Psych 253
Advanced Statistical Modeling

Dimension Reduction

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Unsupervised data analysis

No "labels", just "data".

http://scikit-learn.org/stable/modules/classes.html#module-sklearn.decomposition

Dimension reduction: `sklearn.decomposition`

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Dimension reduction: **`sklearn.decomposition`**

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- Factor Analysis
- Multi-Dimensional Scaling (MDS)
- Independent Components Analysis (ICA)
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Last time

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PCA

Principal Components Analysis

1) Data matrix $\boldsymbol{X}$ of shape (m, n)

PCA

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1) Data matrix $\boldsymbol{X}$ of shape (m, n) — mean centered!

2) Covariance matrix $\boldsymbol{X^T X}$ of shape

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Principal Components Analysis

1) Data matrix $\boldsymbol{X}$ of shape (m, n) — mean centered!

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3) Compute eigenvalues $\boldsymbol{d_1\ d_2\ \ldots d_n}$ and eigenvectors $\boldsymbol{w_1\ w_2\ \ldots w_n}$ of $\boldsymbol{X^TX}$

ordered from biggest to smallest

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$\boldsymbol{w_1}$ = principal axis

$X \cdot \vec{w}_1$ = projection of data onto principal axis

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$\frac{\sum_{i \le k} d_i}{\sum_{i=1}^{n} d_i}$

fraction of variance of original data explained

= projection of data onto top $\boldsymbol{k}$ principal axes

PCA

[Ipynb: principal components analysis]

PCA

Normal projection of PCA is:

$$[p_1, \ldots, p_k] = X \cdot [\vec{w}_1, \ldots, \vec{w}_k]$$

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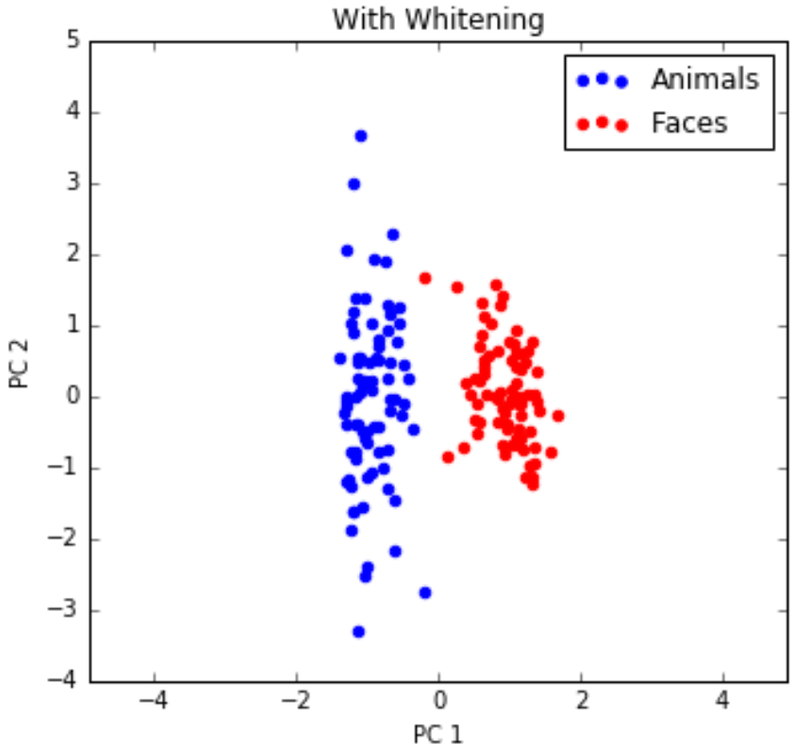

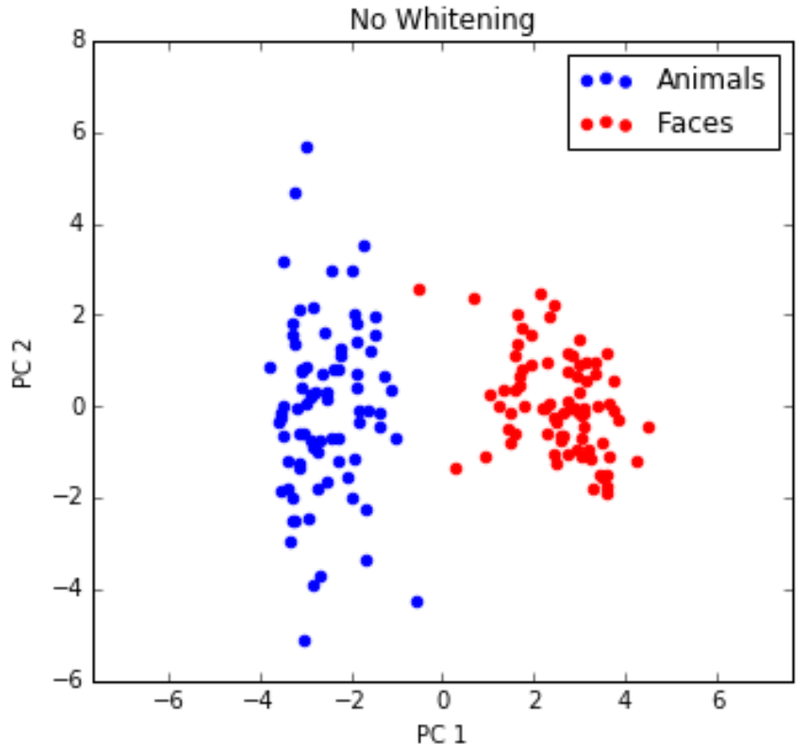

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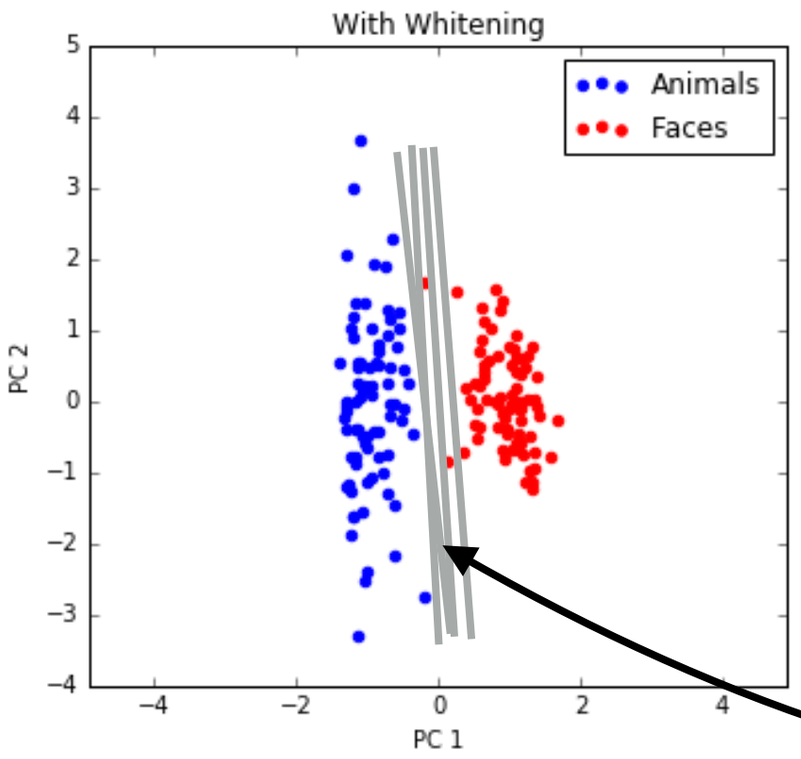

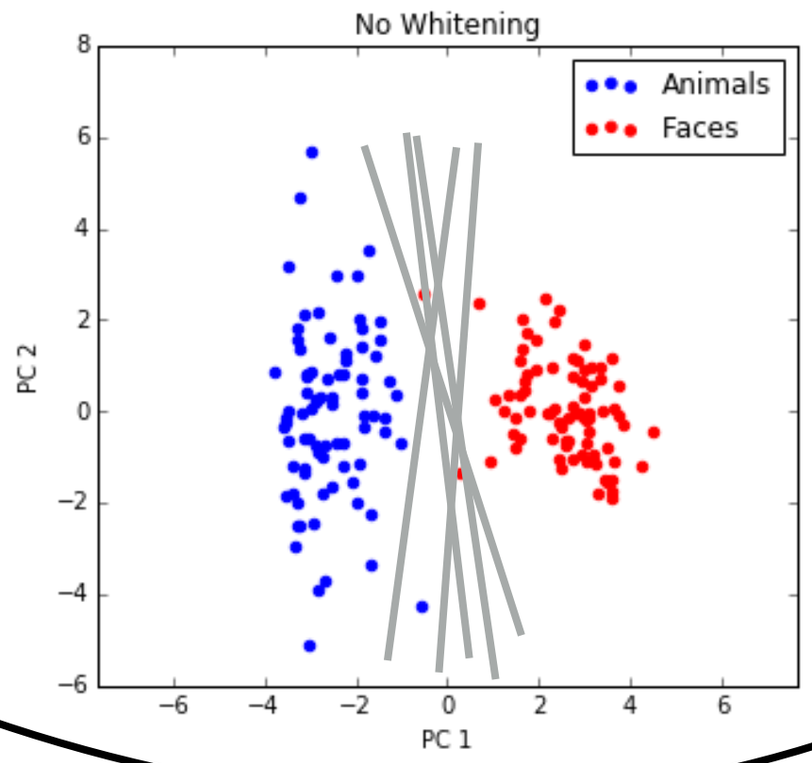

Whitening can make things in downstream operations better.

Such as regularization — less mischief is possible.

Recover Principal Axes of Data

Basic noisy compressive model:

$$X = W \cdot P + \mu + \epsilon$$

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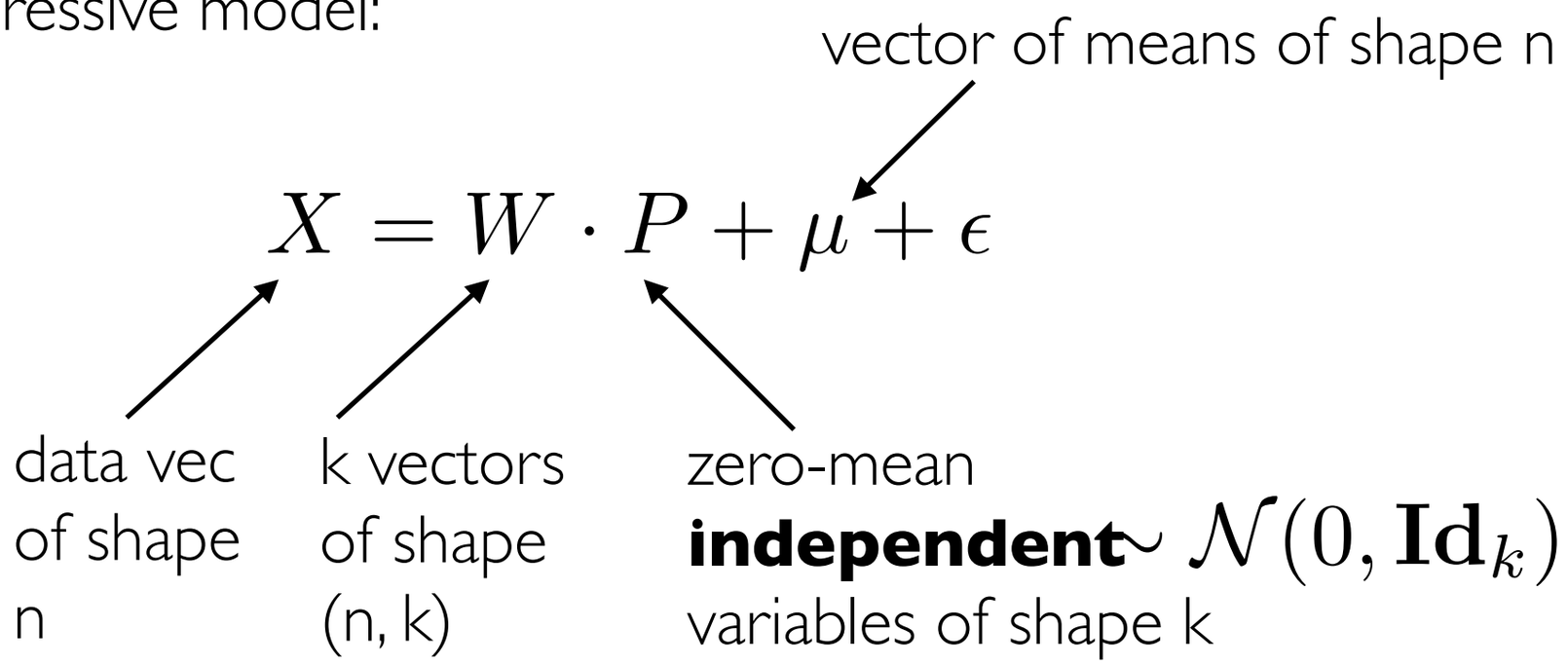

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$$\mathbf{cov} =$$

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$$\mathbf{cov} = (X - \mu)^T (X - \mu)$$

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If you choose like this . . .

$$W = U(D_k - \sigma^2 \mathbf{Id}_k)^{1/2}$$

U = top k eigenvectors of **cov**

D_k = top k eigenvalues of **cov**

. . . then best approx. to X

Recover Principal Axes of Data

Basic noisy compressive model:

$$X = W \cdot P + \mu + \epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{Id}_n)$$

- X: data vec of shape n
- W: k vectors of shape (n, k)
- P: zero-mean **independent** $\sim \mathcal{N}(0, \mathbf{Id}_k)$ variables of shape k
- μ: vector of means of shape n
- ϵ: 0-vector of length n; n **independent** gaussian random variables, all of same variance

$$\mathbf{cov} = (X - \mu)^T (X - \mu) = W^T W + \sigma^2 \mathbf{Id}_n$$

If you choose like this . . .

$$W = U(D_k - \sigma^2 \mathbf{Id}_k)^{1/2}$$

$$\sigma^2 = \frac{1}{n-k} \sum_{i>k} d_i$$

remaining variance is treated as noise

U = top k eigenvectors of **cov**

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. . . then best approx. to X

Factor Analysis

Factor Analysis is the *same* as PCA, except

vector of means of shape n

$$X = W \cdot P + \mu + \epsilon \sim \mathcal{N}(0, \mathbf{\Psi}_n)$$

n independent gaussian random variables, **different** variances

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$\mathbf{\Psi}_n$ = diagonal noise covariance matrix

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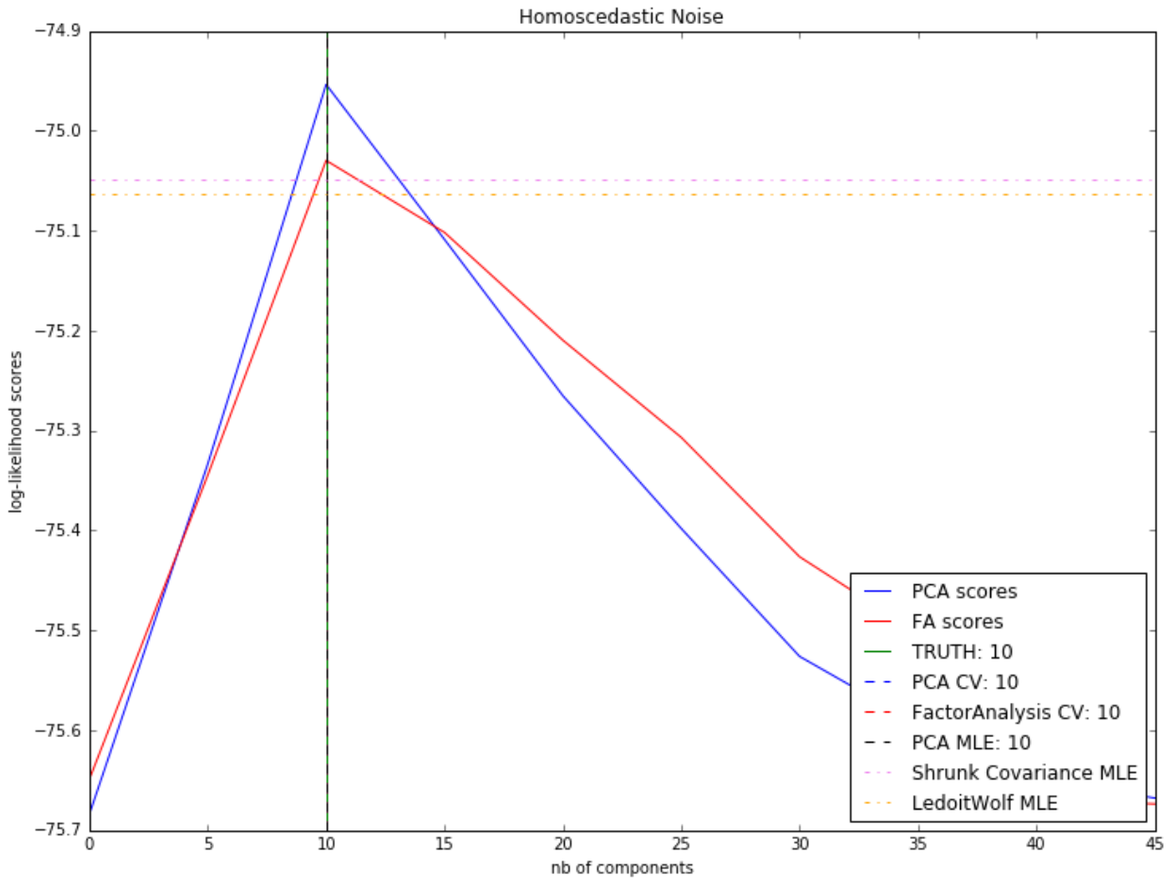
Use Factor Analysis if:

the noise across your prediction dimensions is not the same magnitude

Factor Analysis

"Homoscedastic" noise:

$$\mathcal{N}(0, \sigma^2 \mathbf{Id}_n)$$



"Heteroscedastic" noise:

