ERROR ESTIMATIONS FOR RANDOMIZED LOW-RANK APPROXIMATIONS

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Computational Mathematics Theme - STFC UKRI

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Science and Technology Facilities Council

UNIVERSITY OF OXFORD Mathematical Institute

ERROR ESTIMATIONS FOR RANDOMIZED LOW-RANK APPROXIMATIONS

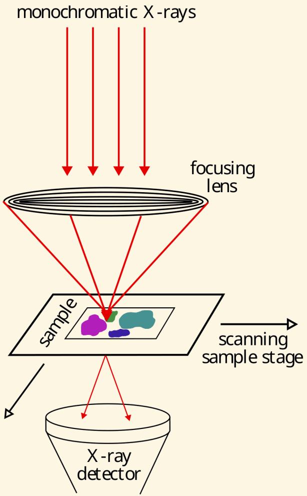
1. (ONE) MOTIVATION: SUBSAMPLING IN SPECTROMICROSCOPY
   with M. Meier (RUG), B. Shustin (STFC), H. Al Daas (STFC), P. Quinn (STFC)

2. A-POSTERIORI ERROR ESTIMATE: GN
   with K. Pearce (UT Austin), N. Pritchard (Oxford)

3. A-POSTERIORI ERROR ESTIMATE: CUR
   with K. Pearce (UT Austin), N. Pritchard (Oxford)

(ONE) MOTIVATION: SUBSAMPLING IN SPECTROMICROSCOPY

SPECTROMICROSCOPY INTRO



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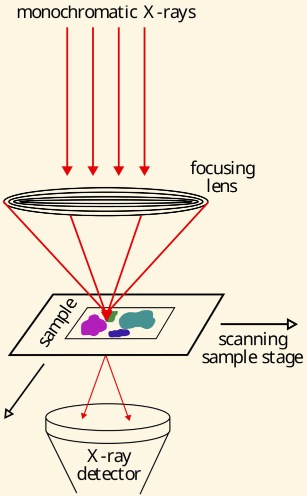

Overall Goal: Determine identity and spacial distributioin of unknown materials contained in the non-homogeneous sample

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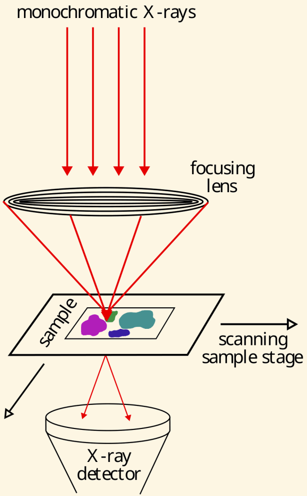

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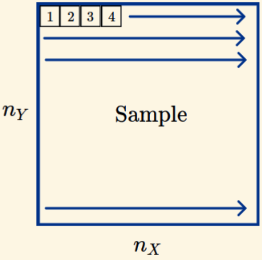

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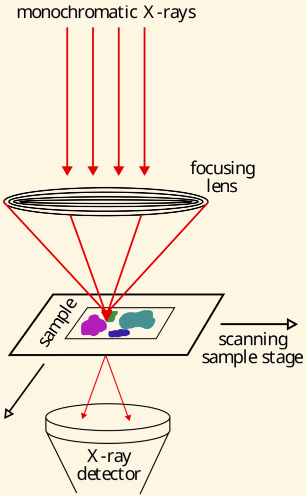

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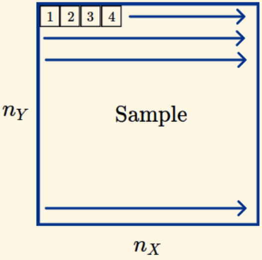

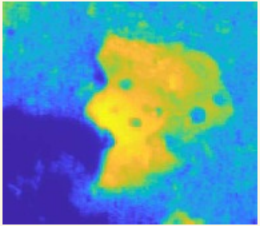

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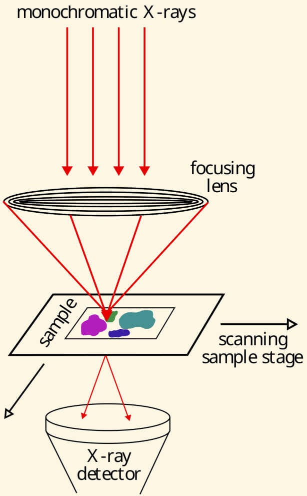

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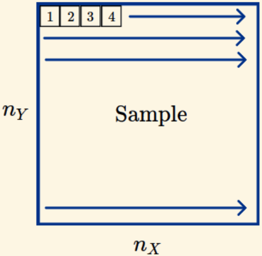
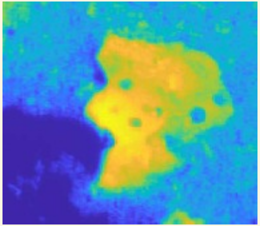
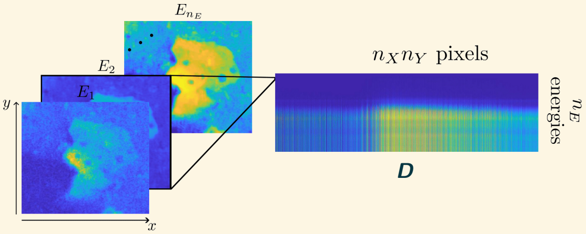
1. (Sub)sampling strategy
2. Analysis





SUBSAMPLING



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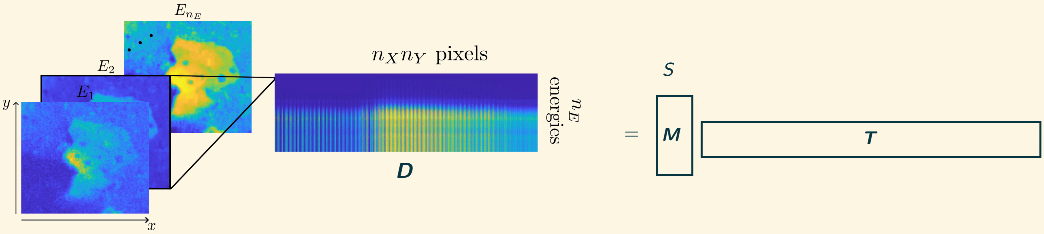

