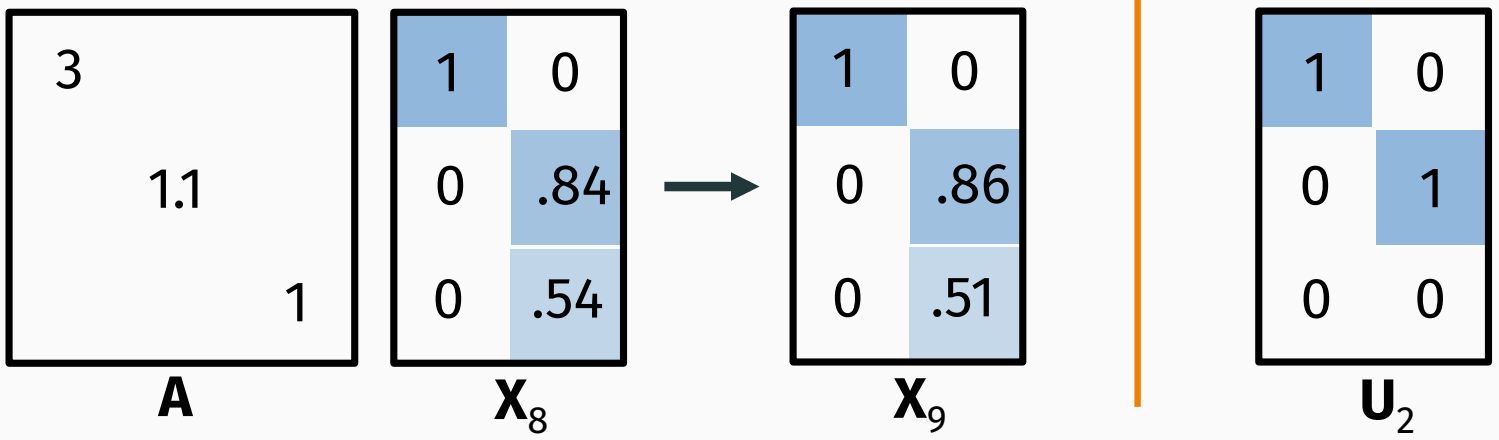

KEY INSIGHT

Convergence becomes less necessary precisely when it is difficult to achieve!

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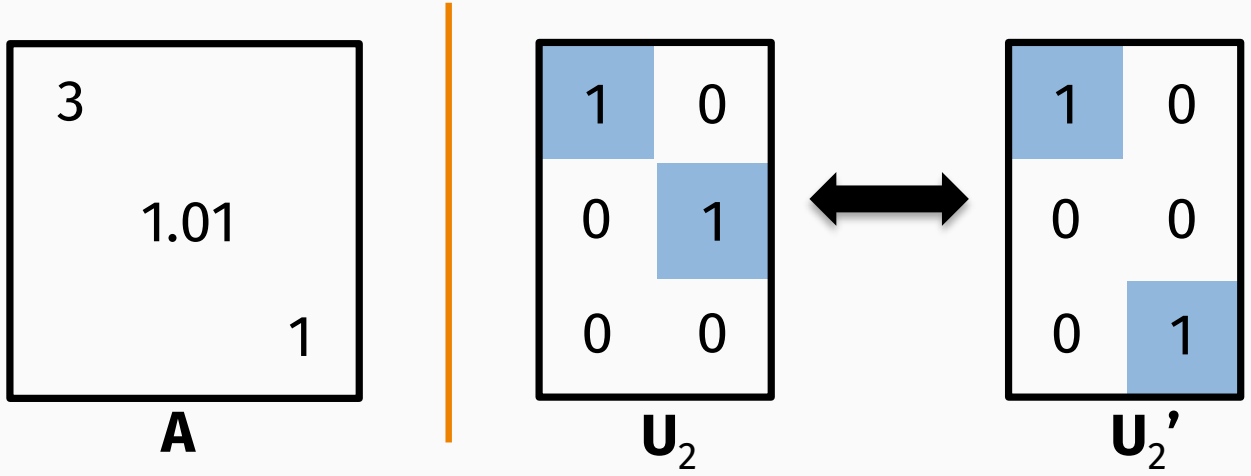

Minimizing $\|u_i - \tilde{u}_i\|_2$ is sufficient, but far from necessary.

