REDUCING ACQUISITION TIME AND RADIATION DAMAGE: DATA-DRIVEN SUBSAMPLING FOR SPECTROMICROSCOPY

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Mathematical Institute - University of Oxford

Computational Mathematics Theme - STFC UKRI

Internal Seminar, 5th June 2025

University of Oxford
Mathematical Institute

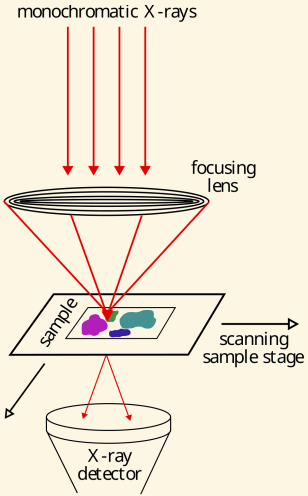
Oxford Mathematics

DATA-DRIVEN SUBSAMPLING FOR SPECTROMICROSCOPY

PROBLEM DESCRIPTION

1

SPECTROMICROSCOPY INTRO



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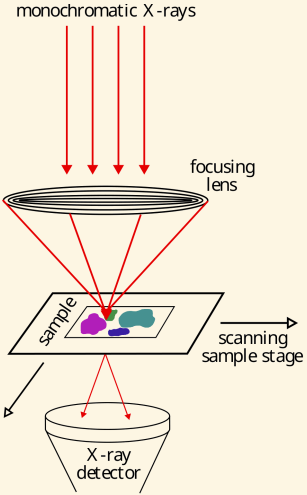

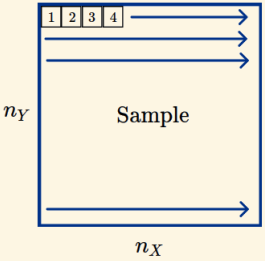

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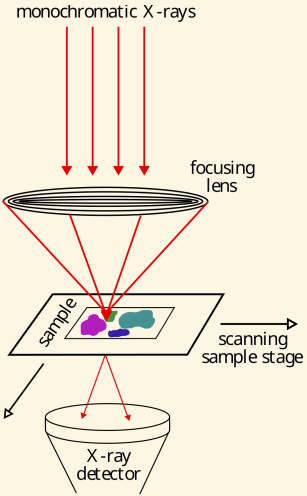
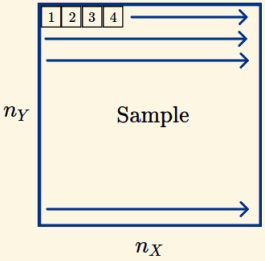


Overall Goal: Determine identity and spacial distributioin of unknown materials contained in the non-homogeneous sample



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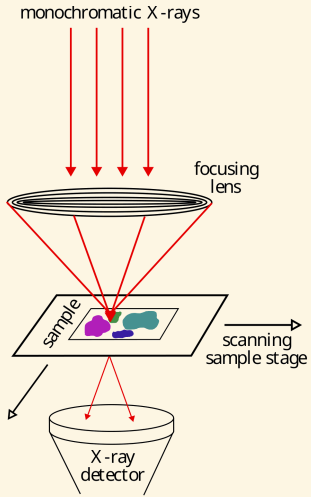

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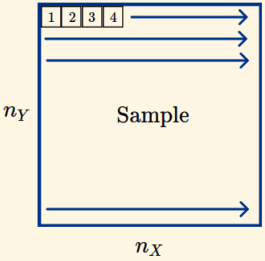
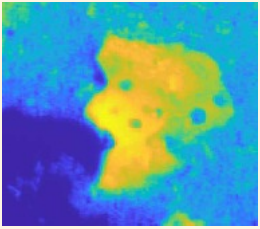
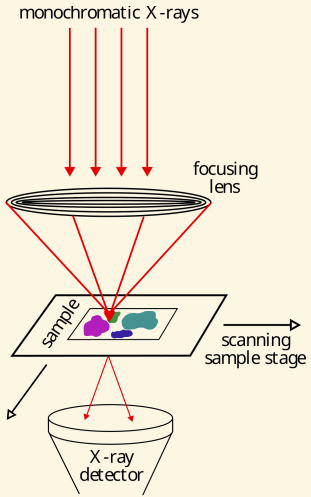




SPECTROMICROSCOPY INTRO *Sub-taks*



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1. (Sub)sampling strategy
2. Analysis