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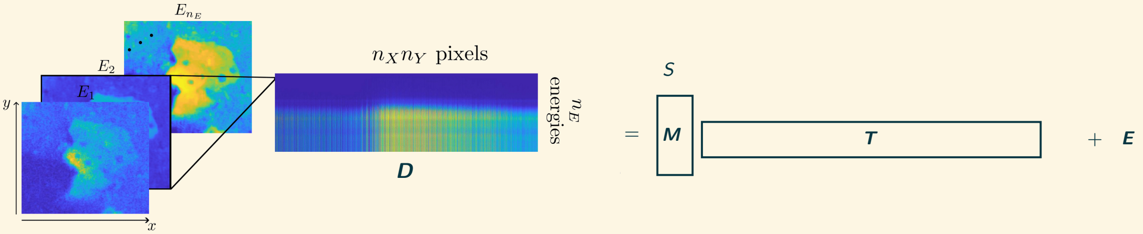

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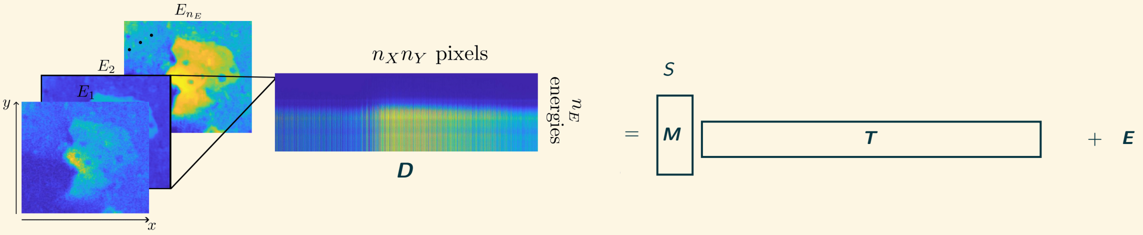
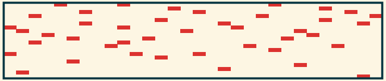


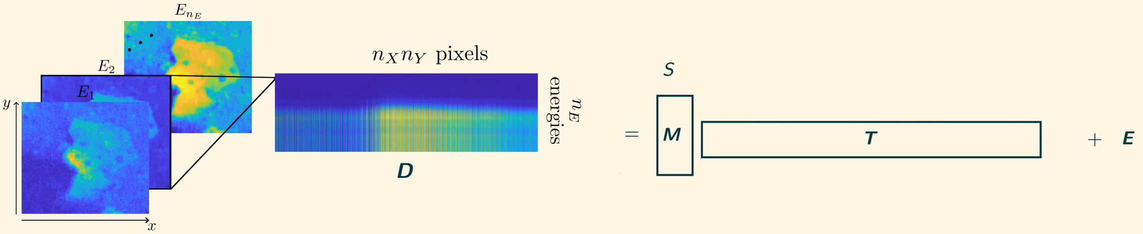
Now

- Uniform Raster sampling



- LoopedASD (Townsend et al, 2022)

SUBSAMPLING



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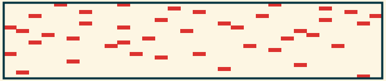


- LoopedASD (Townsend et al, 2022)

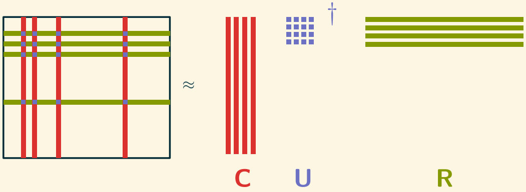
→ Importance Sampling

Leverage scores

$$\ell_i(\boldsymbol{D})^2 := \|\boldsymbol{U}_{\text{dominant}}(i,:)\|_2^2$$

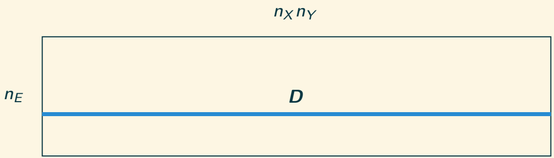
In principle, $\ell(\boldsymbol{D}) \approx \ell(\boldsymbol{M})$

CUR OVERVIEW



- Near optimal low-rank approximation
- "Motivation" of importance distributions (theoretical guarantees)
- Natural fit for experimental design
- Gives matrix completion (with interpolation of rows)

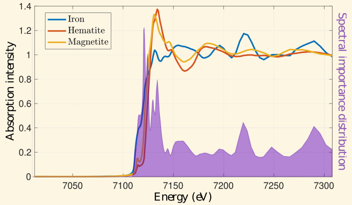
CUR IMPORTANCE SAMPLING FOR SPECTRO-MICROSCOPY (CURISS)



- Determine **spectral** importance distribution and measure accordingly

Data-driven approach: use a small dictionary matrix

$$\ell_i(\boldsymbol{D})^2 \approx \ell_i(\boldsymbol{M}_{\text{dict}})^2$$



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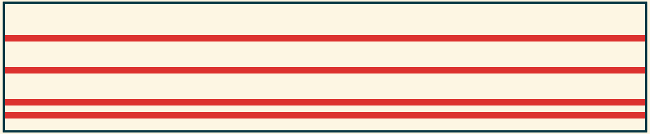
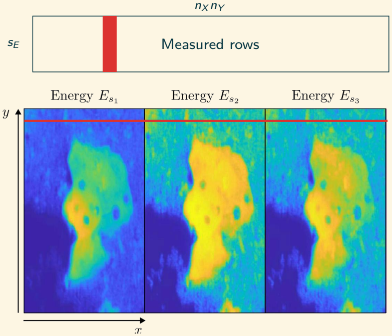


- Determine **spectral** importance distribution and measure accordingly
- Determine **spatial** importance distribution



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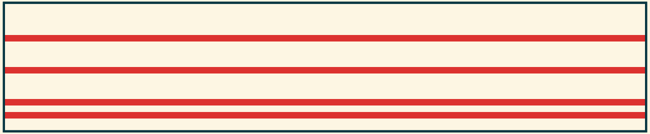

