Unsupervised Learning

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Overview

1. Reminders about previous sessions

2. Unsupervised learning
   - Clustering
     - Clustering with K-means
     - Kernel K-means
   - Density estimation
     - Non parametric kernel densities
     - Mixture model densities
   - Dimensionality reduction
     - Principal component analysis (PCA)
     - Kernel Principal component analysis (PCA)
     - Neural embeddings

Overview

Questions

About previous sessions

Do you have questions or comments about previous sessions

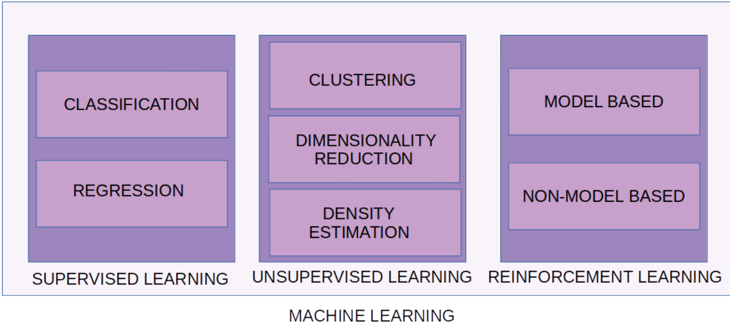
About your projects

- Group project deadline is the **31 of March 2021**
- Do you have questions about the projects' topics
- Personal project will be shared next week in Neoma/Courses
  - You have will two weeks to complete and deliver your work

Projects expectations

- Use what you learned during this class : test many models
- Evaluate your proposals properly : multi-fold cross-validation
- Be creative : it can give extra points

Machine learning approaches overview



Supervised learning methods (last session)

- K-nearest-neighbours : simplicity
- Decision trees and random forests : interpretability
- Kernel methods and support vector machines : solution uniqueness
- Neural networks : efficiency on very large datasets

No single method systematically outperforms : test to find out the best for your problem

Overview

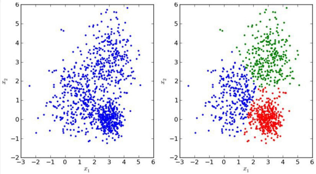
Unsupervised learning

We are given sample data $(\mathbf{x}_n)$, without any labels. The goal is to discover hidden data structure. Unsupervised learning is also called knowledge discovery

Canonical examples

Given data samples $\mathbf{x}_1, ...\mathbf{x}_n, ..., \mathbf{x}_N$

- **Clustering** : cluster samples into K groups
- **Density estimation** : estimate data density $f_{\mathbf{w}}(\mathbf{x}_n) = p(\mathbf{x}_n|\mathbf{w})$
- **Dimensionality reduction** : find lower dimensional embedding space



Unsupervised learning evaluation

- Contrarily to supervised learning, unsupervised learning evaluation is not straightforward
  - There are no associated labels
- Evaluation possible for simulated data
- Evaluation possible on downstream classification tasks where features extracted using unsupervised learning methods are used as input features

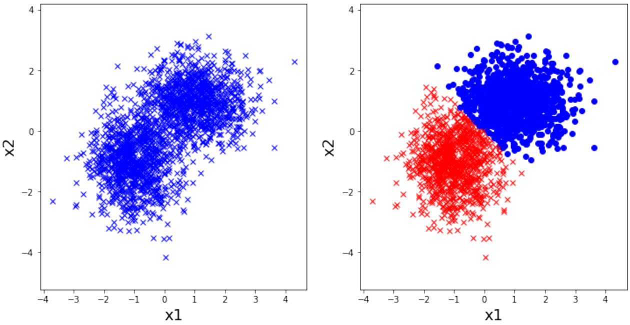
Unsupervised learning in Finance

Why unsupervised learning in finance

- Large amount of unlabelled data is available in most companies
- Data labelling is very costly
- Some applications
  - Cluster customers/assets/portfolio/trend/momentum
  - Infer data generating distribution for stock prices/returns simulation for back-testing
  - Reduce data dimensionality for visualizing high dimensionality data or developping models

Clustering problem

Given a dataset, categorize sample into a pecified number of groups K based on a dissimilarity measure ρ on the sample space.



Samples to the left are clustered into $K = 2$ groups with K-means algorithm based on the the Eucidean distance.