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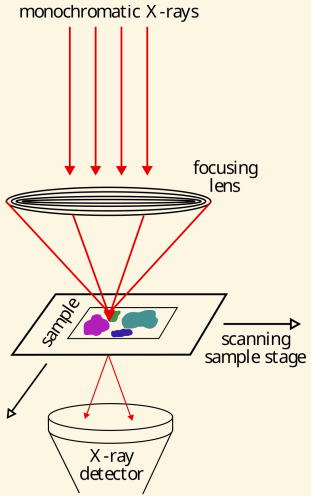

Overall Goal: Determine identity and spacial distribution of unknown materials contained in the non-homogeneous sample

1. (Sub)sampling strategy 2. Analysis

↓

- Measuring the whole dataset takes hours!
- Matrix Completion
- Machinery can't measure a single pixel without measuring its full spatial row/column

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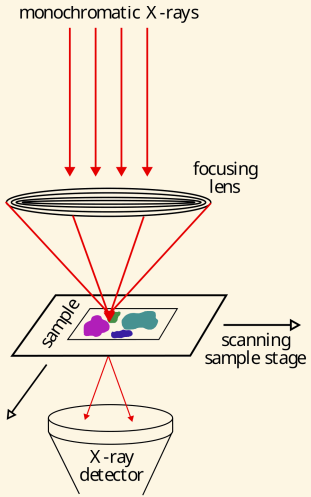

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- Compute SVD of completed matrix → eigenspectra (dominant left singular vectors), eigenimage (dominant right singular vectors)
- Cluster analysis on eigenimages to cluster pixels that have similar eigenspectra
- Average absorption spectra for a cluster found by mean of measured data of the cluster

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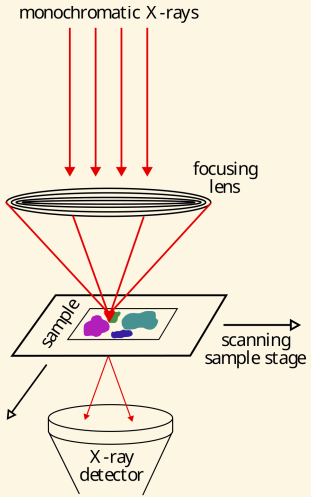

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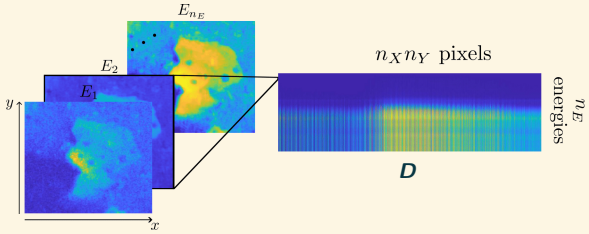

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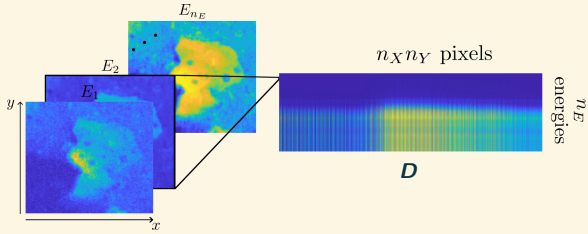
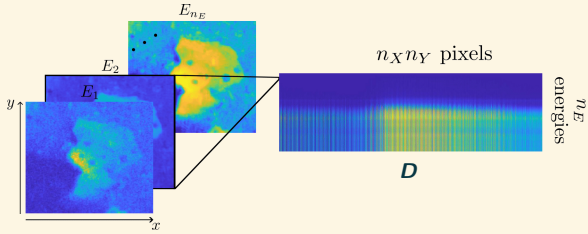


$$= \boxed{M} \quad \boxed{T}$$

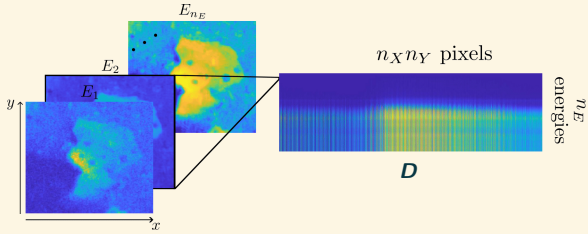
S

SUBSAMPLING



$$S = M \, T + E$$

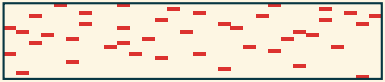
SUBSAMPLING



$$S = M \; T + E$$

Now

- Uniform Raster sampling



- LoopedASD (Townsend et al, 2022)