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.

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This is exactly what Block Power Method does:

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

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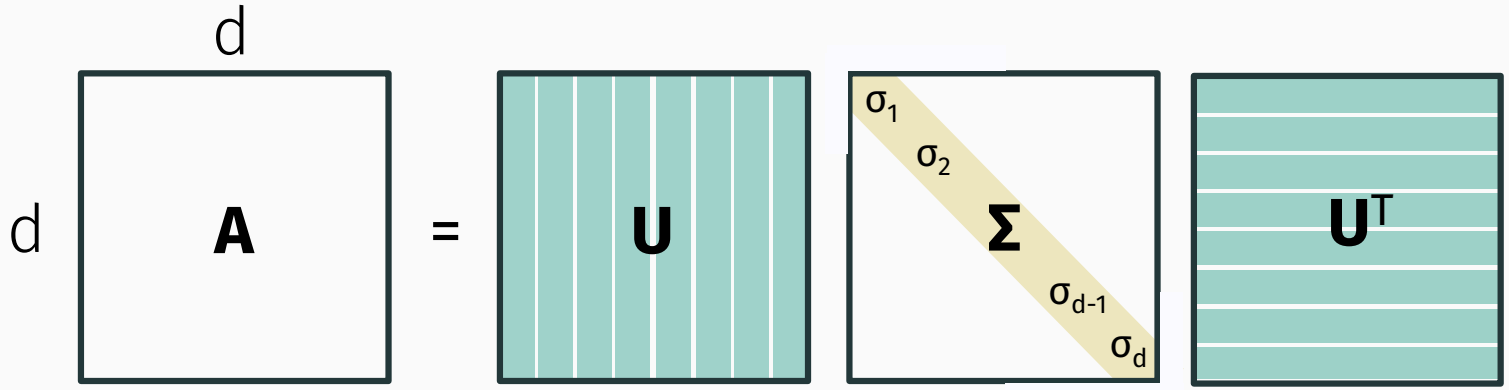
Assuming $\mathbf{A}$ is symmetric, if $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^T$ then $\mathbf{A}^q = \mathbf{U}\mathbf{\Sigma}^q\mathbf{U}^T$.



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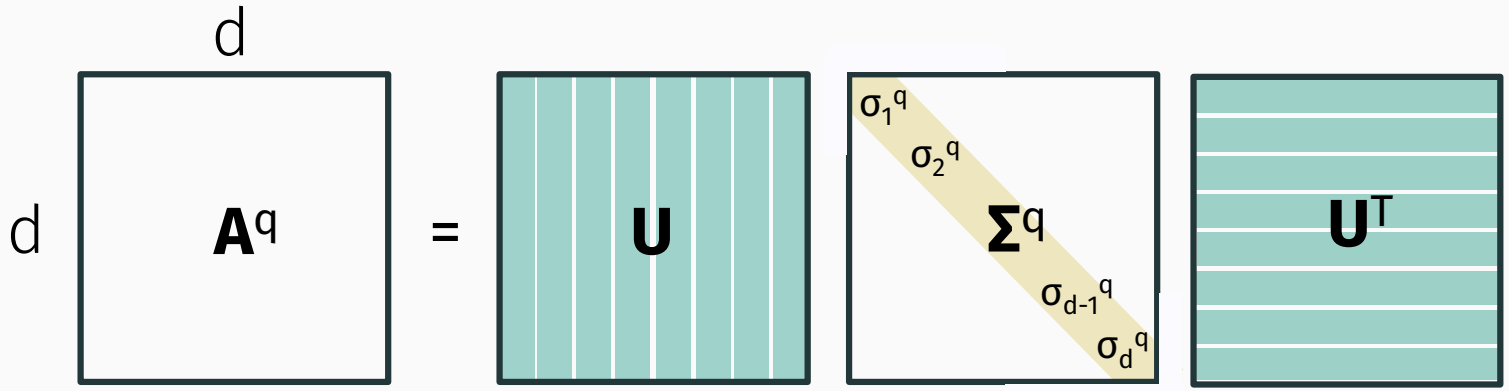