Clustering with K-means

Principle

The goal of the K-means algorithm is to partition a sample set $\{\mathbf{x}_n, n = 1, ..., N\}$ into K sub-sets with assignment variable $s_n, n = 1, ..., N$ minimizing the intra-class distance :

$$\hat{\mathbf{S}} = \arg \min_{s_1,\ldots,s_N} \sum_{n=1}^{N} ||\mathbf{x}_n - \mu_{s_n}||_2$$

where $\mu_k = \frac{1}{|S_k|} \sum_{n \in S_k} \mathbf{x}_n$ with $S_k = \{n | s_n = k\}$

Algorithm

1. Initialize K cluster centroids μ_k : select K samples among the dataset
2. Select a random sample $\mathbf{x}_n$, assign it to the closest centroid's cluster
3. Update the cluster centroid using the new sample $\mathbf{x}_n$
4. loop back to step 2 until convergence

K-means clustering parameters

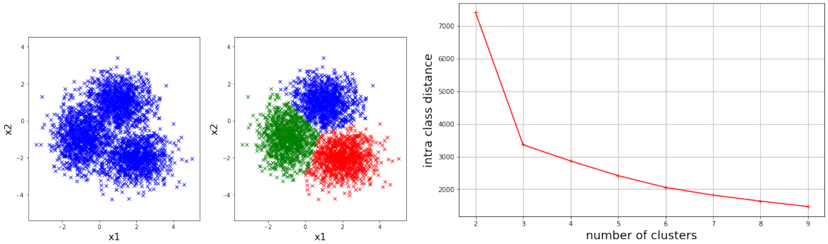
Algorithm requirements

- The number of clusters K
- The dissimilarity measure $\rho(\mathbf{x}_n, \mu_k) = ||\mathbf{x}_n - \mu_k||_2$
- These parameters are specified by the data scientist : you

Specifying the number of cluster K : elbow method

Principle

Run k-mean clustering for varying $K = 1, 2, ..., 10$ and detect inflexion number in the intra class distance curve.



Distance metric definition for K-means

Distance metric choice

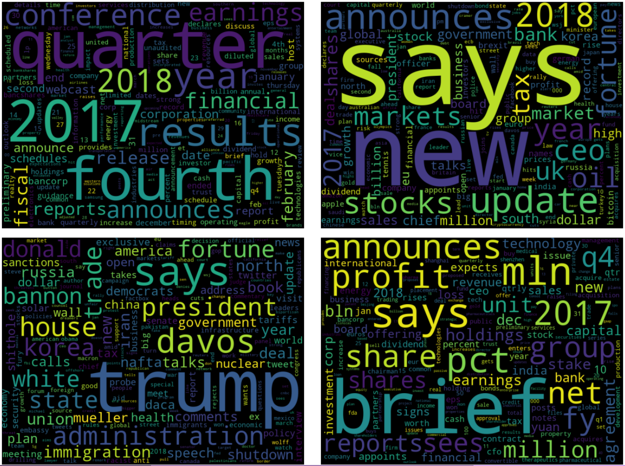
- Classically the Euclidean distance is used with K-means :

$$||\mathbf{x}_n - \mu_k||_2 = \sqrt{\sum_{d=1}^{D}(x_{nd} - \mu_{kd})^2}$$

- Euclidean distance is only suited for vector space elements $\mathbf{x}_n \in \mathbb{R}^D$
- Example : stock return distributions clustering
  - Euclidean distance is not suited to compare distributions
- Important : cluster centroids computation is distance-dependant

K-means example : Finance news corpus clustering

- Build vocabulary : set of wof appearing in documents
- Represent each document as the vector of word occurences
- Apply K-means to word occurence vectors



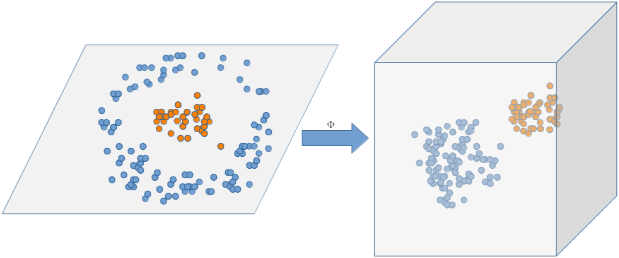
K-means limitations

- Question : why K-means will have trouble on the following problems ?
  - Answer : cluster boundaries are nonlinear
  - Solution : Kernelized K-means

Kernel method for clustering

Principle

Map samples $\mathbf{x}_n$ in a feature space using a map $\phi(\mathbf{x}_n)$ such that in the feature space clustering can be easily solved.



Kernel trick

Exploit the existence of a kernel κ such that $\kappa(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >$.

