Chapter 4

# Column and Column-Row Decompositions

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# Column Decompositions

Boutsidis et al. 2010; Strauch 2014

# Motivation

- SVD is often hard to interpret and yields dense factorizations
  - NMF tries to address these problems with varying success
- But if original data is sparse & easy to interpret, why not use it in the decompositions?

# The CX decomposition

- In the **CX decomposition** we are given a matrix $\boldsymbol{A}$ and a rank $k$, and we need to select $k$ **columns** of $\boldsymbol{A}$ into matrix $\boldsymbol{C}$ and build matrix $\boldsymbol{X}$ s.t. we minimize $\|\boldsymbol{A} - \boldsymbol{C}\boldsymbol{X}\|_\xi$
  - $\xi$ is either $F$ or 2
  - A.k.a. **column subset selection problem** (CSSP)

# Why CX?

- The columns of ***C*** preserve the original interpretation of columns of ***A***
  - Even complex constraints are satisfied if the original data satisfied them
- Feature selection
  - Selects the columns that can be used to explain the rest
  - Compare to the dimensionality reduction

# Alternative target function

- Building $\boldsymbol{C}$ is the hard part of CX decompositions
- Given $\boldsymbol{A}$ and $\boldsymbol{C}$, $\boldsymbol{X}$ can be computed with the pseudo-inverse
  - $\boldsymbol{X} = \boldsymbol{C}^{+}\boldsymbol{A}$
  - Alternative target function for CX: minimize $\|\boldsymbol{A} - \boldsymbol{C}\boldsymbol{C}^{+}\boldsymbol{A}\|_{\xi} = \|\boldsymbol{A} - \boldsymbol{P}_{\boldsymbol{C}}\boldsymbol{A}\|_{\xi}$

# How to select C?

- Exhaustive: try all $\binom{m}{k}$ subsets of columns
  - Not very scalable
- Try to select the columns in a clever way
  - But how?
- Sample columns w.r.t. carefully selected probabilities
  - Avoids deterministic worst-case scenarios

# Related idea: RRQR

- The **rank-revealing QR** (RRQR) factorization of matrix $\boldsymbol{A}$ is

$k$-by-$k$ upper-triangular w/ positive diagonal

$k$-by-$(m–k)$

$n$-by-$n$ orthogonal

$$\boldsymbol{A\Pi} = \boldsymbol{QR} = \boldsymbol{Q}\begin{pmatrix} \boldsymbol{R}_{11} & \boldsymbol{R}_{12} \\ 0 & \boldsymbol{R}_{22} \end{pmatrix}$$

$(n–k)$-by-$(m–k)$

Permutation matrix

that satisfies

$n$-by-$m$

$k$th singular value of $\boldsymbol{A}$

$$\frac{\sigma_k(\boldsymbol{A})}{p_1(k,m)} \leq \sigma_{\min}(\boldsymbol{R}_{11}) \leq \sigma_k(\boldsymbol{A})$$

$$\sigma_{k+1}(\boldsymbol{A}) \leq \sigma_{\max}(\boldsymbol{R}_{22}) \leq p_2(k,m)\sigma_{k+1}(\boldsymbol{A})$$

Some polynomial on $k$ and $m$

# CX and RRQR

- Let $\boldsymbol{A\Pi} = \boldsymbol{QR}$ and let $\boldsymbol{\Pi}_k$ be the first $k$ columns of $\boldsymbol{\Pi}$ and $\boldsymbol{C} = \boldsymbol{A\Pi}_k$ some $k$ columns of $\boldsymbol{A}$
  - Now $||\boldsymbol{A} - \boldsymbol{P_C A}||_\xi = ||\boldsymbol{R}_{22}||_\xi$, $\xi = F$ or 2
  - In particular $||\boldsymbol{A} - \boldsymbol{P_C A}||_2 \leq p_2(k, m)||\boldsymbol{A} - \boldsymbol{A}_k||_2$
    - $\boldsymbol{A}_k = \boldsymbol{U}_k\boldsymbol{\Sigma}_k\boldsymbol{V}_k^T$ (truncated SVD)
    - $\boldsymbol{CX}$ is $p_2(k, m)$-approximation to SVD

