Data Driven Engineering I: Machine Learning for Dynamical Systems

Analysis of Static Datasets II: Dimensionality Reduction

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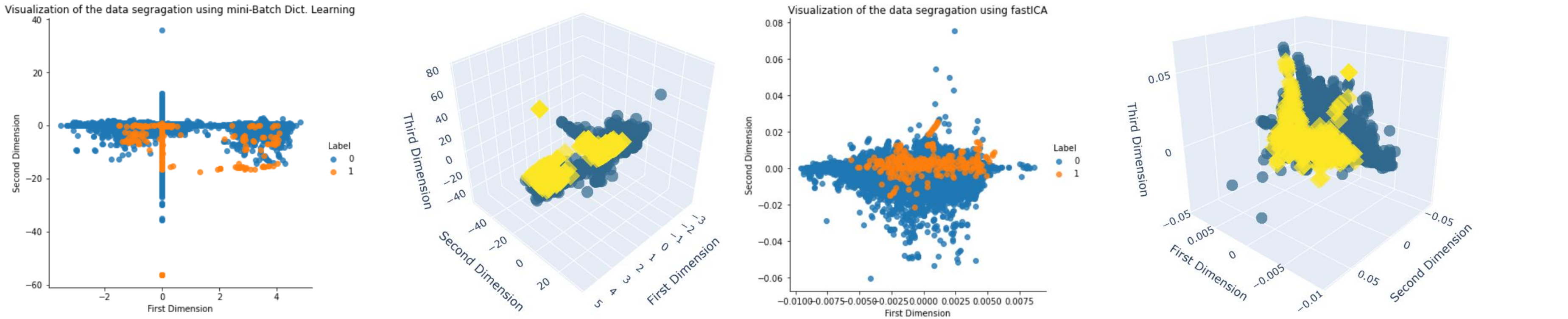


One Page Summary of the Previous Week

* Outlier Detection ⇒ Clustering

* IV Models

(i) k-means ⇒ known structure
(ii) GMM ⇒ known structure
(iii) Hierar. Clustering ⇒ unknown str.
(iv) DBSCAN ⇒ Unknown structure

* Unsupervised Learning ⇒ Model Evalution ?

(i) Silhouette score ⇒ no label
(ii) Homogeneity ⇒ (partial) label
(iii) Custom ⇒ Precision Score

* Data Management ⇒ (local / cloud) uploading ⇒ Label encoding
"text" → [0, 1]

Today’s Agenda

Basic Steps to Follow:

0.) Understand the business / task.
1.) Understand the data.
2.) Explore & prepare the data.

Still valid

3.) Shortlist candidate models. — 2 major type

4.) ~~Training the model~~

5.) Evaluate the model predictions — 3 evaluation tools

6.) "Serve" the model !

Dimensionality Reduction

* When: Data has large number of features (dimensions)

① Computational: compress initial data as a preprocessing step

- e.g. k-Means $\propto (M \times N) \Rightarrow (M' \times N) \quad M' \ll M$

② Feature Extraction: lower dim. representation of the physics

- $M' < M \Rightarrow$ more effective usage of features
- $M' \approx M \Rightarrow$ Coordinate Transformation: $[x, y, z, u, v, w] \Rightarrow [PC_1, PC_2, u', v', w']$

Dimensionality Reduction

* When: Data has large number of features (dimensions)

③ Visualization : exploratory analysis of data (planning phase)

- $M \rightarrow 2 \,//\, 3$ space

Two major branches:

(i) Linear Projection methods
- eg. SVD, PCA, random projection

(ii) Non-linear projection (manifold learning)
- learn the curved distance
- isomap, MDS, LLE, t-SNE, ICA, dictionary learning, Random trees embedding

#0 Understanding the task

- ❑ **Problem**: Manufacturing error in a production line
- ❑ **Modified sensory input:** 28 variables including sensory input
- ❑ 280,000 instances, where only a **small fraction** (~500) of products are **defective**.
- ❑ **Heuristic**: <0.5% is defective