Kernel K-means

Principle

The goal of the Kernel K-means is to partition a sample set $\{\mathbf{x}_n, n = 1, ..., N\}$ into K sub-sets with assignment variables $s_n \in \{1, 2, ..., K\}, n = 1, ..., N$ minimizing the intra-class distance :

$$\text{argmin}_{s_n \in \{1,2,...,K\}} \sum_{n=1}^{N} ||\phi(\mathbf{x}_n) - \mu_{s_n}||_2^2$$

such that $\mu_k = \frac{1}{|S_k|} \sum_{s_n=k} \phi(\mathbf{x}_n)$

Issue

- It is not always possible to compute $\mu_k = \frac{1}{|S_k|} \sum_{s_n=k} \phi(\mathbf{x}_n)$ as $\phi(\mathbf{x}_n)$ can be in some cases an infinite dimension vector
- Exploit kernel trick $\kappa(\mathbf{x}, \mathbf{x}') = <\phi(\mathbf{x}), \phi(\mathbf{x}')>$

Kernel K-means objective with kernel trick

Given relations

- Centroid formula : $\mu_k = \frac{1}{|S_k|} \sum_{s_n=k} \phi(\mathbf{x}_n)$
- Inner product relation $||u - v||_2^2 = ||u||_2^2 - 2 < u, v > + ||v||_2^2$
- Kernel trick : $\kappa(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >$

Objective function

$$||\phi(\mathbf{x}_n) - \mu_{s_n}||_2^2 = \kappa(\mathbf{x}_n, \mathbf{x}_n) - \frac{2}{|S_{s_n}|} \sum_{m \in S_{s_n}} \kappa(\mathbf{x}_n, \mathbf{x}_m) + \frac{1}{|S_{s_n}|^2} \sum_{m, m' \in S_{s_n}} \kappa(\mathbf{x}_m, \mathbf{x}_{m'})$$

Greedy kernel K-means algorithm

- Choose a number of cluster K, and a kernel $\kappa(\mathbf{x}_n, \mathbf{x}_m)$
- Randomly initialized sample cluster assignments $s_n, n = 1, ..., N$
- Repeat until convergence
  1. Select a sample $\mathbf{x}_n$
  2. For $k = 1, 2, ..., K$ compute

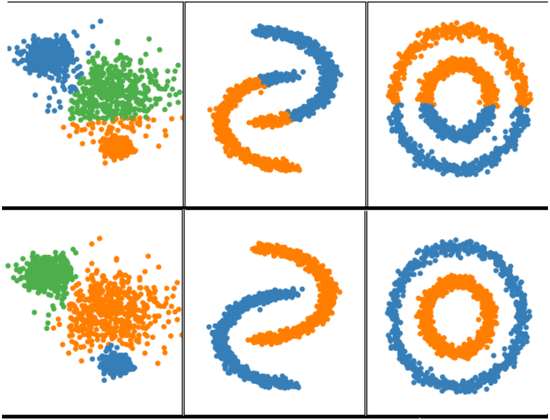
$$L(k) = \kappa(\mathbf{x}_n, \mathbf{x}_n) - \frac{2}{|S_k|} \sum_{m \in S_k} \kappa(\mathbf{x}_n, \mathbf{x}_m) + \frac{1}{|S_k|^2} \sum_{m, m' \in S_k} \kappa(\mathbf{x}_m, \mathbf{x}_{m'})$$

  3. Assign sample $\mathbf{x}_n$ to cluster minimizing $L(k)$:

$$s_n = \arg \min_{k=1,\ldots,K} L(k)$$

K-means vs Kernel K-means

- First row : K-means clustering
- Second row : radial basis function kernel K-means clustering
- Kernel K-means is more efficient at clustering non-spherical samples



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Density representation

What is a density

- Density represents sample probability distributions : Gaussian density
- Machine learning is interested in complex/multi modal densities
  - Non parametric densities : kernel based densities
  - Mixture models : Gaussian mixture models

Applications

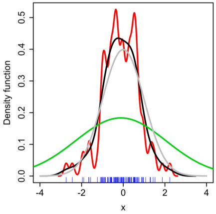
- Outliers detection : finding low probability samples
- Simulations : draw samples from densities

Non parametric kernel densities

Assume $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N$ identically distributed sampled from an unknow density f, at any given point $f(\mathbf{x})$ can be estimated as :

$$\hat{f}(\mathbf{x}) = \frac{1}{C(h, N)} \sum_{n=1}^{N} K_h(\frac{\mathbf{x} - \mathbf{x}_n}{h})$$

- K_h : kernel (as for kernel methods)
- h kernel bandwidth
- $C(h, N)$: normalization factor



Parametric density estimation with E.M. algorithm

Expectation Maximization (E.M.)

