

# ERROR ESTIMATIONS FOR RANDOMIZED LOW-RANK APPROXIMATIONS



Mathematical  
Institute

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*Computational Mathematics Theme - STFC UKRI*

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Oxford  
Mathematics



## ERROR ESTIMATIONS FOR RANDOMIZED LOW-RANK APPROXIMATIONS

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- 2 INTRODUCTION: (RANDOMIZED) LOW-RANK APPROXIMATIONS
- 3 APPROXIMATING SINGULAR VALUES
- 4 A-POSTERIORI ERROR ESTIMATE: GN
- 5 A-POSTERIORI ERROR ESTIMATE: CUR (SPOILER)

## INTRODUCTION: SVD

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1

## NUMERICAL LINEAR ALGEBRA

We devise and analyse methods for:

- Linear System:

$$\begin{array}{|c|} \hline A \\ \hline \end{array} \begin{array}{|c|} \hline x \\ \hline \end{array} = \begin{array}{|c|} \hline b \\ \hline \end{array}$$

- Eigenvalue Problem:

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- (•) Singular Value Decomposition:

- ▶ Find (approximate) singular subspaces
- ▶ Find (approximate) singular values
- ▶ Low-rank approximations

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How?

- ▶ Complexity
- ▶ Accuracy
- ▶ Stability
- ▶ Use of inputs (e.g. Number of passes)

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## NLA TOOLS

$$\triangleright \|A\|_F = \sqrt{\sum_i \sum_j |a_{ij}|^2}, \quad \|A\|_2 = \sup_x \frac{\|Ax\|_2}{\|x\|_2}, \quad \text{with } \|x\|_2 = \sqrt{|x_1|^2 + \dots + |x_n|^2}$$

$$\triangleright \text{Orthogonal matrix: } \begin{matrix} & m \\ m & Q^* \end{matrix} \begin{matrix} m \\ Q \end{matrix} = \begin{matrix} m \\ I_m \end{matrix} = \begin{matrix} m \\ Q \end{matrix} \begin{matrix} m \\ Q^* \end{matrix}$$

$$\triangleright \text{Orthonormal matrix: } \begin{matrix} & m \\ n & Q^* \end{matrix} \begin{matrix} m \\ Q \end{matrix} = \begin{matrix} n \\ I_n \end{matrix}$$

$$\triangleright \text{QR factorization: For any } A \in \mathbb{R}^{m \times n} \text{ there exists a factorization } \begin{matrix} & n \\ m & A \end{matrix} = \begin{matrix} & n \\ m & Q \end{matrix} \begin{matrix} n \\ R \end{matrix}$$

where  $Q$  is orthonormal and  $R$  is upper triangular.

## SINGULAR VALUE DECOMPOSITION

## Singular Value Decomposition (SVD)

Any matrix  $A$  has the decomposition (assume  $m \geq n$ ):

$$\begin{array}{c} m \\ \boxed{A} \end{array} \begin{array}{c} n \\ \end{array} = \begin{array}{c} m \\ \boxed{U} \end{array} \begin{array}{c} n \\ \end{array} \begin{array}{c} n \\ \boxed{\Sigma} \end{array} \begin{array}{c} n \\ \boxed{V^*} \end{array}$$

$$= \sum_{i=1}^n \sigma_i u_i v_i^*$$

where  $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$ , with  $(\sigma_{\max} :=) \sigma_1 \geq \dots \geq \sigma_n \geq 0$ , and  $U, V$  are orthonormal matrices, that is,  $U^* U = V^* V = I_n$ .



Sec. 2.4 (Golub, Van Loan)  
Lect. 4 (Trefethen, Bau, 2022)

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Existence:

Always, from eigenvalues of  $A^*A$

Uniqueness:

- ▶ Singular vectors
  - Can be flipped by signs
  - Multiple singular values
- ▶ Singular values
  - Always unique

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- ▶  $\sigma_i = \sqrt{\lambda_i(A^*A)}$ , for  $i = 1, \dots, n$
- ▶  $\|A\|_2 = \sigma_{\max}$  and  $\|A\|_F^2 = \sum_{i=1}^n \sigma_i^2$
- ▶ "full" SVD:  $A = \begin{bmatrix} U & U_{\perp} \end{bmatrix} \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} V^*$
- ▶  $\sigma_i(A) = \sigma_i(Q_1 A Q_2)$  for any  $Q_1, Q_2$  orthogonal
- ▶ Can be computed by, e.g., Golub-Kahan bi-diagonalization cost  $\mathcal{O}(mn^2)$

# SINGULAR VALUE DECOMPOSITION > *Why do we care?*

## It's beautiful!

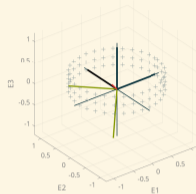
### Theoretical Beauty

- ▶ Existence
- ▶ Info about: norms, rank, subspaces
- ▶ Low-rank optimality
- ▶ Reduces difficulties of problems: Linear system, eigenvalue problem, inverse problem
- ▶ Pseudoinverse

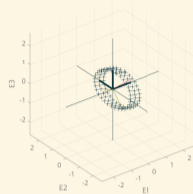


Example by Eric Thomson, definitely worth having a look at  
<http://neurochannels.blogspot.com/2008/02/visualizing-svd.html>

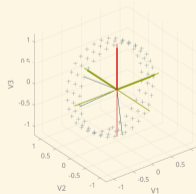
Data in standard basis (black) w/V-basis in green and red


 $Ax$ 

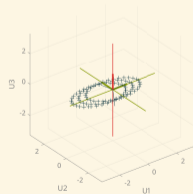
Final output in standard basis (black) w/ U-basis in green/red


 $V^*x \downarrow$ 

Data in V-basis (green and red) w/ standard basis in black


 $\Sigma(V^*x)$ 

Transformed data in U-basis (green/red) w/ standard basis in black



## It's beautiful!

### Applied Beauty

- ▶ Quantum information
- ▶ Immunology
- ▶ Molecular dynamics
- ▶ Information retrieval
- ▶ Pattern Recognition
- ▶ Weather forecast
- ▶ Astrodynamics
- ▶ Small-angle scattering

## It's beautiful!

### Applied Beauty

- ▶ Gene expression data
- ▶ Quantum information
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- ▶ Signal Processing
- ▶ Gene expression data
- ▶ Quantum information
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- ▶ Information retrieval
- ▶ Pattern Recognition
- ▶ Weather forecast

## It's beautiful!

### Applied Beauty

- ▶ Imaging processing and compression
- ▶ Signal Processing
- ▶ Gene expression data
- ▶ Quantum information
- ▶ Immunology
- ▶ Molecular dynamics
- ▶ Information retrieval
- ▶ Pattern Recognition

SINGULAR VALUE DECOMPOSITION > *Why do we care?*

## It's beautiful!

Applied Beauty

## ▶ Choosing a Pizzeria

300 samples measuring 7 features of Pizze  
from 10 different Pizzerie!

Pizzeria	water	protein	fat	ash	sodium	carbohydrates	calories
A	30.49	21.28	41.65	4.82	1.64	1.76	4.67
A	32.20	19.25	43.42	4.62	1.50	0.51	4.70
⋮							
B	50.33	13.96	29.25	3.42	0.96	3.04	3.31
⋮							
C	49.10	24.53	21.08	2.84	0.34	2.45	2.98
⋮							
D	47.45	22.37	20.97	4.06	0.70	5.15	2.99
⋮							
J	44.91	11.07	17.00	2.49	0.66	25.36	2.91



Brilliant example by Joachim Schork, see  
<https://statisticsglobe.com/principal-component-analysis-pca>