# Computing CX by sampling

- Let $\boldsymbol{A} = \boldsymbol{U\Sigma V}^T$ be the input and its SVD and $\boldsymbol{V}_k$ the truncated $\boldsymbol{V}$
- Sample columns of $\boldsymbol{A}$ with replacement
  - Probability $p_j$ for selecting column $j$ is
  $$p_j = \|(\boldsymbol{V}_k^T)_j\|_2^2/k$$
  - Sample $O(k^2 \log(1/\delta)/\epsilon^2)$ columns and repeat $\log(1/\delta)$ times returning the least-error sample

# Notes on sampling

- We can prove that

$$||\boldsymbol{A} - \boldsymbol{P_C}\boldsymbol{A}||_F \leq (1 + \epsilon)||\boldsymbol{A} - \boldsymbol{A}_k||_F$$

with probability at least $1 - \delta$

  - Notice that $\boldsymbol{C}$ has much more than $k$ columns
    - $O(k^2 \log(1/\delta)/\epsilon^2)$ with large hidden constants

# Why does sampling work?

- Intuitively, if $\boldsymbol{A}$ is of low rank ($k \ll n$), $\boldsymbol{A}$ should have many almost-similar columns
- If we sample many columns enough, we should get a representative for each set of similar columns

  ⇒ We need to sample more columns than the rank

  - Or our error depends on the rank…

# CX with exact $k$

- Construct larger-than-$k$ CX decomposition as above for $c$ = O($k$ log $k$) columns (and using rank-$k$ truncated SVD)
  - Let $\boldsymbol{\Pi}_1$ be the $m$-by-$c$ matrix that selects $c$ columns s.t. $\boldsymbol{C} = \boldsymbol{A}\boldsymbol{\Pi}_1$
  - Let $\boldsymbol{D}_1$ be $c$-by-$c$ diagonal s.t. if $j$th column is selected on round $i$, $(\boldsymbol{D}_1)_{ii} = (cp_j)^{-1/2}$

From $\boldsymbol{A} = \boldsymbol{U\Sigma V}^T$

- Run RRQR algorithm for $\boldsymbol{V}_k^T\boldsymbol{\Pi}_1\boldsymbol{D}_1$ to select exactly $k$ columns of $\boldsymbol{V}_k^T\boldsymbol{\Pi}_1\boldsymbol{D}_1$ with matrix $\boldsymbol{\Pi}_2$ ($c$-by-$k$)
  - return $\boldsymbol{C} = \boldsymbol{A}\boldsymbol{\Pi}_1\boldsymbol{\Pi}_2$

# Notes on the exact-$k$ CX

- $\Pr[||\boldsymbol{A} - \boldsymbol{P_C A}||_F \leq \Theta(k \log^{1/2} k)||\boldsymbol{A} - \boldsymbol{A}_k||_F] \geq 0.8$
- The sampling phase still requires really many columns (high hidden constants)
  - But in practice something like $c = 5k$ works
- Any RRQR algorithm can be used for the second step
  - But the analysis depends on the chosen algorithm

# Non-Negative CX

Strauch 2014

# Motivation

- If data is non-negative, so is $\boldsymbol{C}$
  - But $\boldsymbol{X}$ can contain negative values in standard CX
  - Non-negative $\boldsymbol{X}$ yields “parts-of-whole” interpretation similar to NMF
    - Selected columns are “pure” while others are mixtures of the pure columns
  - Non-negativity also improves sparsity

# The non-negative CX decomposition

- In the **non-negative CX decomposition** (NNCX) we are given a non-negative matrix $\boldsymbol{A}$ and a rank $k$, and we need to select $k$ **columns** of $\boldsymbol{A}$ into matrix $\boldsymbol{C}$ and build a non-negative matrix $\boldsymbol{X}$ s.t. we minimize $\|\boldsymbol{A} - \boldsymbol{C}\boldsymbol{X}\|_F$