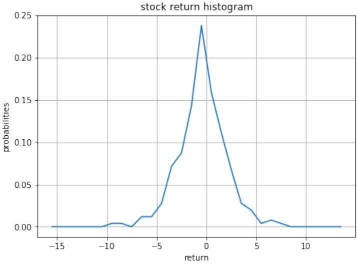
- Data is represented as a mixture of a known distribution (e.g. Gaussian, multinomial, Dirichlet)

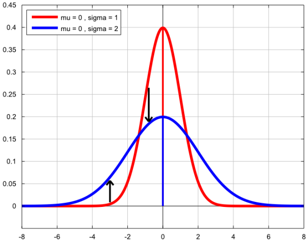
$$p(\mathbf{x}) = \sum_{k=1}^{K} w_k p_k(\mathbf{x})$$

- E.M. produces a density distribution of the given dataset
- For each sample, E.M. produces an assignment score to each mixture
- E.M. is a generalization of k-means algorithm
- **Application** : stock returns modelling beyond Gaussians

Non Gaussian stock return histogram example

- Non Gaussian stock return distribution : too skewed
- Can be modelled by a mixture of two gaussians





Unsupervised learning of a G.M.M. with E.M.

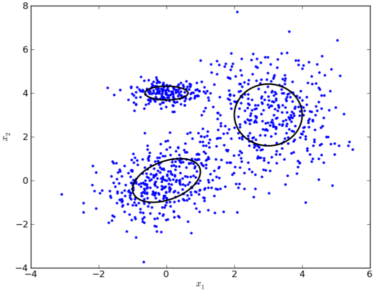
D-dimensional Gaussian density

$$g(\mathbf{x}_n; \mu_k, \Sigma_k) = \frac{1}{\sqrt{(2\pi)^D |\Sigma_k|}} exp - \frac{1}{2}(\mathbf{x}_n - \mu_k)^t \Sigma_k^{-1} (\mathbf{x}_n - \mu_k)$$

Problem

Given a dataset $(\mathbf{x}_n)$, learn using EM a gaussian mixture model (GMM)

$$p(\mathbf{x}_n) = \sum_{k=1}^{K} \alpha_k g(\mathbf{x}_n; \mu_k, \Sigma_k)$$



Learning a GMM with EM algorithm : principle

Latent variables

Introduce assignment variable Z_n such that $p(Z_n = k) = \alpha_k$ is the prior probability sample $\mathbf{x}_n$ being generated by the mixture component k.

Maximum marginal likelihood

Estimate the GMM parameters $\Theta = (\alpha_k, \mu_k, \Sigma_k)$ maximizing likelihood :

$$
\begin{aligned}
p(\mathbf{x}_{1:N}, Z_{1:N}|\Theta) &= \prod_{n=1}^{N} p(\mathbf{x}_n|Z_n)p(Z_n) \\
&= \prod_{n=1}^{N}\prod_{k=1}^{K}[p(\mathbf{x}_n|Z_n = k)p(Z_n = k)]^{\delta_{Z_n}(k)} \\
&= \prod_{n=1}^{N}\prod_{k=1}^{K}[g(\mathbf{x}_n; \mu_k, \Sigma_k)\alpha_k]^{\delta_{Z_n}(k)}
\end{aligned}
$$

Learning a GMM with EM algorithm : the algorithm

Expectation step :

Compute expectation of log-marginal likelihood wrt observations :

$$Q(\Theta|\Theta_{t-1}) = \mathbb{E}_{Z_{1:N}|\mathbf{X}_{1:N},\Theta_{t-1}}[\log p(\mathbf{X}_{1:N}, Z_{1:N}|\Theta)]$$

Maximization step :

Maximize expectation wrt to parameters :

$$\Theta_t = \arg\max_{\Theta} Q(\Theta|\Theta_{t-1})$$

EM Algorithm :

1. Initialize the GMM parameters Θ_0, set $t = 1$
2. Compute log-marginal likelihood expectation $Q(\Theta|\Theta_{t-1})$
3. Compute Θ_t as the arg-maximum of $Q(\Theta|\Theta_{t-1})$
4. Increment t, and loop back to set 2 until convergence

Learning the number of mixtures

As for K-means elbow method on the number of mixture vs the log likelihood curves can be used to estimate the optimal number of mixtures.