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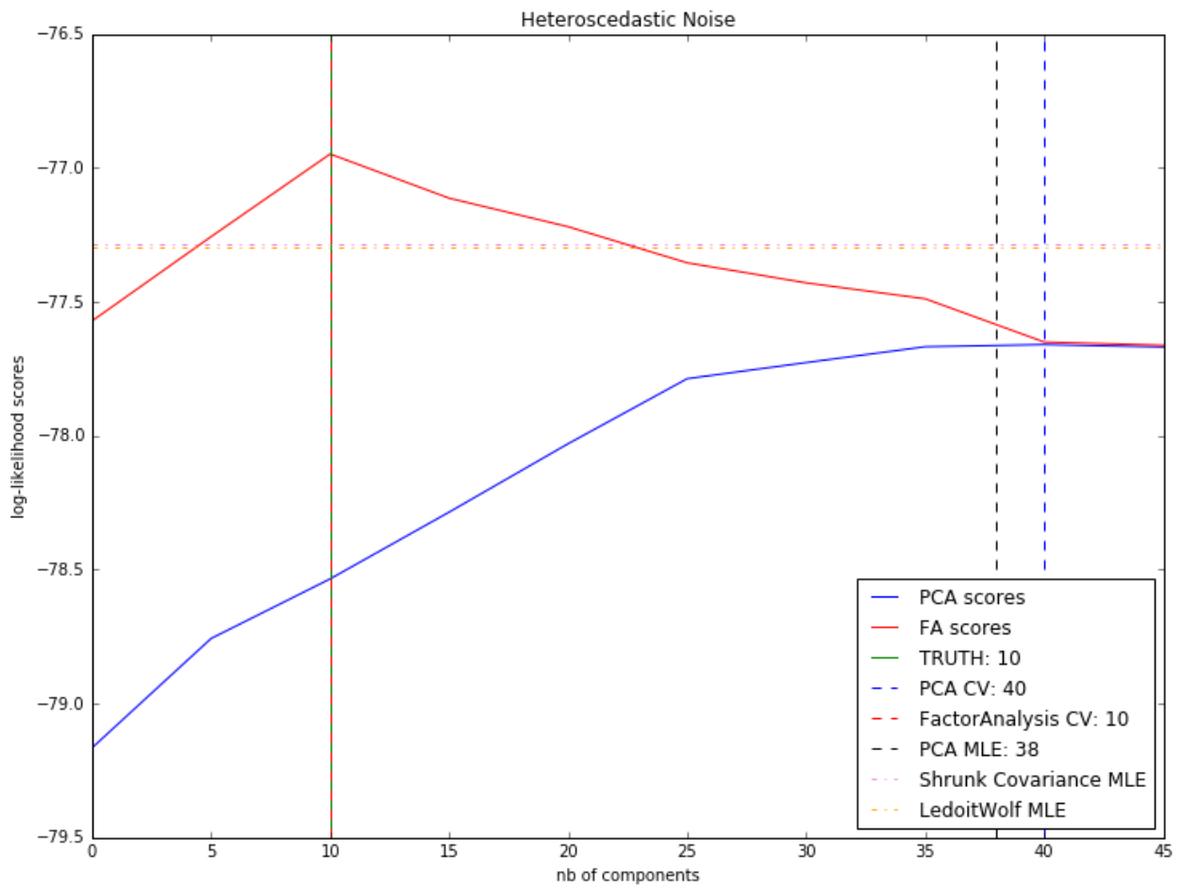

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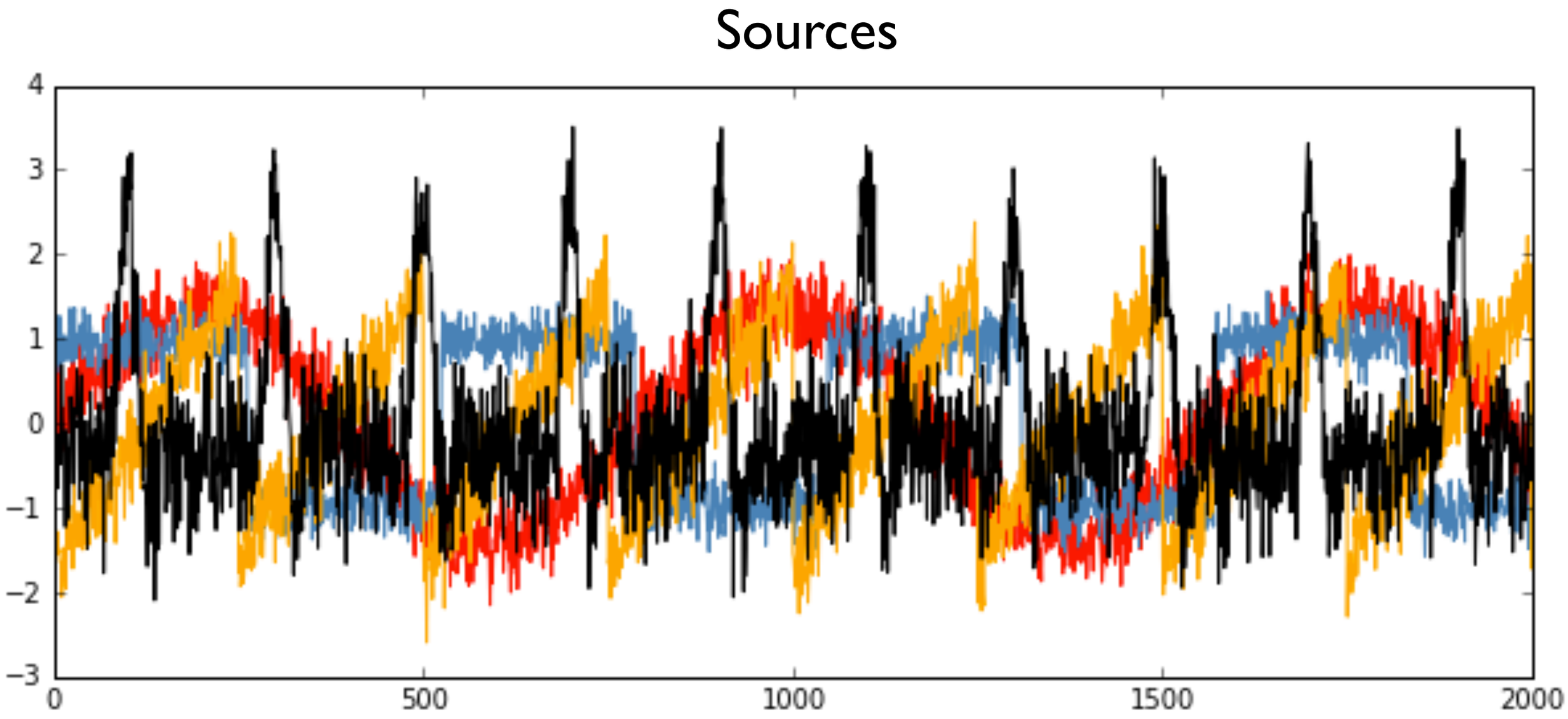
("heteroscadastic" noise)

Independent component analysis



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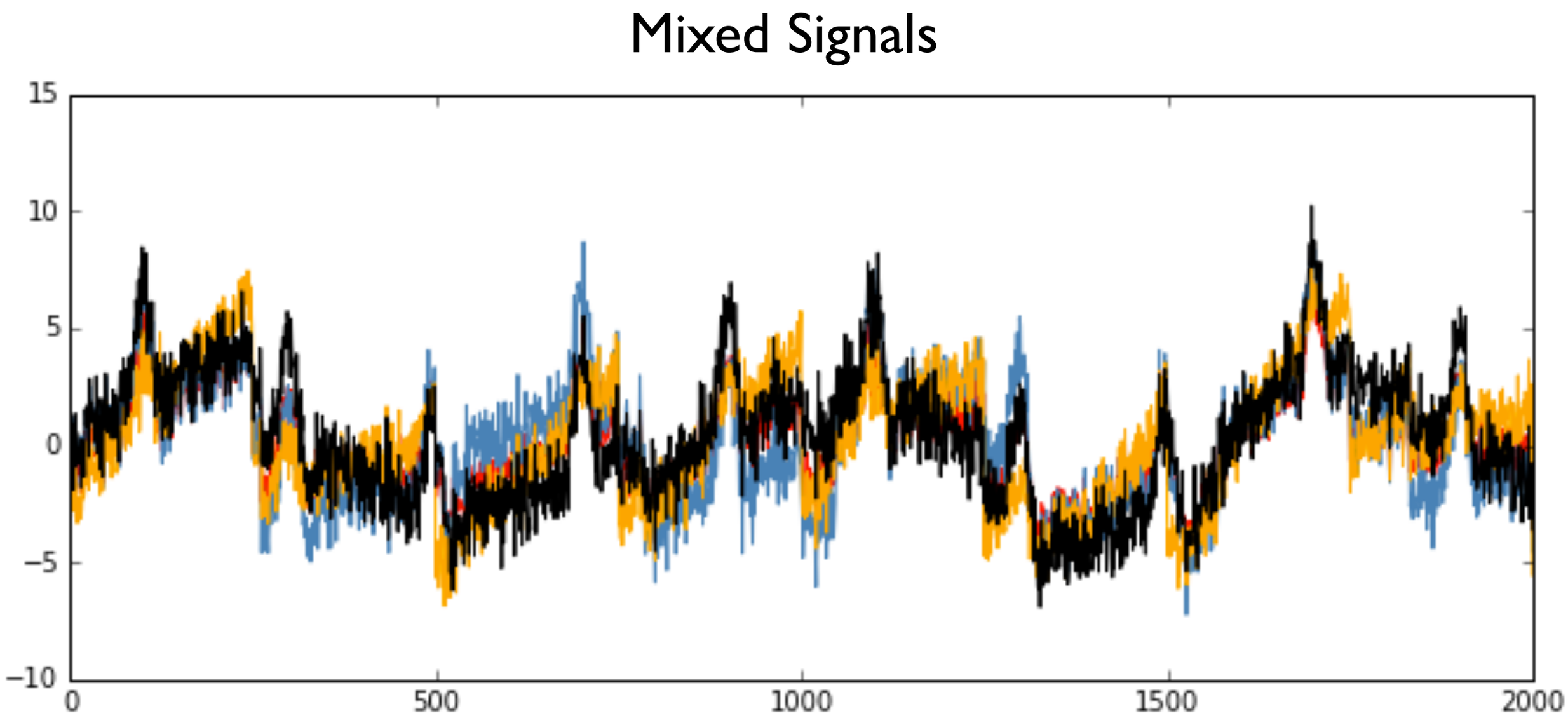


$$X = S \cdot A^T$$

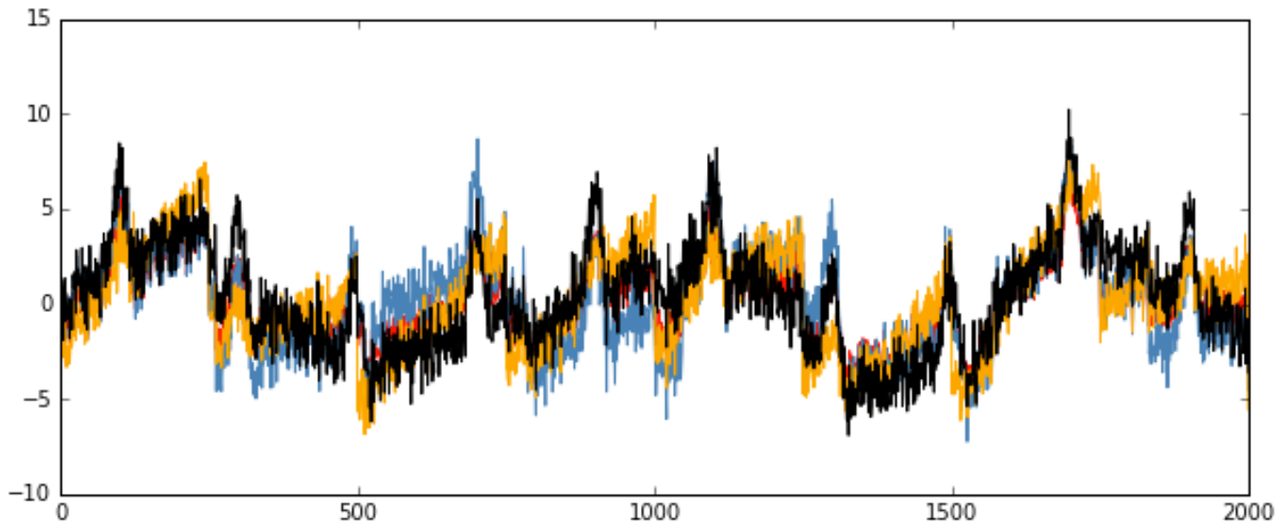
Signals

Sources

Mixing Matrix

Independent component analysis

Signals



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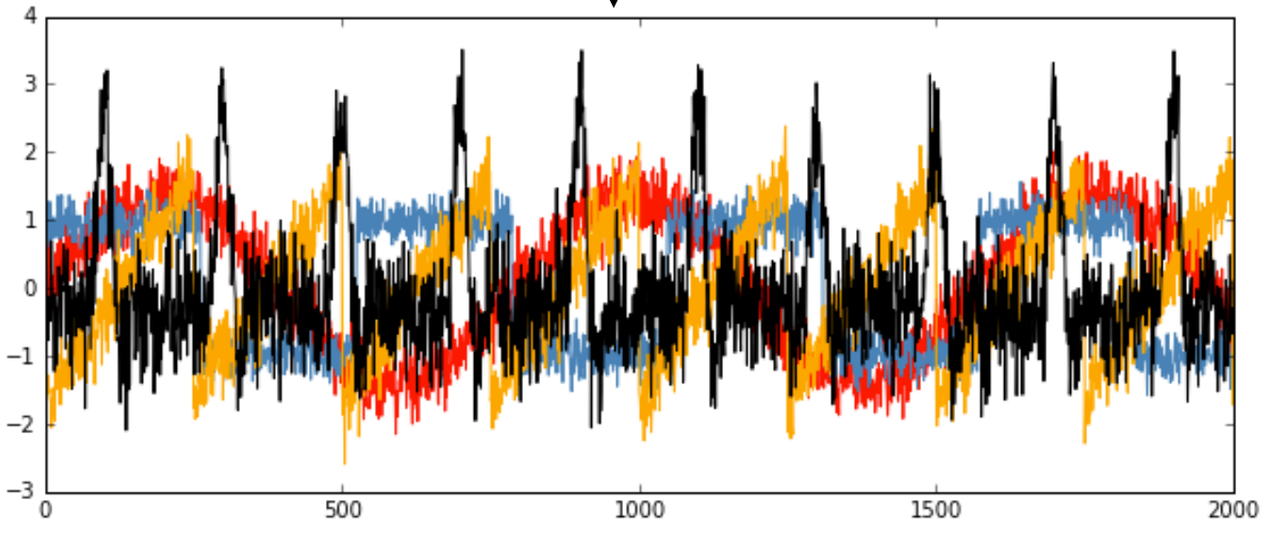
How to recover the sources??



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Independent component analysis

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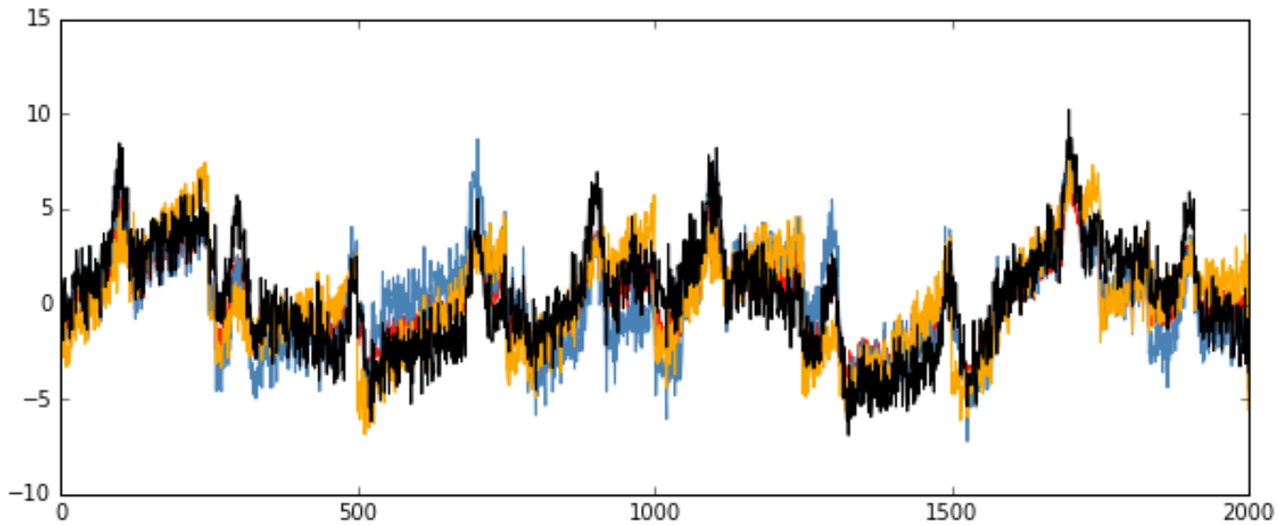

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How to recover the sources??