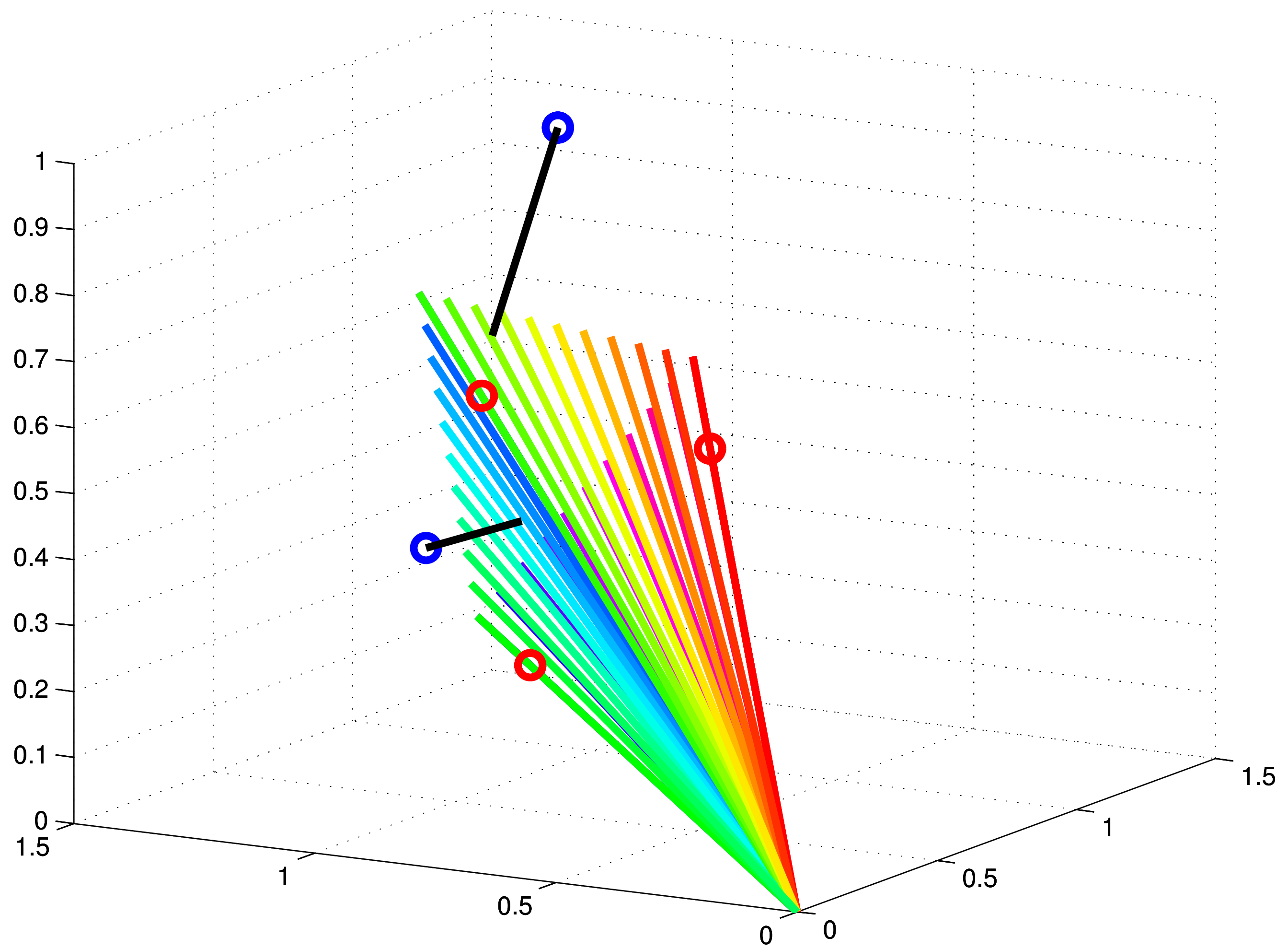
# Geometry of NNCX

Columns in ***C***

Columns not in ***C***

Convex cone

Projections



# Cones and columns

- Consider the cone spanned by columns of $\boldsymbol{A}$, cone($\boldsymbol{A}$)
  - If removing column $j$ of $\boldsymbol{A}$ changes the cone, that column is **extremal**
    - Otherwise it is **internal**
  - Selecting all extremal columns to $\boldsymbol{C}$ gives us $\boldsymbol{A} = \boldsymbol{CX}$ with nonnegative $\boldsymbol{X}$