SINGULAR VALUE DECOMPOSITION > *Why do we care?*

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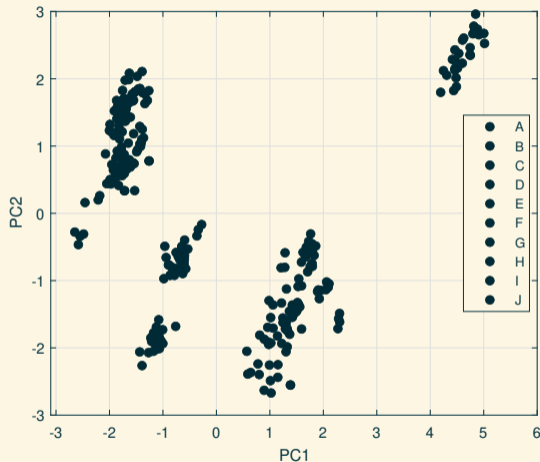
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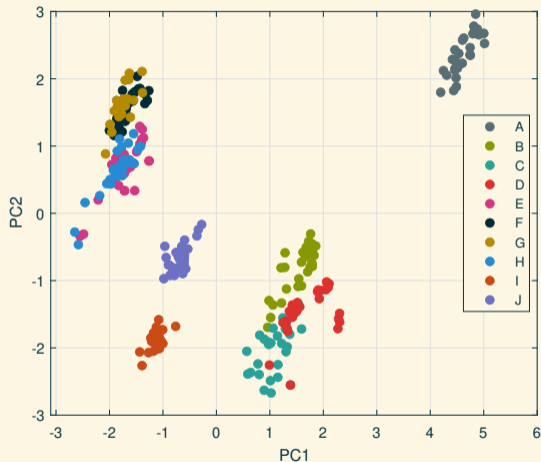
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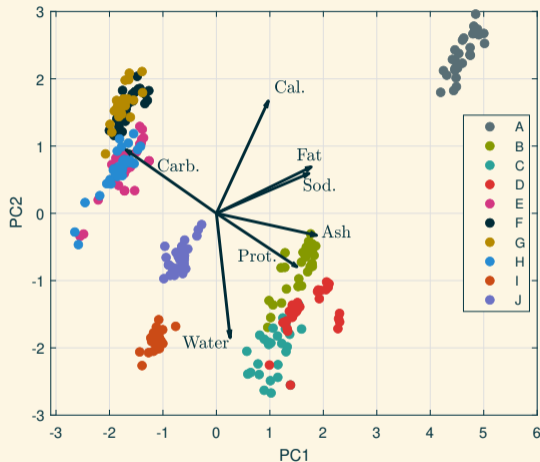
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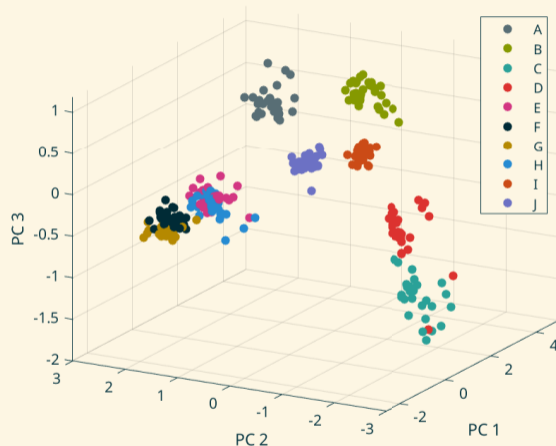
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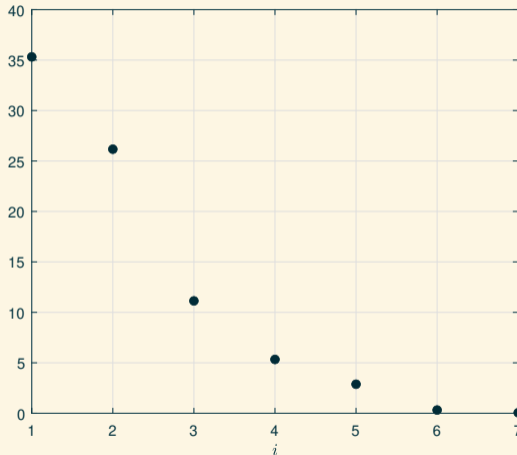
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# INTRODUCTION: (RANDOMIZED) LOW-RANK APPROXIMATIONS

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2

## (NUMERICAL) RANK

▶  $A$  has **rank**  $k$  if there exists  $E$  and  $F$  such that:

$$m \begin{matrix} n \\ \boxed{A} \end{matrix} = m \begin{matrix} k \\ \boxed{E} \end{matrix} k \begin{matrix} n \\ \boxed{F^*} \end{matrix}$$

- rank = number of non-zero singular values

$$A^\dagger := V \operatorname{diag}(\sigma_1^{-1}, \dots, \sigma_k^{-1}, 0, \dots, 0) U^*$$

▶  $A$  has  $\epsilon$ -**rank**  $k$  if there exists  $E$  and  $F$  such that:  $\|A - EF^*\| \leq \epsilon$

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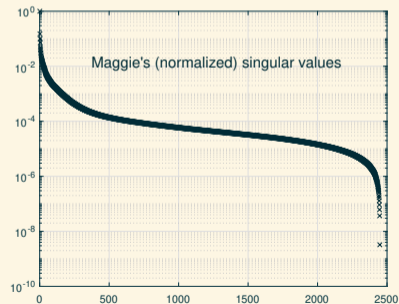
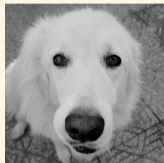
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Maggie -  $2448 \times 2448$ 

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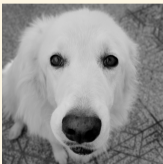
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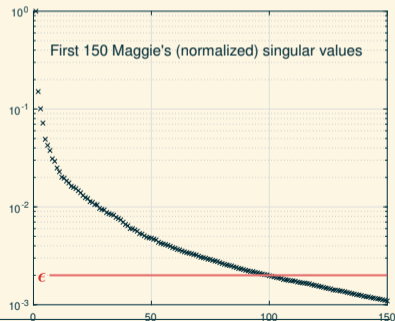
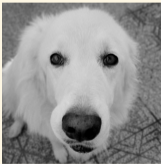
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Maggie - 2448 × 2448



rank 100



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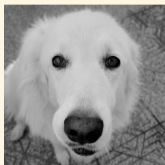
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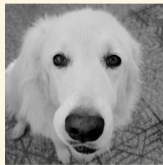
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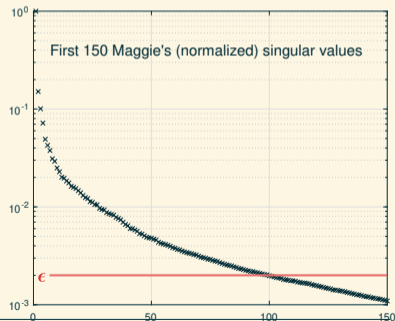
Maggie - 2448 × 2448



rank 100



rank 5



## (RANDOMIZED) LOW-RANK APPROXIMATIONS

Given a fix rank  $r$ , find  $E \in \mathbb{R}^{m \times r}$  and  $F \in \mathbb{R}^{n \times r}$  such that  $A \approx EF^*$

$$A_r = \sum_{i=1}^r \sigma_i u_i v_i^*$$

is the best rank- $r$  approximation of  $A$  in both 2-norm and F-norm

$$\triangleright \|A - A_r\|_2 = \sigma_{r+1}$$

$$\triangleright \|A - A_r\|_F = \sqrt{\sigma_{r+1}^2 + \dots + \sigma_{\text{rank}(A)}^2}$$

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### Classical Approach

$$\|A - A_r\| = \|A - U_r U_r^* A\| = \inf_{P=r\text{-dim orth. proj.}} \|A - PA\|$$

→ Find cheaper (but not optimal) orthogonal projections:

e.g.