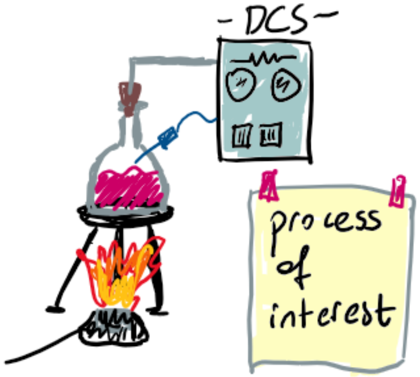
A similar example for you:

"Bosch Production Line Performance
Reduce manufacturing failures"

Dim. Reduction:

- Computational
  - preprocessing -
- Feature Extraction
  - ~ pattern recognition ~
- Visualization

Idea:



$$\Rightarrow X = \begin{bmatrix} \text{———} \\ \text{— product}_n \text{ —} \\ \text{———} \end{bmatrix}$$

→ information m on the production line

Idea:

Assume:

- $\text{product} = \sum_{i=1}^{K} \text{process}_i$
- Features m is correlated to K steps in the production line;

Then:

$$X \rightarrow \boxed{D.R.} \rightarrow \tilde{X} \rightarrow \boxed{DR^T} \rightarrow X'$$

physical coordinates

"latent space"

physical coordinates

Encoding

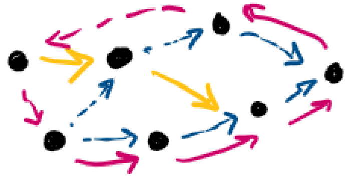
Decoding

if DR is capable of learning the patterns in the physical system;

$$X \approx X'$$

Idea:

Interpretting Patterns



* Physical system is composed of logical steps;
* Logical steps followed ⇒ "Regular product"
* Failure at some point ⇒ "Defect"

"Outlier Detection"

A.I.

"Something is wrong here."

Aim ⇒ Learn enough to detect outliers;

#1 Understanding the data

- Check the data source: understand what the data refers to
- Objective: understand the characteristics of the data
- Look at the feature columns:
  - Any missing values?
  - Any features with NaN values?
  - Uniqueness of the dataset? (“cardinality”)

=> Colab

```
 23   S23       284807 non-null   float64
 24   S24       284807 non-null   float64
 25   S25       284807 non-null   float64
 26   S26       284807 non-null   float64
 27   S27       284807 non-null   float64
 28   S28       284807 non-null   float64
 29   Class     284807 non-null   object
dtypes: float64(29), object(1)
memory usage: 65.2+ MB
time: 54.5 ms
```

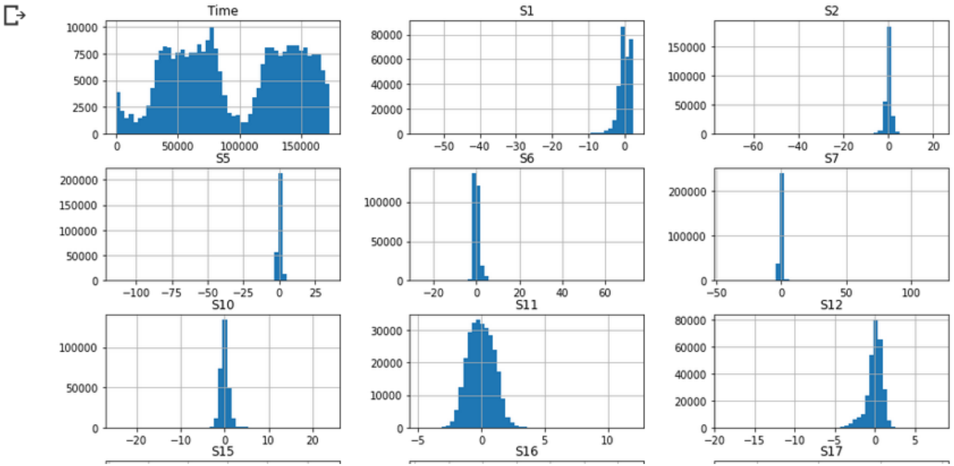
	Time	S1	S2	S3	S4	S5	S6
count	284807.000000	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05	2.848070e+05
mean	94813.859575	1.758743e-12	-8.252298e-13	-9.636929e-13	8.316157e-13	1.591952e-13	4.247354e-13
std	47488.145955	1.958696e+00	1.651309e+00	1.516255e+00	1.415869e+00	1.380247e+00	1.332271e+00
min	0.000000	-5.640751e+01	-7.271573e+01	-4.832559e+01	-5.683171e+00	-1.137433e+02	-2.616051e+01
25%	54201.500000	-9.203734e-01	-5.985499e-01	-8.903648e-01	-8.486401e-01	-6.915971e-01	-7.682956e-01
50%	84692.000000	1.810880e-02	6.548556e-02	1.798463e-01	-1.984653e-02	-5.433583e-02	-2.741871e-01
75%	139320.500000	1.315642e+00	8.037239e-01	1.027196e+00	7.433413e-01	6.119264e-01	3.985649e-01
max	172792.000000	2.454930e+00	2.205773e+01	9.382558e+00	1.687534e+01	3.480167e+01	7.330163e+01

