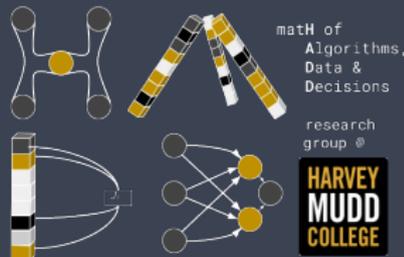


An Interpretable Joint Nonnegative Matrix Factorization-Based Point Cloud Distance Measure

by Jamie Haddock
 (Harvey Mudd College, Department of Mathematics)
on March 23, 2023,
 Conference on Information Sciences and Systems (CISS)

joint with Hannah Friedman, Amani R. Maina-Kilaas, Julianna Schalkwyk, and Hina Ahmed (graduating Harvey Mudd College and Pitzer College seniors)

supported by NSF DMS #2211318



Motivation

» Dataset similarity

... my migraines. Of course I have heart issues too, but the migraines are my main concern right now. My priority is getting

that pain
lightheaded
luck the
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... My doctor was great, realized it was a heart attack really quick. I didn't quite

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... just stress, but my mom had migraines. I told her about what I was feeling and she realized it was exactly what she had.

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... chest pain. I had been feeling lightheaded and nauseous. The pain was definitely there but really I felt more a tightness in my chest than anything. It left me short of breath, which was probably making me lightheaded. The EKG indicated that my heart had several blockages that would need a stent. My cardiologists were able to clear the blockages and I spent one night under watch in the hospital.

After my heart attack, I completely changed my lifestyle. I quit smoking, started an exercise regimen and diet...

... I recently had a minor procedure where I was under anesthesia for it. Whenever I woke up, I had pain in my jaw (which the

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... I woke up with a slightly sore throat, by 12 p.m. I started work at a buddies house.

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... had a lipoma (a bit over an inch around) over my right shoulder blade for years now. Never hurt at all before, until 3 days

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... roughly a year ago I was sitting in the office drinking an energy drink when I started to get this bad tingling sensation in my neck which caused great discomfort. Figuring out the energy drink was causing this I cut it out of my "diet". With that the pain and problems went away. But slowly (over the course of months) one by one different foods and drink have now that same effect mostly being sugars/alcohol/caffeine. The pain I get is very isolated at the left and right occiput. Depending on what I ingest the pain I get might flow down to lower in my neck...

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Understanding the similarities and differences between datasets arises in many contexts: e.g., transfer learning, plagiarism/manipulation detection, and data denoising.

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Patient Surveys

Patients

| | | | | |
|-------------|---|---|---|---|
| heart | 3 | 3 | 0 | 1 |
| weakness | 2 | 0 | 0 | 0 |
| chest | 0 | 2 | 0 | 0 |
| migraine | 0 | 0 | 2 | 3 |
| lightheaded | 0 | 2 | 2 | 1 |
| pain | 3 | 2 | 2 | 4 |

Term-Document Matrix

» Point Cloud Distances

Chamfer's distance:

$$d_{\text{cham}}(X_1, X_2) = \frac{1}{|X_1|} \sum_{\mathbf{x} \in X_1} \min_{\mathbf{y} \in X_2} \|\mathbf{y} - \mathbf{x}\|_2^2 + \frac{1}{|X_2|} \sum_{\mathbf{y} \in X_2} \min_{\mathbf{x} \in X_1} \|\mathbf{x} - \mathbf{y}\|_2^2$$

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- * More robust to outliers.

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- * Utilizes the structure of data.

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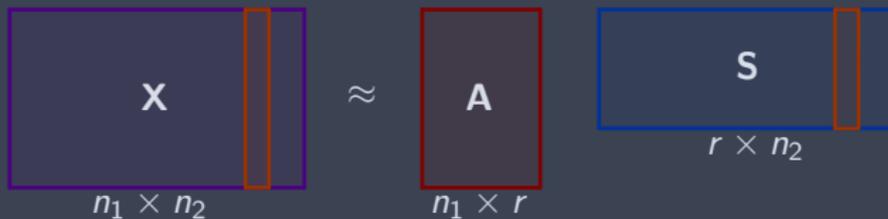
- * More robust to outliers.
- * Utilizes the structure of data.
- * Helps illustrate how the data is similar or dissimilar.