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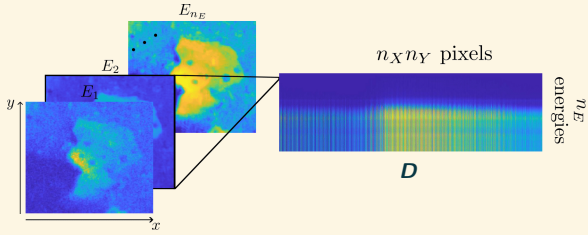

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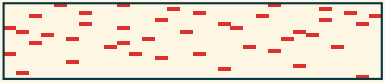

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→ **Importance Sampling**

Leverage scores

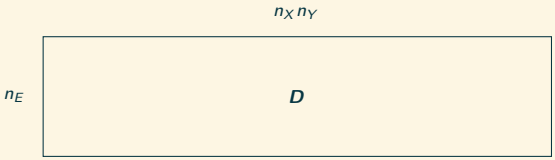
$$\ell_i(\boldsymbol{D})^2 := \|\boldsymbol{U}_{\text{dominant}}(i,:)\|_2^2$$

In principle, $\ell(D) \approx \ell(M)$

FIND IMPORTANCE DISTRIBUTIONS

2

DETERMINING SPECTRAL IMPORTANCE DISTRIBUTION



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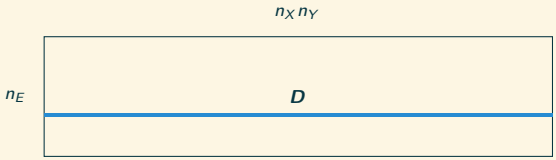

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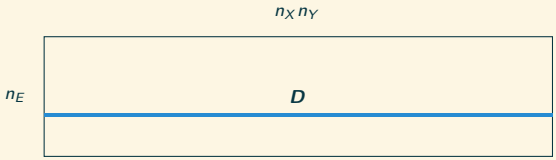

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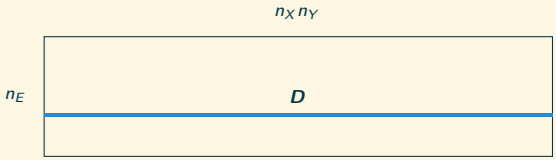

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Our solution: Data-driven approach

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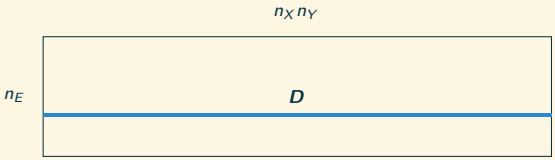

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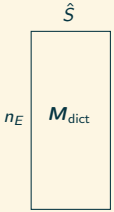

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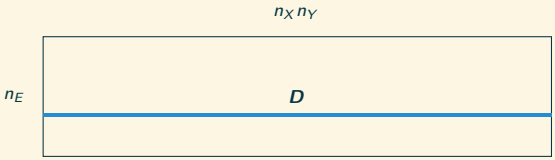

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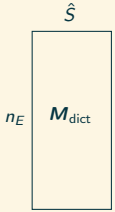

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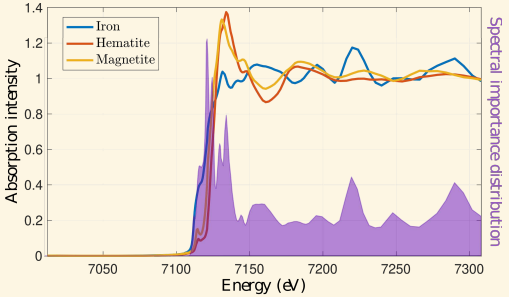

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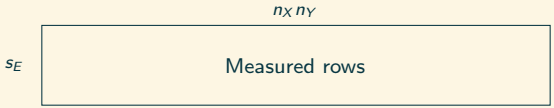

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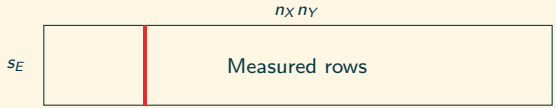

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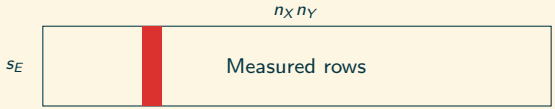

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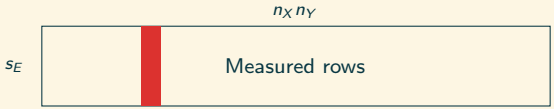