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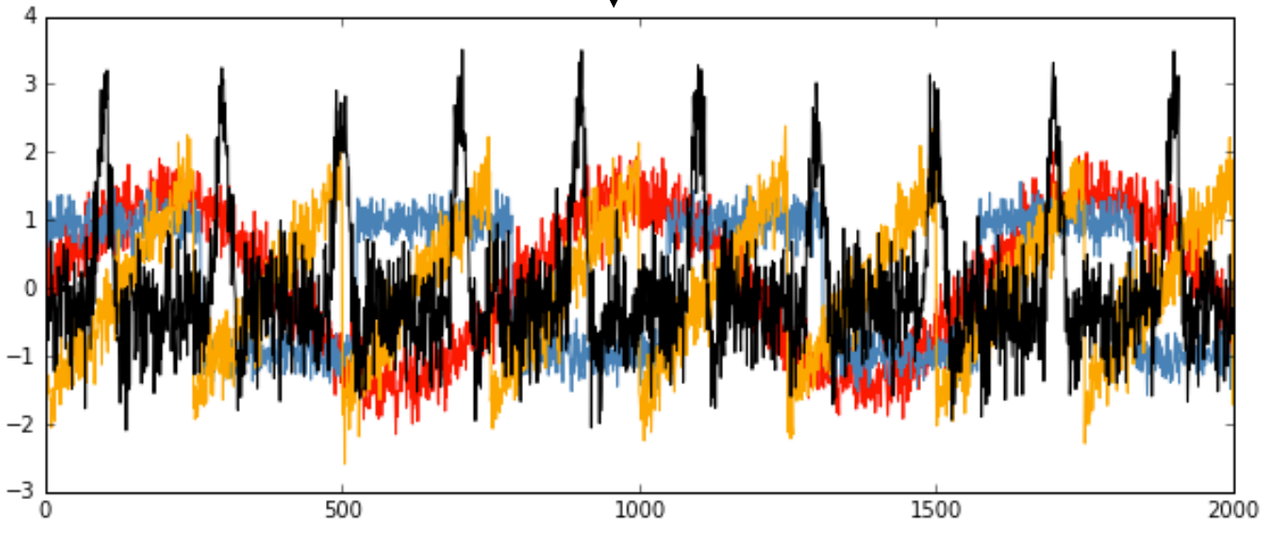

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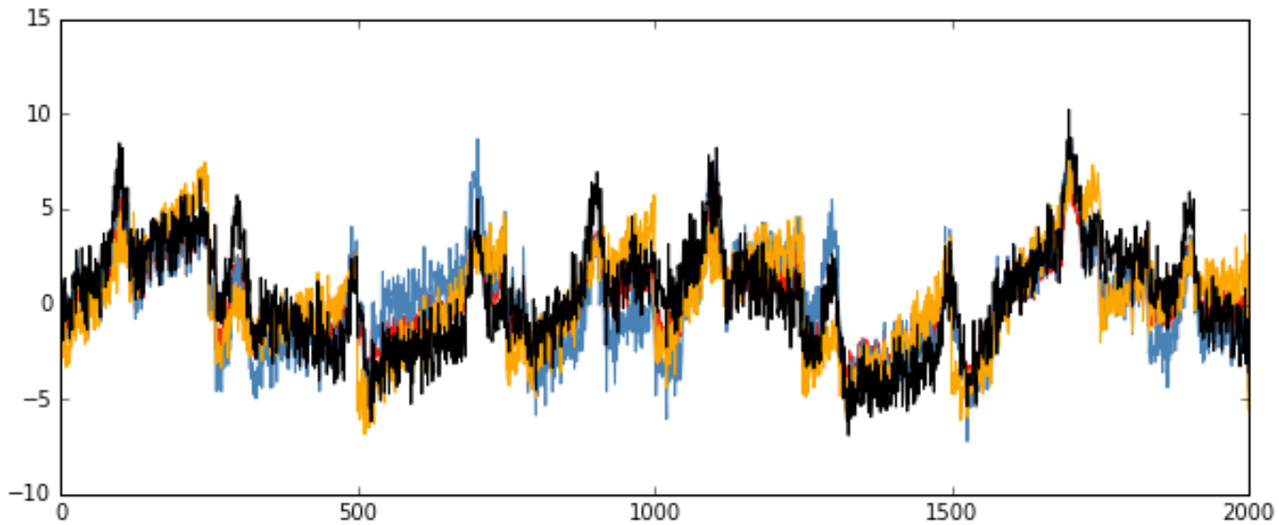

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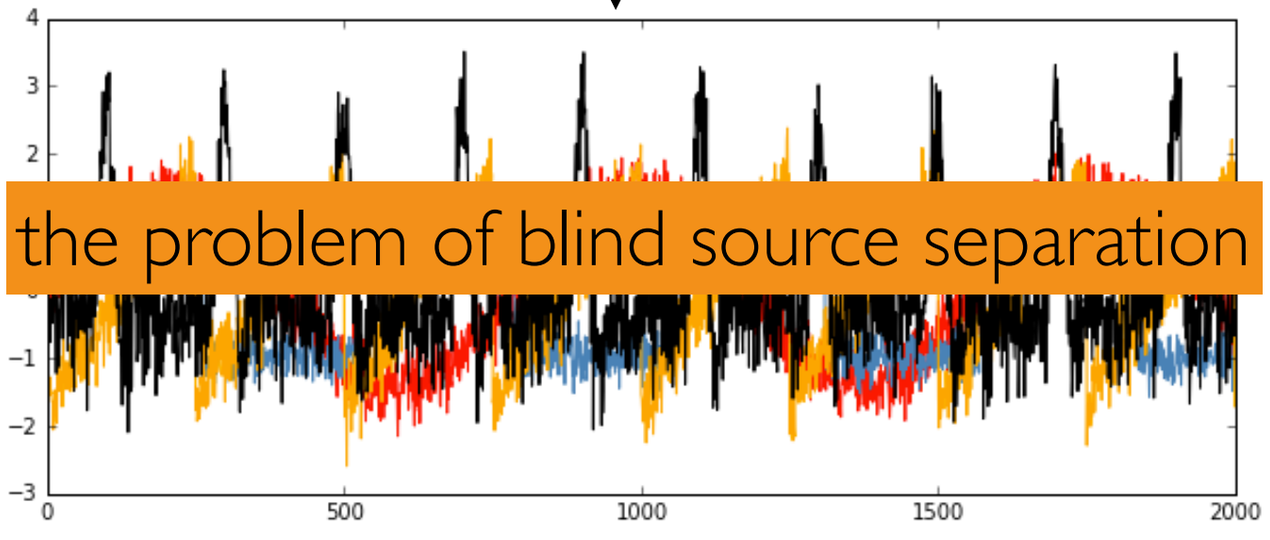
the problem of blind source separation



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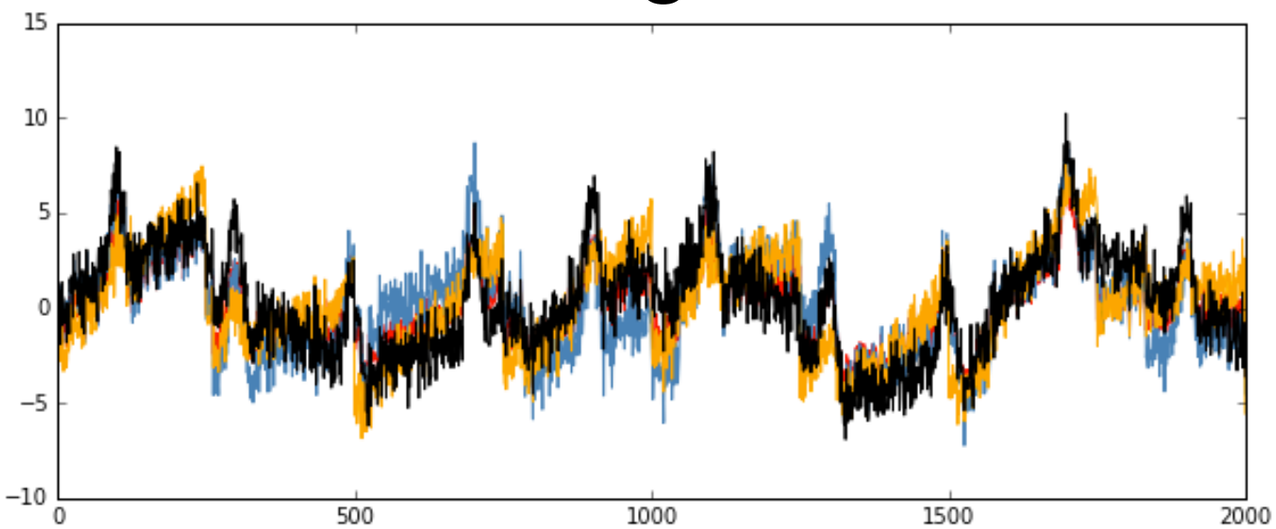

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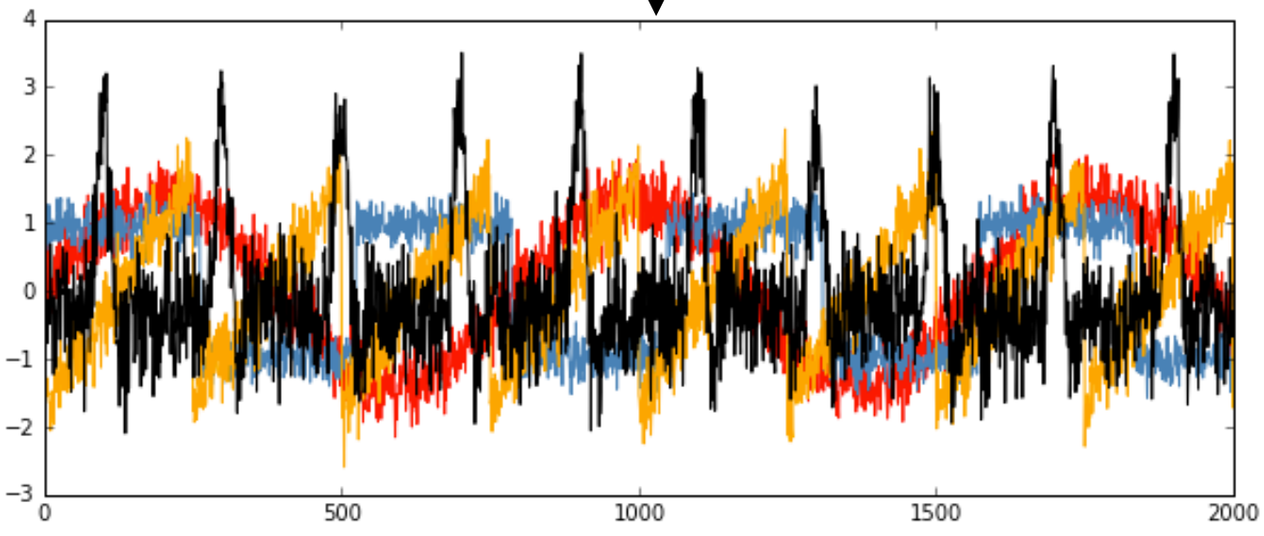

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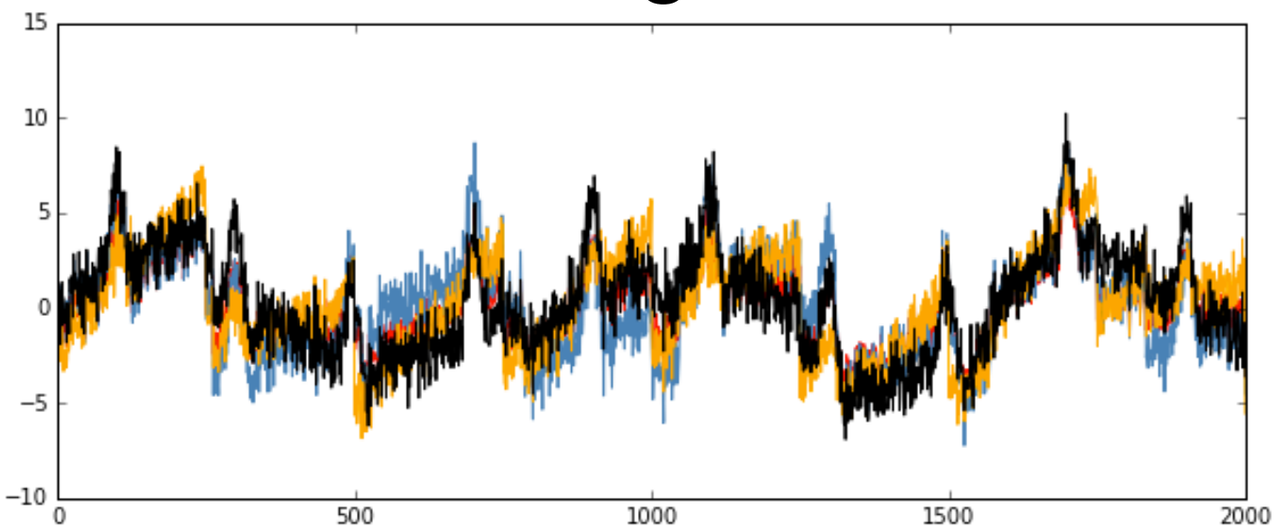
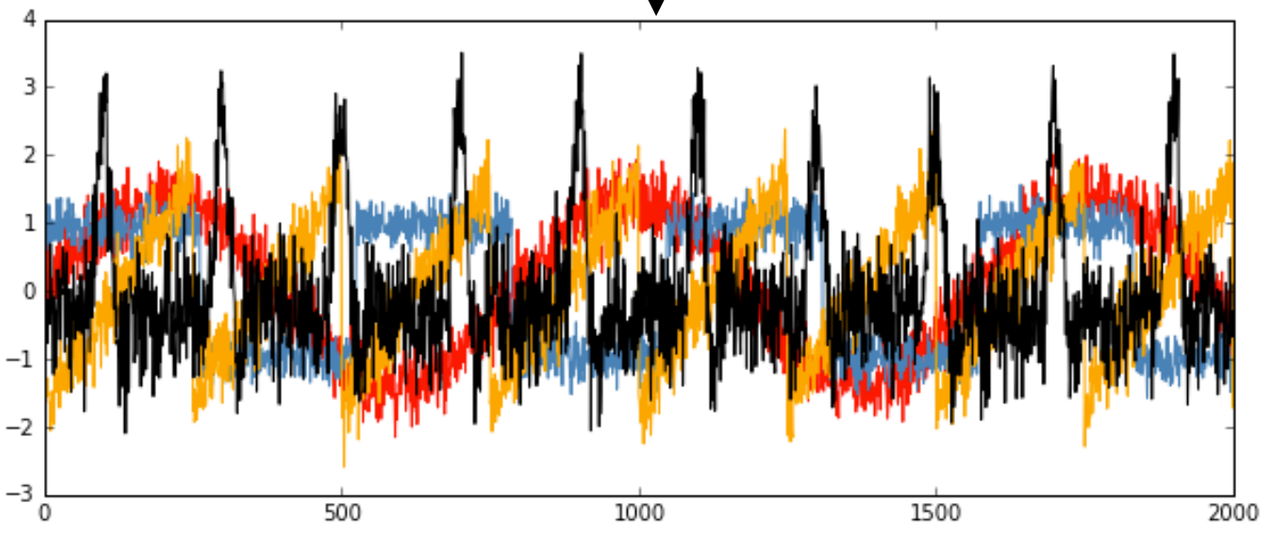


$$X = S \cdot A^T$$

Core Idea: Mixtures are Gaussian …



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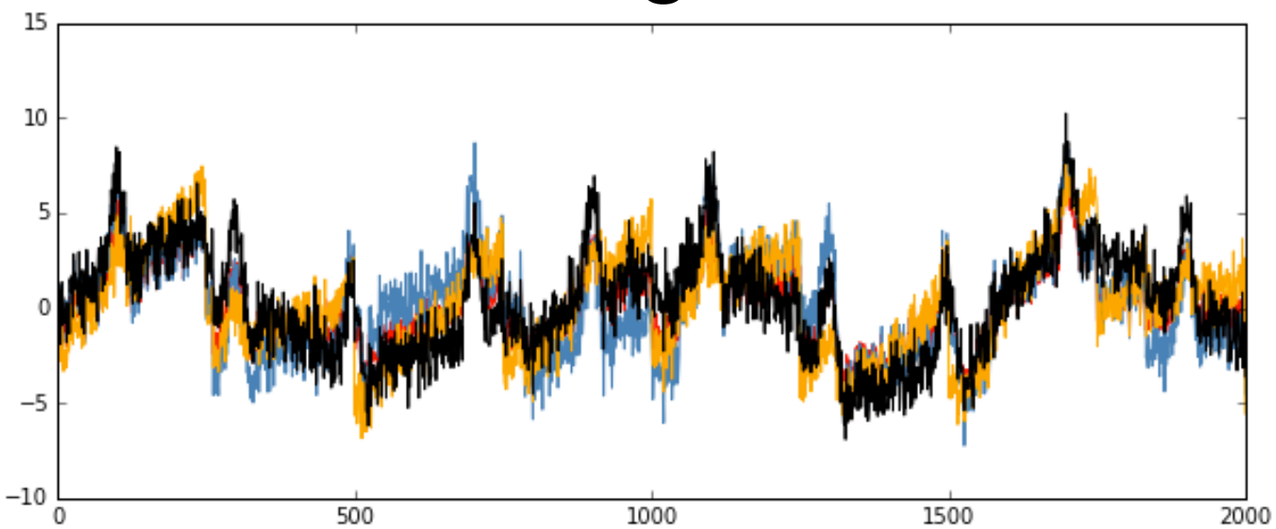