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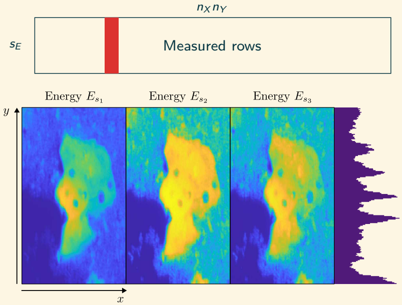

Use ARP (Cortinovis, Kressner, 2024)

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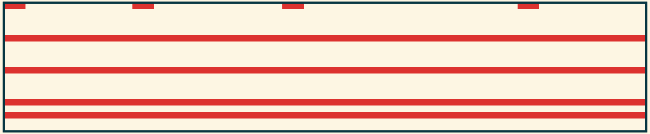

- Determine **spectral** importance distribution and measure accordingly
- Determine **spatial** importance distribution
- Sample spatial rows and measure them at all energies

For the non-measured energies

- Set the beam energy to E.
- Measure the sampled spatial rows

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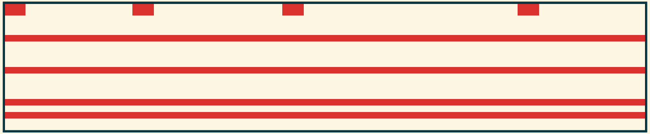

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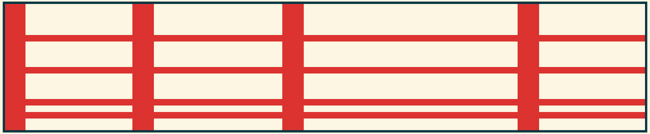

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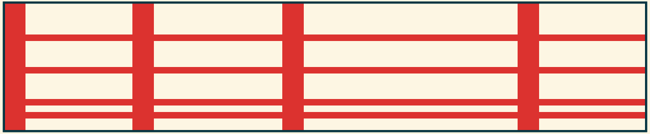
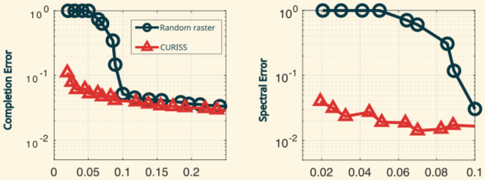


- Determine **spectral** importance distribution and measure accordingly
- Determine **spatial** importance distribution
- Sample spatial rows and measure them at all energies
- Complete the measured dataset using CUR

(Meier, L., Shustin, Al Daas, Quinn, 2026)



ADAPTIVE CURISS (ACURISS)

Goal: Adaptively refine the subsampling, starting from CURISS with initial ratio p_0

Refinement

Stopping Criteria

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Refinement

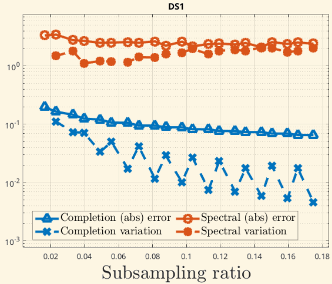
Stopping Criteria

- Completion variation:

$$\|\hat{\boldsymbol{D}}_i - \hat{\boldsymbol{D}}_{i-1}\|_F \leq \eta_{\boldsymbol{D}}$$

- Spectral variation:

$$\|\boldsymbol{M}_{\text{cluster}}(\hat{\boldsymbol{D}}_i) - \boldsymbol{M}_{\text{cluster}}(\hat{\boldsymbol{D}}_{i-1})\|_F \leq \eta_{\boldsymbol{M}}$$



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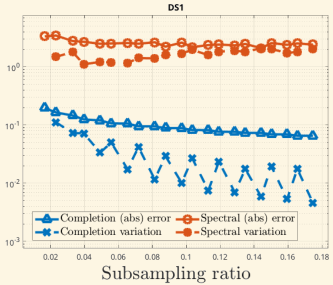
- Problem specific starting point



A-POSTERIORI ERROR ESTIMATE: GN

2

GENERALIZED NYSTRÖM APPROXIMATION

Generalized Nyström

$$A \approx AX(Y^*AX)^\dagger Y^*A =: A_{GN,X,Y}$$

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

1. Choose $X \in \mathbb{R}^{n\times r}$, $Y \in \mathbb{R}^{m\times(r+\ell)}$ 2. Two-side Sketch: AX and Y^*A
3. $[\mathrm{Q},\mathrm{R}] = \mathrm{qr}((Y^*A)X,0)$ 4. $A_{GN,X,Y} = ((AX)R^{-1})(Q^*(Y^*A))$

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3. [Q,R] = qr($(Y^*A)X$,0)
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- $N_{2r+\ell} + \mathcal{O}(r^3 + (m+n)r^2)$
- Single-pass
- 2 multiplications by A

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Accuracy

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

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

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

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

Stability

$$(AX)(Y^*AX)^\dagger_\epsilon Y^*A$$

(Nakatsukasa, 2020)

PROBLEM SETTING AND MAIN IDEA

Generalized Nyström

X, Y random matrix

$$AX(Y^TAX)^\dagger Y^TA$$

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X, Y random matrix

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

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

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

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Sketch the residual

$$G \text{ random}, \quad \|R\| \approx \|RG\|$$

- Good accuracy
- Very small size of G sufficient

- (More) multiplications by R
- G needs to be independent of R

PROBLEM SETTING AND MAIN IDEA

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- ☻ Very small size of G sufficient
- 😐 (More) multiplications by R
- 😐 G needs to be independent of R

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)

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

1.
2.
3.

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1. Remove one column from X
2.
3.