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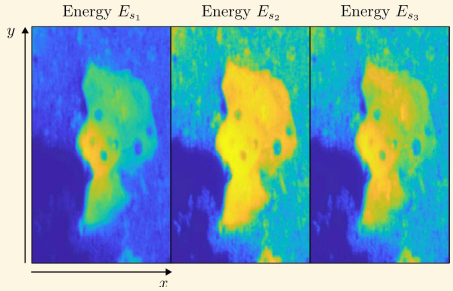

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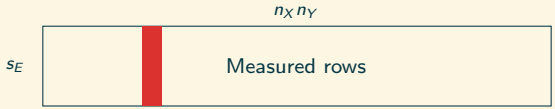

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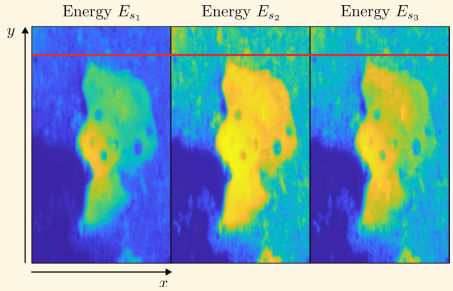

ADAPTIVE RANDOMIZED PIVOTING (ARP)

An algorithm that finds importance distribution by adaptively computing leverage-type scores

(Cortinovis, Kressner, 2024)

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2. Select an index i_1 accordingly
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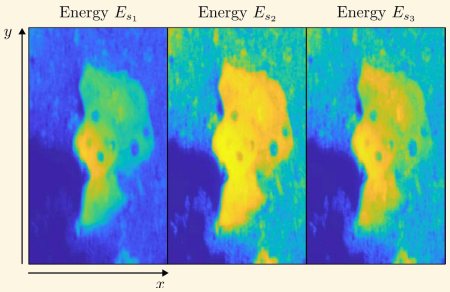

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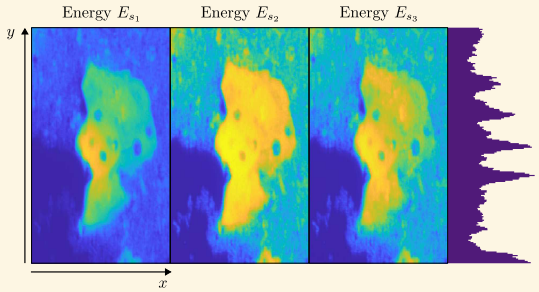

GENERAL SCHEME

Algorithm 1

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2. Sample s_E energies accordingly
3. Change unfolding $\rightarrow \boldsymbol{F}$
4. Use ARP on $\boldsymbol{F}$

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Obtained: Spectral and spatial importance distributions

EXPERIMENT DESIGN

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RASTER IMPORTANCE SAMPLING FOR SPECTRO-MICROSCOPY (RISS)

- Use Algorithm 1 to measure a small number of full energy scans at energies and determine a spatial importance distribution.

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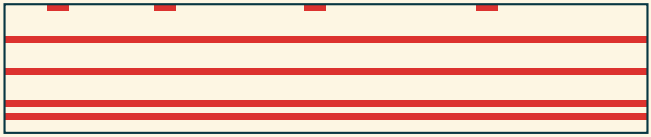

- Use Algorithm 1 to measure a small number of full energy scans at energies and determine a spatial importance distribution.

For the non-measured energies

- Set the beam energy to E.
- Sample s_R spatial rows from the spatial importance distribution
- Measure the sampled spatial rows

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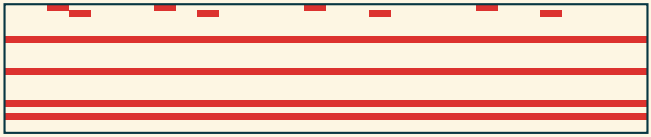

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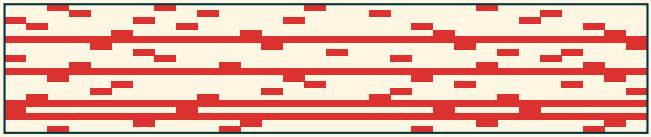

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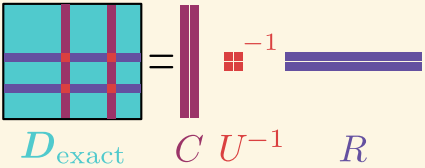
- Complete the measured dataset using loopedASD