- ▶ Gram-Schmidt on the columns/rows of  $A$   
- cost  $\mathcal{O}(mnr)$

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**Randomized Approach**

Use randomization for a model reduction while (approximately) preserving properties of the big problem

Sketching → Random Embedding

- |                                  |                                     |
|----------------------------------|-------------------------------------|
| ☺ Reduced costs                  | ☹ Different outputs                 |
| ☺ (often) near-optimal solutions | ☹ Can fail (with small probability) |

## RANDOMIZED SVD (HMT)

## Randomized SVD

$$A \approx (A\Omega)(A\Omega)^\dagger A =: A_{HMT,\Omega}$$



(Clarkson, Woodruff, 2017)  
(Halko, Martinsson, Tropp, 2011)  
(Rokhlin, Szlam, Tygert, 2009)

1. Choose  $\Omega \in \mathbb{R}^{n \times r}$
2. Sketch:  $X = A\Omega$
3.  $[Q, \sim] = \text{qr}(X, 0)$
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- ▶  $N_r + \mathcal{O}(mr^2) + \tilde{N}_r$
- ▶ Double-pass
- ▶ 2 multiplications by  $A$

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**Accuracy**

$$\hat{r} \leq r - 2$$

$$\mathbb{E} \|A - A_{HMT,\Omega}\|_F \leq \sqrt{1 + \frac{r}{r - \hat{r} - 1}} \|A - A_{best,\hat{r}}\|_F$$

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Stability

Stable under rounding errors if computed with Householder QR

(Connolly, Higham, Pranesh, 2022)

## GENERALIZED NYSTRÖM APPROXIMATION

## Generalized Nyström

$$A \approx A\Omega_1(\Omega_2^*A\Omega_1)^\dagger\Omega_2^*A =: A_{GN,\Omega_1,\Omega_2}$$



(Clarkson, Woodruff, 2009)  
(Nakatsukasa, 2020)  
(Woolfe, Liberty, Rokhlin, Tygert, 2008)

1. Choose  $\Omega_1 \in \mathbb{R}^{n \times r}, \Omega_2 \in \mathbb{R}^{m \times (r+\ell)}$
2. Two-side Sketch:  $X = A\Omega_1$  and  $Y = \Omega_2^*A$
3.  $[Q,R] = \text{qr}(Y\Omega_1, 0)$
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## GENERALIZED NYSTRÖM APPROXIMATION

## Generalized Nyström

$$A \approx A\Omega_1(\Omega_2^*A\Omega_1)^\dagger\Omega_2^*A =: A_{GN,\Omega_1,\Omega_2}$$



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**Accuracy**

$$\hat{r} \leq r - 2$$

$$\mathbb{E}\|A - A_{GN,\Omega_1,\Omega_2}\|_F \leq \sqrt{1 + \frac{r+\ell}{\ell-1}} \sqrt{1 + \frac{r}{r-\hat{r}-1}} \|A - A_{best,\hat{r}}\|_F$$

(Tropp et al., 2017), (Nakatsukasa, 2020)

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Stability

$$(A\Omega_1)(\Omega_2^*A\Omega_1)^\dagger\Omega_2^*A$$

(Nakatsukasa, 2020)

## APPROXIMATING SINGULAR VALUES

---

3

## PROBLEM SETTING

$$A = U\Sigma V^*$$

Given  $\tilde{U}$  and/or  $\tilde{V}$  approximations of the leading singular subspaces of  $A$

$$n \begin{bmatrix} r \\ \tilde{V} \end{bmatrix}, \quad m \begin{bmatrix} r + \ell \\ \tilde{U} \end{bmatrix}$$

**AIM:** Approximate the leading singular values  $\{\sigma_i(A)\}_{i=1}^r$

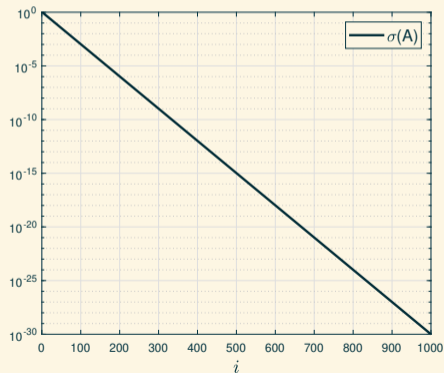
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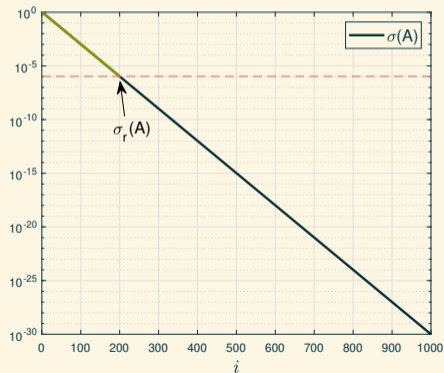
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CLASSICAL APPROACHES > *Rayleigh Ritz and (one-sided) SVD approximations*

## Rayleigh Ritz (RR)

$$\sigma_i(A) \approx \sigma_i(\tilde{U}^* A \tilde{V}) =: \sigma_i(A_{RR, \tilde{V}, \tilde{U}})$$



(Dax, 2012)  
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## CLASSICAL APPROACHES &gt; Rayleigh Ritz and (one-sided) SVD approximations &gt; Accuracy

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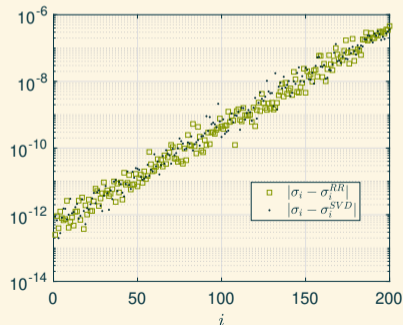
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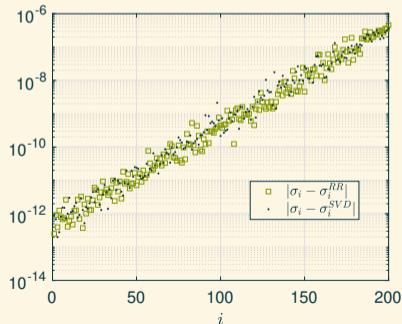


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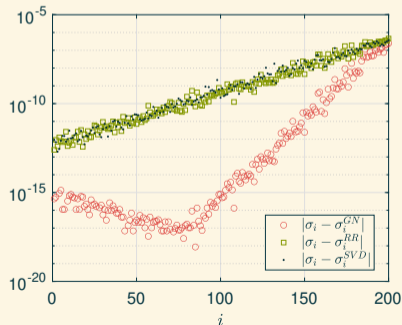


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**BUT,**  
what if we could have this?

## GN APPROXIMATION AND EXTRACTING SINGULAR VALUES

## Generalized Nyström

Given approximations  $\tilde{U}$  and  $\tilde{V}$  to the leading singular subspaces,

$$\sigma_i(A) \approx \sigma_i \left( A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger \tilde{U}^*A \right) =: \sigma_i^{GN}$$

$$\sigma_i \left( \begin{array}{c} \boxed{A\tilde{V}} \end{array} \begin{array}{c} \boxed{\tilde{U}^*A\tilde{V}}^\dagger \end{array} \begin{array}{c} \boxed{\tilde{U}^*A} \end{array} \right)$$

$N_{2r+l}$

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$$\sigma_i \left( \begin{array}{c} \boxed{Q_L} \\ \boxed{R_L} \\ \boxed{\tilde{U}^*A\tilde{V}}^\dagger \\ \boxed{R_R^*} \\ \boxed{Q_R^*} \end{array} \right)$$

$$N_{2r+\ell} + \mathcal{O}((m+n)r^2)$$

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$$\sigma_i \left( \begin{array}{|c|} \hline R_L \\ \hline \end{array} \begin{array}{|c|} \hline \tilde{U}^*A\tilde{V} \\ \hline \end{array}^\dagger \begin{array}{|c|} \hline R_R^* \\ \hline \end{array} \right)$$

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## GN AND MATRIX PERTURBATION THEORY

## GN and Orthogonal Transformations

Consider  $T_1$  and  $T_2$  orthogonal matrices, then

$$T_1^*(M_{GN, \tilde{V}, \tilde{U}})T_2 = (T_1^*MT_2)_{GN, T_2^*\tilde{V}, T_1^*\tilde{U}}$$

For any orthonormal  $\tilde{V}$  and  $\tilde{U}$ , we can:

1. Define  $Q_1 = [\tilde{U} \quad \tilde{U}_\perp]$   $Q_2 = [\tilde{V} \quad \tilde{V}_\perp]$ ;
2. Consider the transformed matrix:  $Q_1^*AQ_2$ ;
3. Consider the transformed GN approximation:

$$Q_1^*A_{GN, \tilde{V}, \tilde{U}}Q_2 = (Q_1^*AQ_2)_{GN, Q_2^*\tilde{V}, Q_1^*\tilde{U}} = (Q_1^*AQ_2)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}}.$$

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$$\rightarrow |\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})| = |\sigma_i(Q_1^*AQ_2) - \sigma_i((Q_1^*AQ_2)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}})|$$