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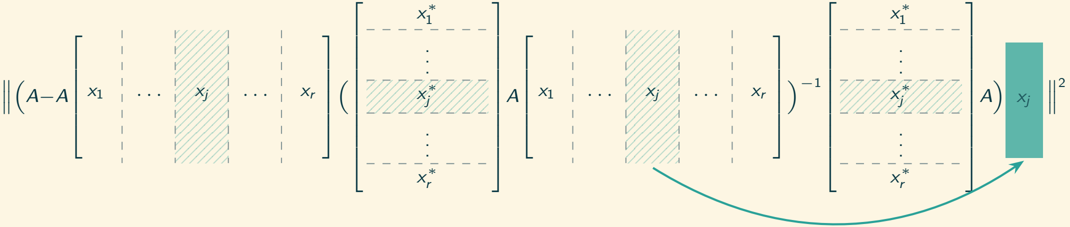

1. Remove one column from X
2. Use it to sketch the error
3.

LEAVE-ONE-OUT FOR SYMMETRIC APPROXIMATIONS

Nyström

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

(Epperly, Tropp, 2024)

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

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

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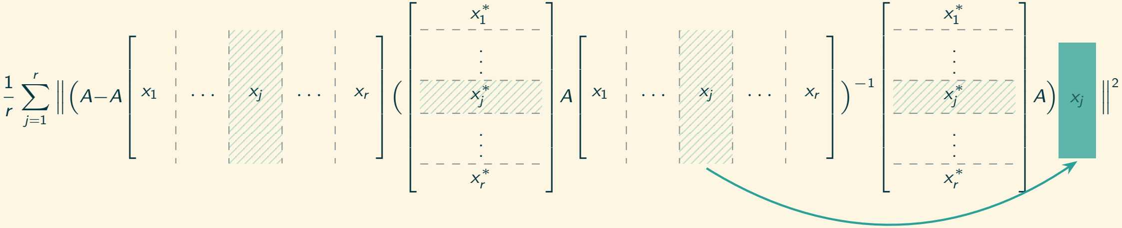

1. Remove one column from X
2. Use it to sketch the error
3. Sum over all possible indices

$$H = X^*AX$$
$$AX = QR$$

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

= Cheap to compute formula!

LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

Generalized Nyström

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

$$AX(Y^TAX)^{\dagger}Y^TA$$

(L., Pearce, Pritchard, 2026)

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$$\left\| A - A \left[\begin{array}{c:c:c:c:c} x_1 & \cdots & x_j & \cdots & x_r \end{array} \right] \left(\left[\begin{array}{c} y_1 \\ \hdashline \vdots \\ \hdashline y_\ell^* \\ \hdashline \vdots \\ \hdashline y_r^* \end{array} \right] A \left[\begin{array}{c:c:c:c:c} x_1 & \cdots & x_j & \cdots & x_r \end{array} \right] \right)^\dagger \left[\begin{array}{c} y_1^* \\ \hdashline \vdots \\ \hdashline y_\ell^* \\ \hdashline \vdots \\ \hdashline y_r^* \end{array} \right] A \right\|^2$$

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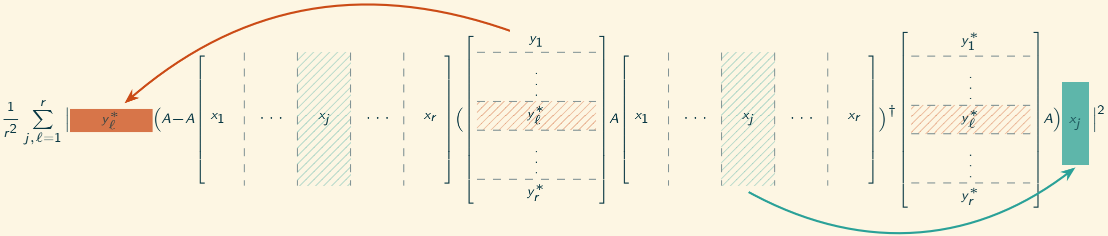

LEAVE-**PAIR**-OUT

LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

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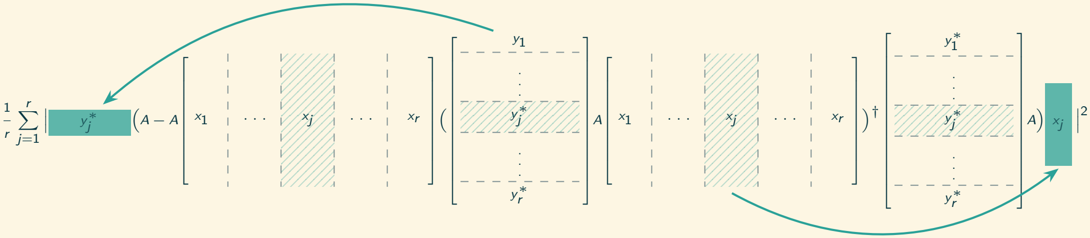
$$AX(Y^TAX)^{\dagger}Y^TA$$

(L., Pearce, Pritchard, 2026)



LEAVE-**TWINS**-OUT

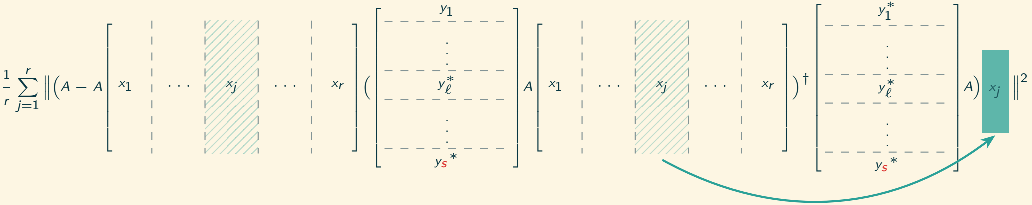
LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM

Generalized Nyström

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

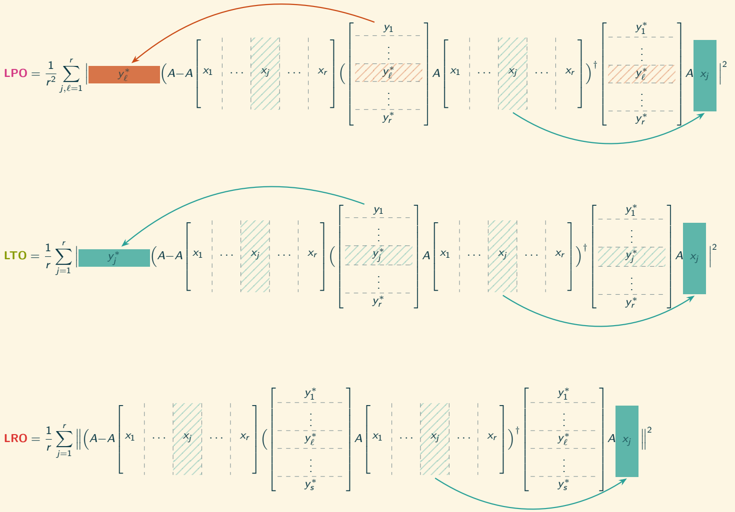
$$AX(Y^TAX)^\dagger Y^TA$$

(L., Pearce, Pritchard, 2026)