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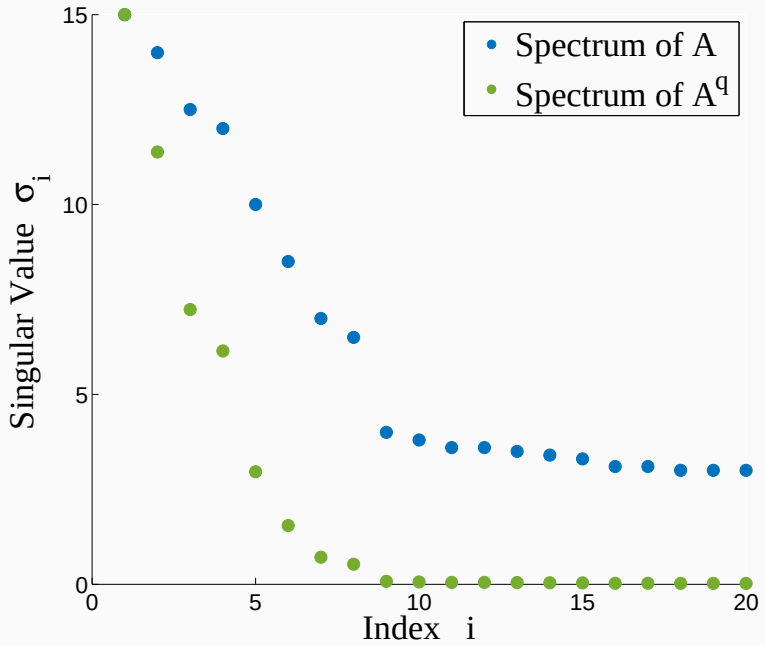

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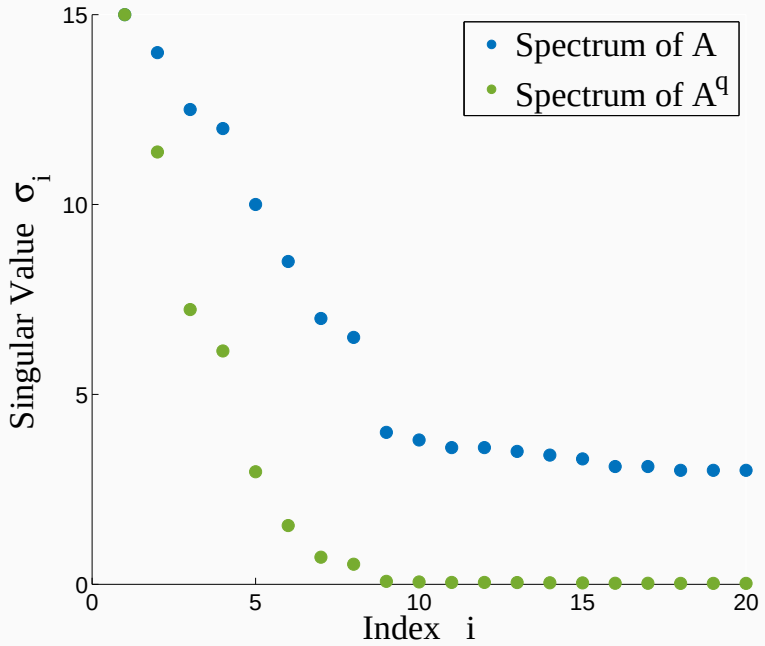

$\|\mathbf{A}^q - \mathbf{A}_k^q\|_F^2 = \sum_{i=k+1}^{d} \sigma_i^{2q}$ is extremely small.