GN AND MATRIX PERTURBATION THEORY > Express  $A_{GN}$  as a perturbation of the original matrix  $A$ 

$$\tilde{V} := \begin{matrix} r & r \\ r & I_r \\ n-r & 0 \end{matrix} \begin{bmatrix} \\ \\ \\ \end{bmatrix}, \quad \tilde{U} := \begin{matrix} r+\ell & r+\ell \\ I_{r+\ell} & \\ m-(r+\ell) & 0 \end{matrix} \begin{bmatrix} \\ \\ \\ \end{bmatrix}, \quad A := \begin{matrix} r & n-r \\ r+\ell & \begin{bmatrix} A_{11} & | & A_{12} \\ \hline & & \end{bmatrix} \\ m-(r+\ell) & \begin{bmatrix} A_{21} & & \\ & A_{22} & \end{bmatrix} \end{matrix} \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$



(Tropp, Webber, 2023)

$$A_{GN, \tilde{V}, \tilde{U}} = A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger \tilde{U}^*A$$

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$$MM^\dagger M = M$$

$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \left[ A_{11} \mid A_{12} \right] = \left[ \begin{array}{c|c} A_{11} A_{11}^\dagger A_{11} & A_{11} A_{11}^\dagger A_{12} \\ \hline A_{21} A_{11}^\dagger A_{11} & A_{21} A_{11}^\dagger A_{12} \end{array} \right]$$

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$M$  has linearly independent columns  
 $\implies M^\dagger M = M^{-1}M = M$

$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \left[ A_{11} \mid A_{12} \right] = \left[ \begin{array}{c|c} \overbrace{A_{11} A_{11}^\dagger A_{11}}^{= A_{11}} & A_{11} A_{11}^\dagger A_{12} \\ \hline A_{21} A_{11}^\dagger A_{11} & A_{21} A_{11}^\dagger A_{12} \end{array} \right]$$

GN AND MATRIX PERTURBATION THEORY > Express  $A_{GN}$  as a perturbation of the original matrix  $A$ 

$$\tilde{V} := \begin{matrix} r \\ n-r \end{matrix} \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \quad \tilde{U} := \begin{matrix} r+\ell \\ m-(r+\ell) \end{matrix} \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}, \quad A := \begin{matrix} r & n-r \\ r+\ell & \\ m-(r+\ell) & \end{matrix} \left[ \begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right]$$

$$A_{GN, \tilde{V}, \tilde{U}} = \begin{bmatrix} A_{11} \\ - \\ A_{21} \end{bmatrix} (A_{11})^\dagger \left[ \begin{array}{c|c} A_{11} & A_{12} \end{array} \right] = \left[ \begin{array}{c|c} A_{11} & A_{11} A_{11}^\dagger A_{12} \\ \hline \underbrace{A_{21} A_{11}^\dagger A_{11}}_{= A_{21}} & A_{21} A_{11}^\dagger A_{12} \end{array} \right]$$

**GN AND MATRIX PERTURBATION THEORY** > Express  $A_{GN}$  as a perturbation of the original matrix  $A$ 

$$\tilde{V} := \begin{matrix} r \\ n-r \end{matrix} \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \quad \tilde{U} := \begin{matrix} r+\ell \\ m-(r+\ell) \end{matrix} \begin{bmatrix} I_{r+\ell} \\ 0 \end{bmatrix}, \quad A := \begin{matrix} r & n-r \\ r+\ell & \\ m-(r+\ell) & \end{matrix} \left[ \begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right]$$

$$A_{GN, \tilde{V}, \tilde{U}} = A - \left[ \begin{array}{c|c} 0 & A_{12} - A_{11}A_{11}^\dagger A_{12} \\ \hline 0 & A_{22} - A_{21}A_{11}^\dagger A_{12} \end{array} \right] =: A - E_{GN}$$

GN AND MATRIX PERTURBATION THEORY > Express  $A_{GN}$  as a perturbation of the original matrix  $A$ 

$$\tilde{V} := \begin{matrix} r \\ n-r \end{matrix} \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \quad \tilde{U} := \begin{matrix} r \\ m-r \end{matrix} \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \quad A := \begin{matrix} r & n-r \\ m-r \end{matrix} \left[ \begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right]$$

No-oversample ( $\ell = 0$ )  
 $\rightarrow A_{12} - A_{11}A_{11}^\dagger A_{12} = 0$ , but change of  
 block sizes!

$$A_{GN, \tilde{V}, \tilde{U}} = A - \left[ \begin{array}{c|c} 0 & 0 \\ \hline 0 & A_{22} - A_{21}A_{11}^\dagger A_{12} \end{array} \right] =: A - E_{GN}$$

## Weyl's Theorem

For any matrix  $M$  we have that

$$|\sigma_i(M) - \sigma_i(M + E)| \leq \|E\|_2$$



Cor. 7.3.5 (Horn, Johnson, 2012)  
Cor. 1.4.31 (Stewart, 1998)

## Weyl's Theorem

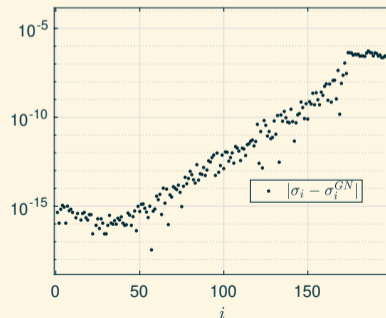
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Cor. 7.3.5 (Horn, Johnson, 2012)  
Cor. 1.4.31 (Stewart, 1998)

$$|\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})|$$



## Weyl's Theorem

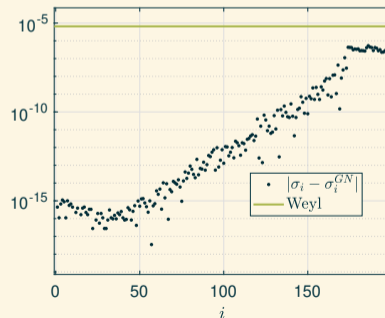
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Cor. 7.3.5 (Horn, Johnson, 2012)  
Cor. 1.4.31 (Stewart, 1998)

$$|\sigma_i(A) - \sigma_i(A_{GN, \tilde{V}, \tilde{U}})| \leq \|E_{GN}\|_2$$



BOUND ON GN APPROXIMATION ERROR > Derivation
 

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- $A, \tilde{V}, \tilde{U} \rightarrow A_{GN} = A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger\tilde{U}^*A$

- Define

$$\bar{A} = [\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp], \quad \bar{A}_{GN} = \left( [\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp] \right)_{GN, \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \begin{bmatrix} I_r \\ 0 \end{bmatrix}}$$

$$\implies \bar{A}_{GN} = \bar{A} - \begin{bmatrix} 0 & 0 \\ 0 & \bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger\bar{A}_{12} \end{bmatrix} =: \bar{A} - E_{GN}$$

**BOUND ON GN APPROXIMATION ERROR** > *Derivation*

- $A, \tilde{V}, \tilde{U} \rightarrow A_{GN} = A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger\tilde{U}^*A$

- Define

$$\bar{A} = [\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp], \quad \bar{A}_{GN} = \left([\tilde{U} \ \tilde{U}_\perp]^* A [\tilde{V} \ \tilde{V}_\perp]\right)_{GN, \begin{bmatrix} l_r \\ 0 \end{bmatrix}, \begin{bmatrix} l_r \\ 0 \end{bmatrix}}$$

$$\Rightarrow \bar{A}_{GN} = \bar{A} - \begin{bmatrix} 0 & 0 \\ 0 & \bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger\bar{A}_{12} \end{bmatrix} =: \bar{A} - E_{GN}$$



Corollary 5.1  
(L., Al Daas, Nakatsukasa, 2024)

Define

$$\tau_i = \frac{\max\{\|\bar{A}_{12}\|_2, \|\bar{A}_{21}\|_2\}}{\min_j |\sigma_i(\bar{A}) - \sigma_j(\bar{A}_{22})| - 2\|E_{GN}\|_2}.$$

