Interpretable Nonnegative Matrix Decompositions

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Outline

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A Motivating Problem

A dialectologist has some dialectal information in a matrix $A = (a_{ij})$

- rows correspond to dialectal features
- columns correspond to areas (e.g., municipalities)
- $a_{ij} = 1$ if feature is present in the dialect spoken in the area.

Dialectologist wants to solve the following two problems:

1. What are the k main characteristic features of dialects?
2. What are the k characteristic areas for dialects?
    - To make more studies on few selected areas.

Some type of matrix decomposition is sought.

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First Idea: NMF

Dialectologist don't want to see negative values in the decomposition.

- "Dialect spoken in area A contains 1.2 of feature X and -0.2 of feature Y" vs. "Dialect spoken in area A contains 0.7 of feature Z and 0.3 of feature V."
  - Negative values can yield negative features
- She considers **Nonnegative Matrix Factorization**.
  - A is represented as $A \approx WH$ where W and H are nonnegative and their inner dimension is k.

But the columns of W and rows of H are just some nonnegative vectors

$\Rightarrow$ They don't give the Dialectologist her characteristic areas and features.

Second Idea: CX and CUR Decompositions

Dialectologist could use **Column (CX)** and **Column-Row (CUR) decompositions**.

CX
: Matrix A is represented as $A \approx CX$ with C containing k columns of A (while X is arbitrary).

CUR
: Matrix A is represented as $A \approx CUR$ with C as above and R containing r rows of A (while U is arbitrary).

Columns of C and rows of R now give the desired characteristic areas and features.
But now X and U can have negative values.

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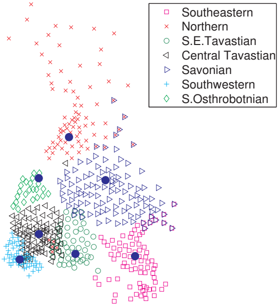
Solution: Nonnegative CX and CUR Decompositions

Dialectologist's solution is to force also X and U be nonnegative.
Thus

- Characteristic areas are given by columns of C.
- Characteristic features are given by rows of R (or, by columns of C when CX decomposition is done to A^T).
- Other features and areas are represented using only nonnegative linear combinations.



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The Nonnegative CX Decomposition

Problem (Nonnegative CX Decomposition, NNCX)

Given a matrix $A \in \mathbb{R}_+^{m \times n}$ *and an integer* k, *find an* $m \times k$ *matrix* C *of* k *columns of* A *and a matrix* $X \in \mathbb{R}_+^{k \times n}$ *minimizing*

$$\|A - CX\|_F.$$

Example:

$$A = \begin{pmatrix} 0.6 & 0.9 & 0.6 & 0.4 & 0.7 \\ 1.0 & 0.7 & 0.9 & 1.0 & 0.9 \\ 0.6 & 0.5 & 0.2 & 0.4 & 1.0 \end{pmatrix}$$

$$C = \begin{pmatrix} 0.6 & 0.9 & 0.6 \\ 1.0 & 0.7 & 0.9 \\ 0.6 & 0.5 & 0.2 \end{pmatrix} X = \begin{pmatrix} 1.0 & 0.0 & 0.0 & 0.9 & 1.7 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.5 \\ 0.0 & 0.0 & 1.0 & 0.5 & 0.0 \end{pmatrix}$$

The Nonnegative CUR Decomposition

Problem (Nonnegative CUR Decomposition, NNCUR)

Given a matrix $A \in \mathbb{R}_+^{m \times n}$ *and integers* k *and* r, *find an* $m \times k$ *matrix* C *of* k *columns of* A, *an* $r \times n$ *matrix* R *of* r *rows of* A, *and a matrix* $U \in \mathbb{R}_+^{k \times r}$ *minimizing* $\|A - CUR\|_F$.