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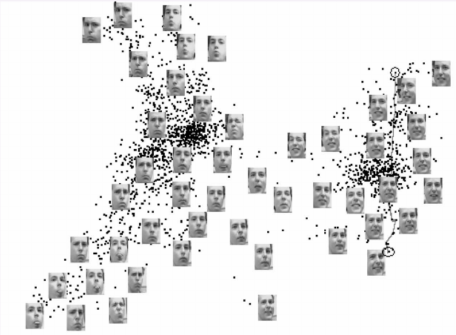
What and why dimensionality

What

- Finding a lower dimensional representation of samples

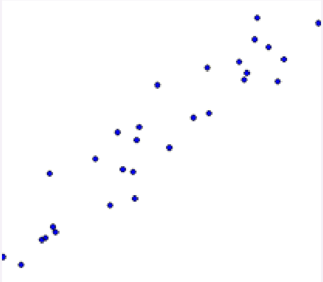


Why

- Additional dimension can je just ud to noise in data
- Models can be easier to build on lower dimensional

Problem statement

Principal component analysis (PCA) can be defined as the orthogonal projection of the data on a lower dimensional linear space such that the variance of the projected data is maximized.



Dimensionality reduction with PCA : principle (1/2)

- Consider samples $\mathbf{x}_1$, $\mathbf{x}_2$, ..., $\mathbf{x}_N$ with $\mathbf{x}_n \in \mathbb{R}^D$
- Goal : project samples on M-dimension linear space ($M < D$) while maximizing projected sample variance

Case $M = 1$

- Principal sub-space is defined vector $\mathbf{u}_1$ with $||\mathbf{u}_1||_2^2 = \sqrt{\mathbf{u}_1^\top \mathbf{u}_1} = 1$
- Covariance matrix of a centered sample set ($\bar{\mathbf{x}} = 0$) is defined as :

$$S = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^\top$$

- Projected samples on subspace spanned by $\mathbf{u}_1$ are given by $\tilde{x}_n = \mathbf{u}_1^\top \mathbf{x}_n$
- Projected samples variance is defined as :

$$\frac{1}{N} \sum_{n=1}^{N} (\mathbf{u}_1^\top \mathbf{x}_n)^2 = \mathbf{u}_1^\top S \mathbf{u}_1$$

Dimensionality reduction with PCA : principle (2/2)

- Problem : find vector $\mathbf{u}_1$ maximizing $\mathbf{u}_1^\top S \mathbf{u}_1$ with $\mathbf{u}_1^\top \mathbf{u}_1 = 1$
- Introducing Langrange multiplier λ_1 optimization problem is :

$$J(\mathbf{u}_1) = \mathbf{u}_1^\top S \mathbf{u}_1 + \lambda_1(1 - \mathbf{u}_1^\top \mathbf{u}_1)$$

- Computing gradient of $J(\mathbf{u}_1)$ wrt $\mathbf{u}_1$ and setting to 0

$$S\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$$

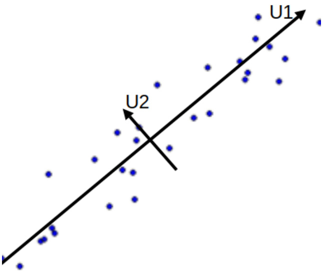
Solution

- $\mathbf{u}_1$ is an eigenvector of covariance matrix S with eigenvalue λ_1
- $\mathbf{u}_1^\top S \mathbf{u}_1 = \lambda_1$: is maximized if λ_1 is the largest eigenvalue, and $\mathbf{u}_1$ its eigenvector

$M > 1$

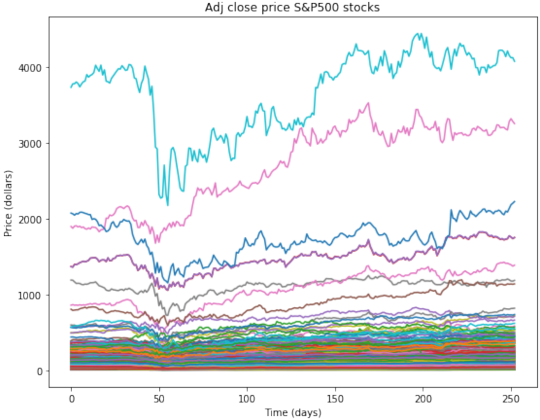
Select the M eigen vectors corresponding to the largest eigenvalues