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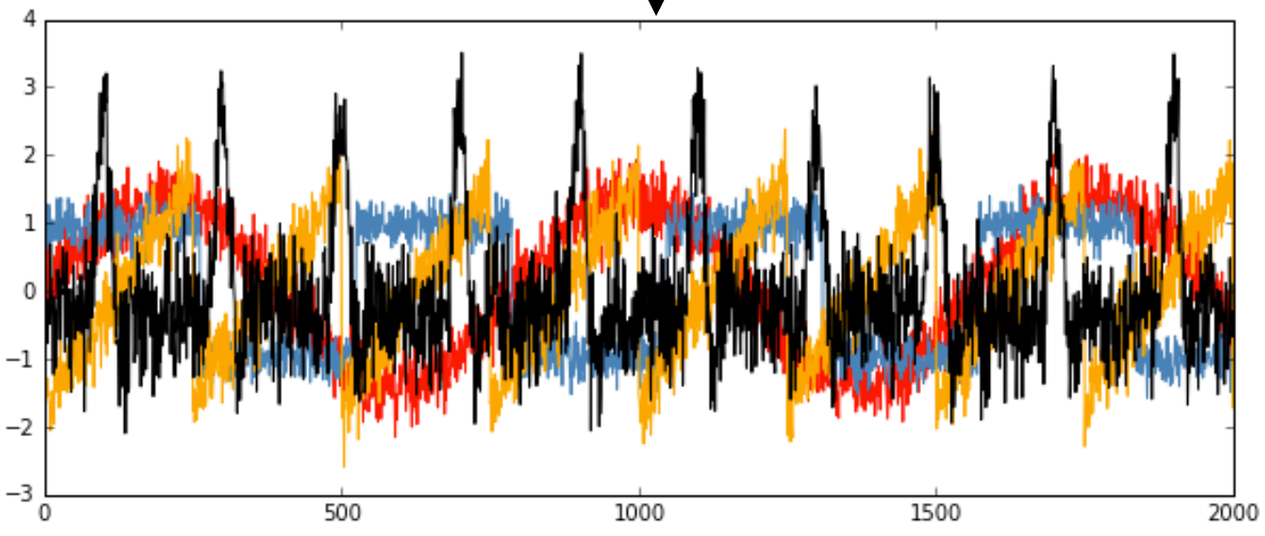
Core Idea: Mixtures are Gaussian …

So sources should **not** be.

"Non-gaussian is independent."



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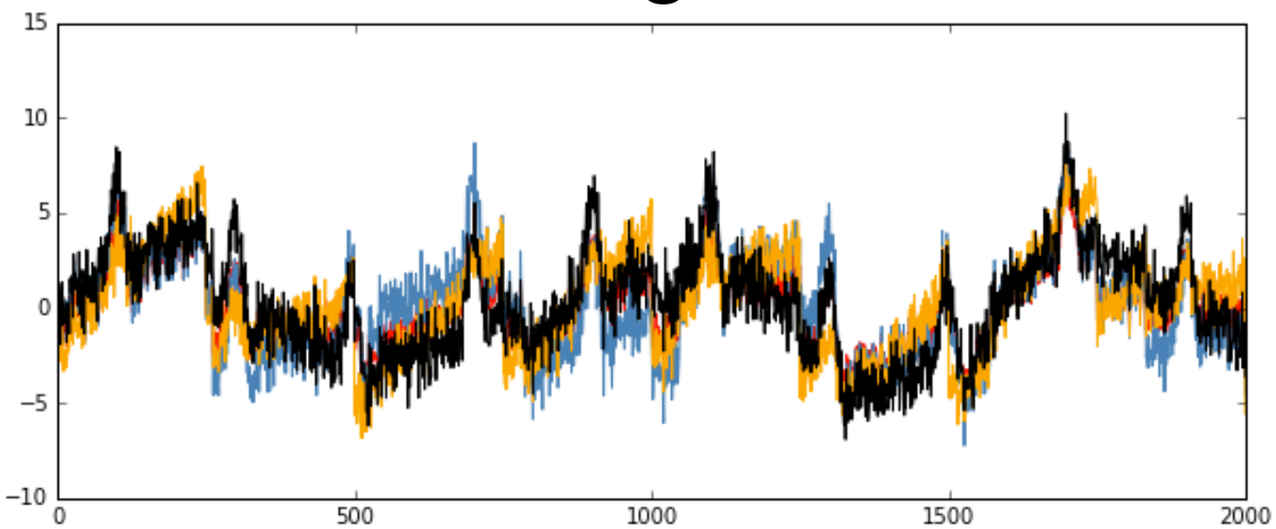


$$X = S \cdot A^T$$

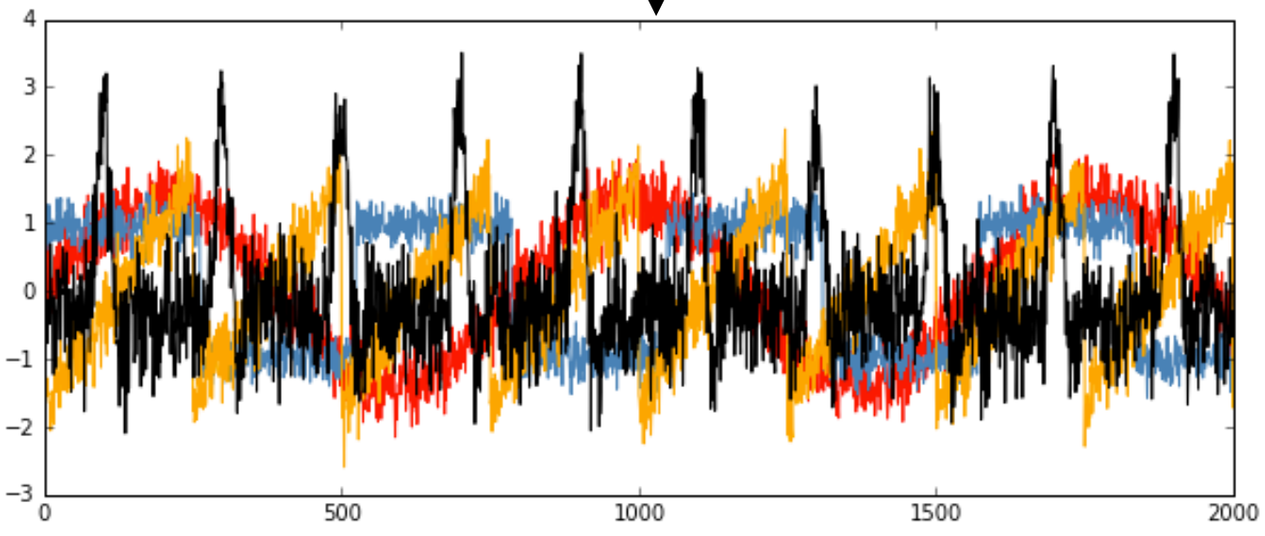
Core Idea: Mixtures are Gaussian …

Specifically: find ***w*** that maximizes non-Gaussianity of

$$w^T X$$

So sources should **not** be.

"Non-gaussian is independent."



Sources

Independent component analysis

Specifically: find ***w*** that maximizes non-Gaussianity of $w^T X$

How to measure non-Gaussianity?

Independent component analysis

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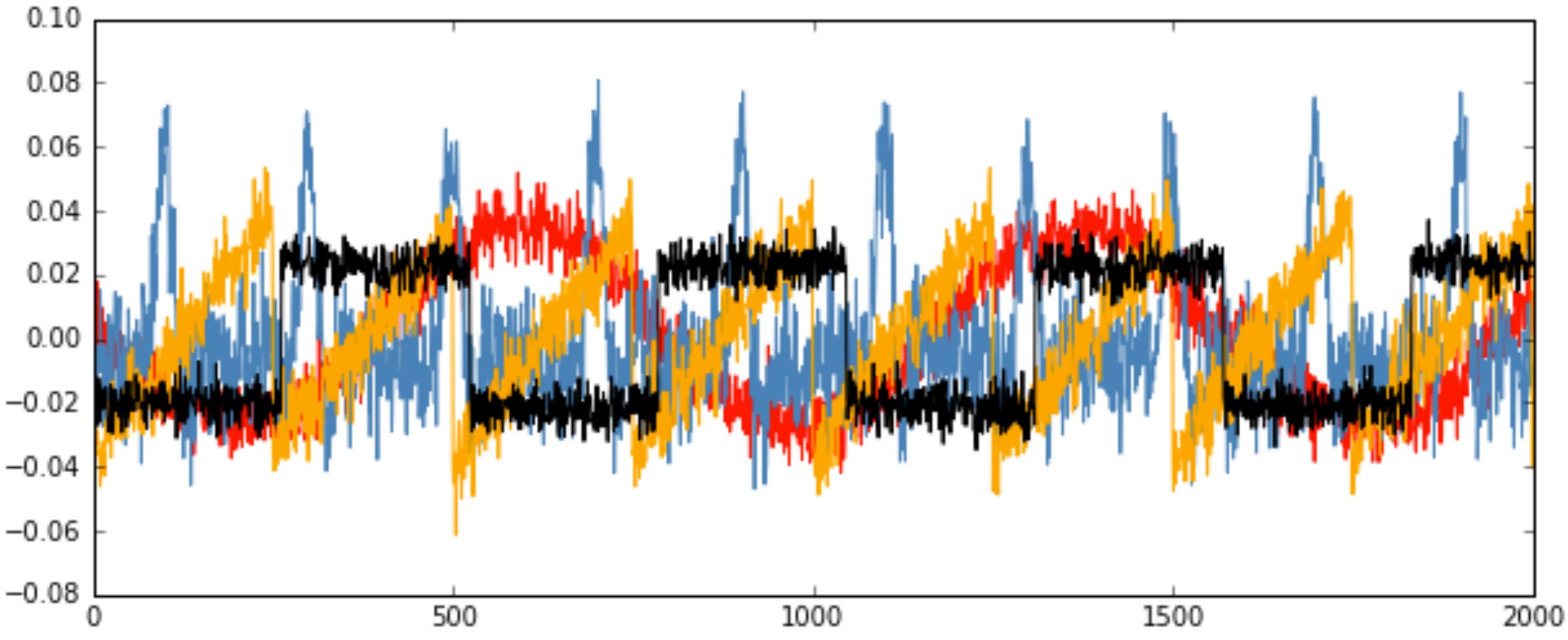
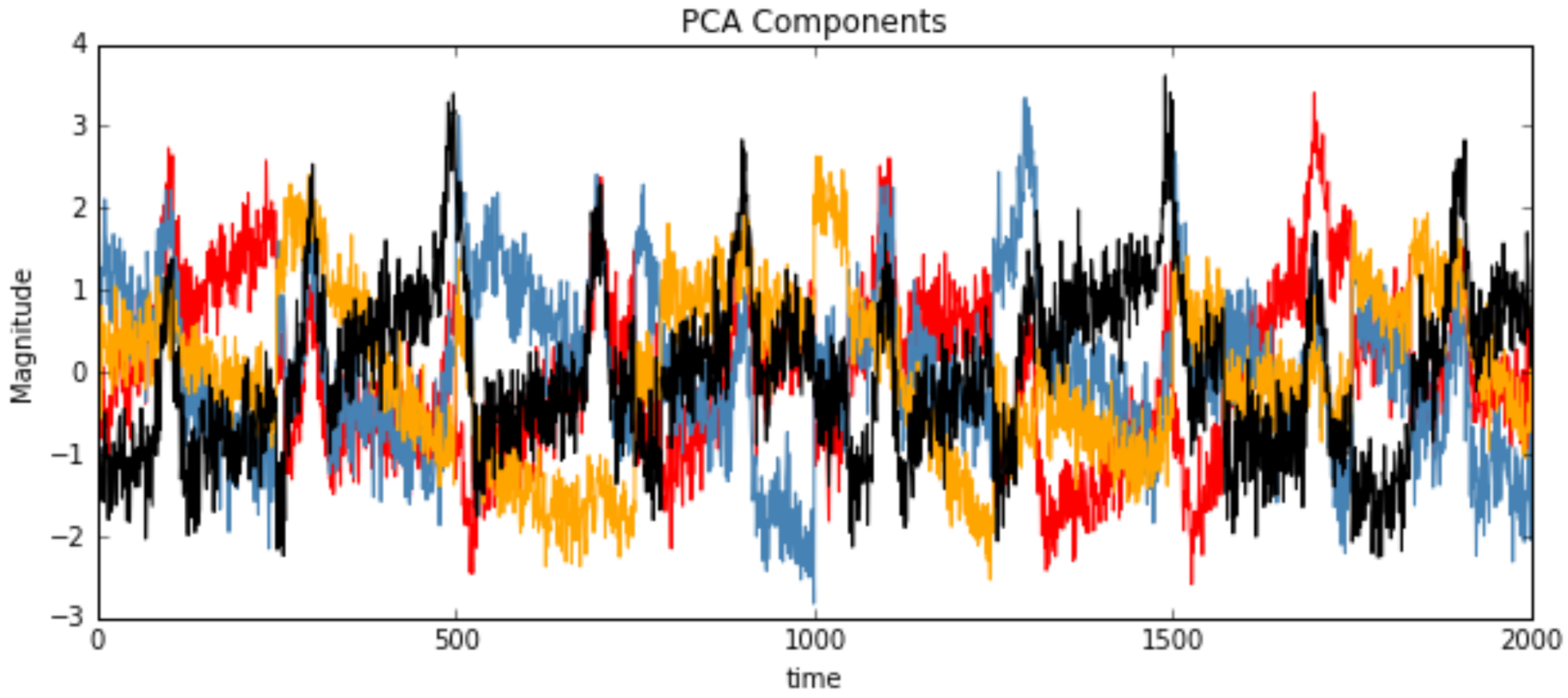
Independent component analysis

[Ipynb: FastICA algorithm]