Example:

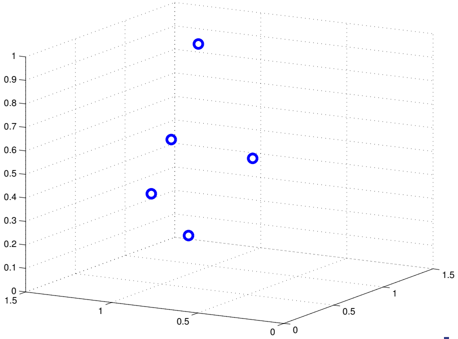
$$A = \begin{pmatrix} 0.6 & 0.9 & 0.6 & 0.4 & 0.7 \\ 1.0 & 0.7 & 0.9 & 1.0 & 0.9 \\ 0.6 & 0.5 & 0.2 & 0.4 & 1.0 \end{pmatrix}$$

$$C = \begin{pmatrix} 0.6 & 0.9 & 0.6 \\ 1.0 & 0.7 & 0.9 \\ 0.6 & 0.5 & 0.2 \end{pmatrix} U = \begin{pmatrix} 0.0 & 1.3 \\ 2.2 & 0.0 \\ 0.0 & 0.7 \end{pmatrix} R = \begin{pmatrix} 0.6 & 0.9 & 0.6 & 0.4 & 0.7 \\ 1.0 & 0.7 & 0.9 & 1.0 & 0.9 \end{pmatrix}$$

NNCX as a Convex Cone

- Columns of A represent points in space.

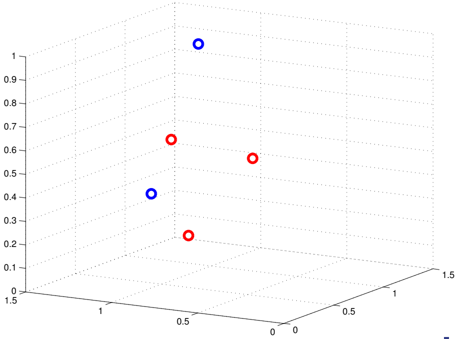
$$\begin{pmatrix} 0.6 & 0.9 & 0.6 & 0.4 & 0.7 \\ 1.0 & 0.7 & 0.9 & 1.0 & 0.9 \\ 0.6 & 0.5 & 0.2 & 0.4 & 1.0 \end{pmatrix}$$



NNCX as a Convex Cone

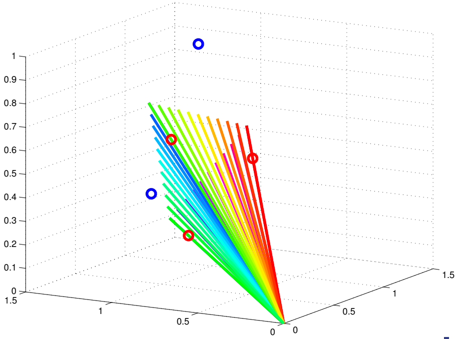
- C selects some of these points.

$$\begin{pmatrix} \color{red}{0.6} & \color{red}{0.9} & \color{red}{0.6} & 0.4 & 0.7 \\ \color{red}{1.0} & \color{red}{0.7} & \color{red}{0.9} & 1.0 & 0.9 \\ \color{red}{0.6} & \color{red}{0.5} & \color{red}{0.2} & 0.4 & 1.0 \end{pmatrix}$$



NNCX as a Convex Cone

- Points in C generate some **convex cone** $\mathcal{C}$.
  - $v \in \mathcal{C}$ if there is $x \in \mathbb{R}^k_+$ s.t. $v = Cx$.

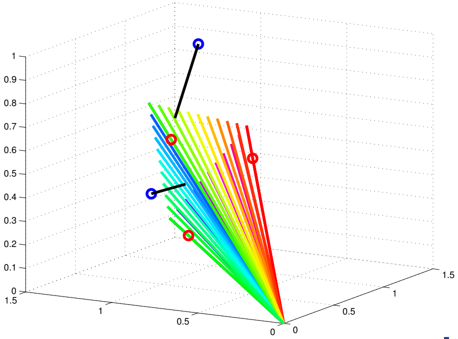


NNCX as a Convex Cone

- $\|A - CX\|_F^2$ equals to the sum of squared shortest distances from A's columns to cone's points.

$$\left\| \begin{pmatrix} 0.6 & 0.9 & 0.6 \\ 1.0 & 0.7 & 0.9 \\ 0.6 & 0.5 & 0.2 \end{pmatrix} \begin{pmatrix} 0.6 \\ 0 \\ 0.3 \end{pmatrix} - \begin{pmatrix} 0.4 \\ 1.0 \\ 0.4 \end{pmatrix} \right\|_2^2$$