Introduction

» Nonnegative Matrix Factorization (NMF)

Model: Given nonnegative data \mathbf{X} , compute nonnegative \mathbf{A} and \mathbf{S} of lower rank so that

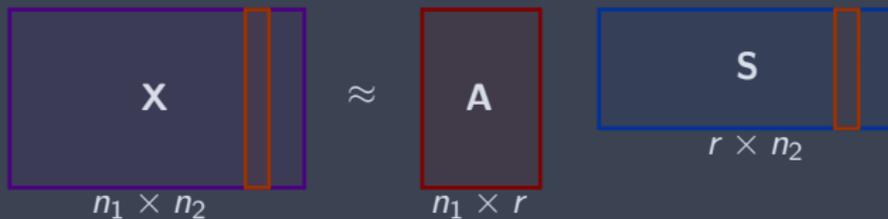
$$\mathbf{X} \approx \mathbf{AS}.$$



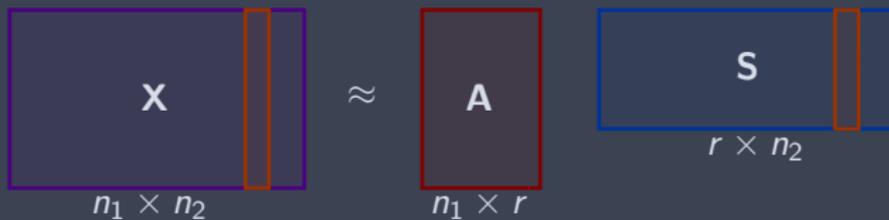
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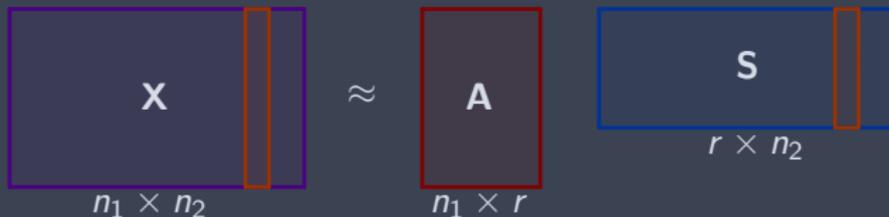


» Nonnegative Matrix Factorization (NMF)



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Motivation

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Introduction

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Our Method and Distance

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Experiments

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Conclusions

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» Nonnegative Matrix Factorization (NMF)



- ▷ Popularized by [Lee & Seung 1999]
- ▷ Employed for dimensionality-reduction and topic modeling
- ▷ Often formulated as

$$\min_{\mathbf{A} \in \mathbb{R}_{\geq 0}^{n_1 \times r}, \mathbf{S} \in \mathbb{R}_{\geq 0}^{r \times n_2}} \|\mathbf{X} - \mathbf{AS}\|_F^2 \quad \text{or} \quad \min_{\mathbf{A} \in \mathbb{R}_{\geq 0}^{n_1 \times r}, \mathbf{S} \in \mathbb{R}_{\geq 0}^{r \times n_2}} D(\mathbf{X} \|\mathbf{AS}).^1$$

¹information divergence $D(\mathbf{A} \|\mathbf{B}) = \sum_{i,j} \left(\mathbf{A}_{ij} \log \frac{\mathbf{A}_{ij}}{\mathbf{B}_{ij}} - \mathbf{A}_{ij} + \mathbf{B}_{ij} \right)$

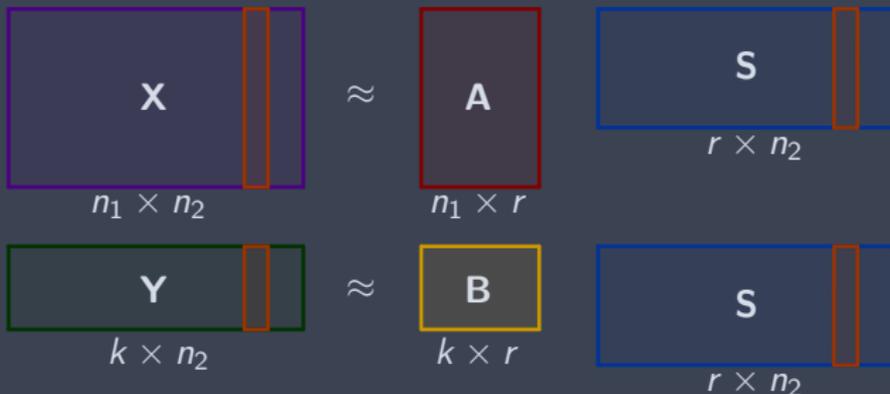
» Joint NMF

Model: Jointly factorize two nonnegative matrices \mathbf{X}_1 and \mathbf{X}_2 , sharing one factor matrix between the factorizations.