time: 447 ms

#2 Exploring the data

- ❑ **Objective**: generate a data quality report

- ❑ Using standard statistical measures of central tendency and variation
  - ❑ tabular data and visual plots
  - ❑ mean, mode, and median
  - ❑ standard deviation and percentiles
  - ❑ bars, histograms, box and violin plots



- ✓ Missing values,
- ✓ Irregular cardinality problems,
  - ▪ 1 or comparably small
- ✓ Outliers
  - ▪ invalid outliers and valid outliers

#2 Exporing the data: Correlation Matrix

- Shows the correlation between each pair of features

$$\mathrm{Cov}(a,b) = \frac{1}{n-1}\sum_{i=1}^{n}\left[(a_i-\bar{a})\times(b_i-\bar{b})\right]$$

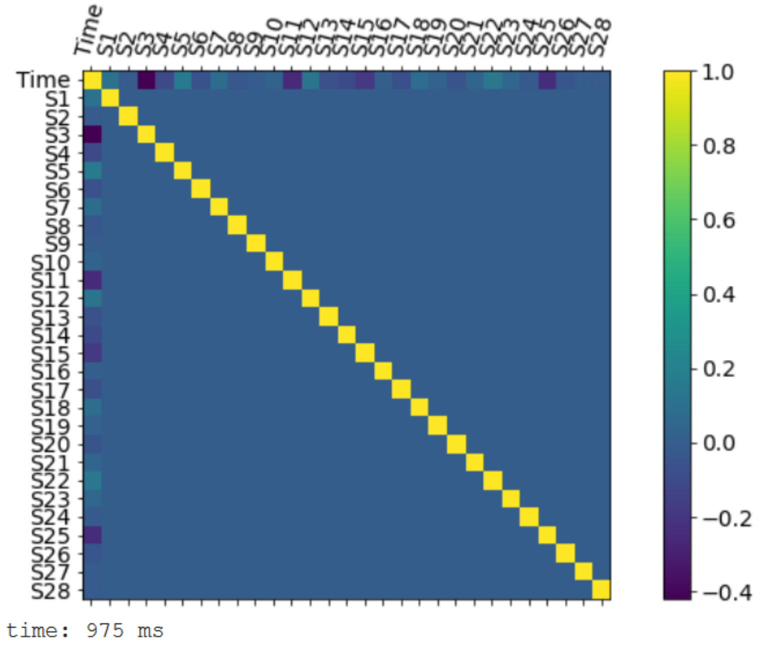
Features — instance — mean — mean

- Normalized form of "covariance"

$$\Downarrow$$

$$\mathrm{Corr}(a,b) = \frac{\mathrm{Cov}(a,b)}{SD(a)\times SD(b)}$$

* Normalized
* Dimensionless
Easy to interpret



- Ranges between −1 and +1

#2 Preparing the Data

- Clustering >> unsupervised >> **training & test split not needed**

- We will use it to **reduce the volume of the data** when needed:

```
[ ] X_train, X_test, y_train, y_test = train_test_split(dataX,
    dataY, test_size=0.9,
    random_state=2020, stratify=dataY)

    time: 188 ms
```