Independent component analysis

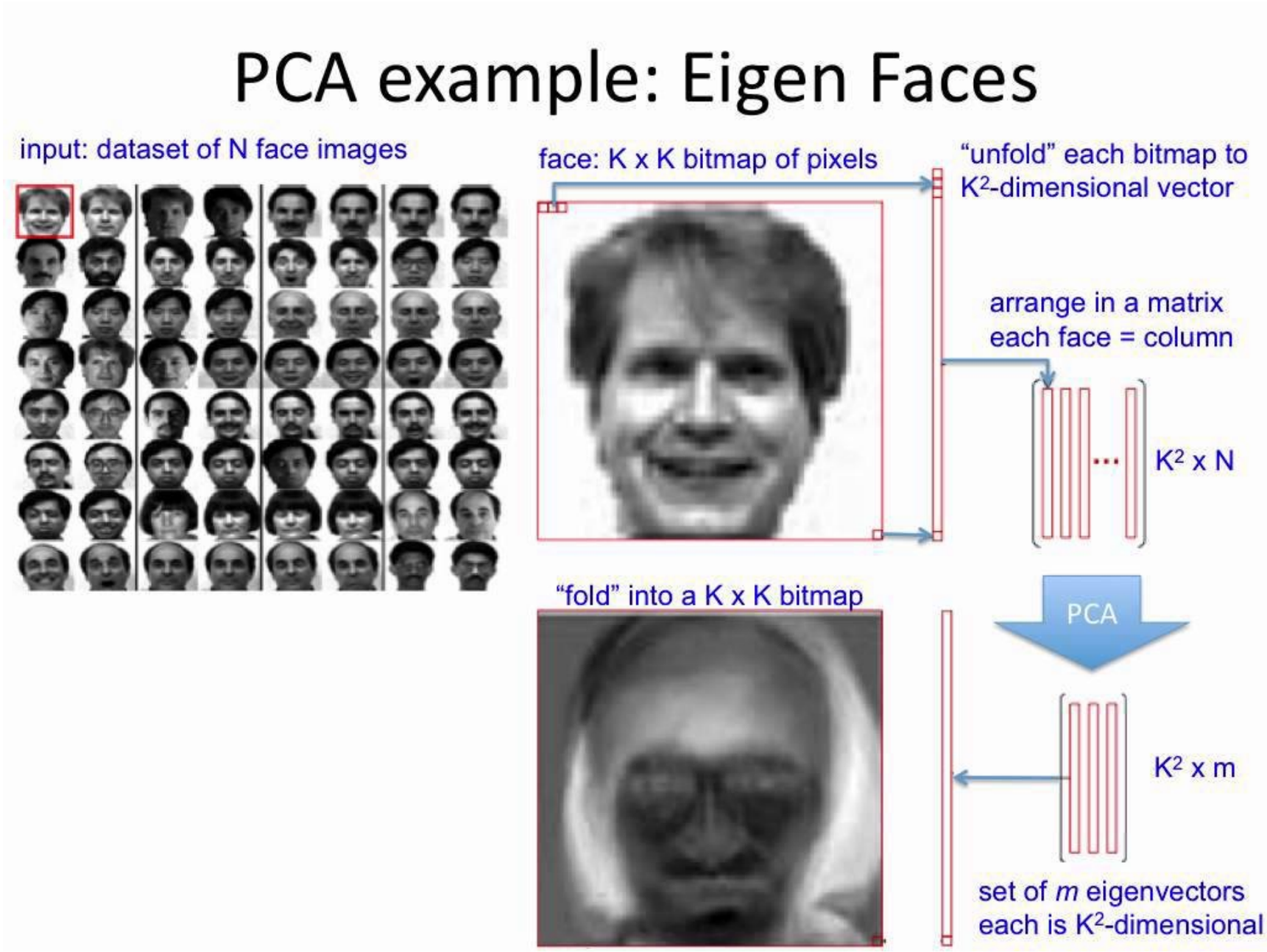


PCA results


PCA Components
Magnitude
time
4
3
2
1
0
−1
−2
−3
0
500
1000
1500
2000

Independent component analysis

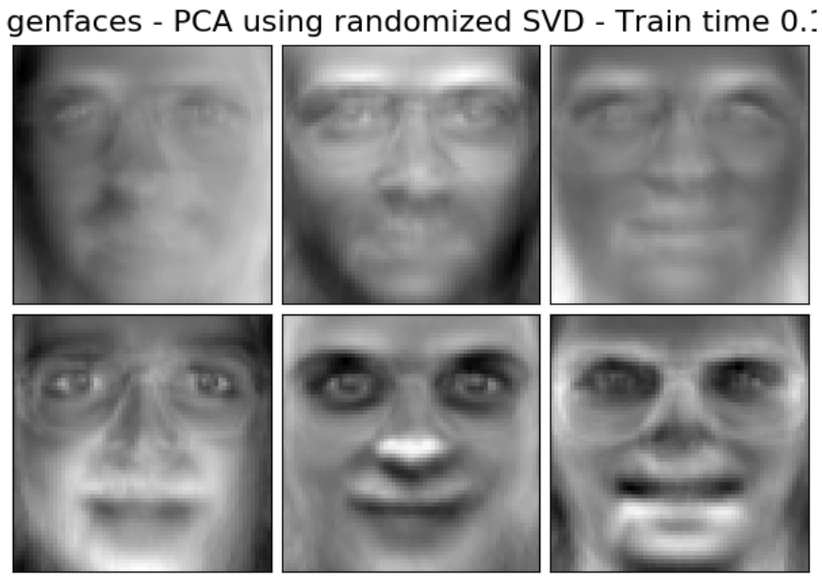
PCA

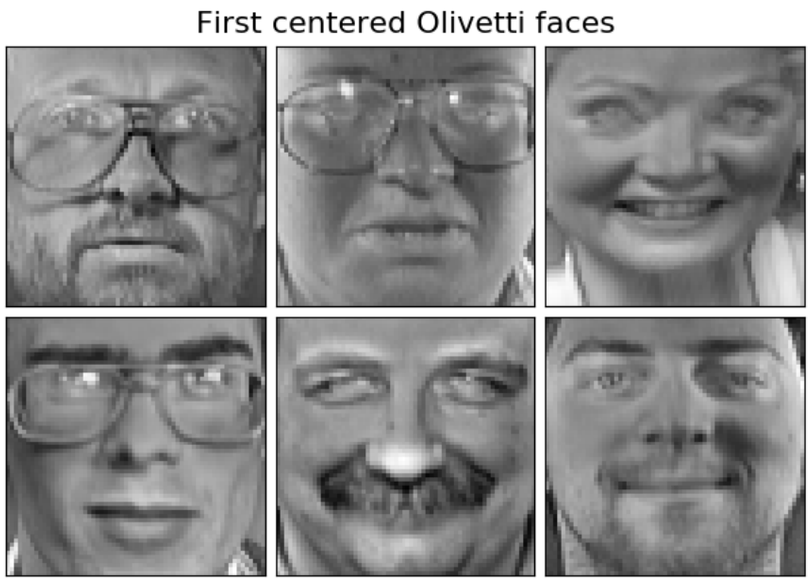


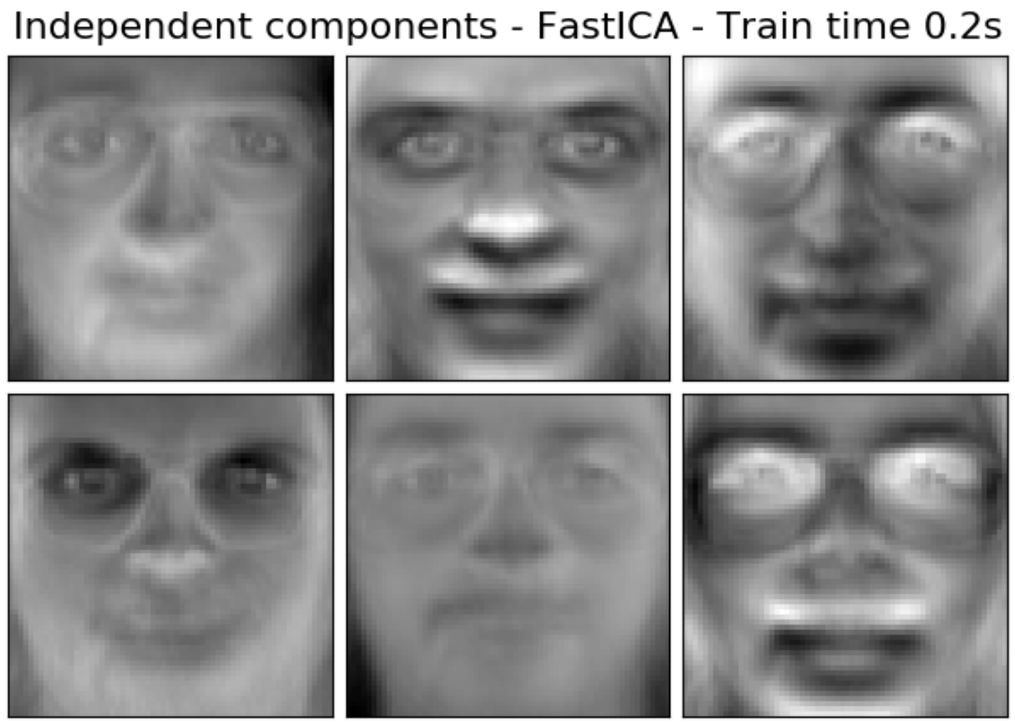
Independent component analysis

$$x = A \cdot s$$

where the s_i are statistically independent signals







Independent component analysis

fMRI response data collected* on 165 commonly heard natural sound stimuli.

Man speaking
Flushing toilet
Pouring liquid
Tooth-brushing
Woman speaking
Car accelerating
Biting and chewing
Laughing
Typing
Car engine starting
Running water
Breathing
Keys jangling
Dishes clanking
Ringtone
Microwave
Dog barking

Road traffic
Zipper
Cellphone vibrating
Water dripping
Scratching
Car windows
Telephone ringing
Chopping food
Telephone dialing
Girl speaking
Car horn
Writing
Computer startup sound
Background speech
Songbird
Pouring water
Pop song
Water boiling

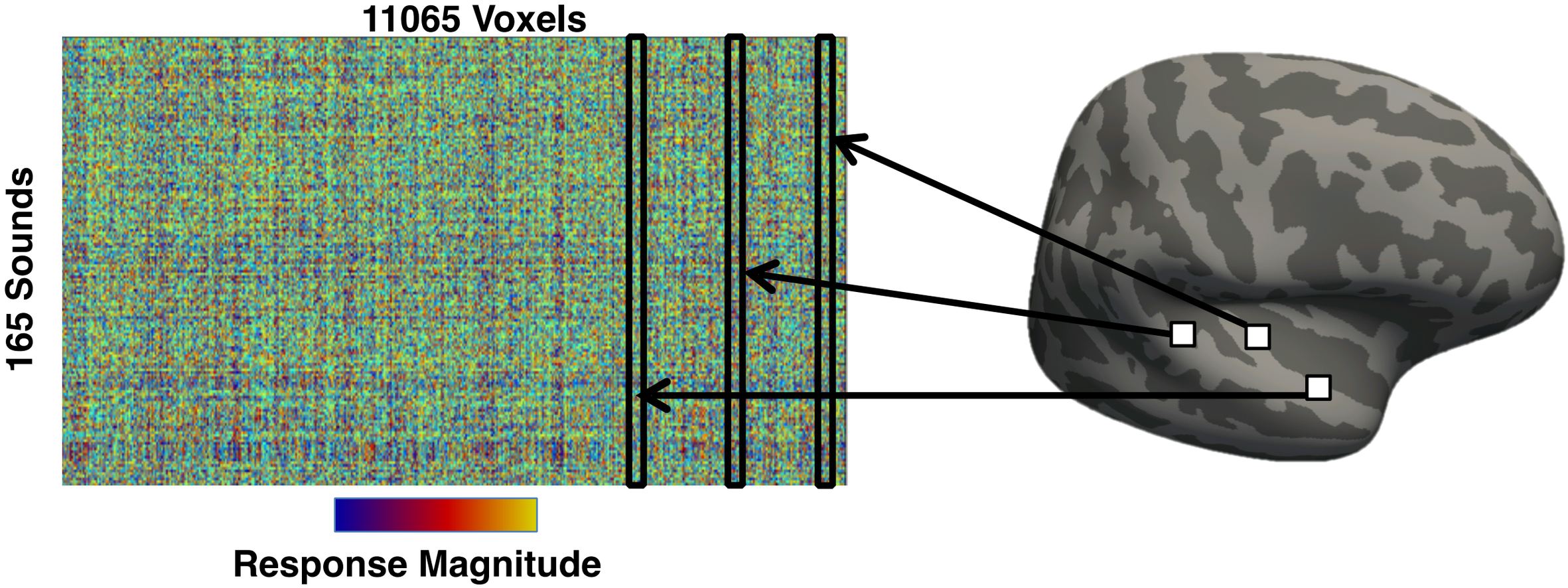
Guitar
Coughing
Crumpling paper
Siren
Splashing water
Computer speech
Alarm clock
Walking with heels
Vacuum
Wind
Boy speaking
Chair rolling
Rock song
Door knocking

•
•
•

*Sam Norman-Haignere, Nancy Kanwisher, and Josh McDermott

Independent component analysis

For each voxel, measured average response to each sound:



Data matrix: voxels X sounds.

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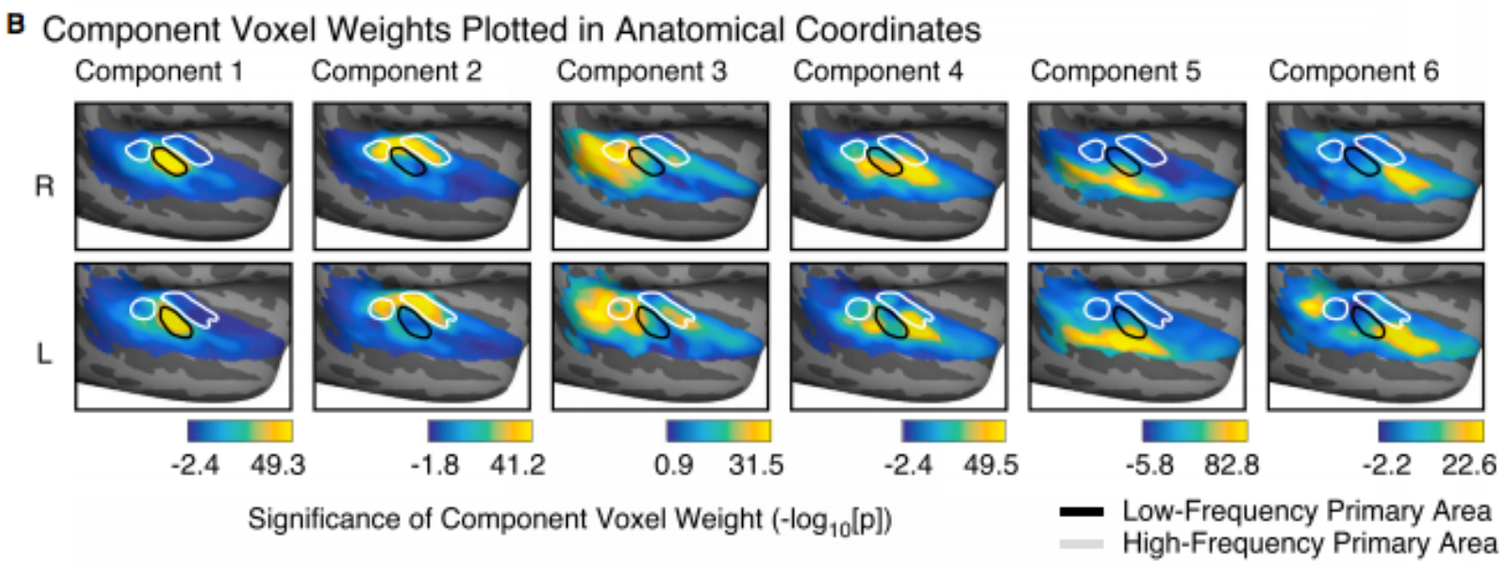
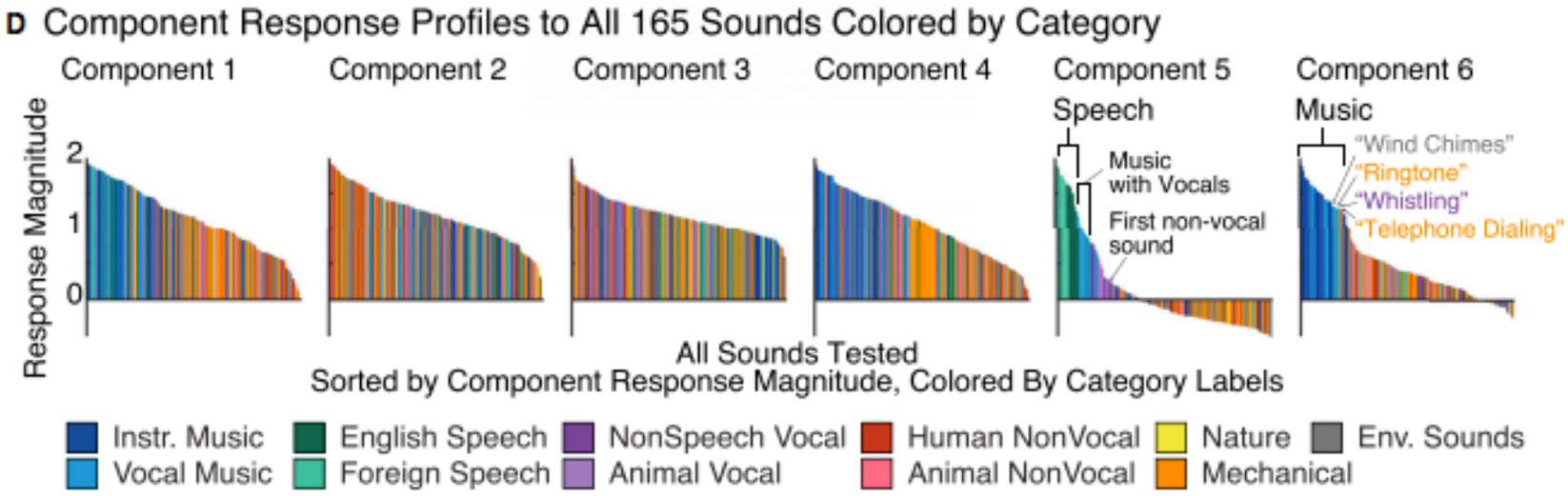