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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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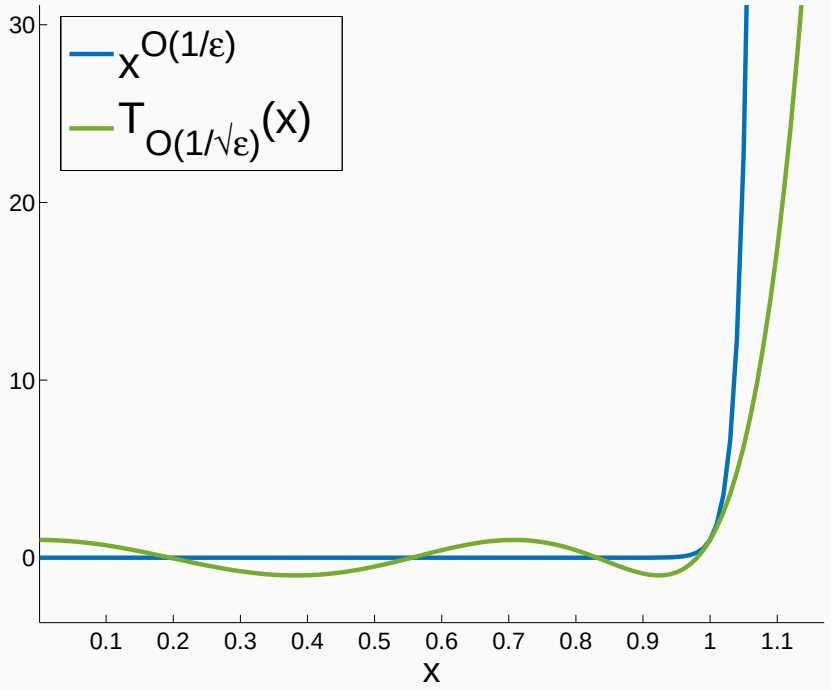

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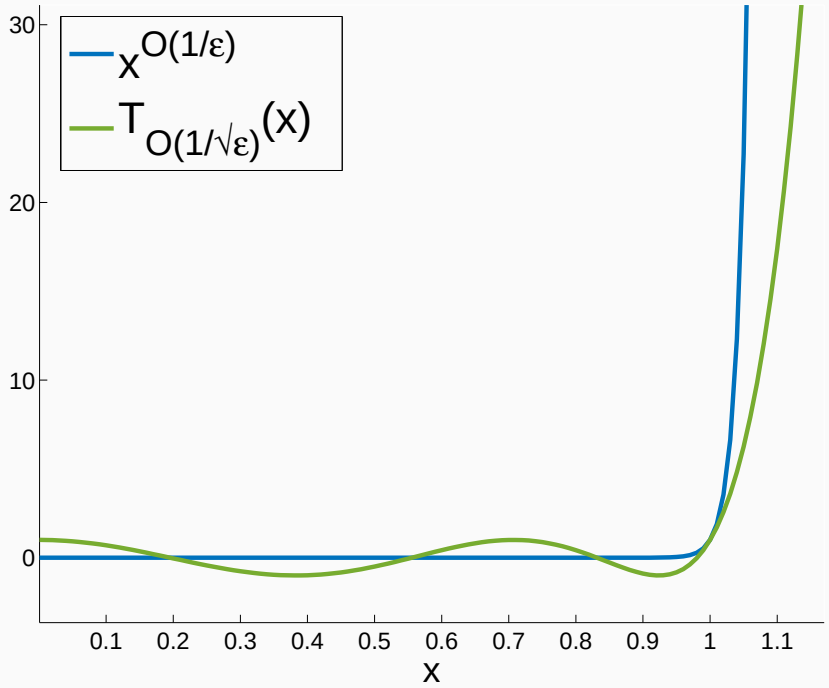