PCA : two dimensions example

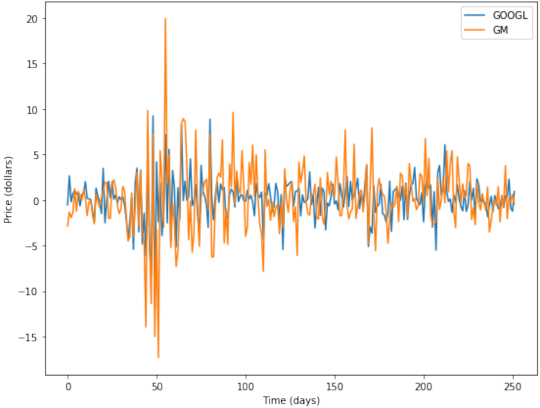


- Two principal linear subspaces $\mathbf{u}_1$ and $\mathbf{u}_2$
  - $\mathbf{u}_1$: first principal sub-space corresponding to largest eigenvalues
  - $\mathbf{u}_2$: second principal sub-space
- Data can be considered unidimensional according to first eigenspace

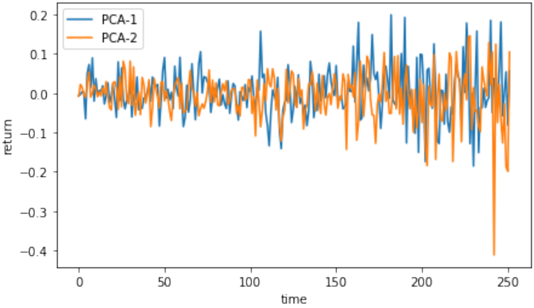
Stock return trajectories PCA analysis : stock prices



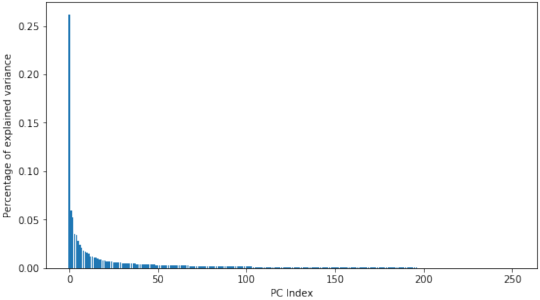
$$\text{return}_t = \frac{\text{price}_t - \text{price}_{t-1}}{\text{price}_{t-1}}$$



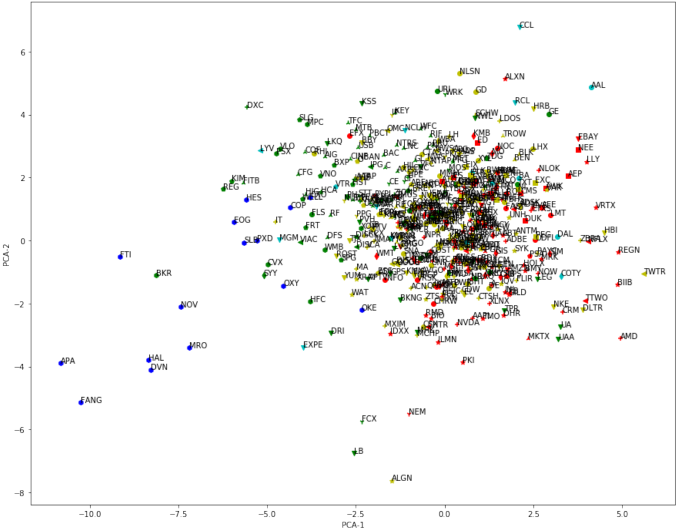
Stock return trajectories PCA analysis : two first PCs



Stock return trajectories PCA analysis : explained variance



Stock return trajectories PCA analysis : embedding



PCA applied to stock returns : eigen portfolios

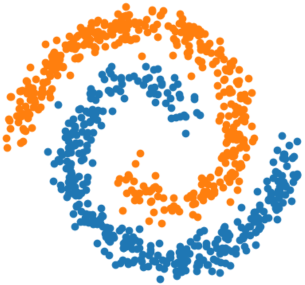
- Compute PCA stock returns decomposition
- First PC corresponds to market trend
- Portfolio with weights corresponding coordinate wrt the first PC

$$w_k \propto < \mathrm{PC}_1, \mathrm{S}_k >$$

is strongly correlated to S&P index

Issues with linear principal component analysis

- Favorable case : samples have a linear span.