#3 Candidate Models: PCA

Principal Component Analysis

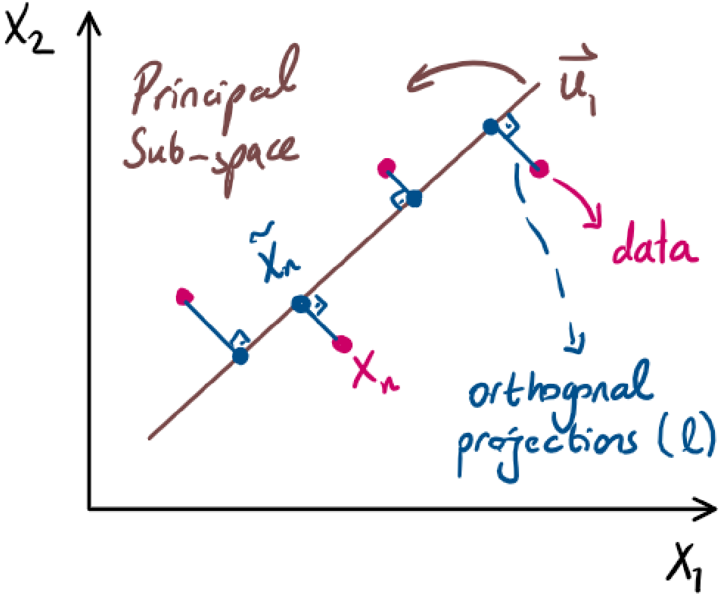
- [x] Looks into the correlation between features
- [x] Combines highly correlated ones.
- [x] New combined features ⇒ "Principal Components"

- Features $\rightleftarrows$ PC$_i$ } Reconstruction is possible

Obj: minimum information loss

[info. ≡ Variance]

How PCA works?



Objective:

* max. the variance of the • points

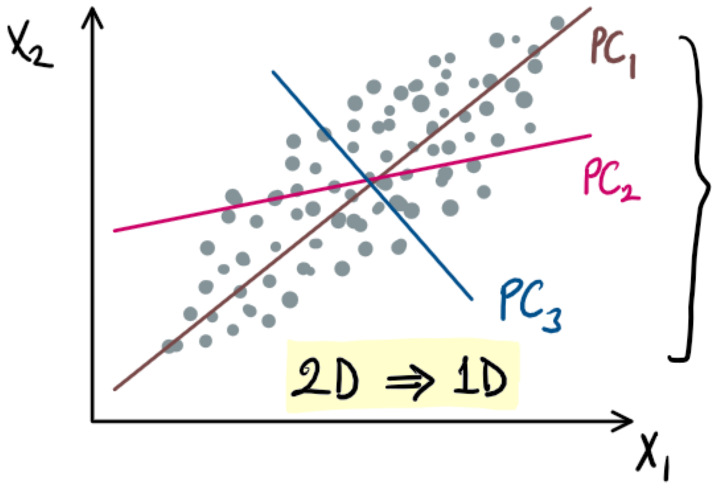
"maximum variance formulation"

$\Updownarrow$

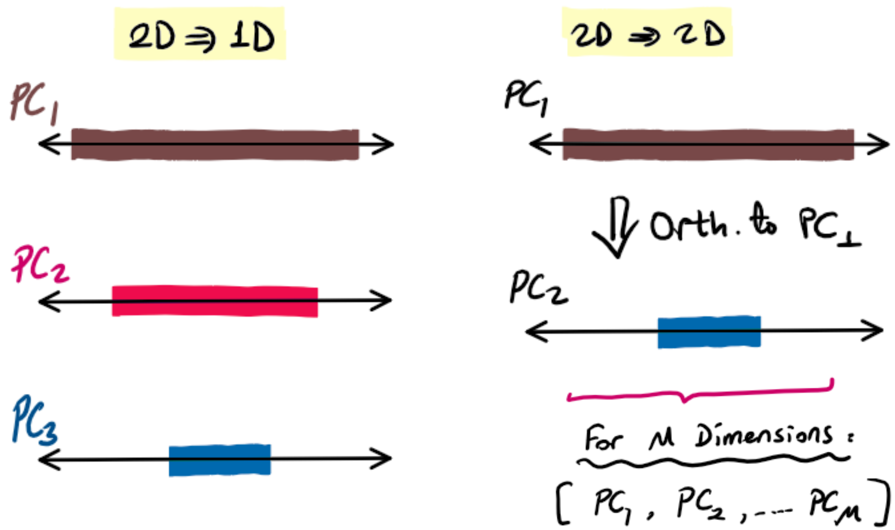
* Minimize the sum-of-squares of projection errors $\sum \ell_i$

"minimum error formulation"

Max. Correlation: how does it work?