LEAVE-**RIGHT**-OUT

LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM › *Cheap to compute formula*



LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM › *Cheap to compute formula*

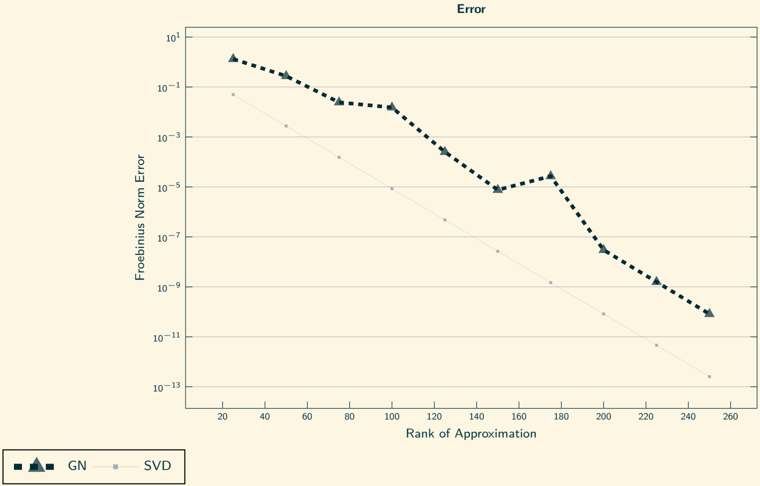
$$\textbf{LPO} = \frac{1}{r^2}\sum_{j,\ell=1}^{r}\left| y_\ell^* \Big(A - A\begin{bmatrix} x_1 & \cdots & x_j & \cdots & x_r \end{bmatrix}\Big(\begin{bmatrix} y_1 \\ \vdots \\ y_\ell^* \\ \vdots \\ y_r^* \end{bmatrix} A \begin{bmatrix} x_1 & \cdots & x_j & \cdots & x_r \end{bmatrix}\Big)^{\dagger} \begin{bmatrix}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

$$H = Y^* AX$$
$$AX = QR$$

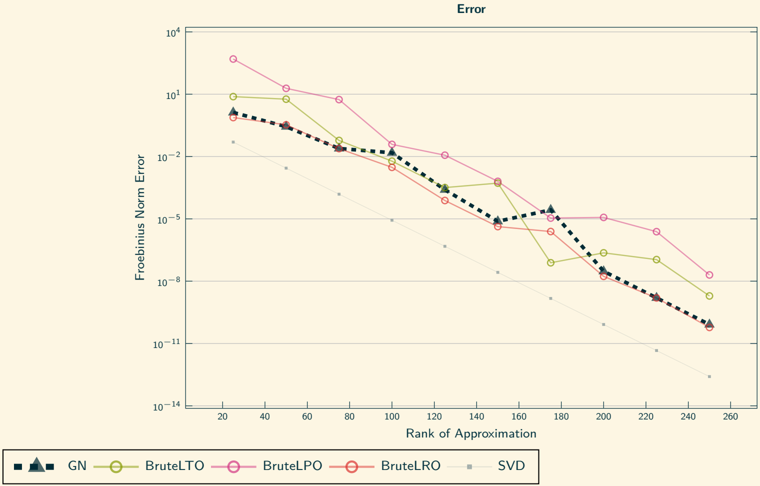
$$\textbf{LTO} = \frac{1}{r}\sum_{j=1}^{r}\left| y_j^* \Big(A - A\begin{bmatrix} x_1 & \cdots & x_j & \cdots & x_r \end{bmatrix}\Big(\begin{bmatrix} y_1 \\ \vdots \\ y_j^* \\ \vdots \\ y_r^* \end{bmatrix} A \begin{bmatrix} x_1 & \cdots & x_j & \cdots & x_r \end{bmatrix}\Big)^{\dagger} \begin{bmatrix}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

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

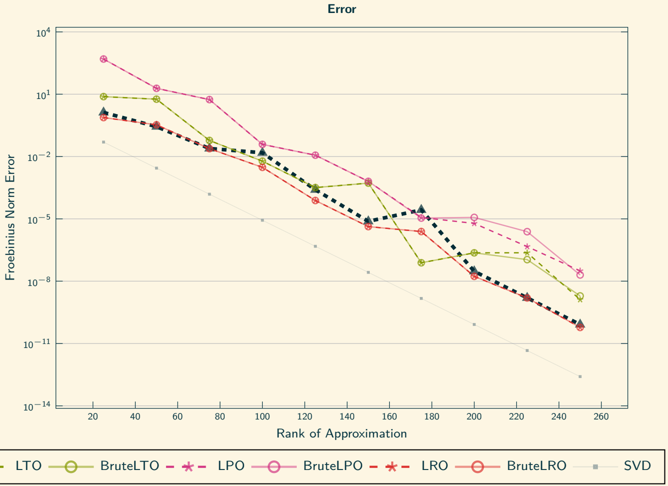
LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM › *Experiments*



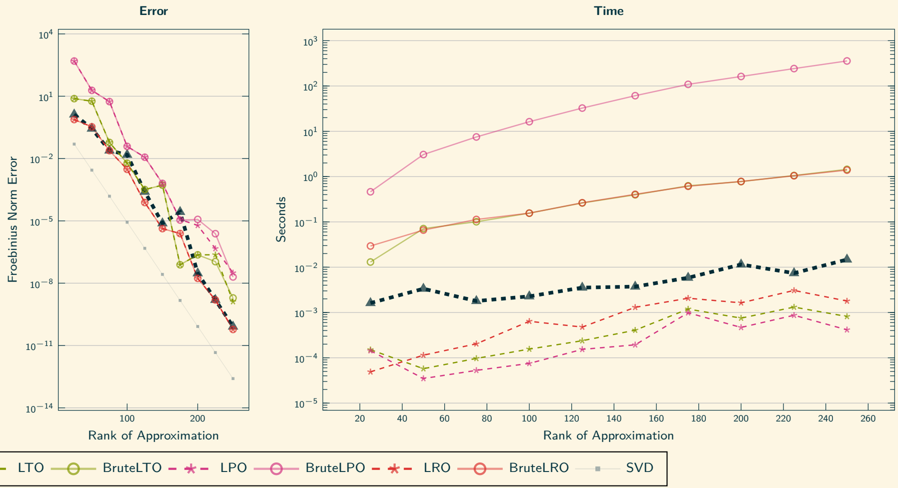
LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM › *Experiments*



LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM › *Experiments*



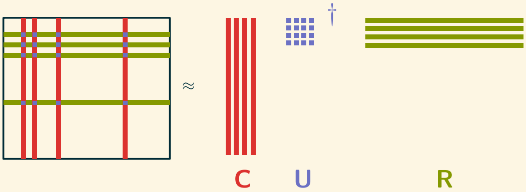
LEAVE-ONE-OUT FOR GENERALIZED NYSTRÖM › *Experiments*



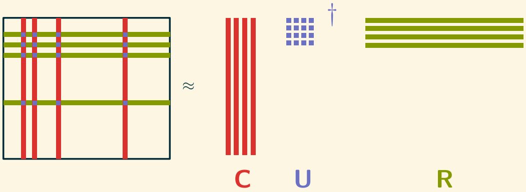
A-POSTERIORI ERROR ESTIMATE: CUR

3

MAIN CHARACTER AND PROBLEM SETTING



MAIN CHARACTER AND PROBLEM SETTING

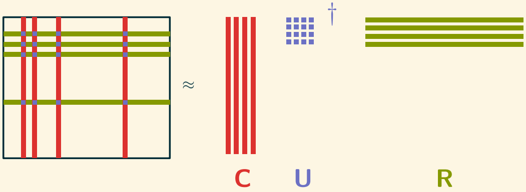


Goal

Estimate the approximation error blindly

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

MAIN CHARACTER AND PROBLEM SETTING



Goal

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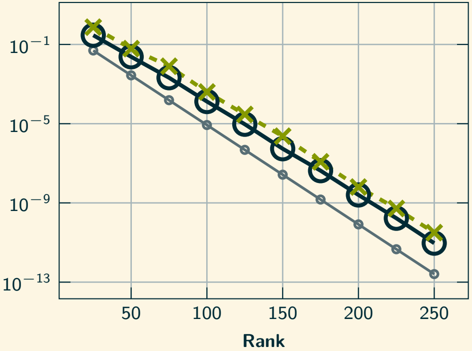
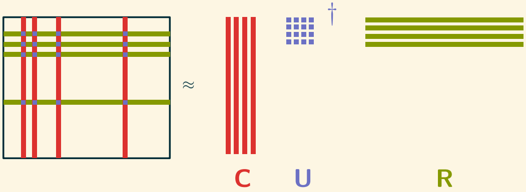
$$\|A - CUR\|_F^2$$



Leave-right-out for CUR

MAIN CHARACTER AND PROBLEM SETTING



Goal

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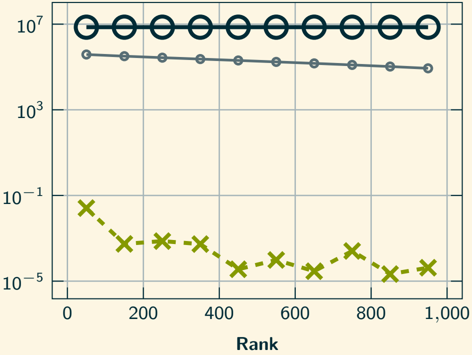
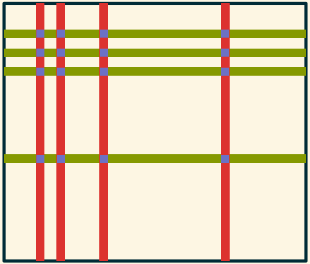


Leave-right-out for CUR

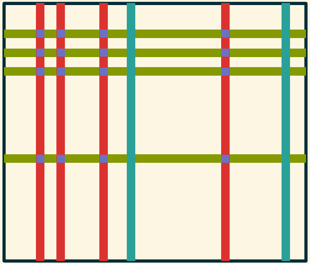
- Biased estimator
- Problem with "lack of randomness"
- Not reliable in general (we'll see it later)

BLIND ERROR ESTIMATE FOR CUR



Proposed estimator

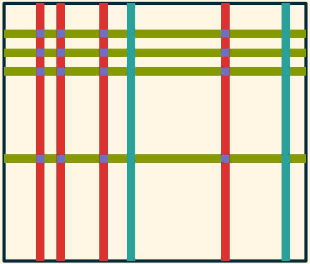
BLIND ERROR ESTIMATE FOR CUR



Proposed estimator

1. Select extra columns

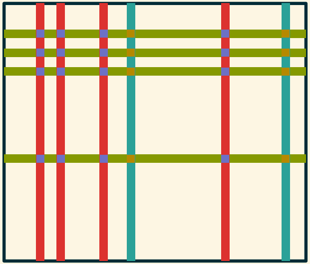
BLIND ERROR ESTIMATE FOR CUR



Proposed estimator

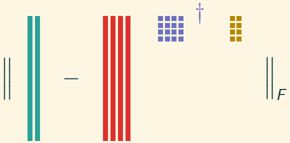
1. Select extra columns
   - Which extra columns?
   - How many extra columns?