CUR OVERVIEW



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

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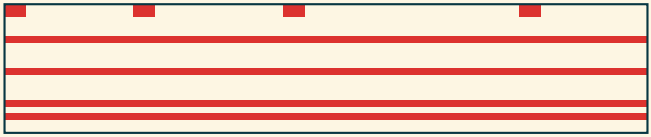

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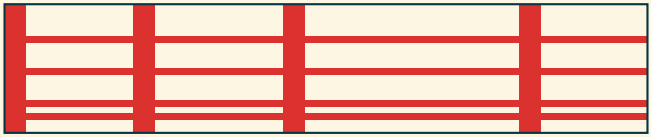
CUR IMPORTANCE SAMPLING FOR SPECTRO-MICROSCOPY (CURISS)



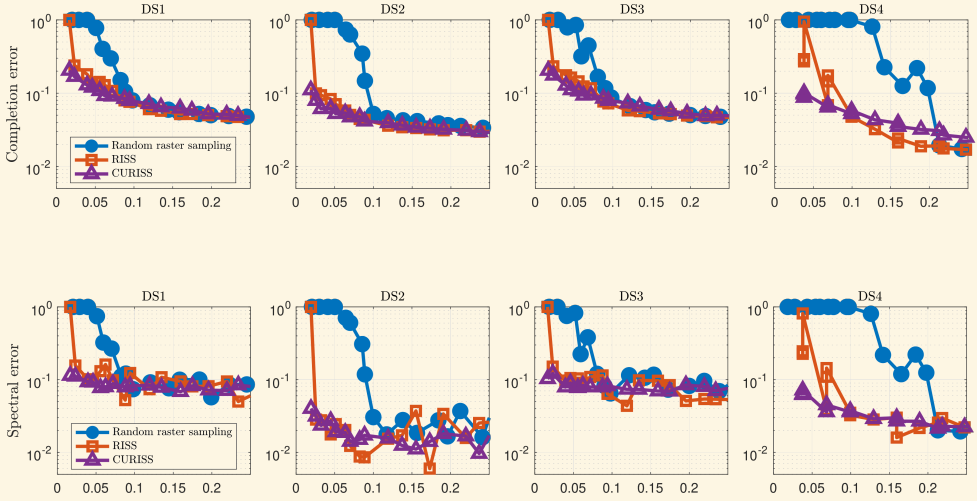
- Use Algorithm 1 to measure a small number of full energy scans at energies and determine a spatial importance distribution.
- Sample s_R spatial rows from the spatial importance distribution

For the non-measured energies

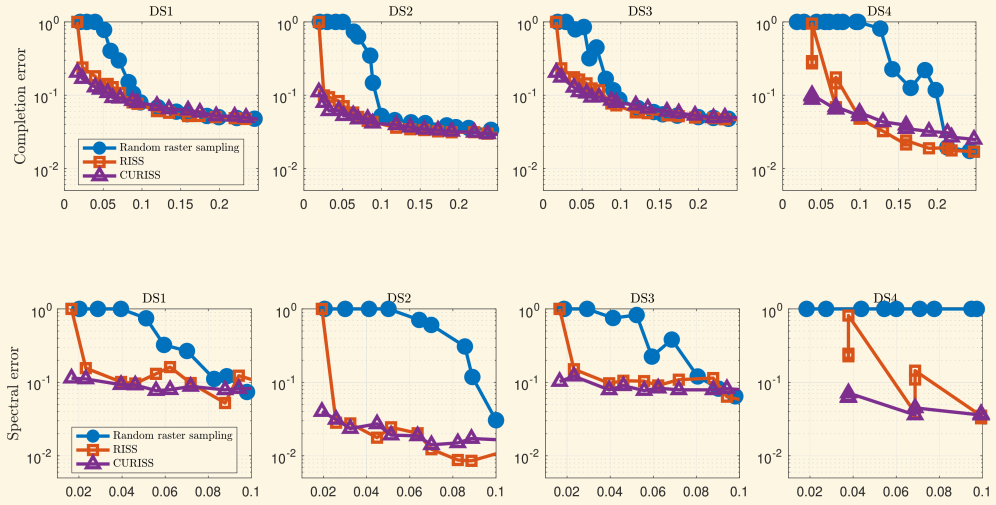
- Set the beam energy to E.
- Measure the sampled spatial rows

- Complete the measured dataset using CUR

RESULTS


DS1
DS2
DS3
DS4
Completion error
Spectral error
Random raster sampling
RISS
CURISS
10^0
10^{-1}
10^{-2}
0
0.05
0.1
0.15
0.2