$= 0.0369$



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The Two Subproblems of [NN]CX

Finding matrix C (aka Column Subset Selection problem)

Finding matrix X when some matrix C is given

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Finding matrix C (aka Column Subset Selection problem)

- more combinatorial on its nature
- nonnegativity constraint, in general, does not have any effects
- computational complexity is unknown (assumed to be NP-hard)

Finding matrix X when some matrix C is given

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Finding matrix X when some matrix C is given

- constrained (in NNCX) least squares fitting problem
- well-known methods to solve the problem in polynomial time
  - for CX one can use Moore–Penrose pseudo-inverse for $X = C^{\dagger}A$
  - for NNCX the problem is a convex quadratic program (solved using, e.g., quasi-Newtonian methods).

The $\texttt{Local}$ Algorithm for NNCX

Assume we can find X when C is given. $\texttt{Local}$ performs a standard greedy local search to select C.

$\texttt{Local}$

1. initialize C randomly and compute X
2. **while** reconstruction error decreases
    1. select c, a column of C, and a, a column of A not in C such that if c is replaced with a the reconstruction error decreases most
    2. replace c with a
3. compute X and **return** C and X

N.B. We need to solve X in step 2.1.

The ALS Algorithm

The ALS algorithm uses the alternating least squares method often employed in NMF algorithms.

ALS

1. initialize $\tilde{C}$ randomly
2. **while** reconstruction error decreases
   1. find nonnegative X to minimize $\|A - \tilde{C}X\|_F$
   2. find nonnegative $\tilde{C}$ to minimize $\|A - \tilde{C}X\|_F$
3. match columns of $\tilde{C}$ to their nearest columns in A
4. let C be those columns, compute X and **return** C and X

- $\tilde{C}$ does not contain A's columns.
- Matching can be done in polynomial time.

How to Use Columns: Convex Quadratic Programming

Given C, we can find nonnegative X minimizing $\|A - CX\|_F$ in polynomial time

- convex quadratic programming
- quasi-Newton methods (L-BFGS)
- also convex optimization methods are possible

But these methods can take quite some time.

- $\texttt{Local}$ needs to solve X $k(n-k)$ times for a single local swap.
- When final C is selected, they can be used as a post-processing step.

How to Use Columns: Projection Method

We employ a simple **projection method**:

1. let $X = C^{\dagger}A$ (Moore–Penrose pseudo-inverse)
2. for $x_{ij} < 0$ let $x_{ij} = 0$

This method is fast in practice and is often used in NMF algorithms. However, no guarantees on its performance can be given.

In experiments, we used only this method for a fair comparison.

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Algorithms for NNCUR Decomposition

Let Alg be an algorithm for NNCX.
Algorithm for NNCUR:

1. $C = \text{Alg}(A)$
2. $R = \text{Alg}(A^T)$
3. find nonnegative U s.t. $\|A - CUR\|_F$ is minimized

For 3 we can use $U = C^\dagger A R^\dagger$ and use the projection method.
Same method is used also for standard CUR.

Outline

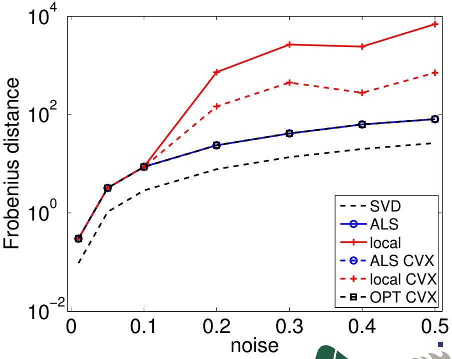
Algorithms Used

- `Local`
- `ALS`
- `844` by Berry, Pulatova, and Stewart (ACM Trans. Math. Softw. 2005)
- `DMM` by Drineas, Mahoney, and Muthukrishnan (ESA, APPROX, and arXiv 2006–07)
  - based on sampling, approximates SVD within $1 + \varepsilon$ w.h.p., but needs lots of columns in C.
- `K-means`, which selects C using k-means
- NMF
  - theoretical lower bound for NNCX and NNCUR
- SVD
  - lower bound for all methods