- Unfavorable case : samples have a curvilinear span.
- Solutions :
  - Kernel PCA
  - Neural embedding

Kernel PCA : principles

Feature map and associated kernel

Let $\phi : \mathbb{R} \longleftrightarrow \mathcal{H}$ be a feature map and κ its associated kernel :

$$\kappa(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >_{\mathcal{H}}$$

Principles

Given dataset $\mathbf{x}_n, n = 1, ..., N$:

- Map samples in a feature space using feature map ϕ
- Apply PCA to the mapped samples $\phi(\mathbf{x}_n), n = 1, ..., N$
- Exploit kernel trick $\kappa(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >$ to simplify computations

Kernel PCA : the optimization problem

Orthogonal projection in feature space

Let f be a direction in the feature space, the orthogonal projection of mapped feature on direction f is given by :

$$h_f(\mathbf{x}) = < \phi(\mathbf{x}), \frac{f}{||f||} >$$

Orthogonal projection's variance is given by :

$$\text{var}[h_f] = \frac{1}{N} \sum_{n=1}^{N} \frac{< \phi(\mathbf{x}_n), f >^2}{||f||^2}$$

Principal components in feature space are solutions of the problem :

$$f_i = \begin{cases} \arg\max_{f \perp \{f_1, \ldots, f_{i-1}} \text{var}[h_f] \\ \text{with } ||f|| = 1 \end{cases}$$

Kernel PCA : eigenvalue problem (1/2)

The representer theorem

for all $\mathbf{x}$ there exist $\alpha_i = (\alpha_{i1}, ..., \alpha_{iN})$ such that $f_i(\mathbf{x}) = \sum_{n=1}^{N} \alpha_{in}\kappa(\mathbf{x}_n, \mathbf{x})$

$$||f_i||^2 = \sum_{n,m}^{N} \alpha_{in}\alpha_{im}\kappa(\mathbf{x}_n, \mathbf{x}_m) = \alpha_i^\top K \alpha_i$$

$$\sum_{n=1}^{N} f_i(\mathbf{x}_n)^2 = \alpha_i^\top K^2 \alpha_i$$

$$< f_i, f_j >= \alpha_i^\top K \alpha_j$$

$$\alpha_i = \begin{cases} arg\max_{\alpha \in \mathbf{R}^N} \alpha^\top K \alpha \\ \alpha_i^\top K \alpha_j = 0, j = 1, ..., i-1 \\ \alpha_i^\top K \alpha_i = 1 \end{cases}$$

Kernel PCA : eigenvalue problem (2/2)

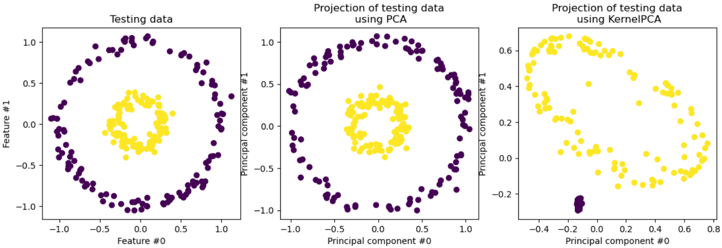
- Decomposing $K = U\Delta U^\top$ with eigenvalues $\Delta_1, ..., \Delta_N \geq 0$
- setting $\beta = K^{\frac{1}{2}}\alpha$ with $K^{\frac{1}{2}} = U\Delta^{\frac{1}{2}}U^\top$

Eigenvalues problem

$$\beta_i = \begin{cases} \mathit{arg}\,\max_{\beta\in\mathbf{R}^N} \beta^\top K\beta \\ \beta_i^\top\beta_j = 0, j = 1, ..., i-1 \\ \beta_i^\top\beta_i = 1 \end{cases}$$

Kernel PCA : scikit learn example

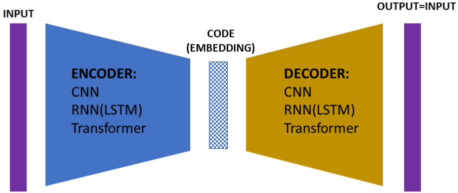
- Model comparison over a non-spherical dataset
- Projection on two first principal components
- Kernel PCA efficiently identifies the two curves of variation

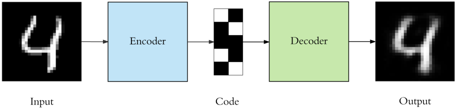


Neural embeddings

Auto-encoders

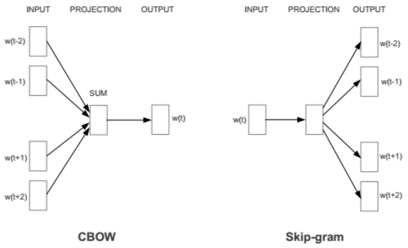
- Networks trained to replicate their inputs through a bottleneck layer
- Bottleneck forces encoder to compress input into low dimension code
- Decoder reconstructs input from low dimension code
- Code contain all information required to reconstruct into inputs