RESULTS


DS1
DS2
DS3
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RESULTS

What if $\boldsymbol{M}_{\text{dict}}$ is not available? $\rightarrow$ Uniform sampling for energy scans

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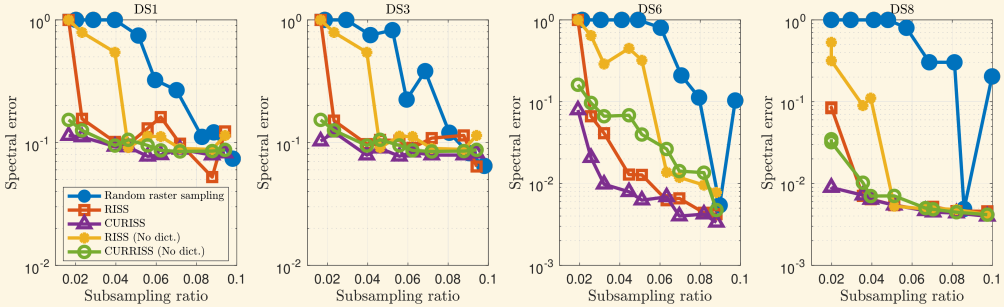
What if $\boldsymbol{M}_{\text{dict}}$ is not available? → Uniform sampling for energy scans



ADAPTIVE STRATEGY

4

ADAPTIVE CURISS (ACURISS)

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

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Refinment

- How to update the importance distributions?

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

Refinment

- How to update the importance distributions?

Stopping Criteria

- How can we evaluate the accuracy of the refined CUR and understand when to stop?

ACURISS *Refinment*

1. Initial CUR by CURISS with p_0
2. Alternate addition of a full energy scan (row of $\boldsymbol{D}$) and a spatial row scan (block of columns of $\boldsymbol{D}$)

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New energy scan

- Leverage scores of $\boldsymbol{M}_{\text{dict}}$ already computed
- Set to zero for already measured energies

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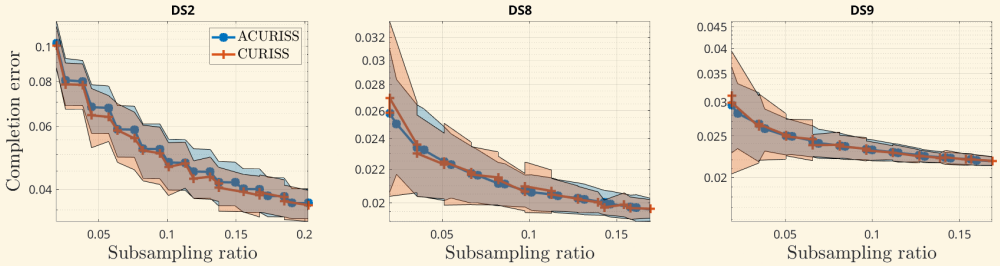
New energy scan

- Leverage scores of $\boldsymbol{M}_{\text{dict}}$ already computed
- Set to zero for already measured energies

New spatial row scan

- Create new $\boldsymbol{F}$
- Do ARP knowing already selected indices

ACURISS VS CURISS



ACURISS *Stopping Criteria*

Goal: Obtain an indicator of the accuracy BUT **Problem:** The full matrix $\boldsymbol{D}$ is not available!!

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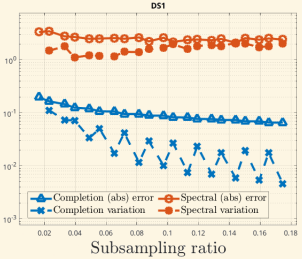
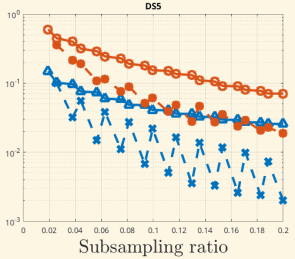
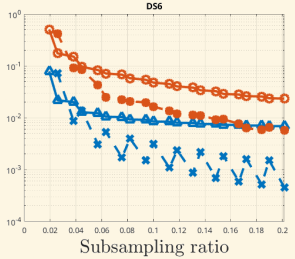
Spectral variation: At each refinement, compute spectral analysis, compare with previous step

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

ACURISS *Stopping Criteria*







THANK YOU!

REDUCING ACQUISITION TIME AND RADIATION DAMAGE: DATA-DRIVEN SUBSAMPLING FOR SPECTROMICROSCOPY

Maike Meier, Lorenzo Lazzarino, Boris Shustin, Hussam Al-Daas, and Paul Quinn