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Example: Semi-supervised NMF



Often applied in classification!

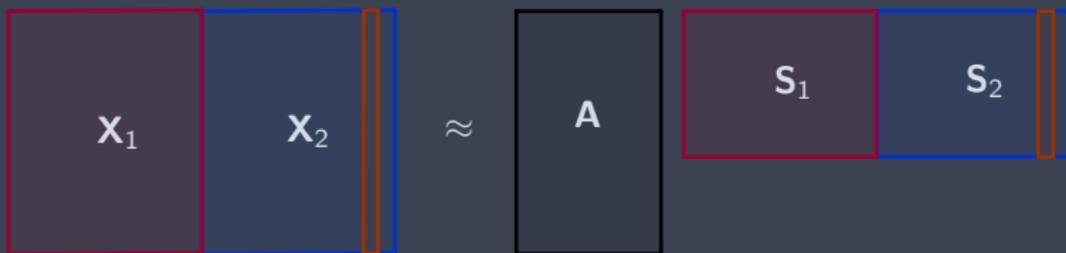
¹Lee, H., Yoo, J., and Choi, S. "Semi-supervised nonnegative matrix factorization." IEEE Signal Processing Letters 17.1 (2009): 4-7.

H., et al. "Semi-supervised Nonnegative Matrix Factorization for Document Classification." 2021 55th Asilomar Conference on Signals, Systems, and Computers. IEEE, 2021.

» Joint NMF

Model: Jointly factorize two nonnegative matrices \mathbf{X}_1 and \mathbf{X}_2 , sharing one factor matrix between the factorizations.

Example: Joint NMF/Guided NMF

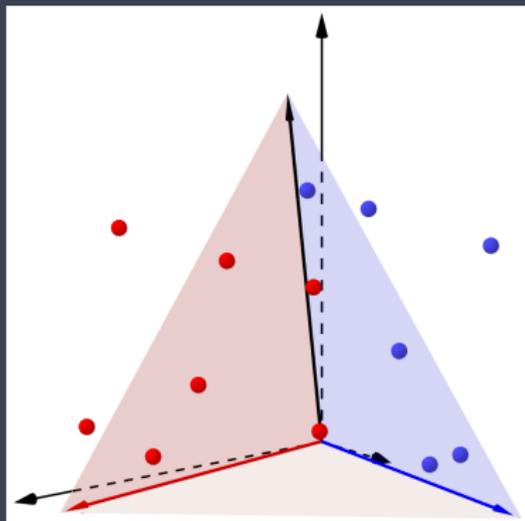


Intuition: many columns of \mathbf{A} used in representing \mathbf{X}_1 and \mathbf{X}_2 indicates dataset similarity.

¹Kim, H., et al. "Simultaneous discovery of common and discriminative topics via joint nonnegative matrix factorization." Proc. ACM SIGKDD Int. Conf. Knowl. Disc. Data Mining. 2015.

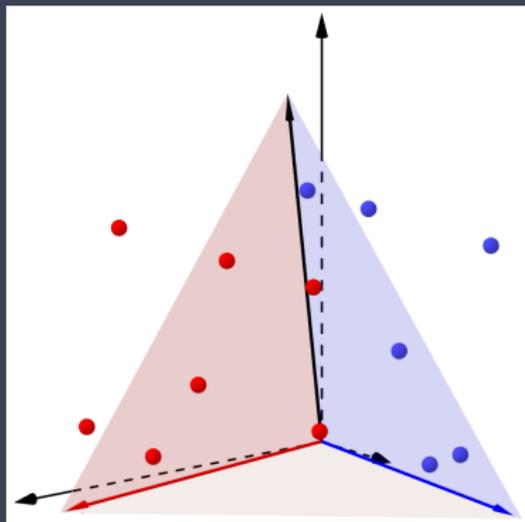
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» Joint NMF (jNMF) for Similarity



NMF learns a conic
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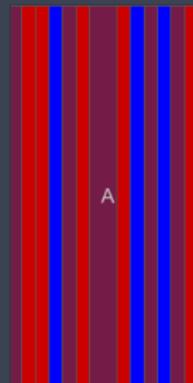
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Similar



Different

Our Method and Distance

» Our jNMF Similarity Method

Intuition: use the entries of S_1 and S_2 to measure how much topics are shared between datasets.