Checking Variance



Key Property of PCA: Hierarchical coordinate system

$$PC_1 > PC_2 > PC_3 > \dots > PC_M \quad \Rightarrow \quad \sum_{i=1}^{M'} PC_i \approx \sum_{i=1}^{M} PC_i$$

Solution Method: SVD

$$X = \begin{array}{ccccc} & & & \text{feature } j & \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{array}$$

1. Evaluation of the mean $\bar{X}$
2. Finding covariance matrix S for dataset X.
3. Finding M' eigenvectors of S corresponding to M' largest eigenvalues.

Solution Method: SVD

① X must be scaled $\Rightarrow \bar{X}_j = 0$; $\underbrace{[-1, 1]}_{\text{whitened}}$
"mean centered data".

$$\bar{X} = \frac{1}{N} \sum_{n=1}^{N} X_n$$

② Calculate the covariance matrix for data:

$$S = \frac{1}{N} \sum_{n=1}^{N} (X_n - \bar{X})(X_n - \bar{X})^T$$

③ Variance of the projected data on $\vec{u}_1$

$$\frac{1}{N} \sum_{n=1}^{N} \{ u_1^T X_n - u_1^T \bar{X} \}^2 = u_1^T S u_1$$

④ Maximize the projected variance wrt u_1:

$\boxtimes$ Take derivative wrt u_1; equal to zero.

$\Downarrow$

we need to prevent $\|u_1\| \to \infty$.

☑ Introduce a Lagrangian multiplier

⑤ $u_1^T S u_1 + \lambda_1 (1 - u_1^T u_1)$

⑥ $\frac{\partial}{\partial u_1} \to \emptyset \Rightarrow S u_1 = \lambda_1 u_1$

Solution Method : SVD

⑦ $\| u_1^T \Rightarrow \boxed{u_1^T S u_1 = \lambda_1}$

$\Downarrow$

⑧ Variance will be maximum when u_1 is equal to the eigenvector having the largest eigen value λ_1.

$\Downarrow$

"First principal component"

How PCA works?

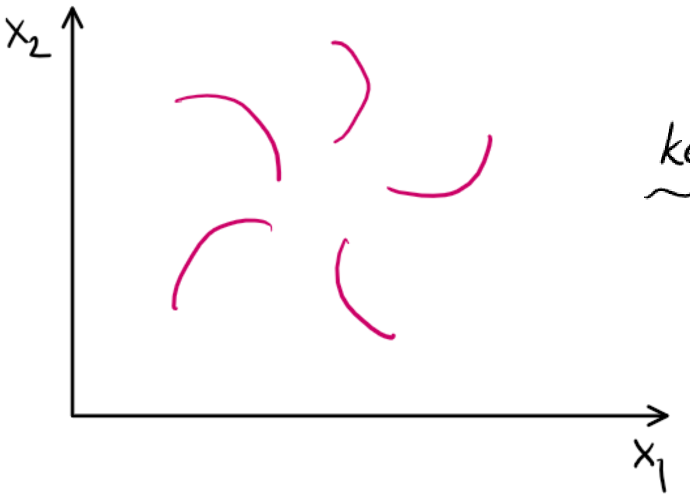
* eigen-decomposition of the covariance matrix