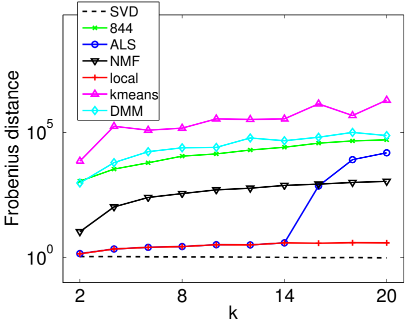
To Find Optimal X or Not

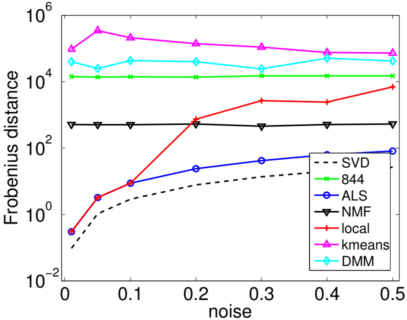
We used convex optimization (CVX) to solve optimal X.

- SVD's distance to optimal CX decomposition (OPT CVX)
- `ALS` is optimal even without CVX (ALS, ALS CVX, and OPT CVX coincide everywhere)
- `Local` benefits somewhat from convex optimization post-processing



Noise and Decomposition Size





Left: `Local` is the best (ex. SVD).

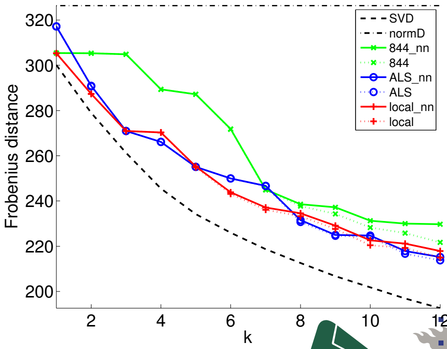
Right: `ALS` is the best (ex. SVD).

CUR and NNCUR Decompositions of the Newsgroup Data

Newsgroup data with CUR and NNCUR decompositions.
`Local` and `ALS` are the two best methods.
Only very small increase in reconstruction error when nonnegativity is required

- ∴ data has latent NNCUR structure.

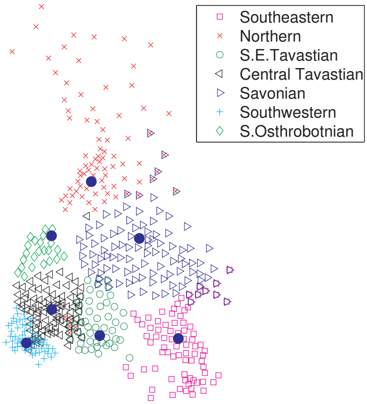
`DMM` is not included due to its bad performance.



The Dialect Data

Dialect data with NNCUR decomposition using ALS.

- Symbols show the spread of the features (rows) selected.
- Solid dots mark the representative municipalities (columns) selected.
- Spread of features coincides well with current understanding of Finland's dialects.



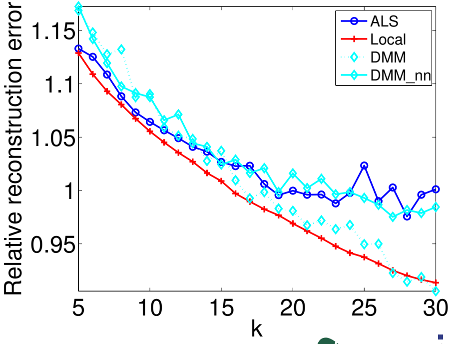
How Many Columns Are Needed to Beat SVD?

Relative error against SVD:

$$\mathrm{error}/\mathrm{SVD}(5)$$

Jester joke dataset, similar experiment done in Drineas et al. (arXiv), [NN]CX decomposition

- $\mathtt{Local}$ is mostly best – better than $\mathtt{DMM}$ without nonnegativity
- It takes $k = 16$ for $\mathtt{Local}$ to be better than SVD with $k = 5$.



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Conclusions

- We studied nonnegative variants of CX and CUR decompositions.
- Several real-world datasets seem to have such structure.
- Very simple algorithms were able to find good decompositions.
  - Our algorithms can be better than general CX and CUR algorithms.
- Better algorithms are sought.
  - Perhaps the convex cone interpretation helps.
- Model-selection issue: how big C and R should be?
- CX and CUR decompositions are still relatively little studied in CS (esp. data mining) community.

Thank You!

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