Method:

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Method:

- * Scale each column in X_1, X_2 to be mean one.
- * Learn rank- k jNMF approximation, $[X_1 \ X_2] \approx A[S_1 \ S_2]$.

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- * For $i = 1, \dots, k$, define

$$s_i = \max \left(\{s_{ij}^{(1)}\}_{j=1}^{n_1} \cup \{s_{ij}^{(2)}\}_{j=1}^{n_2} \right)$$

where $s_{i1}^{(1)}, s_{i2}^{(1)}, \dots, s_{in_1}^{(1)}$ and $s_{i1}^{(2)}, s_{i2}^{(2)}, \dots, s_{in_2}^{(2)}$ are the entries of the i th rows of S_1 and S_2 , respectively.

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- * For $j = 1, \dots, K$
 - * Choose $T_i \sim \text{unif}([0, s_i])$ for $i = 1, 2, \dots, k$.
 - * Compute $\mathbf{p}_i^{(j)} := F_i^{(2)}(T_i) - F_i^{(1)}(T_i)$, where

$$F_i^{(1)}(T_i) := \frac{1}{n_1} \sum_{j=1}^{n_1} \mathbf{1}[s_{ij}^{(1)} < T_i] \text{ and } F_i^{(2)}(T_i) := \frac{1}{n_2} \sum_{j=1}^{n_2} \mathbf{1}[s_{ij}^{(2)} < T_i].$$

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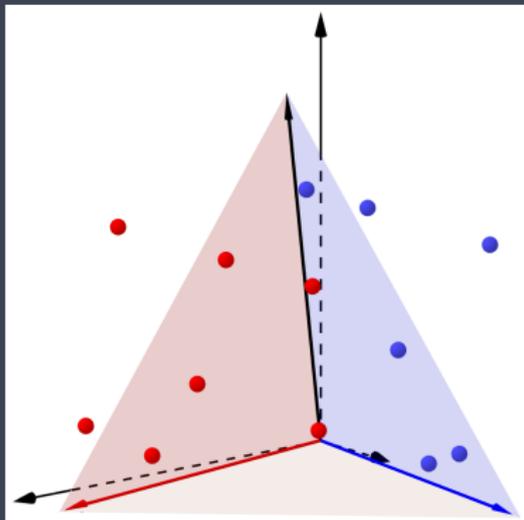
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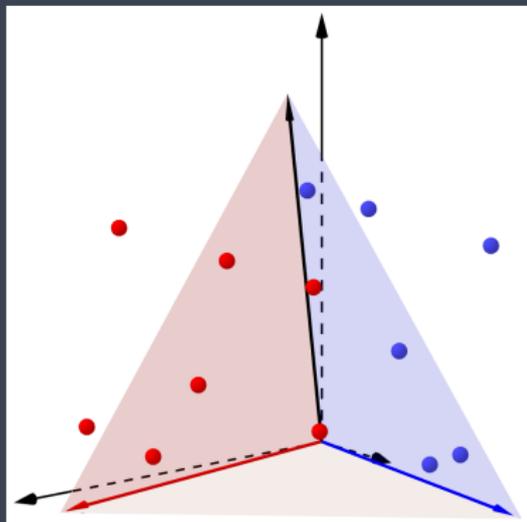
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- * Return $\bar{\mathbf{p}} = \frac{1}{K} \sum_{j=1}^K \mathbf{p}^{(j)}$