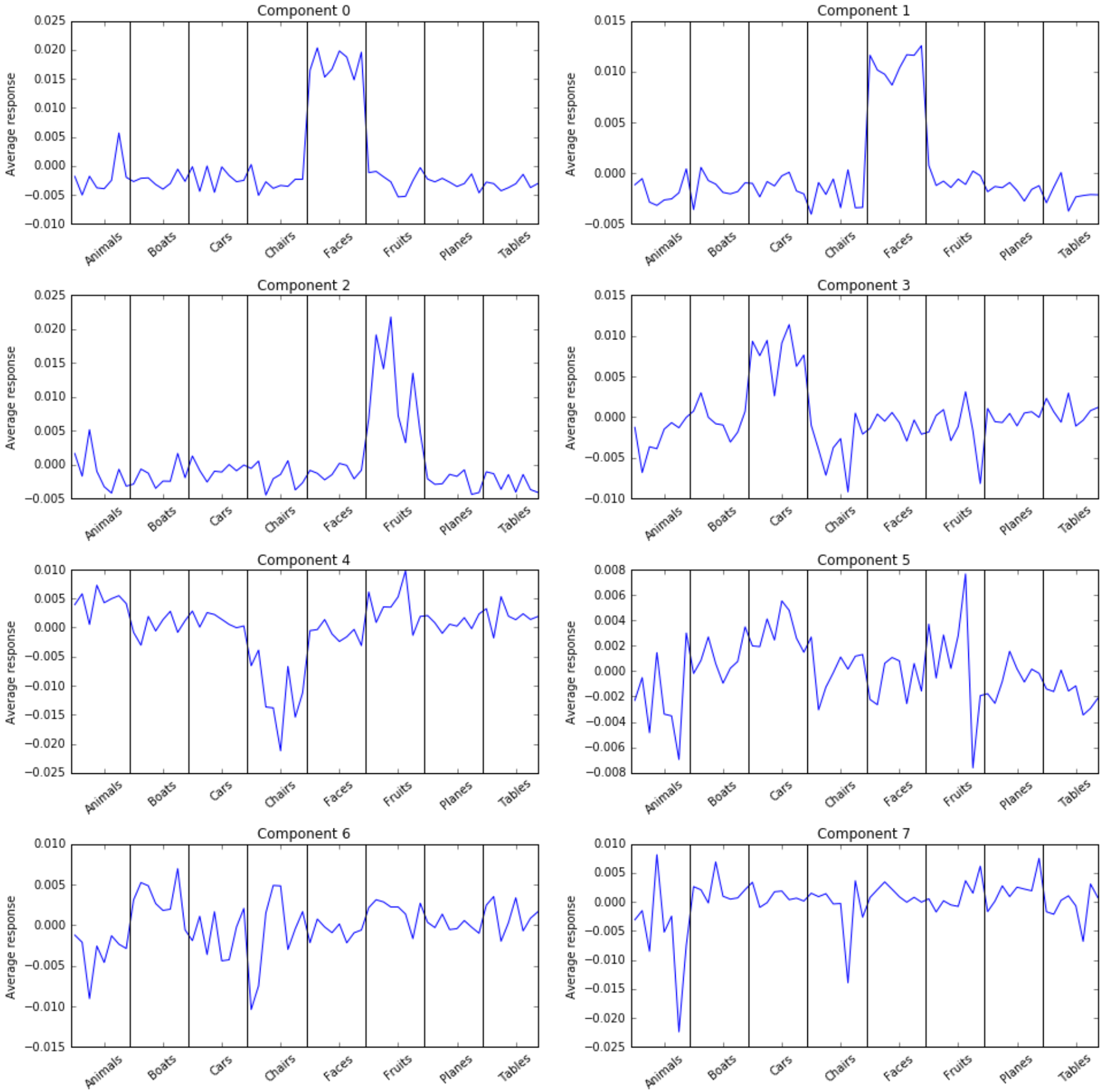


Norman-Haigniere, et. al. 2015

Independent component analysis

[Ipynb: ICA on neural data]

Independent component analysis



Other Factorization Methods

Non-negative Matrix Factorization (NMF)

Sebastian Seung

$$X \sim W \cdot H \qquad\qquad W, H \geq 0$$

minimize: $$\frac{1}{2} \sum_{ij} (X_{ij} - (W \cdot H)_{ij})^2$$

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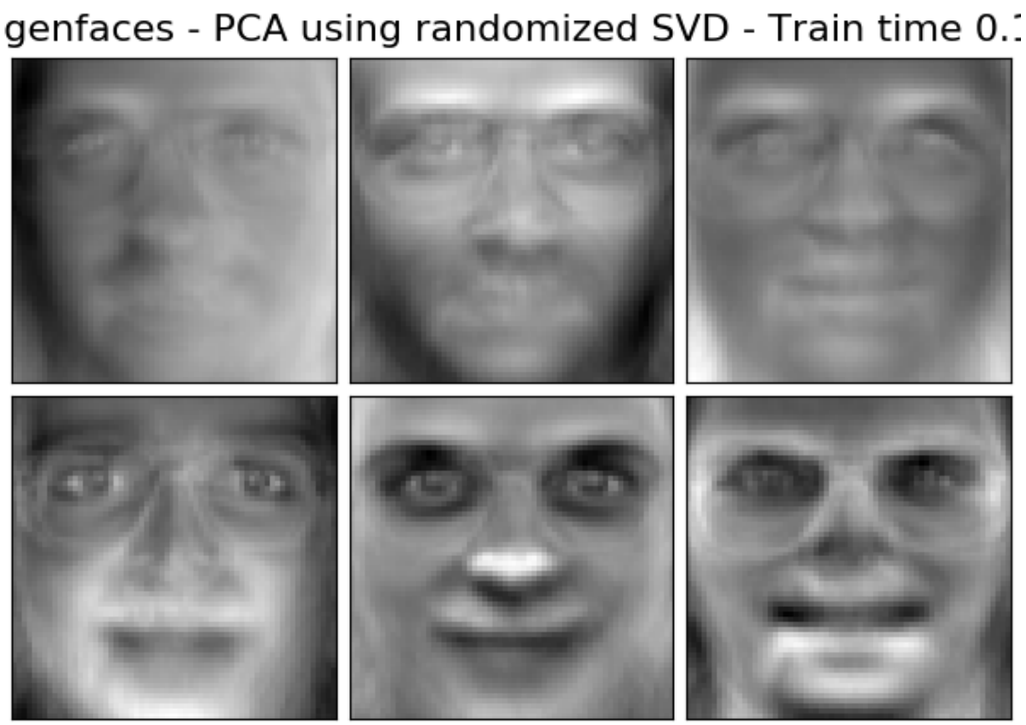

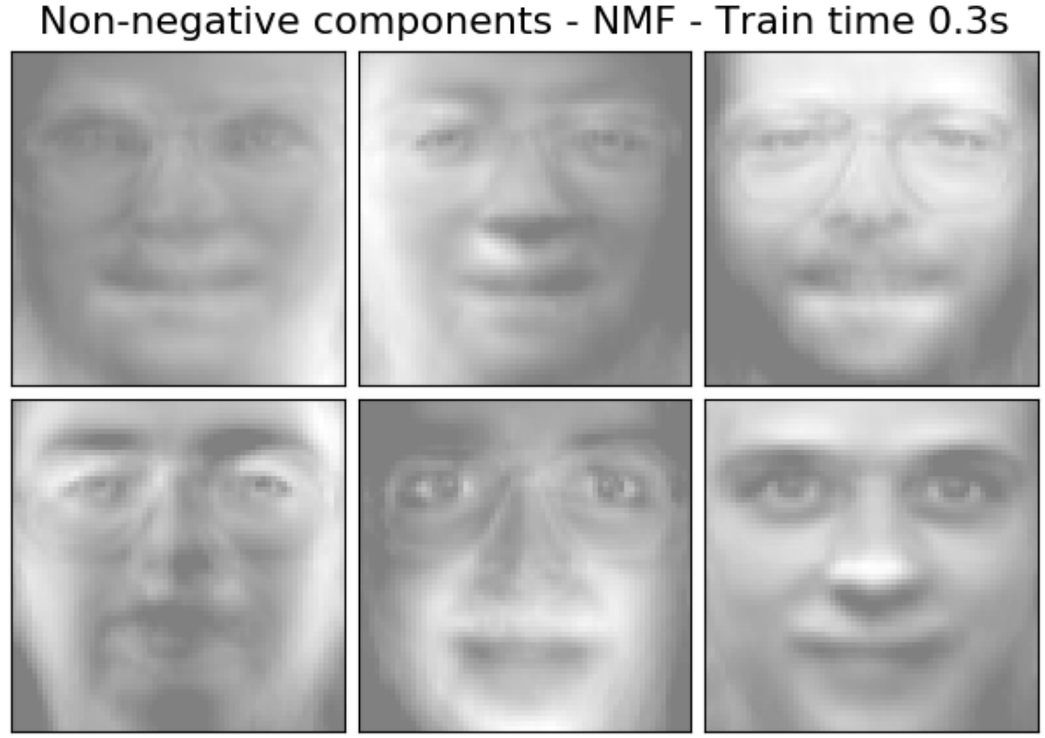

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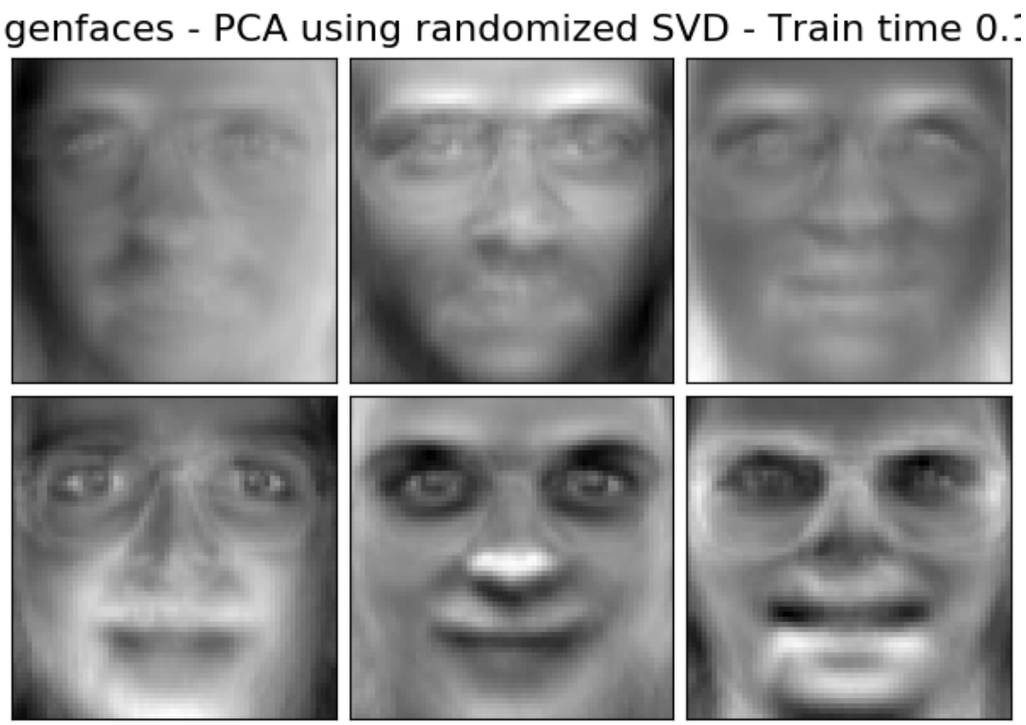
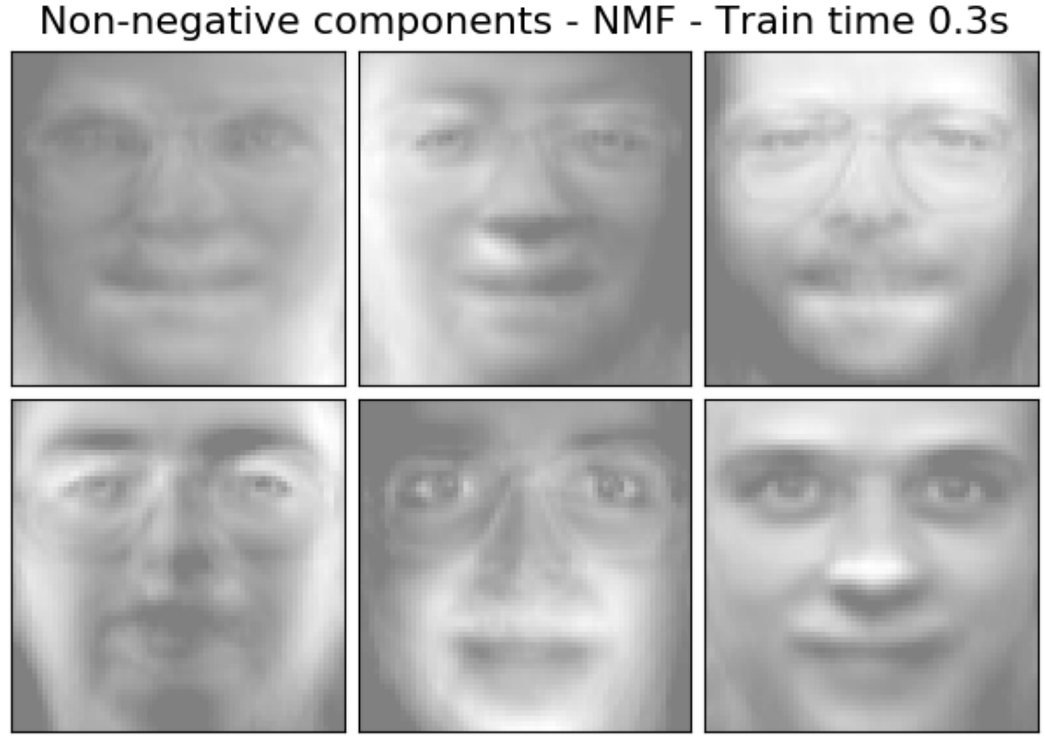




regularization: $$\frac{1}{2}\sum_{ij}(X_{ij} - (W \cdot H)_{ij})^2 + \alpha(||W||_1 + ||H||_1)$$

Other Factorization Methods

Non-negative Matrix Factorization (NMF)

NEURORESOURCE

Simultaneous Denoising, Deconvolution, and Demixing of Calcium Imaging Data

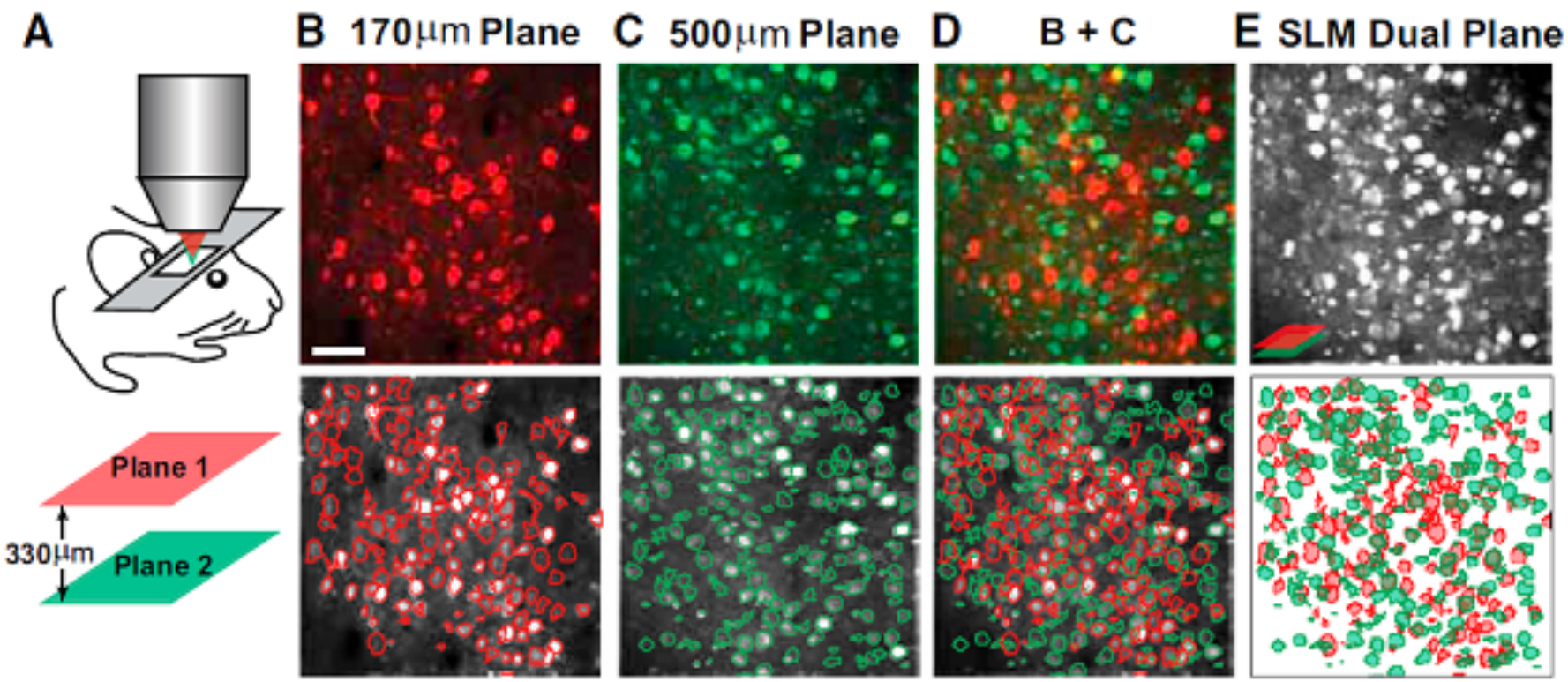
Eftychios A. Pnevmatikakis, Daniel Soudry, Yuanjun Gao, Timothy A. Machado, Josh Merel, David Pfau, Thomas Reardon, Yu Mu, Clay Lacefield, Weijian Yang, Misha Ahrens, Randy Bruno, Thomas M. Jessell, Darcy S. Peterka, Rafael Yuste, Liam Paninski