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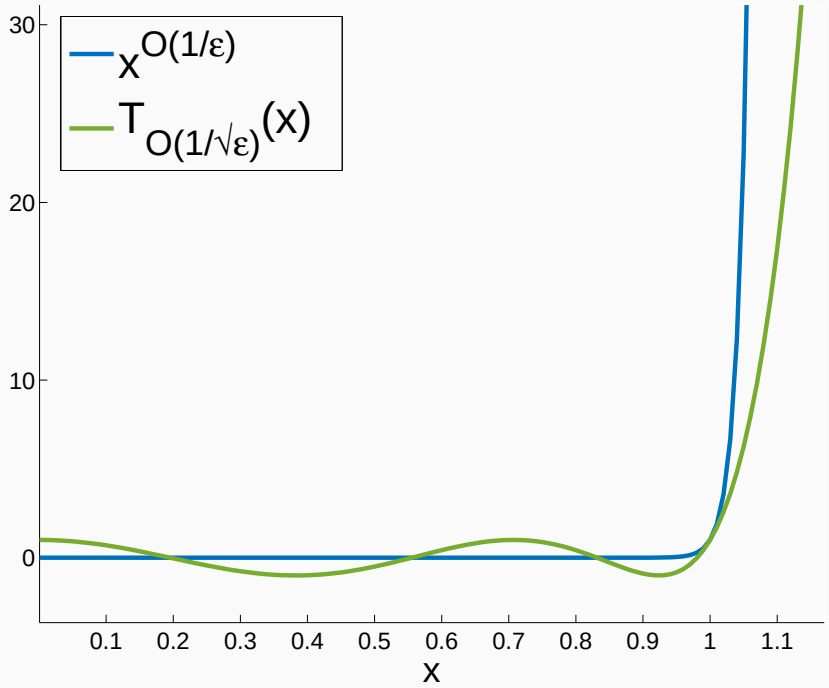

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Implicit use of acceleration polynomial

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

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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.

RAYLEIGH-RITZ POST-PROCESSING

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

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

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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).