Then, for each  $i$ , if  $\tau_i > 0$

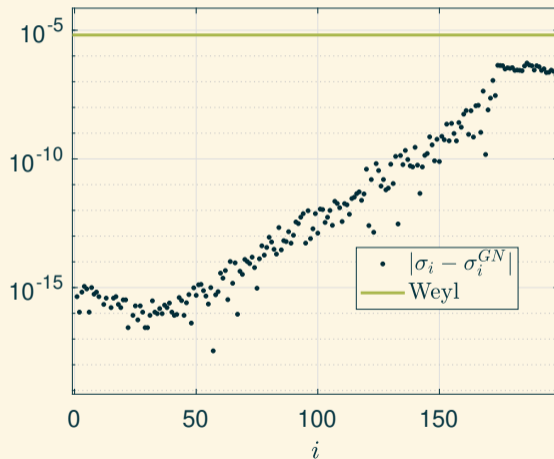
$$|\sigma_i(A) - \sigma_i(A_{GN})| = |\sigma_i(\bar{A}) - \sigma_i(\bar{A}_{GN})| \leq \left\| \bar{A}_{22} - \bar{A}_{21}\bar{A}_{11}^\dagger\bar{A}_{12} \right\|_2 \tau_i^2$$

▶  $\tau_i < 1$  necessary to be better than Weyl. If  $\sigma_i(\bar{A})$  is far from the spectrum of  $\bar{A}_{22}$  then  $\tau_i \ll 1$

## BOUND ON GN APPROXIMATION ERROR &gt; Numerical illustration

- $\ell = 0$
- $A \in \mathbb{R}^{1000 \times 1000}$
- $U_{ex}, V_{ex}$  Haar Matrices
- $\sigma_i(A)$  exponentially decaying
- $[\tilde{V}, \sim] = \text{qr}(A^* \Omega, 0)$
- $[\tilde{U}, \sim] = \text{qr}(A \Omega, 0)$
- $\tilde{V} \in \mathbb{R}^{1000 \times 200}$
- $\tilde{U} \in \mathbb{R}^{1000 \times 200}$
- Compute pseudoinverses by QR factorization

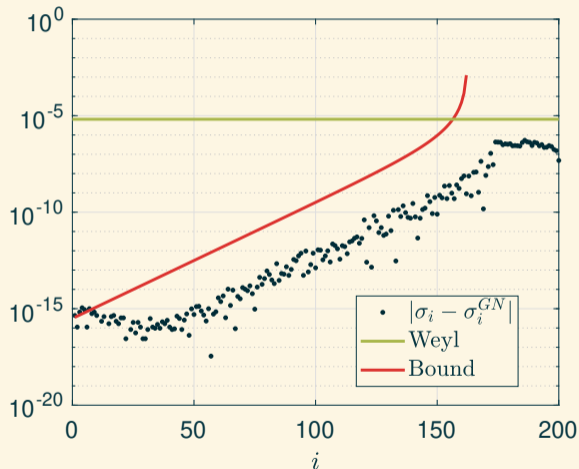
$$\sigma_i(A_{GN, \tilde{V}, \tilde{U}}) = \sigma_i(A \tilde{V} (\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A)$$



## BOUND ON GN APPROXIMATION ERROR &gt; Numerical illustration

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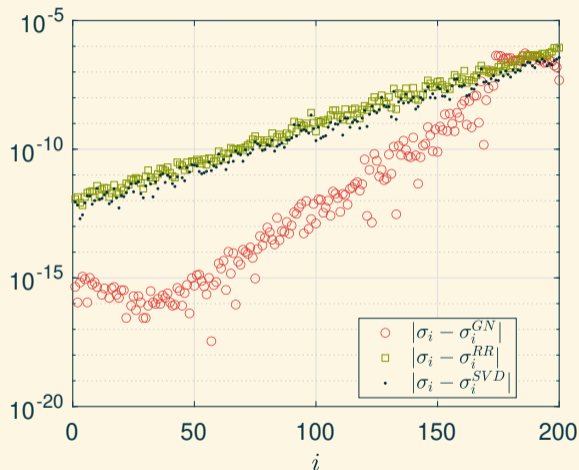
$$\sigma_i(A_{GN, \tilde{V}, \tilde{U}}) = \sigma_i(A \tilde{V} (\tilde{U}^* A \tilde{V})^\dagger \tilde{U}^* A)$$



## COMPARISON OF METHODS &gt; Idea

Single-pass methods

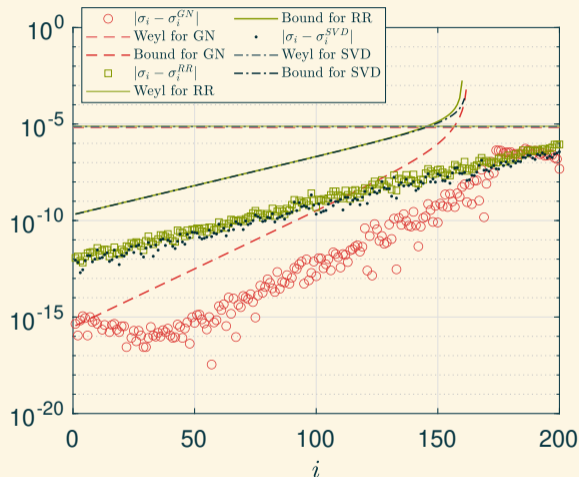
- ▶  $\sigma_i^{SVD} = \sigma_i(A\tilde{V})$
- ▶  $\sigma_i^{RR} = \sigma_i(\tilde{U}^*A\tilde{V})$
- ▶  $\sigma_i^{GN} = \sigma_i(A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger\tilde{U}^*A)$



## COMPARISON OF METHODS &gt; Idea

Single-pass methods

- ▶  $\sigma_i^{SVD} = \sigma_i(A\tilde{V})$
- ▶  $\sigma_i^{RR} = \sigma_i(\tilde{U}^*A\tilde{V})$
- ▶  $\sigma_i^{GN} = \sigma_i(A\tilde{V}(\tilde{U}^*A\tilde{V})^\dagger\tilde{U}^*A)$



## A-POSTERIORI ERROR ESTIMATE: GN

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4

## PROBLEM SETTING AND MAIN IDEA

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### Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$

## PROBLEM SETTING AND MAIN IDEA

## Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$

Goal: Estimate the approximation error using only what you already have

$$\|A - AX(Y^*AX)^\dagger Y^*A\|^2$$

## PROBLEM SETTING AND MAIN IDEA

### Generalized Nyström

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### Certificate of Accuracy

$G$  random,  $\|M\| \approx \|MG\|$

- ☺ Good accuracy
- ☺ Very small size of  $G$  sufficient
- ☹ (More) multiplications by  $M$
- ☹  $G$  needs to be independent of  $M$

## PROBLEM SETTING AND MAIN IDEA

### Generalized Nyström

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(Epperly, Tropp, 2024)

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### Certificate of Accuracy

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- ☹ (More) multiplications by  $M$
- ☹  $G$  needs to be independent of  $M$

### Leave-one-out

Remove one sample column and use it to sketch the error

- ☺ We use only what we have already computed
- ☹ Need fast formula

## LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

A **SPSD** matrix, **X** random matrix

$$AX(X^TAX)^{-1}X^TA$$



(Epperly, Tropp, 2024)

## LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

A **SPSD** matrix, **X** random matrix

$$AX(X^TAX)^{-1}X^TA$$



(Epperly, Tropp, 2024)

$$\left\| A - A \begin{bmatrix} | & & | & & | \\ x_1 & \cdots & x_j & \cdots & x_r \\ | & & | & & | \end{bmatrix} \left( \begin{bmatrix} \text{---} & x_1^* & \text{---} \\ \vdots & \vdots & \vdots \\ \text{---} & x_j^* & \text{---} \\ \vdots & \vdots & \vdots \\ \text{---} & x_r^* & \text{---} \end{bmatrix} A \begin{bmatrix} | & & | & & | \\ x_1 & \cdots & x_j & \cdots & x_r \\ | & & | & & | \end{bmatrix} \right)^{-1} \begin{bmatrix} \text{---} & x_1^* & \text{---} \\ \vdots & \vdots & \vdots \\ \text{---} & x_j^* & \text{---} \\ \vdots & \vdots & \vdots \\ \text{---} & x_r^* & \text{---} \end{bmatrix} A \right\|^2$$

- 1.
- 2.
- 3.

## LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

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(Epperly, Tropp, 2024)

$$\left\| A - A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \begin{bmatrix} x_1^* & \dots & x_j^* & \dots & x_r^* \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix}^{-1} \begin{bmatrix} x_1^* & \dots & x_j^* & \dots & x_r^* \end{bmatrix} A \right\|^2$$

1. Remove one column from  $X$
- 2.
- 3.

## LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

A **SPSD** matrix, **X** random matrix

$$AX(X^TAX)^{-1}X^TA$$



(Epperly, Tropp, 2024)

$$\left\| \left( A - A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \begin{bmatrix} x_1^* \\ \vdots \\ x_j^* \\ \vdots \\ x_r^* \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \right)^{-1} \begin{bmatrix} x_1^* \\ \vdots \\ x_j^* \\ \vdots \\ x_r^* \end{bmatrix} A \begin{bmatrix} x_j \end{bmatrix} \right\|^2$$

The diagram illustrates the leave-one-out error estimate. It shows a matrix expression where the column  $x_j$  is removed from the matrix  $X$  (indicated by a hatched box). The resulting matrix is inverted, and the error is measured by the norm of the product of the inverse matrix and the column  $x_j$  (indicated by a teal box). A green arrow points from the teal box to the list below.

1. Remove one column from  $X$
2. Use it to sketch the error
- 3.

## LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

A **SPSD** matrix, **X** random matrix

$$AX(X^TAX)^{-1}X^TA$$



(Epperly, Tropp, 2024)

$$\frac{1}{r} \sum_{j=1}^r \left\| \left( A - A \begin{bmatrix} x_1 & \dots & \text{---} & x_j & \dots & x_r \end{bmatrix} \begin{bmatrix} x_1^* \\ \vdots \\ x_j^* \\ \vdots \\ x_r^* \end{bmatrix} A \begin{bmatrix} x_1 & \dots & \text{---} & x_j & \dots & x_r \end{bmatrix} \right)^{-1} \begin{bmatrix} x_1^* \\ \vdots \\ x_j^* \\ \vdots \\ x_r^* \end{bmatrix} A \begin{bmatrix} x_j \end{bmatrix} \right\|^2$$

The diagram illustrates the leave-one-out error estimation process. It shows a sequence of matrices and vectors. On the left, a matrix  $(A - A X_j X_j^T A)$  is formed by subtracting the rank-1 approximation  $A x_j x_j^T A$  from  $A$ . The column  $x_j$  in  $X$  and the corresponding row  $x_j^*$  in  $X^T$  are highlighted with diagonal hatching. This matrix is inverted and multiplied by the vector  $A x_j$  to produce the error vector  $x_j$ , which is shown in a teal box on the right. A green arrow points from the  $x_j$  box back to the  $x_j$  column in the  $X$  matrix, indicating the feedback loop in the error estimation.

1. Remove one column from  $X$
2. Use it to sketch the error
3. Sum over all possible indices

## LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

A **SPSD** matrix, **X** random matrix

$$AX(X^TAX)^{-1}X^TA$$



(Epperly, Tropp, 2024)

$$\frac{1}{r} \sum_{j=1}^r \left\| \left( A - A \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \begin{bmatrix} x_1^* \\ \vdots \\ x_j^* \\ \vdots \\ x_r^* \end{bmatrix} A \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \right)^{-1} \begin{bmatrix} x_1^* \\ \vdots \\ x_j^* \\ \vdots \\ x_r^* \end{bmatrix} A \begin{bmatrix} x_j \end{bmatrix} \right\|^2$$

1. Remove one column from  $X$
2. Use it to sketch the error
3. Sum over all possible indices

$$H = X^*AX$$

$$AX = QR$$

$$= \frac{1}{r} \|RH \text{diag}\left(\frac{1}{[H^{-1}]_{ii}}, i = 1, \dots, r\right)\|_F^2$$

= Cheap to compute formula!

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

### Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$



(L., Pearce, Pritchard, 2026)

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

## Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$



(L., Pearce, Pritchard, 2026)

$$\|A - A \begin{bmatrix} | & & | & & | \\ x_1 & \cdots & x_j & \cdots & x_r \\ | & & | & & | \end{bmatrix} \left( \begin{bmatrix} \text{---} y_1 \text{---} \\ \vdots \\ \text{---} y_\ell^* \text{---} \\ \vdots \\ \text{---} y_r^* \text{---} \end{bmatrix} A \begin{bmatrix} | & & | & & | \\ x_1 & \cdots & x_j & \cdots & x_r \\ | & & | & & | \end{bmatrix} \right)^\dagger \begin{bmatrix} \text{---} y_1^* \text{---} \\ \vdots \\ \text{---} y_\ell^* \text{---} \\ \vdots \\ \text{---} y_r^* \text{---} \end{bmatrix} A \|^2$$

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

## Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$



(L., Pearce, Pritchard, 2026)

$$\frac{1}{r^2} \sum_{j,\ell=1}^r \left\| y_\ell^* \left( A - A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_\ell^* \\ \vdots \\ y_r \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix}^\dagger \begin{bmatrix} y_1^* \\ \vdots \\ y_\ell^* \\ \vdots \\ y_r^* \end{bmatrix} A \right) x_j \right\|^2$$

The diagram illustrates the leave-one-out error estimation for the Generalized Nyström approximation. It shows the matrix  $A$  being approximated by  $AX(Y^TAX)^\dagger Y^T A$ . The matrix  $X$  is composed of columns  $x_1, \dots, x_j, \dots, x_r$ , and the matrix  $Y$  is composed of rows  $y_1, \dots, y_\ell^*, \dots, y_r$ . The approximation is shown with a red arrow pointing to the  $y_\ell^*$  term in the sum, and a green arrow pointing to the  $x_j$  term in the norm, indicating the leave-one-out process.

## LEAVE-PAIR-OUT

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

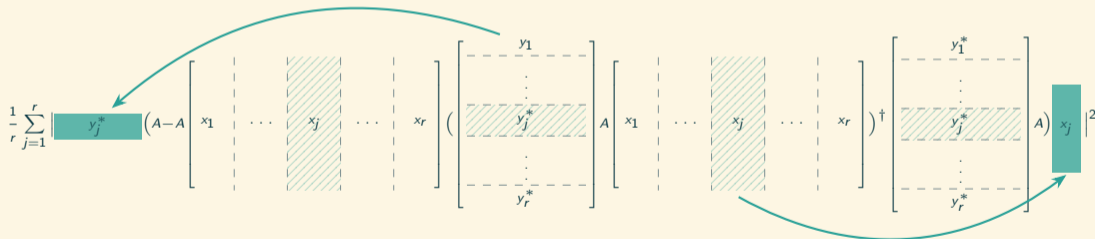
## Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$



(L., Pearce, Pritchard, 2026)



## LEAVE-TWINS-OUT

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

## Generalized Nyström

Low-rank approximation:  $A$  general matrix,  $X, Y$  random matrix

$$AX(Y^TAX)^\dagger Y^T A$$



(L., Pearce, Pritchard, 2026)

$$\frac{1}{r} \sum_{j=1}^r \left\| \left( A - A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_\ell^* \\ \vdots \\ y_s^* \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix}^\dagger \begin{bmatrix} y_1^* \\ \vdots \\ y_\ell^* \\ \vdots \\ y_s^* \end{bmatrix} A \right) x_j \right\|^2$$

The diagram illustrates the leave-one-out error estimate. It shows the Frobenius norm of the error matrix  $(A - AXY^\dagger AX)X$  squared, averaged over  $r$  columns  $x_j$ . The matrix  $X$  is represented as a row of columns  $x_1, \dots, x_j, \dots, x_r$ , with the  $j$ -th column shaded with diagonal lines. The matrix  $Y$  is a column vector of rows  $y_1, \dots, y_\ell^*, \dots, y_s^*$ . The matrix  $Y^T A X$  is a square matrix with rows  $y_1, \dots, y_\ell^*, \dots, y_s^*$ . The matrix  $(Y^T A X)^\dagger$  is its pseudoinverse. The matrix  $AX(Y^T A X)^\dagger Y^T A$  is the low-rank approximation. The error matrix is  $(A - AXY^\dagger AX)X$ . The  $j$ -th column of this error matrix is  $(A - AXY^\dagger AX)x_j$ , which is the quantity whose squared norm is being averaged.