Published Online: January 07, 2016

Open Archive | PlumX Metrics

DOI: http://dx.doi.org/10.1016/j.neuron.2015.11.037 | CrossMark

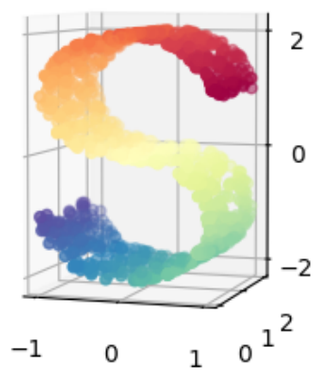
Article Info

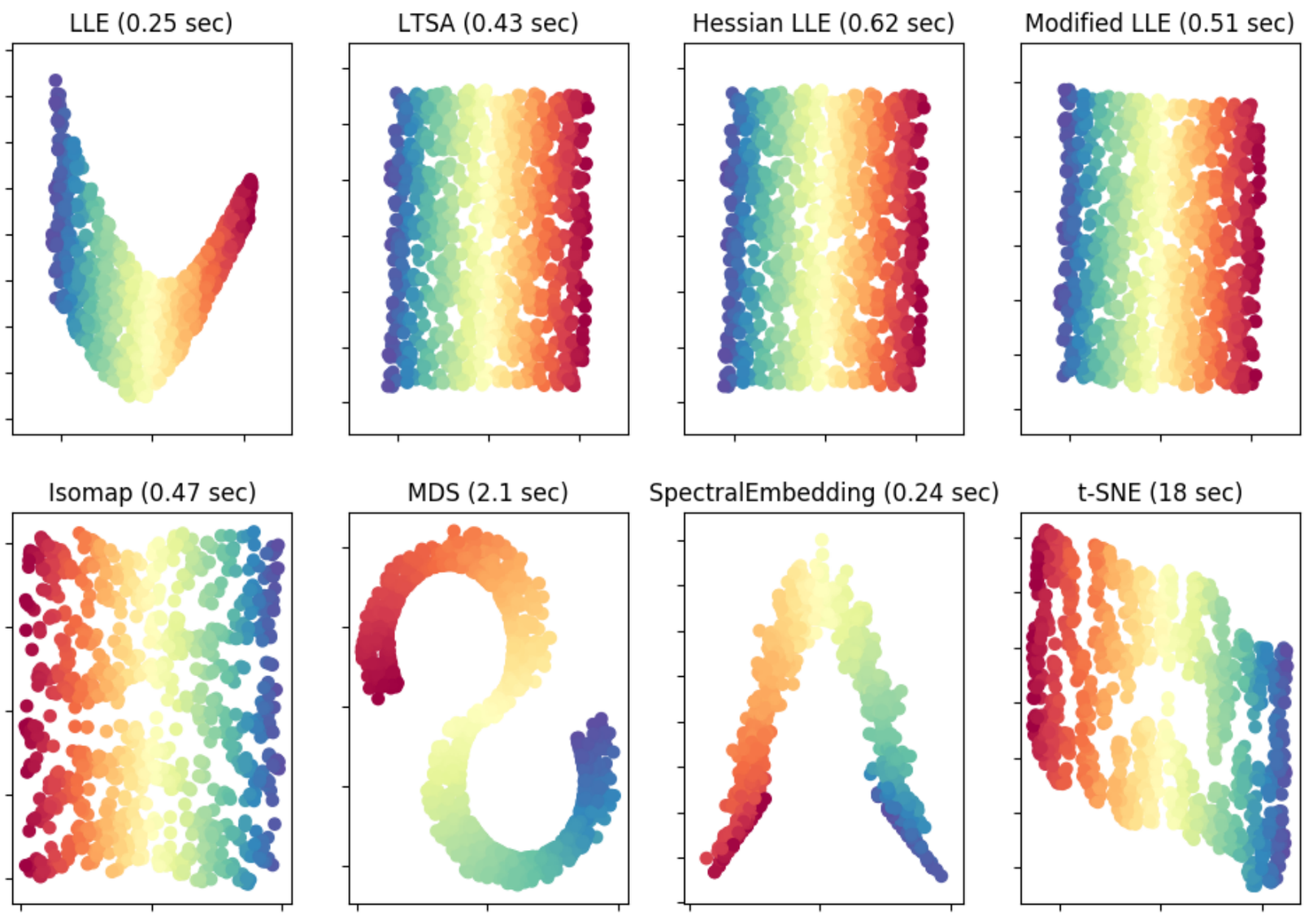


Manifold Learning

Arrange the data so that values fill out "nice" coordinates on a "nicely-shaped" manifold

True 3D data





Various embeddings in 2D

Manifold Learning

Multi-Dimensional Scaling (MDS)

Goal: find an "embedding function"

$$F : \mathbb{R}^k \longrightarrow \mathbb{R}^l$$

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but such that distances have been preserved:

$$d(F(x_i), F(x_j)) \sim d(x_i, x_j)$$

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distance in reduced-dim embedding

distance in original space

Manifold Learning

Multi-Dimensional Scaling (MDS)

$$F : \mathbb{R}^k \longrightarrow \mathbb{R}^l; l \ll k; d(F(x_i), F(x_j)) \sim d(x_i, x_j)$$

Loss function:

$$\text{Stress}(F(x_1), \ldots, F(x_N)) = \left(\sum_{i \neq j} (d(x_i, x_j) - ||F(x_i) - F(x_j)||)^2 \right)^{\frac{1}{2}}$$

Optimization by seeking to minimize stress.

Manifold Learning

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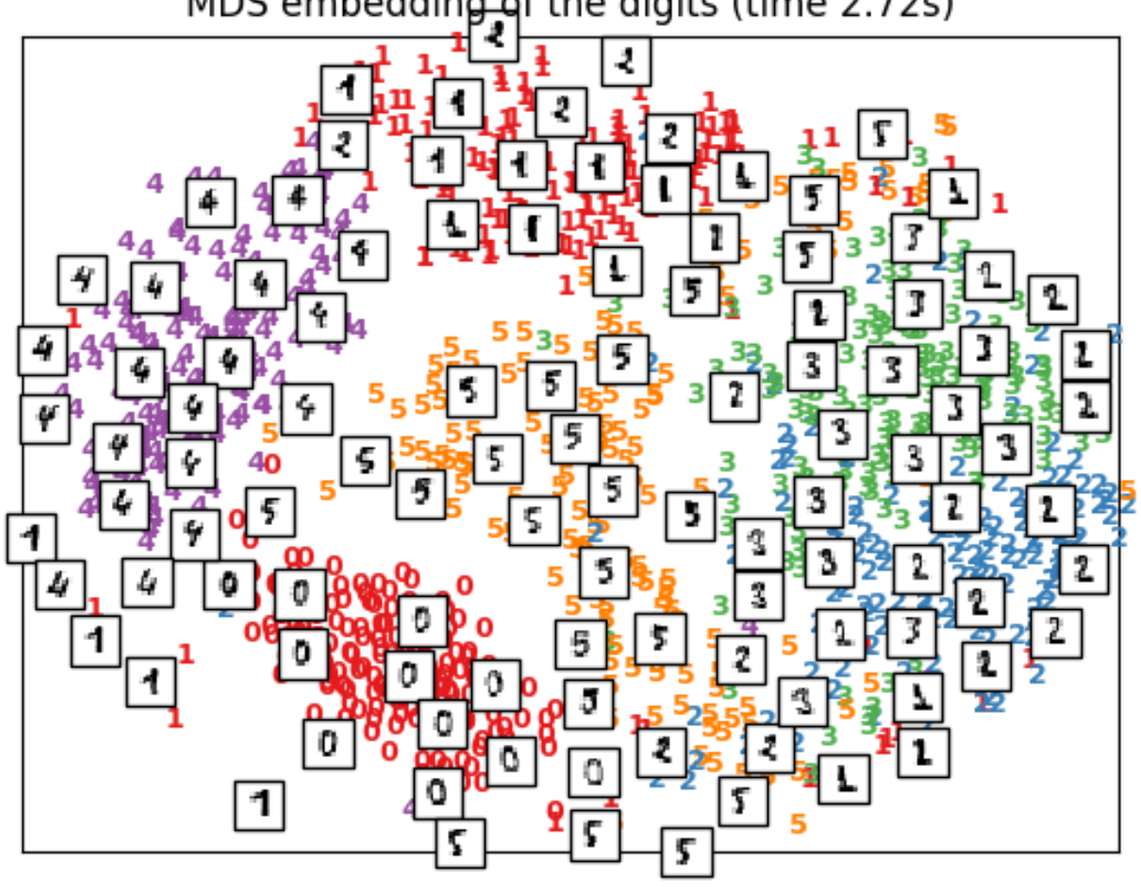
A selection from the 64-dimensional digits dataset

MDS embedding of the digits (time 2.72s)



number of dimensions / learned via supervision.

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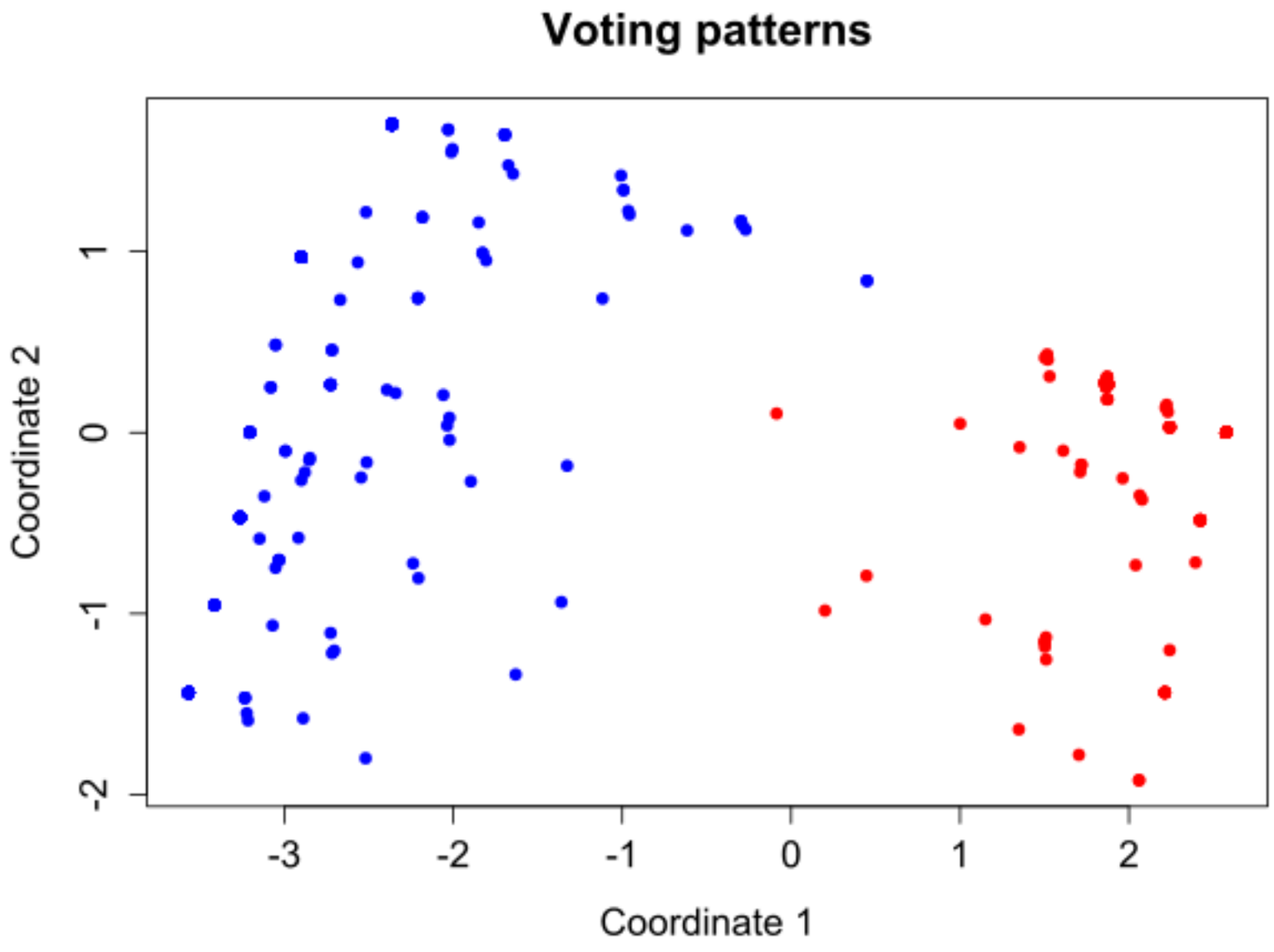

"An example of classical multidimensional scaling applied to voting patterns in the United States House of Representatives. Each red dot represents one Republican member of the House, and each blue dot one Democrat."

from Wikipedia

Independent component analysis

[Ipynb: MDS on neural data]

Manifold Learning

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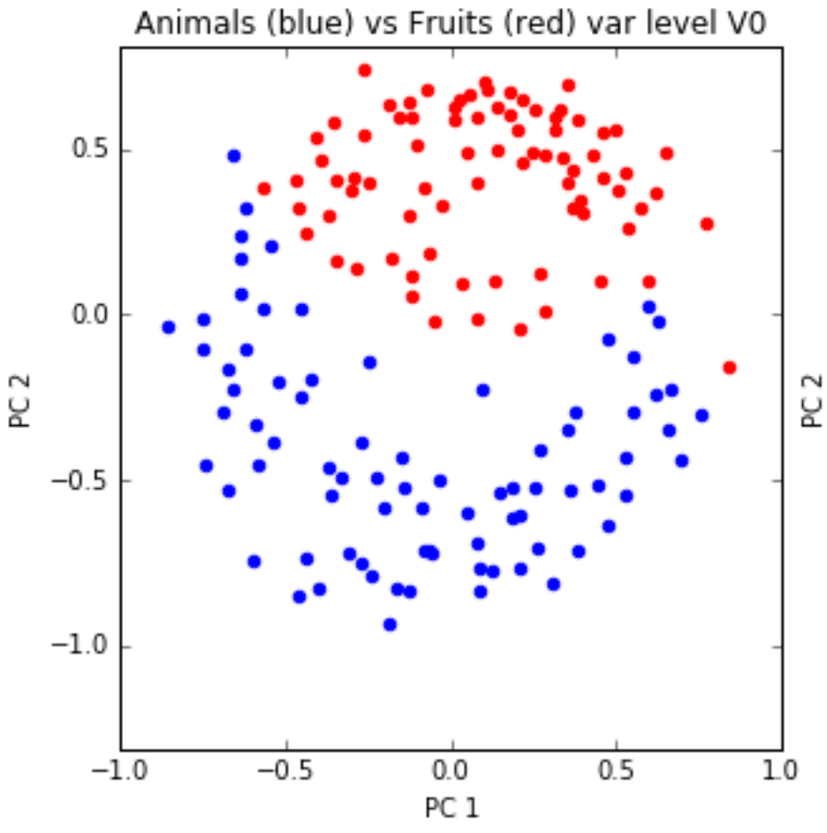
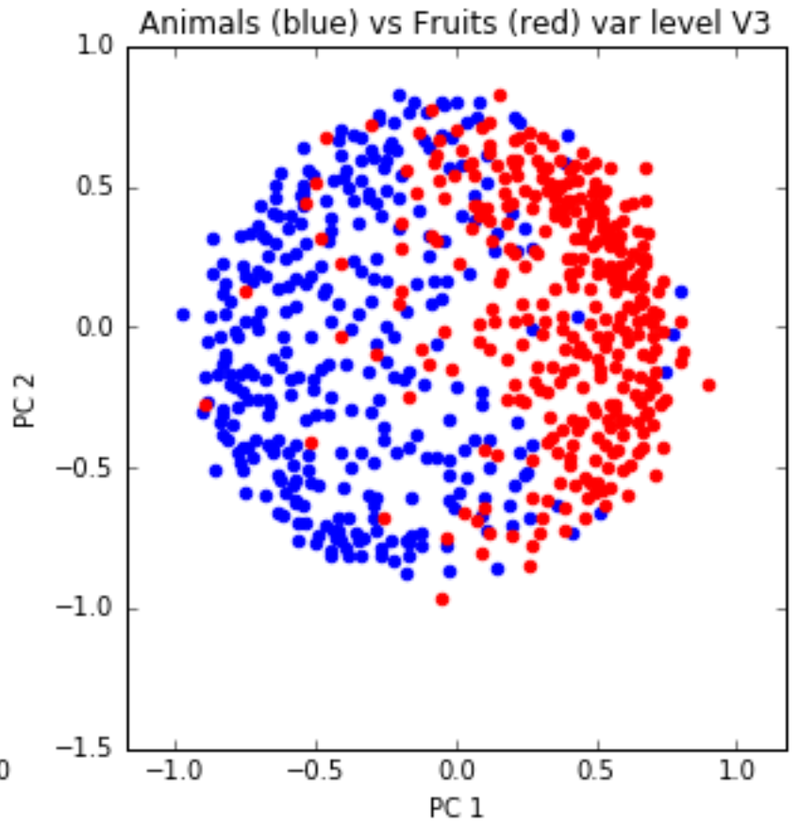
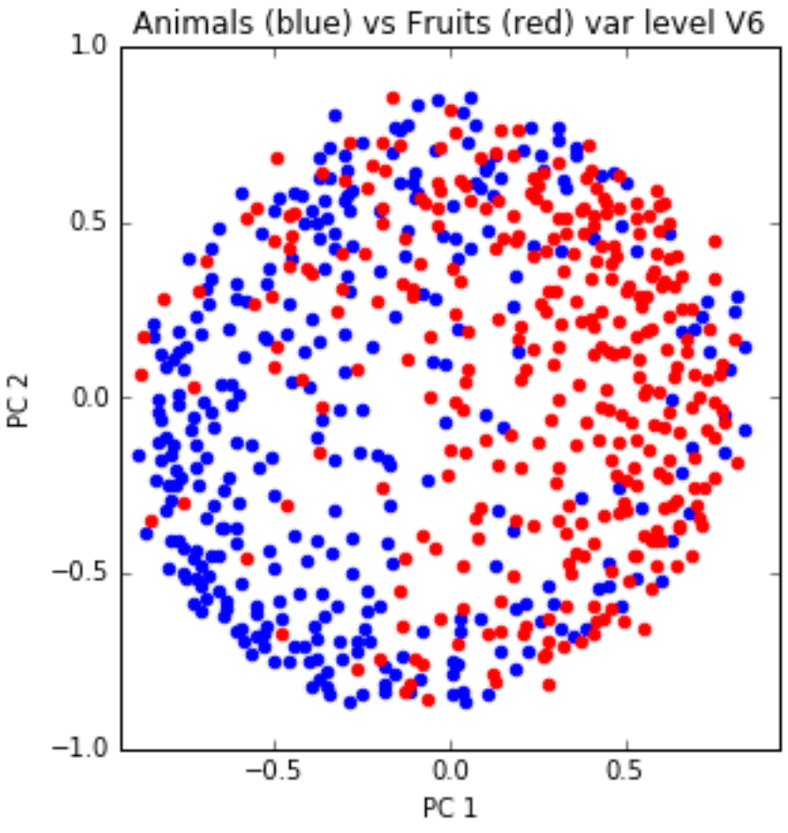
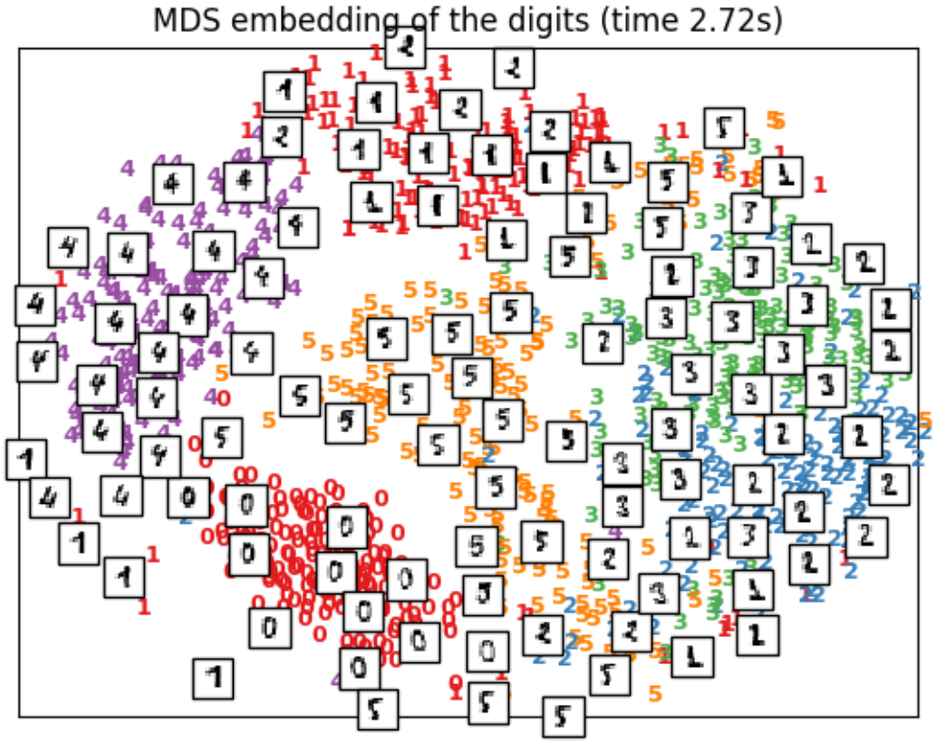