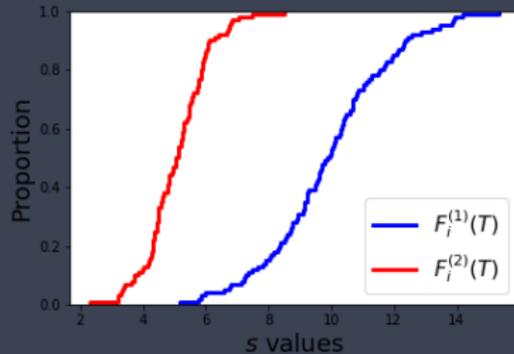
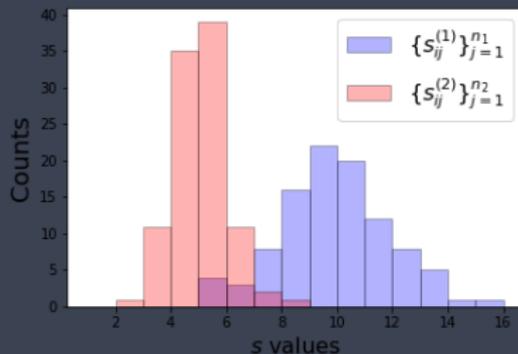
» jNMF Similarity Method



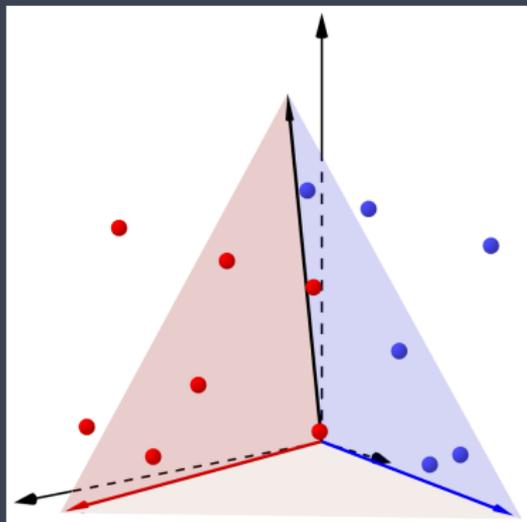
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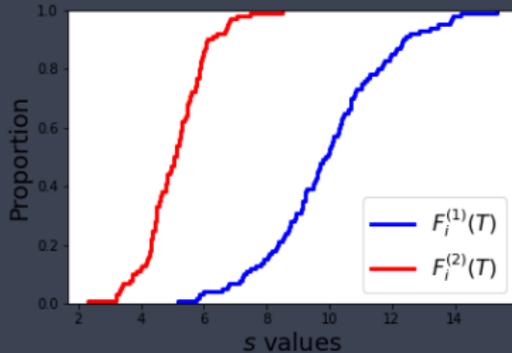
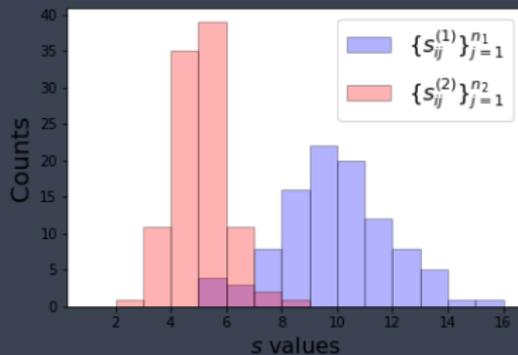


» jNMF Similarity Method



$$d(X_1, X_2) := \|\bar{\mathbf{p}}\|_1$$

$$\mathbf{p}_i^{(j)} := F_i^{(2)}(T_i) - F_i^{(1)}(T_i)$$



Experiments

» Swimmer Image Dataset

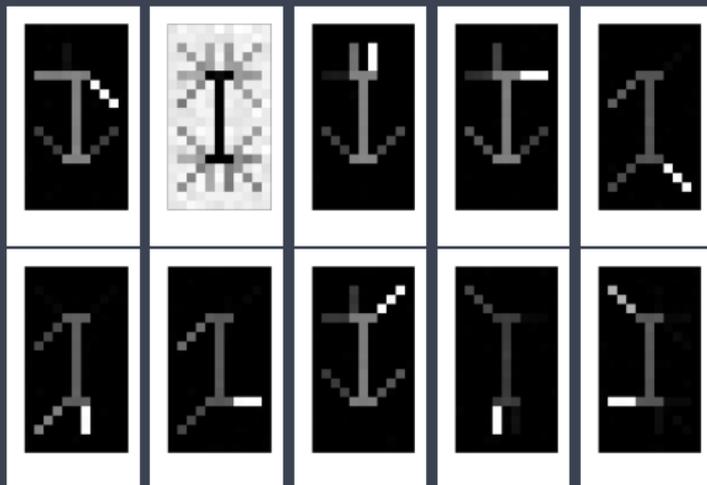
Swimmer Images



¹Donoho, D., and Stodden, V. "When does non-negative matrix factorization give a correct decomposition into parts?." NeurlPS (2003).