  ↳ PCs are orthogonal ⇒ uncorrelated to each other

  ↳ PCs have maximum correlation with measurements

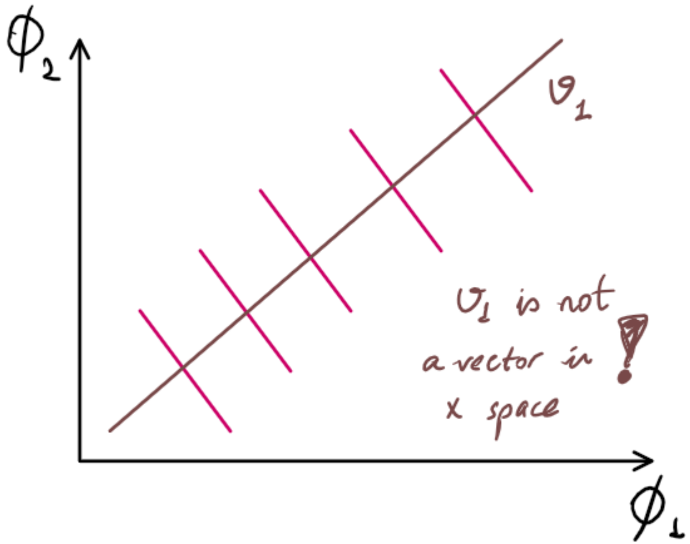
#3 Candidate Models: kernel PCA

kPCA



kernel trick:

$x \rightarrow \phi(x)$



#5 Evaluating the Results: Reconstruction error

Encoding Decoding

$$X \rightarrow \boxed{D.R.} \rightarrow \tilde{X} \rightarrow \boxed{DR^T} \rightarrow X'$$

physical coordinates "latent space" physical coordinates

if DR is capable of learning the patterns in the physical system;

$$X \approx X'$$

* $loss = \sum_{m=1}^{M} (x_m - x'_m)^2 \Rightarrow N$ elements

Normalization:

* $loss' = \dfrac{loss - \min(loss)}{\max(loss) - \min(loss)} \Rightarrow [0, 1]$

Interpretation:

* $loss' \rightarrow 0 \Rightarrow$ Regular Product

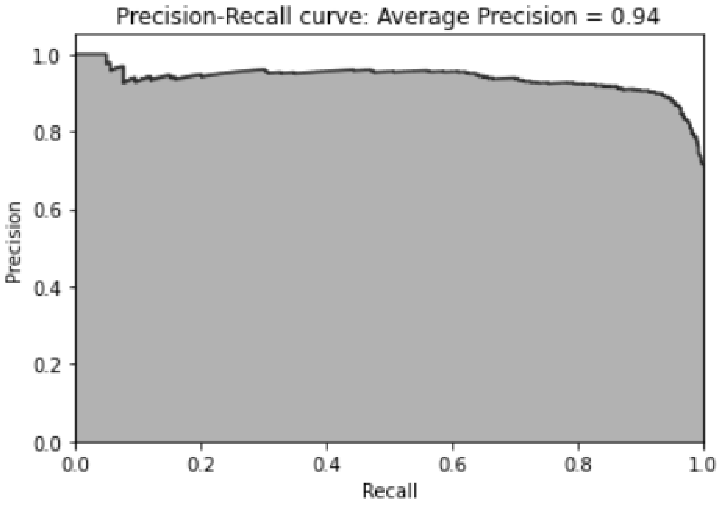
$loss' \rightarrow 1 \Rightarrow$ Anomaly, defective

#5 Evaluation of the predictions

Precision Recall Curve (for imbalanced data)

$$\text{Precision} := \frac{\text{True Positive}}{\text{TP} + \text{False Positive}} \Rightarrow \frac{\text{It is positive}}{\text{“It is positive”}}$$

$$\text{Recall} := \frac{\text{True Positive}}{\text{TP} + \text{False Negative}} \Rightarrow \frac{\#\,\text{Correct Predict.}}{\#\,\text{True Cases}}$$



- **Precision** captures how often, when a model makes a positive prediction, this prediction turns out to be correct.
- **Recall** tells us how confident we can be that all the instances with the positive target level have been found by the model.