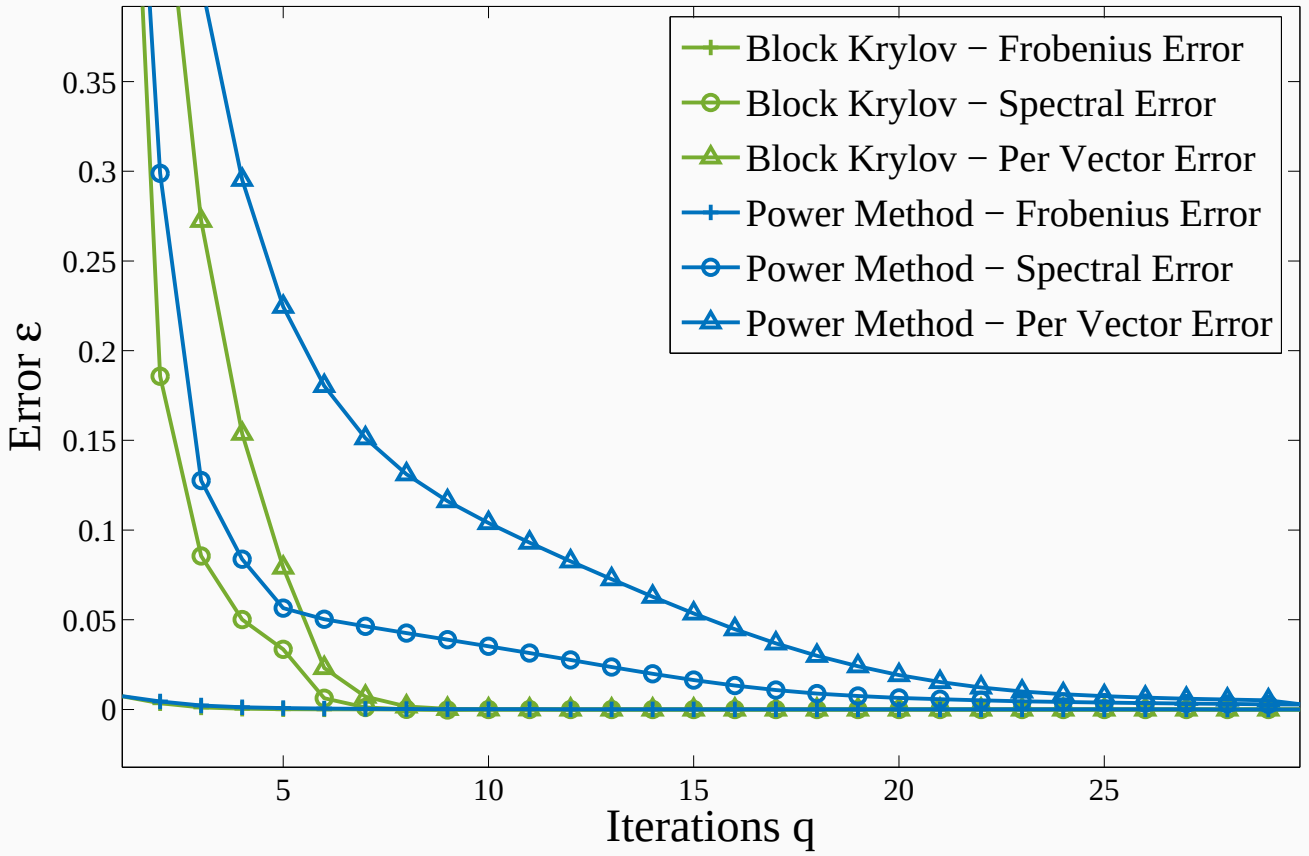
Block Power Method

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

Block Krylov Iteration

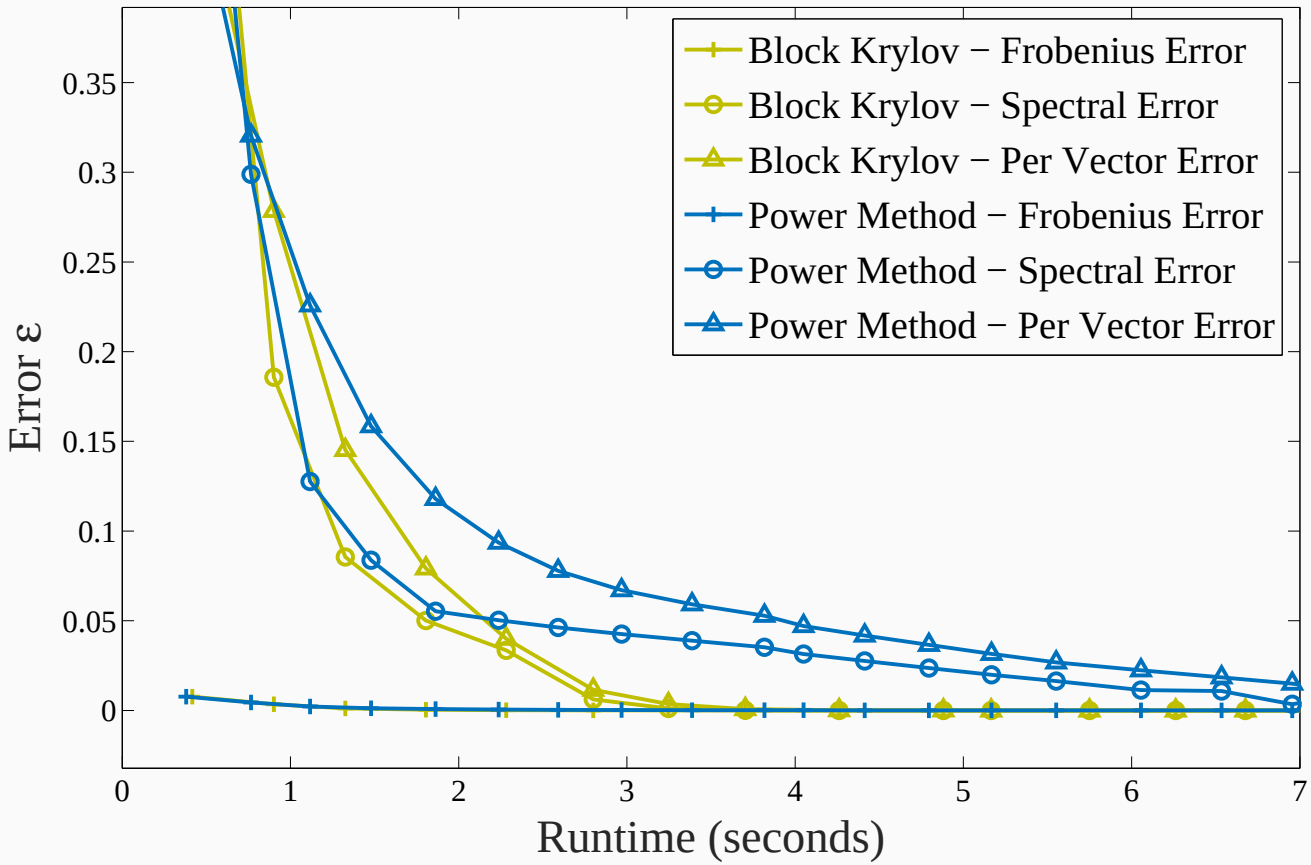
```
X = randn(d,k);
K = zeros(d,k*iter);
for i=1:iter
    [X,R] = qr(A*X);
    K(:,(i-1)*k+1:i*k) = X;
end
[Q,R] = qr(K);
[U,S] = svd(Q'*A,'econ');
U = Q*U(:,1:k);
```