LEAVE-**RIGHT**-OUT

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM &gt; Cheap to compute formula

$$\text{LPO} = \frac{1}{r^2} \sum_{j,\ell=1}^r \left\| y_\ell^* (A-A) \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \left( \begin{bmatrix} y_1 \\ \vdots \\ y_\ell^* \\ \vdots \\ y_r \end{bmatrix} A \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \right)^\dagger \begin{bmatrix} y_1^* \\ \vdots \\ y_\ell^* \\ \vdots \\ y_r^* \end{bmatrix} A x_j \right\|^2$$

$$\text{LTO} = \frac{1}{r} \sum_{j=1}^r \left\| y_j^* (A-A) \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \left( \begin{bmatrix} y_1 \\ \vdots \\ y_j^* \\ \vdots \\ y_r \end{bmatrix} A \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \right)^\dagger \begin{bmatrix} y_1^* \\ \vdots \\ y_j^* \\ \vdots \\ y_r^* \end{bmatrix} A x_j \right\|^2$$

$$\text{LRO} = \frac{1}{r} \sum_{j=1}^r \left\| (A-A) \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \left( \begin{bmatrix} y_1^* \\ \vdots \\ y_\ell^* \\ \vdots \\ y_s^* \end{bmatrix} A \begin{bmatrix} x_1 \\ \vdots \\ x_j \\ \vdots \\ x_r \end{bmatrix} \right)^\dagger \begin{bmatrix} y_1^* \\ \vdots \\ y_\ell^* \\ \vdots \\ y_s^* \end{bmatrix} A x_j \right\|^2$$

## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM &gt; Cheap to compute formula

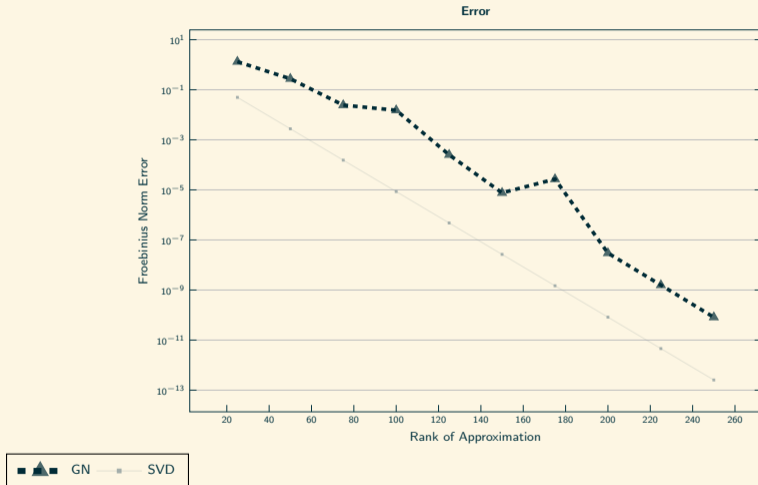
$$\text{LPO} = \frac{1}{r^2} \sum_{j,\ell=1}^r \left| y_\ell^* (A-A) \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \left( \begin{bmatrix} y_1 \\ \dots \\ y_\ell^* \\ \dots \\ y_r \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \right)^\dagger \begin{bmatrix} y_1^* \\ \dots \\ y_\ell^* \\ \dots \\ y_r^* \end{bmatrix} A x_j \right|^2 = \frac{1}{r^2} \sum_{j=1}^r \sum_{\ell=1}^r \left| \frac{1}{[H^{-1}]_{j,\ell}} \right|^2$$

$$\begin{aligned}
 H &= Y^* A X \\
 A X &= Q R
 \end{aligned}$$

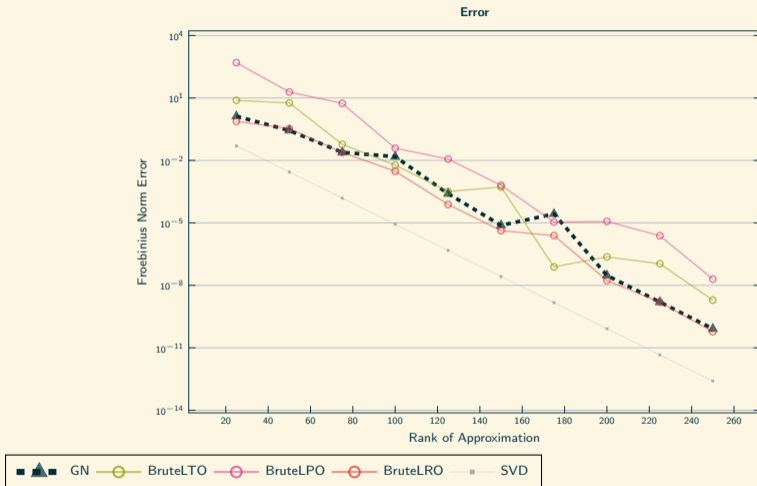
$$\text{LTO} = \frac{1}{r} \sum_{j=1}^r \left| y_j^* (A-A) \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \left( \begin{bmatrix} y_1 \\ \dots \\ y_j^* \\ \dots \\ y_r \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \right)^\dagger \begin{bmatrix} y_1^* \\ \dots \\ y_j^* \\ \dots \\ y_r^* \end{bmatrix} A x_j \right|^2 = \frac{1}{r} \sum_{j=1}^r \left| \frac{1}{[H^{-1}]_{j,j}} \right|^2$$

$$\text{LRO} = \frac{1}{r} \sum_{j=1}^r \left\| (A-A) \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \left( \begin{bmatrix} y_1^* \\ \dots \\ y_\ell^* \\ \dots \\ y_s^* \end{bmatrix} A \begin{bmatrix} x_1 & \dots & x_j & \dots & x_r \end{bmatrix} \right)^\dagger \begin{bmatrix} y_1^* \\ \dots \\ y_\ell^* \\ \dots \\ y_s^* \end{bmatrix} A x_j \right\|^2 = \frac{1}{r} \|R(H^* H)^{-1} \text{diag}(\frac{1}{[(H^* H)^{-1}]_{i,i}}, i=1, \dots, s)\|_F^2$$

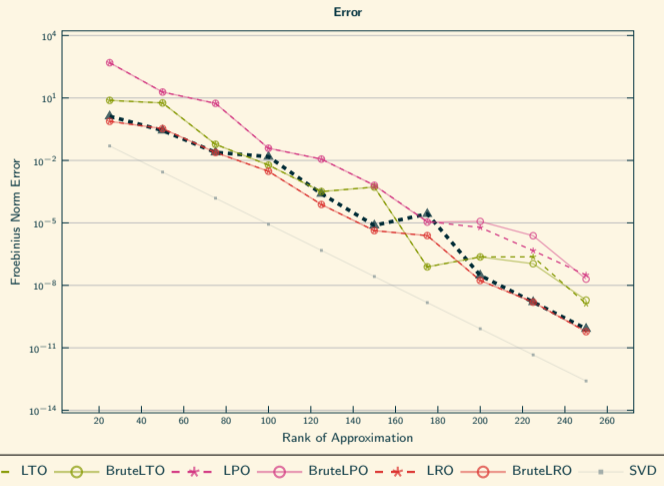
## LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM &gt; Experiments



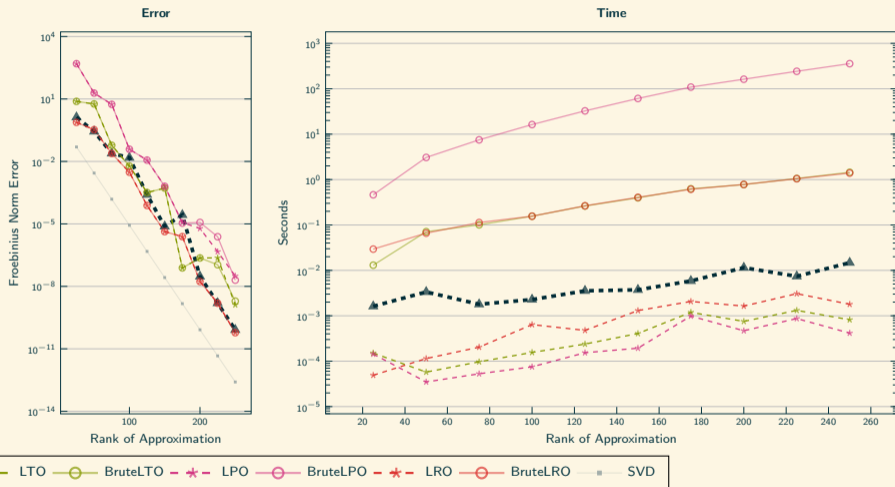
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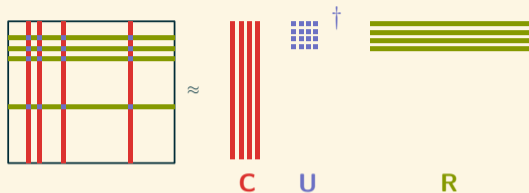