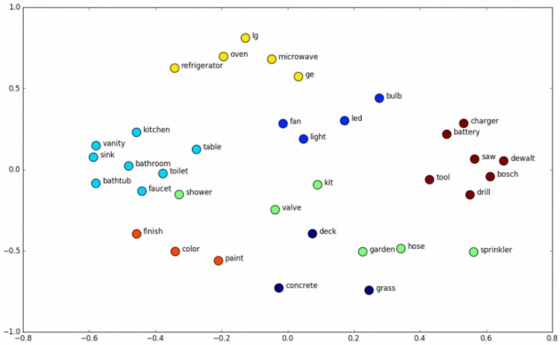


Definition

- A word embeddding model is trained to predict a word through a bottleneck (embedding) using the word context (or vice versa)
- Allows to go beyond linear PCA dimensionality reduction



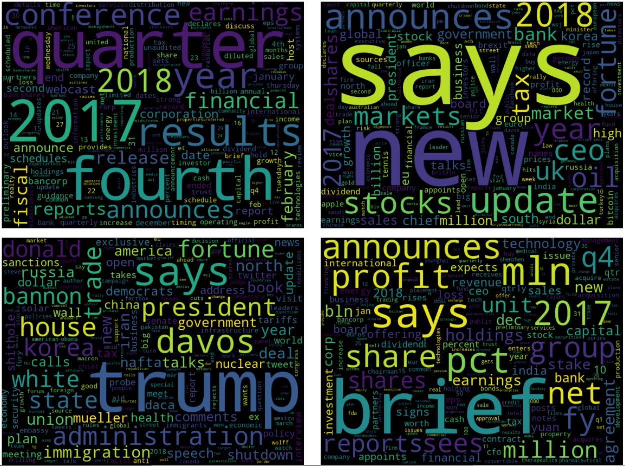
Word embedding results



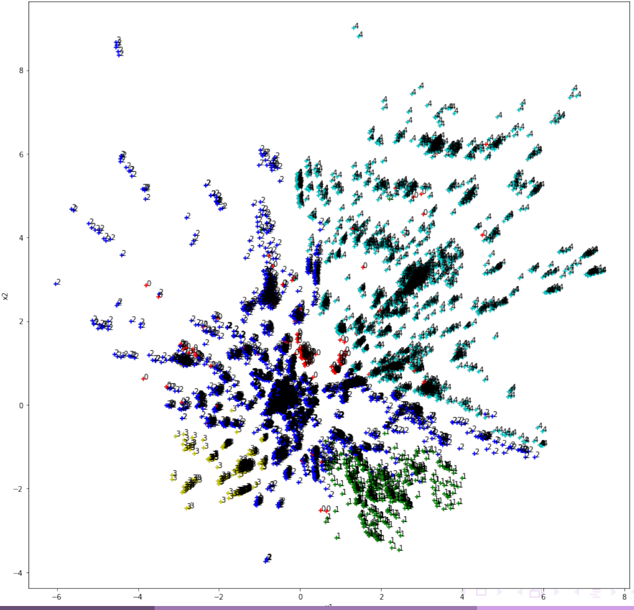
In the embedding space, semantically related words are close

Finance news corpus document embedding : clustering

- Build vocabulary : set of wof appearing in documents
- Represent each document as the vector of word occurences
- Apply K-means to word occurence vectors

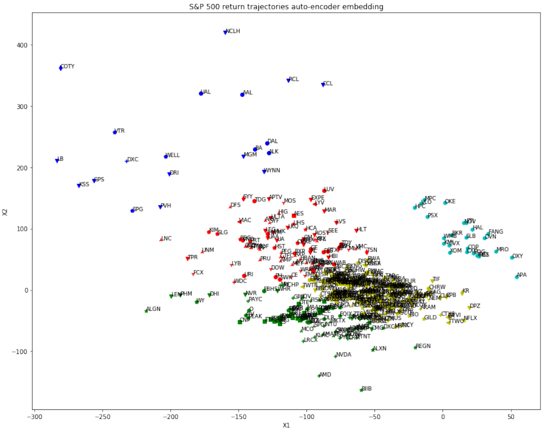


Finance news corpus document embedding



Stock return trajectories neural embedding (1/2)

- An auto-encoder is train to replicated stock returns trajectories through a 2 dimension bottleneck
- Initial trajectories is compressed into 2 dimensions



Stock return trajectories neural embedding (2/2)

- Stocks returns in plot according to mean return vs volatility
- Neural embedding captured well mean return volatility structure