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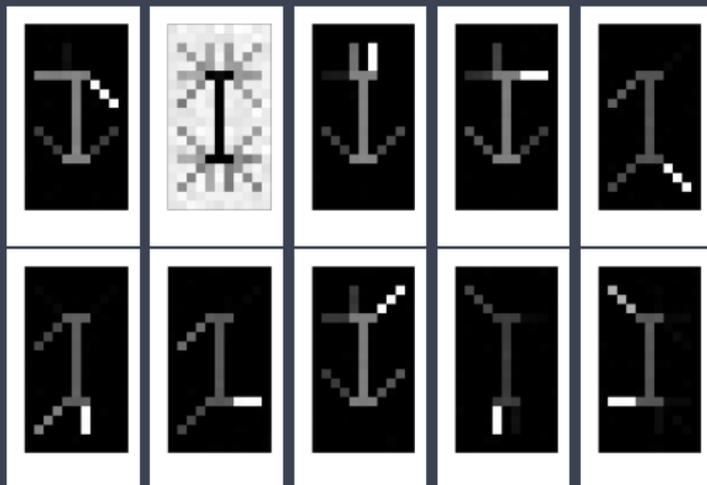


Basis vectors learned by jNMF on Swimmer dataset $X_1, X_1 + N$ where N is uniform noise.

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» Swimmer Image Dataset

Swimmer Images



Basis vectors learned by jNMF on Swimmer dataset $X_1, X_1 + N$ where N is uniform noise.

$$\bar{p} = [0.063, -0.901, 0.076, 0.065, 0.069, \\ 0.058, 0.058, 0.069, 0.079, 0.079]$$

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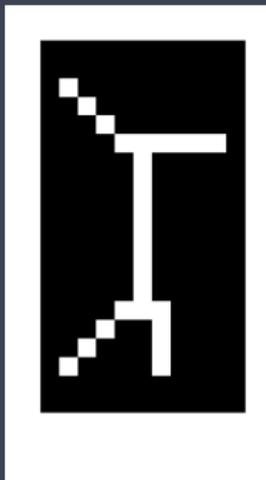
Swimmer Images



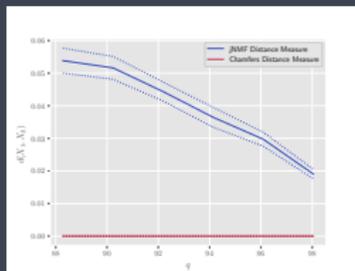
| X_2 | X_1 | $X_1 P_\pi$ | λX_1 | \bar{X}_1 | $X_1 + N$ | N |
|-----------------------------|-------|-------------|---------------|-------------|-----------|-------|
| $d(X_1, X_2)$ | 0.000 | 0.000 | 0.000 | 0.052 | 1.509 | 2.297 |
| $d_{\text{cham}}(X_1, X_2)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.741 | 1.560 |

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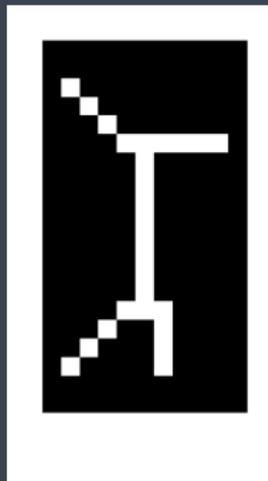


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| $d_{\text{cham}}(X_1, X_2)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.741 | 1.560 |