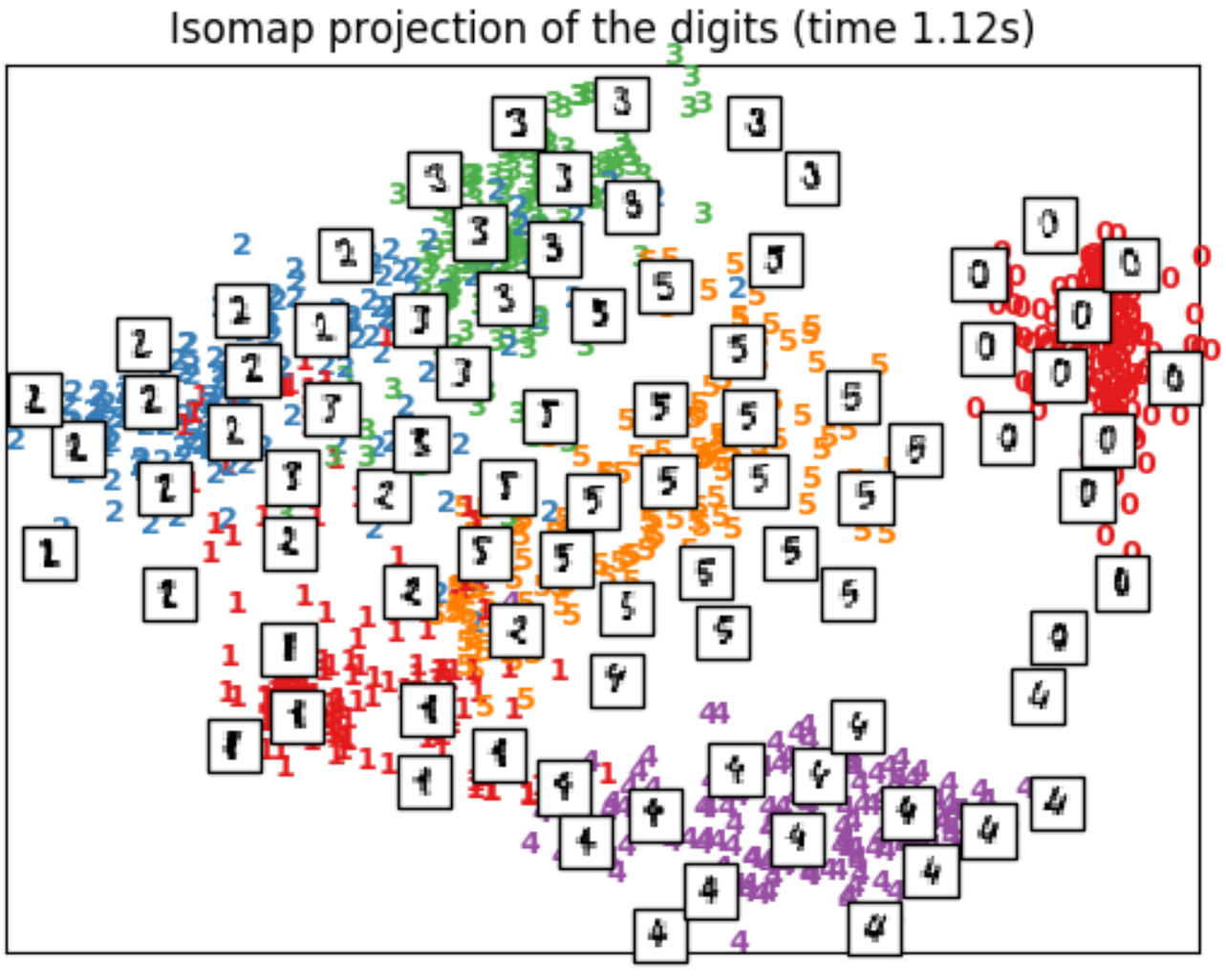




Manifold Learning

IsoMap: extends MDS by using computing distances relative to k-nearest neighbor graph in the high-dimensional space (e.g "manifold geodesics" rather than straight-line distance).





number of dimensions *l* and neighborhood *k* learned via supervision.

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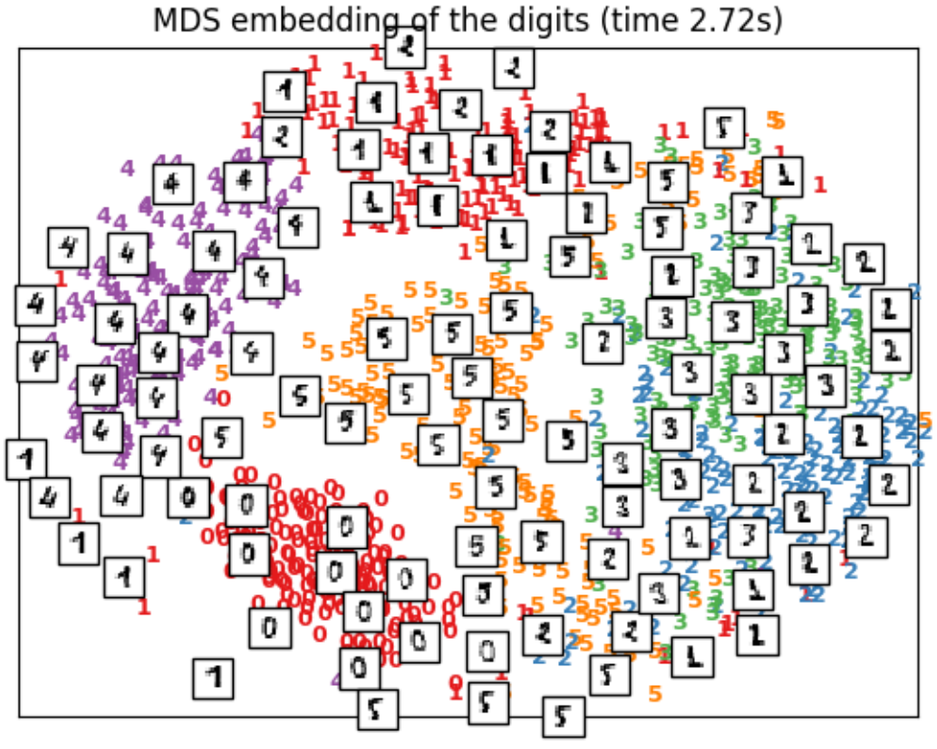

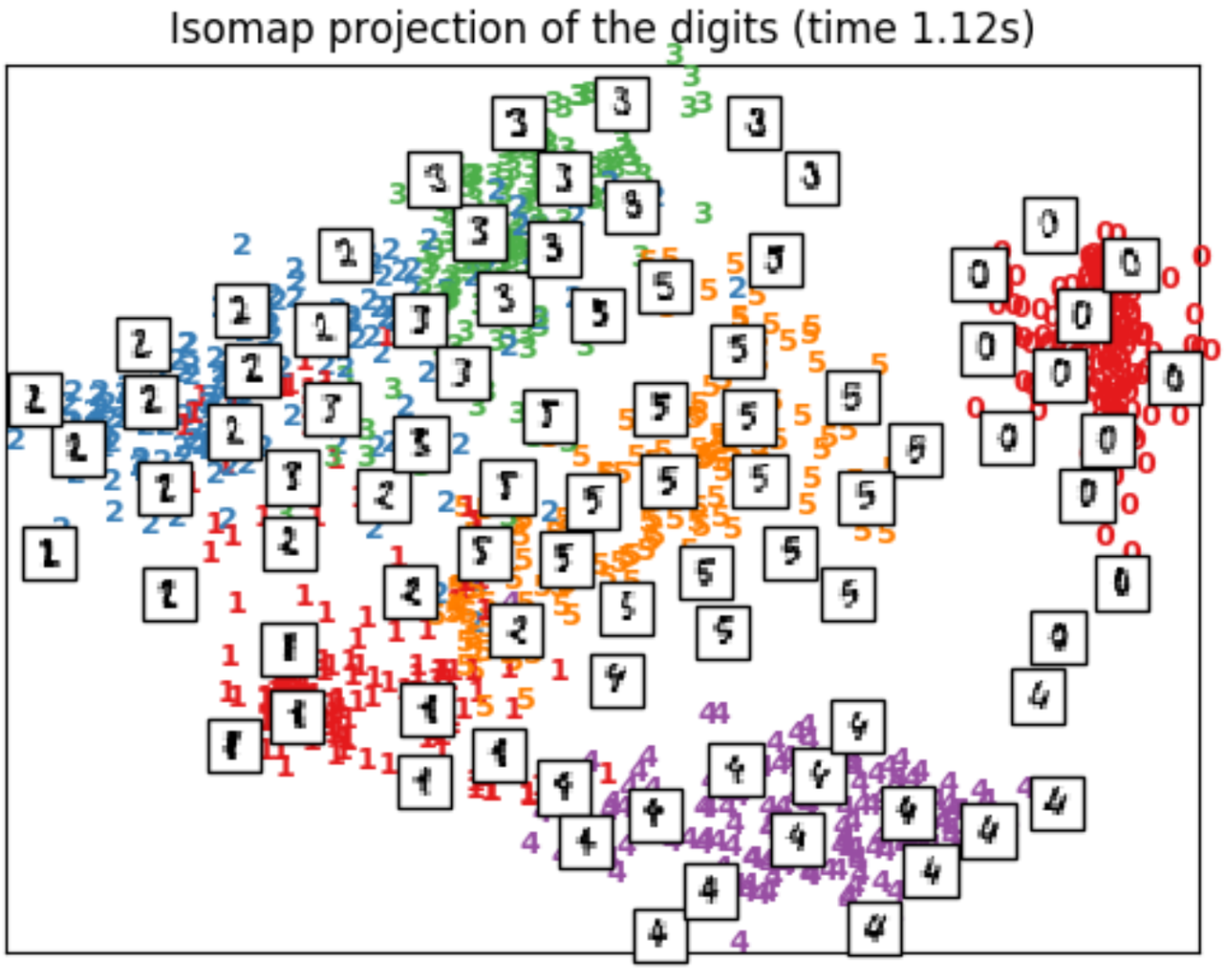

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Manifold Learning

t-SNE chooses a particular generative model for data and for the compression

$$x \in \mathbb{R}^k; y \in \mathbb{R}^l; l \ll k; F(x) \longmapsto y$$

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$$x \in \mathbb{R}^k; y \in \mathbb{R}^l; l \ll k; F(x) \longmapsto y$$

$$d(x_i, x_j) = \frac{exp(-|x_i - x_j|^2/2\sigma_i^2)}{\sum_{k \neq i} exp(-|x_i - x_k|^2/2\sigma_i^2)} + \text{symmetric term}$$

as if generated from gaussian joint probability

Manifold Learning

t-SNE chooses a particular generative model for data and for the compression

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$$d(y_i, y_j) = \frac{1/(1 + (y_i - y_j)^2)}{\sum_{k \neq i} 1/(1 + (y_i - y_k)^2)}$$

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Manifold Learning

t-SNE chooses a particular *generative model* for data and for the compression

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as if generated from student t distribution

minimize $\sum_{i,j} d(x_i, d_j) log \left[\frac{d(x_i, x_j)}{d(y_i, y_j)} \right]$

KL-divergence

Manifold Learning

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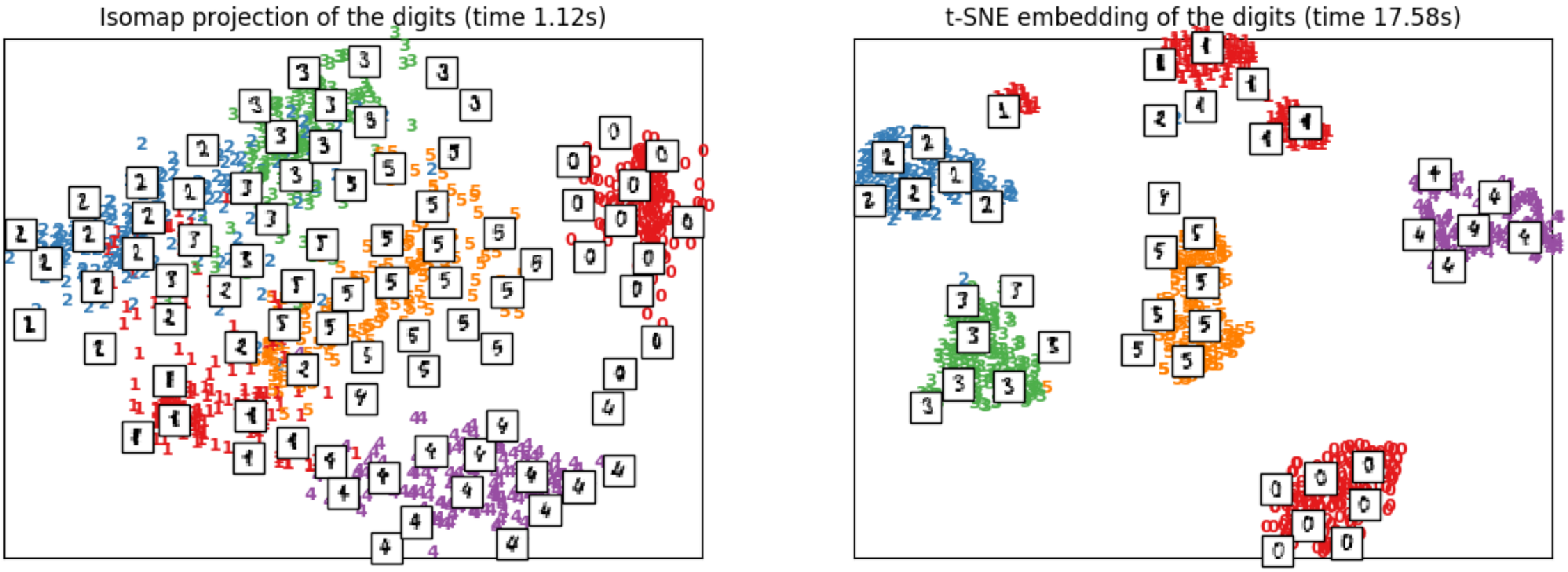

2 parameters: *l*, perplexity (related to sigmas).