BLIND ERROR ESTIMATE FOR CUR

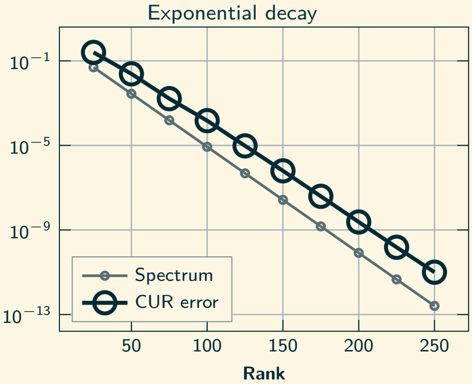


Proposed estimator

1. Select extra columns
   - Which extra columns?
   - How many extra columns?
2. Compute the error "on the extra column"

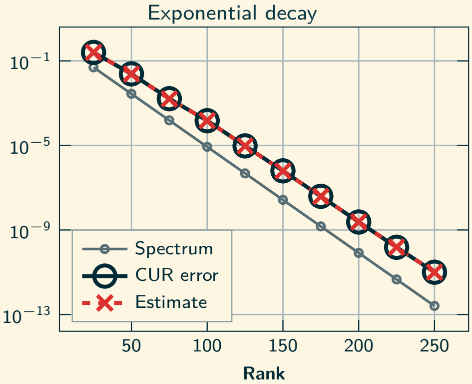


BLIND ERROR ESTIMATE FOR CUR › *Does it work?*



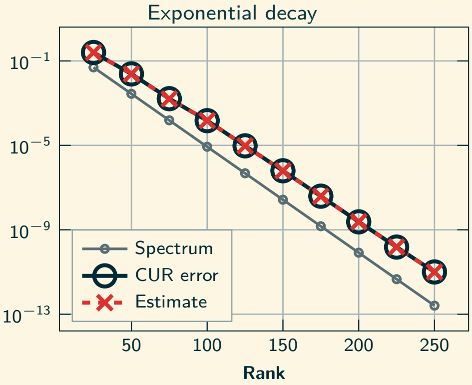
- Haar distributed singular vectors
- CUR via Sketch QR

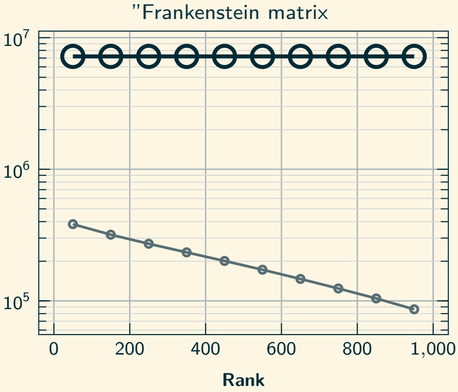
BLIND ERROR ESTIMATE FOR CUR › *Does it work?*



- Haar distributed singular vectors
- CUR via Sketch QR
- 5 uniform sampled extra columns
- 10 trials

BLIND ERROR ESTIMATE FOR CUR › *Does it work?*





- Haar distributed singular vectors
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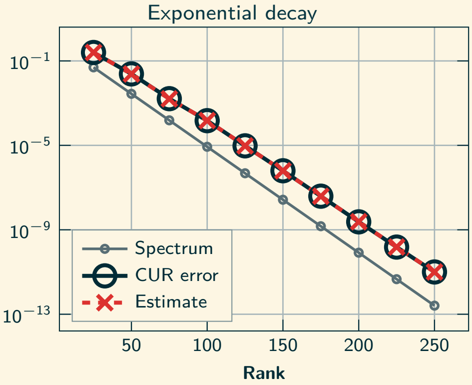
- 10 trials

- $A = \text{blockdiag}\{\text{cauchy}, \text{golub}, \text{randcorr}, \text{hilb}\}$
- CUR with first columns/rows

BLIND ERROR ESTIMATE FOR CUR › *Does it work?*



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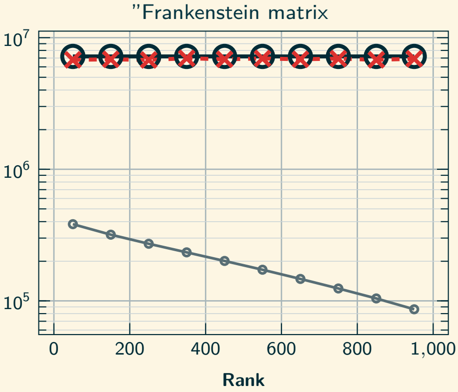
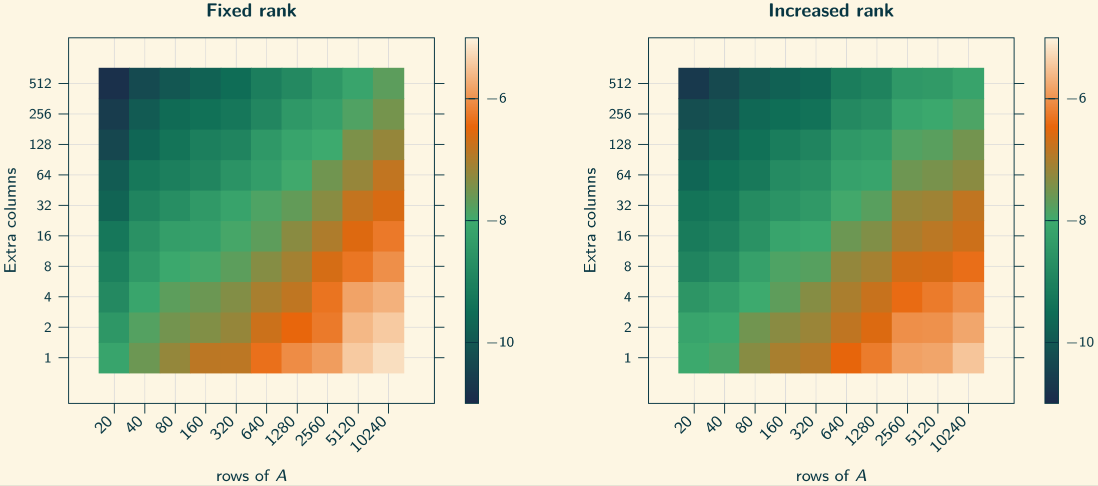


- $A = \text{blockdiag}\{\text{cauchy}, \text{golub}, \text{randcorr}, \text{hilb}\}$
- CUR with first columns/rows
- 5 uniform sampled extra columns
- 10 trials

BLIND ERROR ESTIMATE FOR CUR › *How many extra columns?*

A with algebraically decay singular values, Haar distributed singular vectors;
target rank = 10, exact rank = 15 (fixed or doubled)