# Algorithm for NNCX

- When we cannot select all extremal columns, we must choose which of them to select
  - Our goal is to maximize the volume of the convex cone
  - Finding the extremal columns is not easy
  - Given the columns, we must compute the non-negative projection

# The convex_cone algorithm

- Set $\boldsymbol{R} \leftarrow \boldsymbol{A}$
- **repeat**
  - Select column $\boldsymbol{c}$ with highest norm in the residual $\boldsymbol{R}$
    - Normalize $\boldsymbol{c}$ to unit norm
  - Solve nonnegative $\boldsymbol{x}$ that minimizes $||\boldsymbol{R} - \boldsymbol{c}\boldsymbol{x}^T||$
  - Set $\boldsymbol{R} \leftarrow \boldsymbol{R} - \boldsymbol{c}\boldsymbol{x}^T$
- **until** $k$ columns are selected
- Set $\boldsymbol{C}$ to the columns of $\boldsymbol{A}$ corresponding to the selected $\boldsymbol{c}$ and solve nonnegative $\boldsymbol{X}$ minimizing $||\boldsymbol{A} - \boldsymbol{C}\boldsymbol{X}||_F$

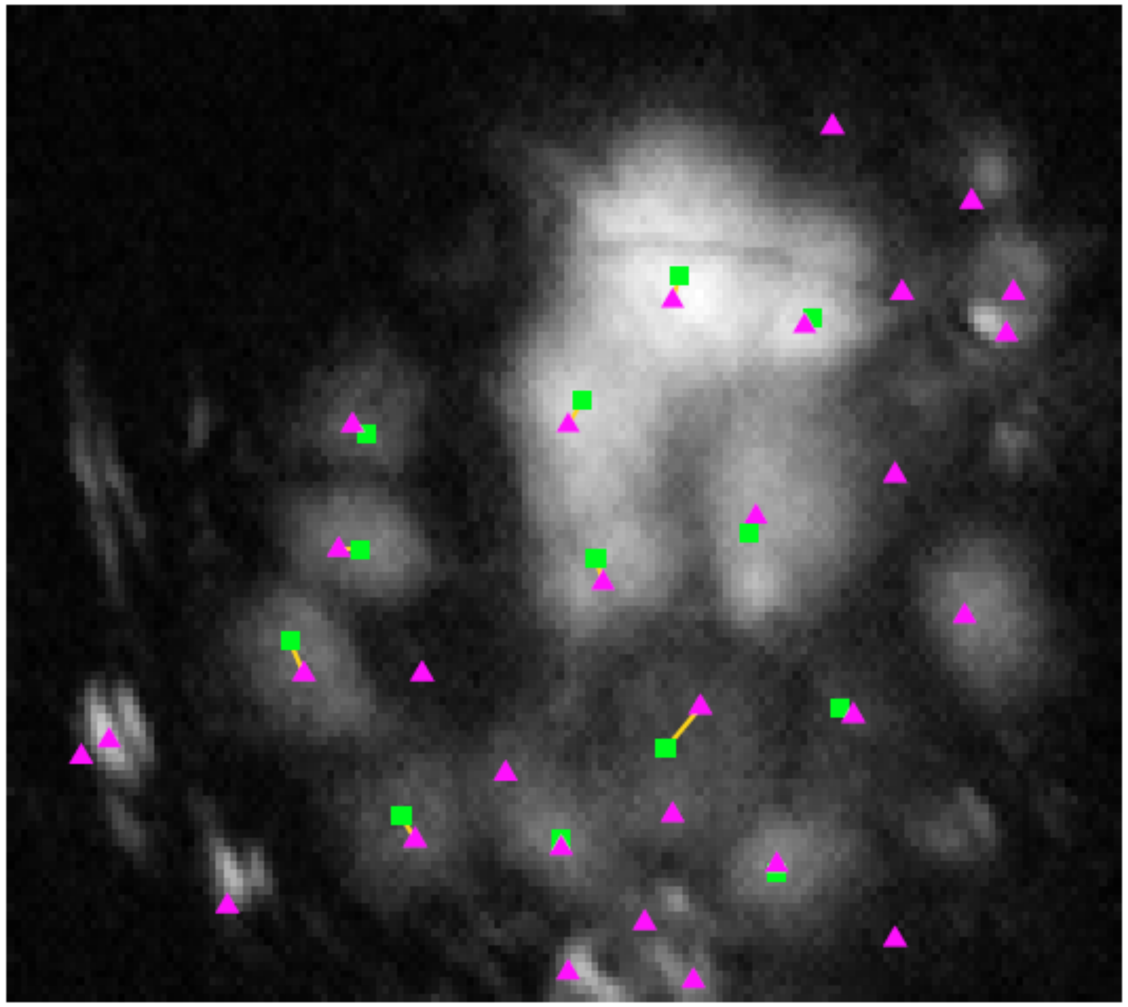
# Solving for non-negative *X*

- Given ***C***, finding non-negative ***X*** is the same as with NMF
  - Convex optimization with linear constraints
  - Or truncated-to-zero pseudo-inverse

# Application: Neuroimaging

- Record brain cell activity over time
  - Every row is one frame
- Assume some columns contain the pure glomerulus signal
  - ***C*** identifies these signals
  - ***X*** explains how the signals are mixed in the brain images

Movie frame with real and found locations marked

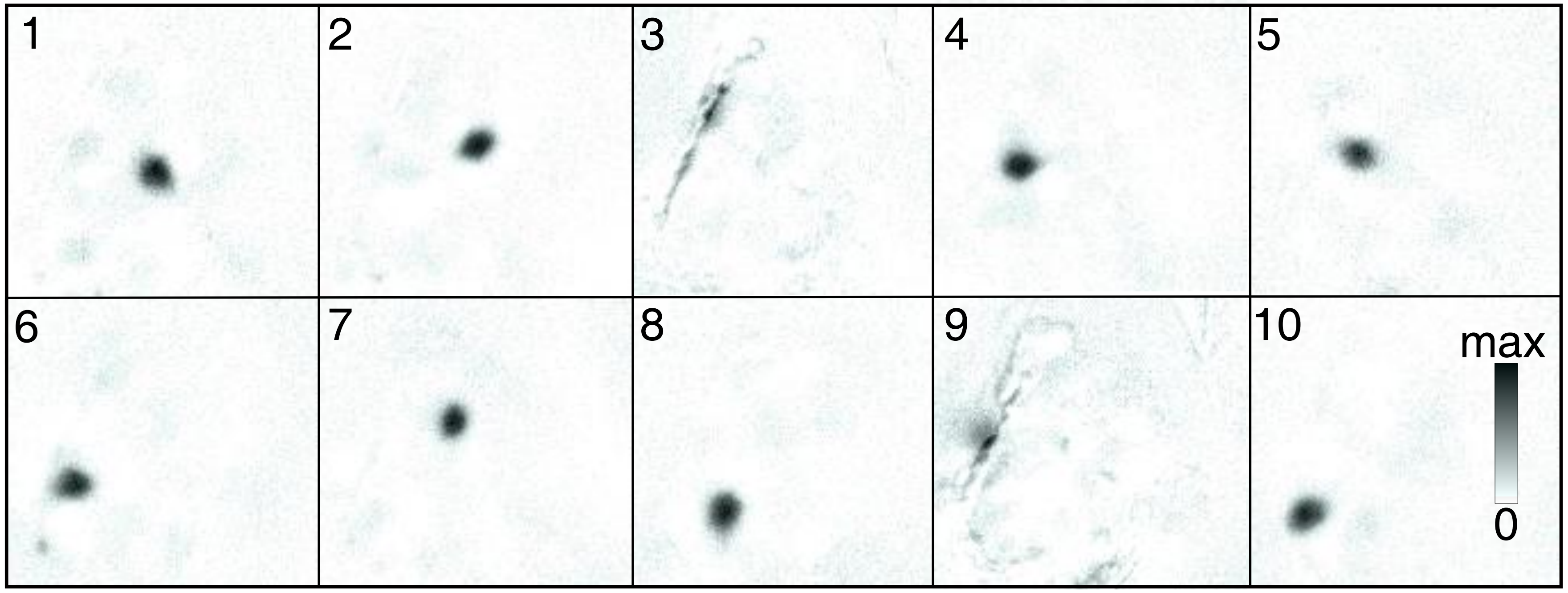


Human expert

Algorithm

Strauch 2014

# Application cont’d




Top-10 rows of X from NNCX decomposition shows the shape and location of glomeruli