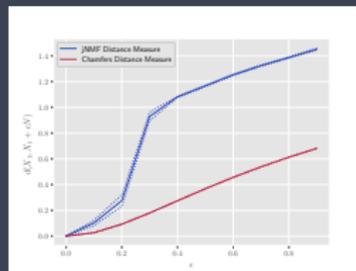
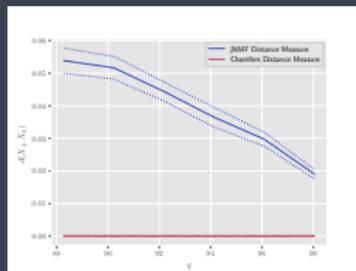


» Swimmer Image Dataset

Swimmer Images

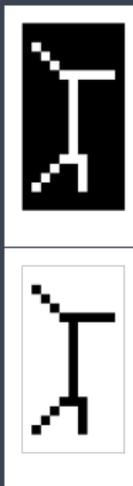


| X_2 | X_1 | $X_1 P_\pi$ | λX_1 | \bar{X}_1 | $X_1 + N$ | N |
|-----------------------------|-------|-------------|---------------|-------------|-----------|-------|
| $d(X_1, X_2)$ | 0.000 | 0.000 | 0.000 | 0.052 | 1.509 | 2.297 |
| $d_{\text{cham}}(X_1, X_2)$ | 0.000 | 0.000 | 0.000 | 0.000 | 0.741 | 1.560 |



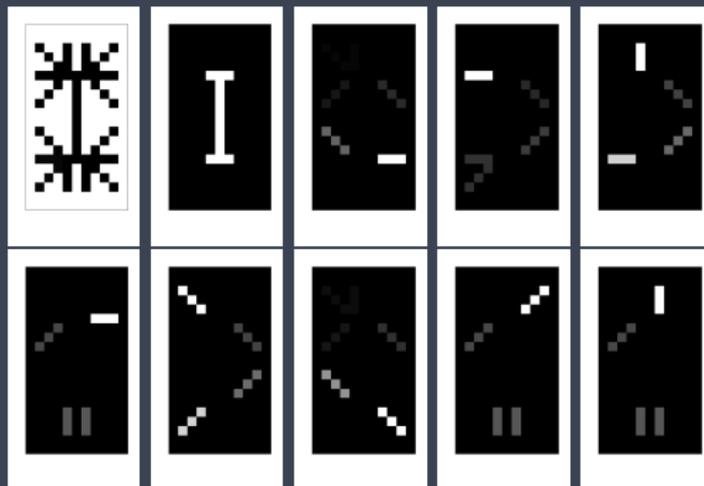
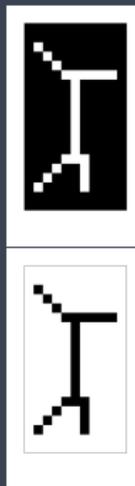
» Swimmer Image Dataset

Swimmer and
Inverse Swimmer:



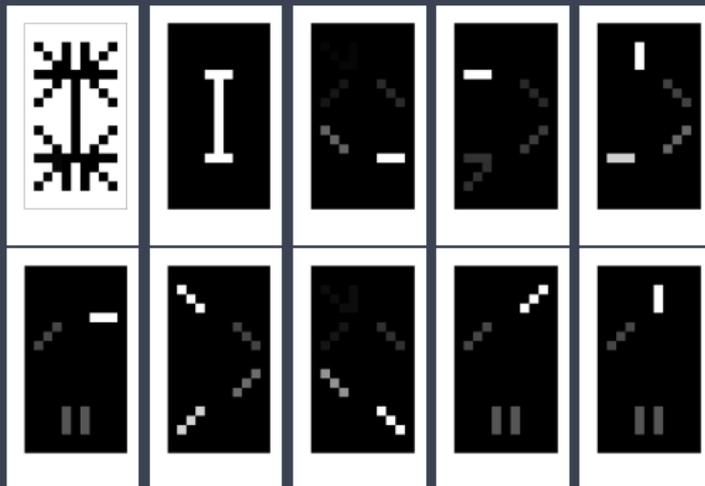
» Swimmer Image Dataset

Swimmer and
Inverse Swimmer:



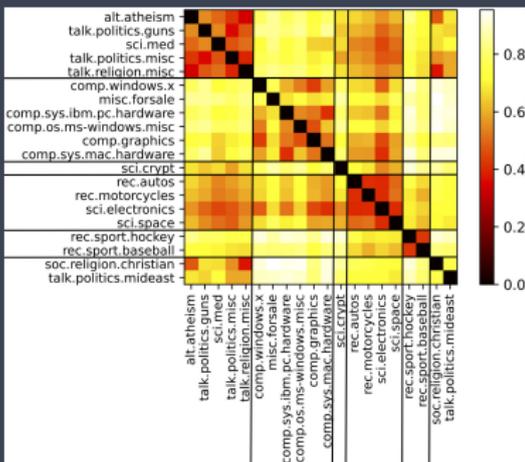
» Swimmer Image Dataset

Swimmer and
Inverse Swimmer:



$$\bar{\mathbf{p}} = [-0.999, 1.000, 0.010, -0.017, 0.003, -0.004, 0.015, 0.004, -0.001, -0.000]$$

» 20 Newsgroups Dataset

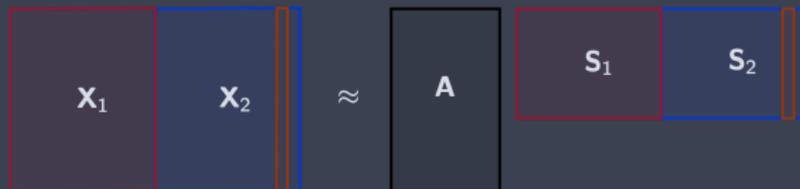


jNMF Distance

Conclusions

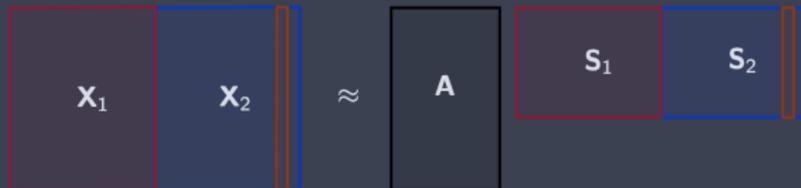
» Conclusions

- ▷ jNMF provides information about dataset similarity and dissimilarity



» Conclusions

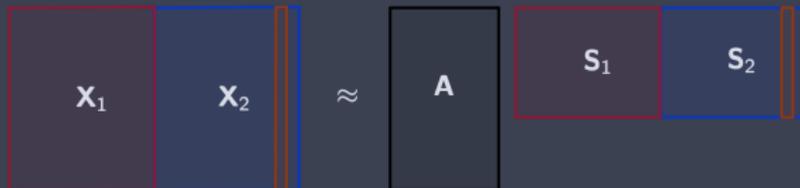
- ▷ jNMF provides information about dataset similarity and dissimilarity



- ▷ we can aggregate this information using samples from the empirical distribution function to form a vector indicating which dataset learned basis vectors represent, \bar{p}

» Conclusions

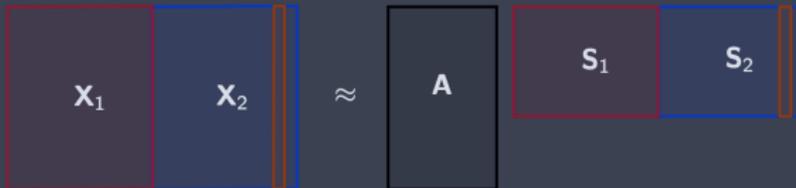
- ▷ jNMF provides information about dataset similarity and dissimilarity



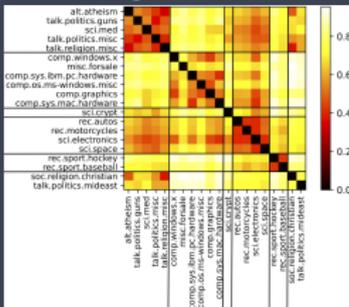
- ▷ we can aggregate this information using samples from the empirical distribution function to form a vector indicating which dataset learned basis vectors represent, \bar{p}
- ▷ the information can be further aggregated to yield a distance, $d(X_1, X_2) = \|\bar{p}\|_1$

» Conclusions

- ▷ jNMF provides information about dataset similarity and dissimilarity



- ▷ we can aggregate this information using samples from the empirical distribution function to form a vector indicating which dataset learned basis vectors represent, \bar{p}
- ▷ the information can be further aggregated to yield a distance, $d(X_1, X_2) = \|\bar{p}\|_1$
- ▷ initial experiments are promising



» **Thanks for listening!**

Questions?

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