Block Krylov beats Block Power Method definitively for small ϵ.



20 NEWSGROUPS, $k = 20$

Block Krylov beats Block Power Method definitively for small ϵ.



20 NEWSGROUPS, $k = 20$

Main Takeaway: First gap independent bound for Krylov methods.

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

Open Questions

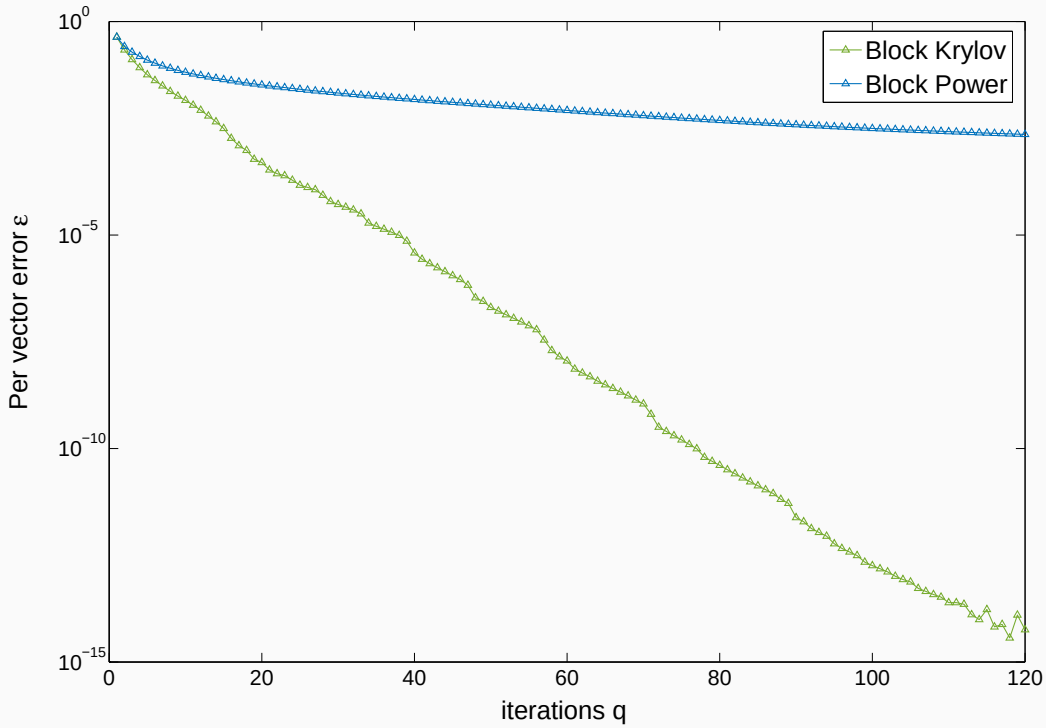
- Full stability analysis.
- 'Master' error metric for gap independent results.
- Gap independent bounds for other methods (e.g. online and stochastic PCA).
- Analysis for small space/restarted block Krylov methods?

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 $k = 10$, $\kappa = 100{,}000$