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#3 Candidate Models: Dictionary Learning

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Dictionary learning

* Obj: Sparse representation of original data
* Inspired from how visual cortex operates → image, sound, signal

- "Dict. Matrix" ← Sparse Matrices "atom"
- atom ← Binary vectors [0 0 1 .. 0 1]
- Each Instance := Weighted sum of atoms

} performs well for sparse systems

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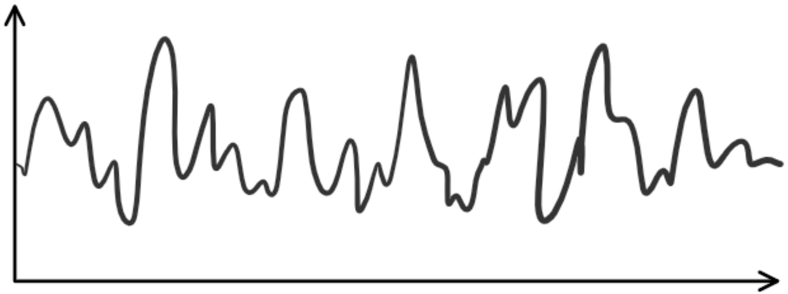
#3 Candidate Models: ICA

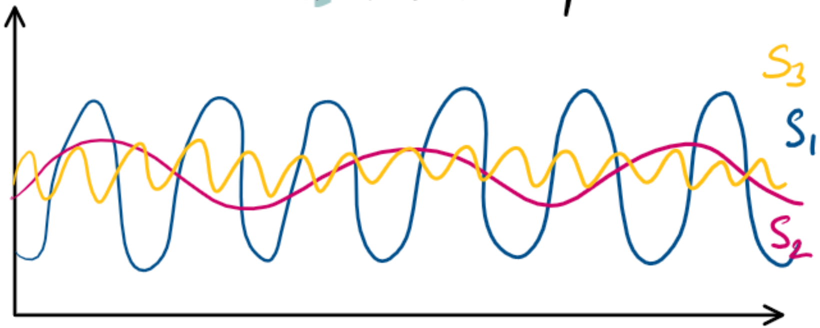
Independent Component Analysis

* Bell & Sejnowski (1995)
* latent distribution is non-gaussian

Blind Source Separation

* Optical imaging
* Face recognition
* time series predictions
* gene expressions
* industrial processes



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#3 Candidate Models: Nonlinear Projections

① Multidimensional Scaling (MDS)

* Obj: preserve the pairwise distance between datapoints as closely as possible.
* Pairwise ⇒ Computationally expensive
* eigenvectors of "distance matrix"
* distance := Euclidean ⇒ "Expensive PCA"

#3 Candidate Models: Nonlinear Projections

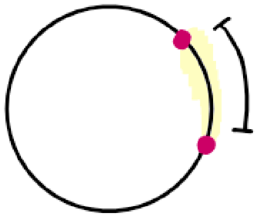
(2) Locally Linear Embedding (LLE)

* Obj: preserve the distance with local neighbours
* Computes set of coeff. that best reconstruct the data from neighbouring points.
* Dimensions are reduced while preserving these coeff.

#3 Candidate Models: Nonlinear Projections

③ Isometric Feature Mapping (isomap)

* project data using MDS.
* uses geodesic distances;



arc length → distance

(i) First defines the neighbours for each data point.

(ii) List all neighb. points & distances (Euc.)

(iii) Find geodesic distances ($\sum_i$ arc_length$_i$)

(iv) MDS is applied.

#3 Candidate Models: Nonlinear Projections

④ Stochastic Neighbour Embedding (t-SNE)

* Obj. Convert the affinites of datapoints into joint probabilities.

* Good for identifying local structures.

Others ⇒ suitable for continuous manifolds.

* Good for visualizing high dimensional data.

(–) typically ~ $10^3 - 10^4$ times slower than PCA.

(–) Stochastic ⇒ Different seeds will give different clusters.

(–) Global structure may not be preserved if initiated randomly.

↳ you can intialize with PCA.

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Additional Notes

Content

(*) SVD & PCA

(i) PCA (ii) iPCA (iii) kPCA

(*) Anomaly Score

(*) PR-Curve

(*) 2D & 3D scatter plots.

(*) isomap

(*) LLE approach

(*) t-SNE

(*) MDS

reduce the dimensions.

(*) Dictionary Learning

(*) ICP