A-POSTERIORI ERROR ESTIMATE: CUR (SPOILER)

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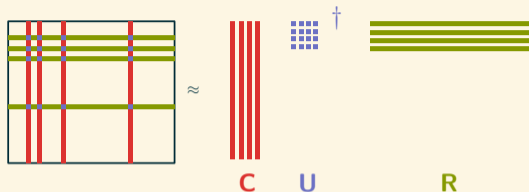
5

## MAIN CHARACTER AND PROBLEM SETTING



- ▶ Near optimal low-rank approximation
- ▶ Interpretable
- ▶ Suitable for experiments design

## MAIN CHARACTER AND PROBLEM SETTING



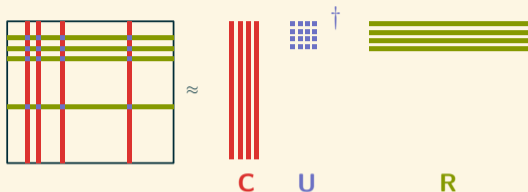
- ▶ Near optimal low-rank approximation
- ▶ Interpretable
- ▶ Suitable for experiments design

### Goal

Estimate the approximation error blindly

$$\|A - CUR\|_F^2$$

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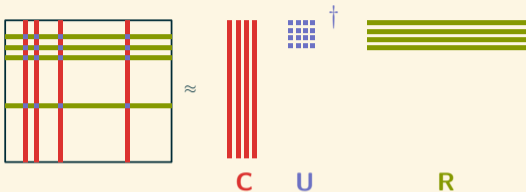
### Goal

Estimate the approximation error blindly

$$\|A - CUR\|_F^2$$

Why: You may not have  $A$  at all,  
 e.g., Spectro-microscopy experiments  
 (Meier, L., Shustin, Al Daas, Quinn, 2026)

## MAIN CHARACTER AND PROBLEM SETTING



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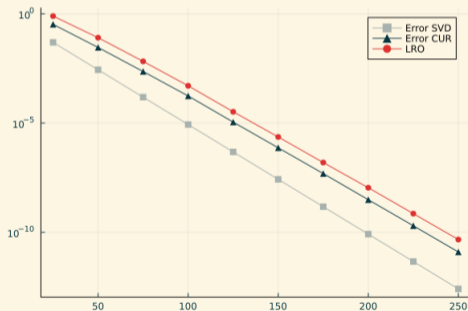
### Goal

Estimate the approximation error blindly

$$\|A - CUR\|_F^2$$

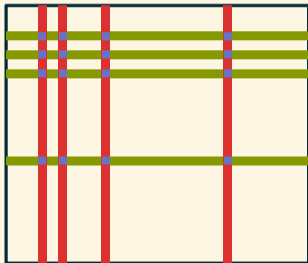
Why: You may not have  $A$  at all,  
e.g., Spectro-microscopy experiments  
(Meier, L., Shustin, Al Daas, Quinn, 2026)

### Leave-right-out for CUR



## BLIND ERROR ESTIMATE FOR CUR

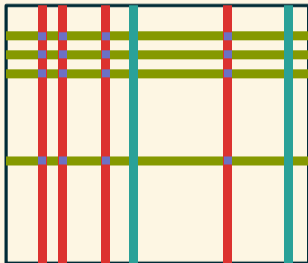
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- 1.
- 2.

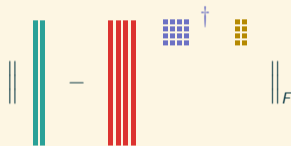
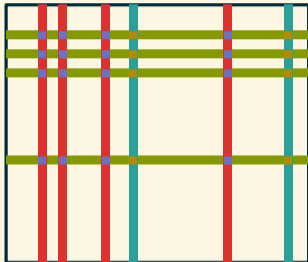
## BLIND ERROR ESTIMATE FOR CUR

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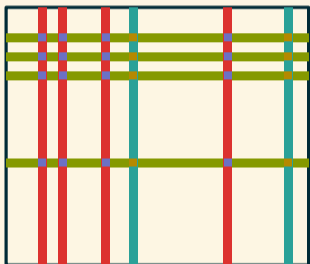
1. Select extra columns
- 2.

## BLIND ERROR ESTIMATE FOR CUR



1. Select extra columns
2. Compute the error "on the extra column"

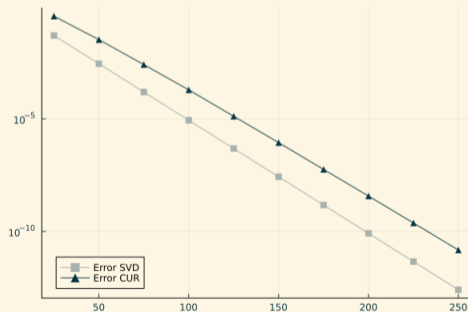
## BLIND ERROR ESTIMATE FOR CUR



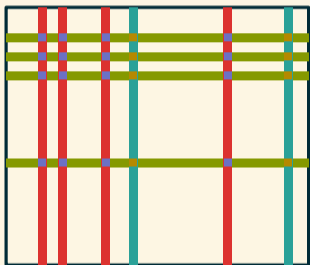
1. Select extra columns
2. Compute the error "on the extra column"

$$\| \begin{matrix} \text{teal columns} \\ \text{red columns} \end{matrix} - \begin{matrix} \text{blue grid} \\ \text{orange grid} \end{matrix} \|_F$$

Exponential decay



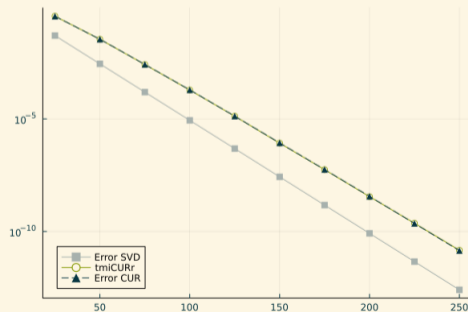
## BLIND ERROR ESTIMATE FOR CUR



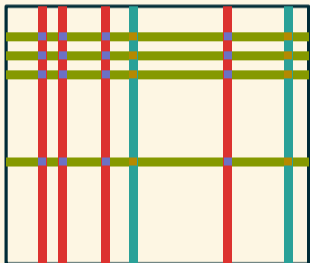
1. Select extra columns
2. Compute the error "on the extra column"

$$\| \begin{matrix} \text{teal columns} \\ \text{red columns} \end{matrix} - \begin{matrix} \text{blue grid} \\ \text{orange grid} \end{matrix} \|_F$$

Exponential decay

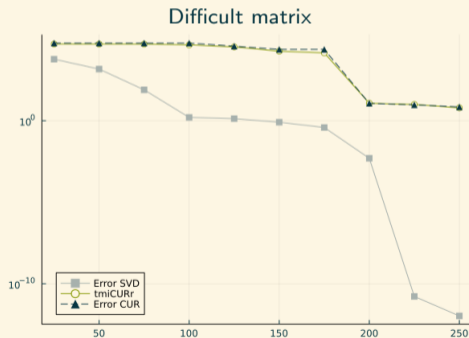


## BLIND ERROR ESTIMATE FOR CUR



1. Select extra columns
2. Compute the error "on the extra column"

$$\| \begin{matrix} \text{Teal columns} \\ \text{Red columns} \end{matrix} - \begin{matrix} \text{Blue grid} \\ \text{Yellow grid} \end{matrix} \|_F$$



# THANK YOU!

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## ERROR ESTIMATIONS FOR RANDOMIZED LOW-RANK APPROXIMATIONS

LORENZO LAZZARINO

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- [1] Matrix perturbation analysis of methods for extracting singular values from approximate singular subspaces, L.L., H. Al Daas, Y. Nakatsukasa, 2024, SIMAX
- [2] Reducing acquisition time and radiation damage: data-driven subsampling for spectro-microscopy, M. Meier, L. L., B. Shustin, H. Al Daas, P. Quinn, 2026, Arxiv
- [3] Efficient error estimators for generalized Nystrom, L. L., K. Pearce, N. Pritchard, 2026, Arxiv
- [4] Blind error estimator for CUR, L. L., K. Pearce, N. Pritchard, Hopefully soon!