BLIND ERROR ESTIMATE FOR CUR › *Quality of estimator*

Theory

- Unbiased estimator
- Let J be the set of indices corresponding to selected columns in the CUR. Let I be a random subset of $\{1, \dots, n\} \setminus I$, and $p_k > 0$ be the probability of $k \in I$. Let S_I be the matrix whose columns are scaled canonical vectors indexed by I, with scaling $\omega_k > 0$ for the column corresponding to the index $k \in I$. Then,

$$\frac{\|(A - CUR)S_I\|_F^2 - \mathbb{E}\left[\|(A - CUR)S_I\|_F^2\right]}{\|(A - CUR)S_I\|_F^2} \sim SE\left(\frac{\max_i \omega_k^2}{2 \min_k p_k \omega_k^2}, 0\right)$$

- Also,

$$\frac{\mathbb{E}[\|A - CUR\|_F^2 - \|(A - CUR)S_I\|_F^2]^2}{\|A - CUR\|_F^4} \leq (\max_k(1 - p_k))^2.$$

BLIND ERROR ESTIMATE FOR CUR › *Quality of estimator*

Practice

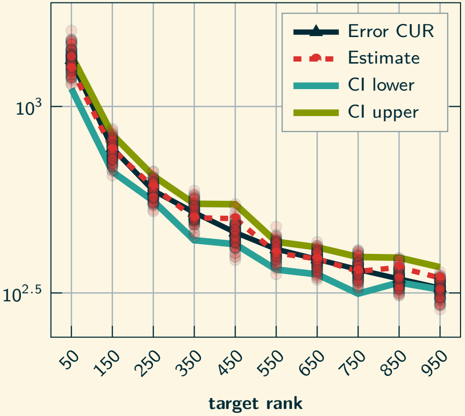
Bootstrap

Provide uncertainty sets for the estimate by:

- Repeatedly resample from observed data to create many simulated datasets
- Compute statistic on each one to build an empirical distribution of it

Experiment: Chan 10000 × 10000 matrix

Bootstrap: Column norm of residual at the extra columns on first trial



BLIND ERROR ESTIMATE FOR CUR › *Quality of estimator*

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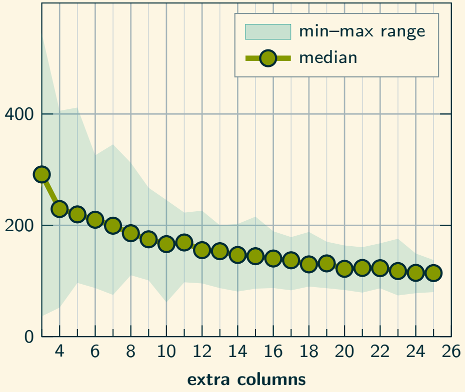
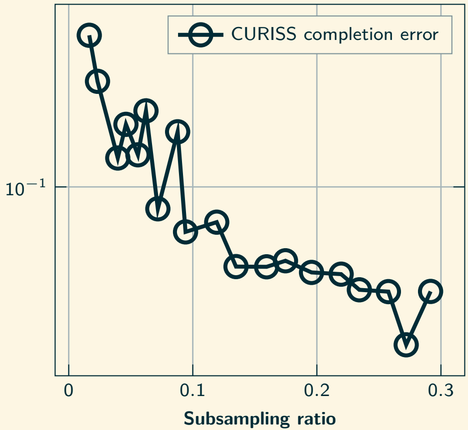
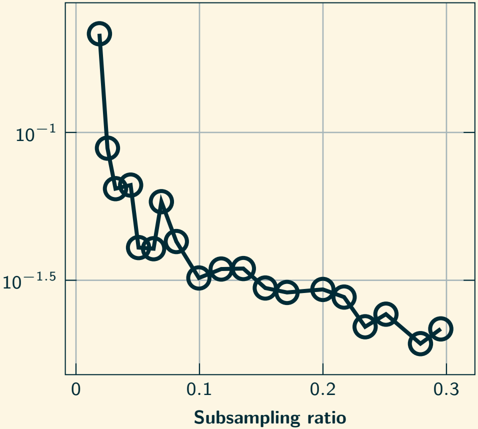


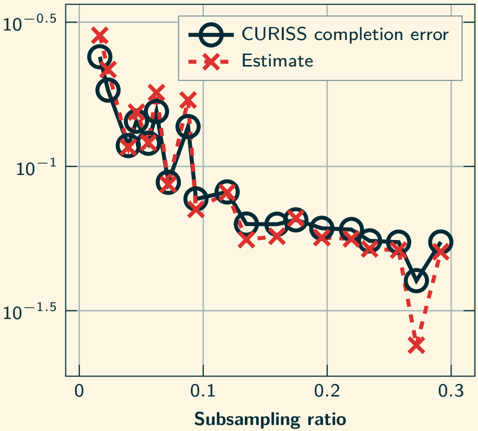
BLIND ERROR ESTIMATE FOR CUR › *Spectromicroscopy*





- Spectromicroscopy datasets
- CUR via CURISS (presented at the start)

BLIND ERROR ESTIMATE FOR CUR › *Spectromicroscopy*



- Spectromicroscopy datasets
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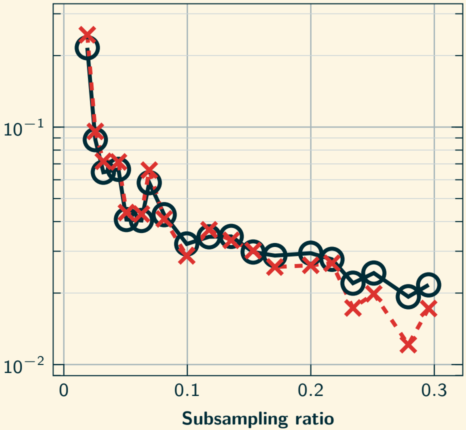

- 2 extra spatial rows
- 100 trials

THANK YOU!

😊

ERROR ESTIMATIONS FOR RANDOMIZED LOW-RANK APPROXIMATIONS

Lorenzo Lazzarino

[1] 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

[2] Efficient error estimators for generalized Nystrom, L. L., K. Pearce, N. Pritchard, 2026, Arxiv

[3] Blind error estimator for CUR, L. L., K. Pearce, N. Pritchard, Hopefully soon!