# Column-Row Decompositions

Leskovec et al. chapter 11.4; Skillicorn chapter 3.6.2

# The CUR decomposition

- In the **CUR decomposition** we are given matrix $\boldsymbol{A}$ and integers $c$ and $r$, and our task is to select $c$ columns of $\boldsymbol{A}$ to matrix $\boldsymbol{C}$ and $r$ rows to matrix $\boldsymbol{R}$, and build $c$-by-$r$ matrix $\boldsymbol{U}$ minimizing $||\boldsymbol{A} - \boldsymbol{CUR}||_F$
  - Often $c = r = k$

# Why CUR?

- If selecting the actual columns in CX is good, selecting the actual columns and rows must be even better
  - We find prototypical columns *and rows*
  - $\boldsymbol{U}$ is usually small, so if $\boldsymbol{C}$ and $\boldsymbol{R}$ are sparse, storing CUR takes little space

# Solving CUR: general idea

- CUR is two-sided CX
- Simple algorithm idea:
  - Solve CX for $\boldsymbol{A}$ and $\boldsymbol{A}^T$ and solve for $\boldsymbol{U}$ given $\boldsymbol{C}$ and $\boldsymbol{R}$
    - $\boldsymbol{U} = \boldsymbol{C}^+\boldsymbol{A}\boldsymbol{R}^+$
- Better algorithms take into account the columns selected to $\boldsymbol{C}$ when computing $\boldsymbol{R}$

# Simple CUR algorithm

- Sample columns proportional to their $L_2$-norm
- Sample rows proportional to their $L_2$-norm
- Build $\boldsymbol{W} = \boldsymbol{A}[R,C]$ (the sub-matrix of columns in $\boldsymbol{R}$ and rows in $\boldsymbol{C}$)
  - Let $\boldsymbol{W} = \boldsymbol{X\Sigma Y}^T$ be an SVD of $\boldsymbol{W}$, and set $\boldsymbol{U} \leftarrow \boldsymbol{Y}(\boldsymbol{\Sigma}^{+})^2\boldsymbol{X}^T$

# Fancier CUR algorithm

- Find $\boldsymbol{C}$ similar to exact-$k$ CX earlier
  - Sample $O(k/\epsilon)$ additional columns
- Find $\boldsymbol{Z} \in \text{span}(\boldsymbol{C})$, $\boldsymbol{Z}^T\boldsymbol{Z} = \boldsymbol{I}$, such that $||\boldsymbol{A}^T - \boldsymbol{A}^T\boldsymbol{Z}\boldsymbol{Z}^T||_F \leq (1 + O(\epsilon))||\boldsymbol{A} - \boldsymbol{C}\boldsymbol{X}^*||_F$

Optimal X

  - Use $\boldsymbol{Z}$ to get the probabilities for sampling O($k$ log $k$) rows of $\boldsymbol{A}$ and reduce that to O($k$) rows
  - Sample $O(k/\epsilon)$ additional rows
- Set $\boldsymbol{U} = \boldsymbol{X}^*\boldsymbol{Z}^T\boldsymbol{A}\boldsymbol{R}^+$

Boutsidis & Woodruff 2014

# Comments on the Boutsidis & Woodruff algorithm

- Slight variations of the above algorithm achieve:
  - selects the smallest number of rows and columns for $(1+\epsilon)$ approximation
  - matrix $\boldsymbol{U}$ has the smallest possible rank

# CX and CUR summary

- Rows and columns of the original data should be interpretable
  - Also admit local constraints in the data
- CX and CUR decompositions are forms of feature selection
  - Applications when we need “prototypical” rows and columns

# Literature


- Drineas, Mahoney & Muthukrishnan (2006): *Subspace sampling and relative-error matrix approximation: Column-based methods*. In APPROX/RANDOM ’06
- Boutsidis, Mahoney & Drineas (2010): *An improved approximation algorithm for the column subset selection problem*. arXiv:0812.4293v2
- Boutsidis & Woodruff (2014): *Optimal CUR matrix decompositions*. arXiv:1405.7910v2
- Strauch (2014): *Column subset selection with applications to neuroimaging data.* PhD thesis, U. Konstanz