Dimension reduction: PCA, tSNE

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Outline

Mean and variance

- n samples of dimension 1 (scalars) : $\{x^0, x^1 \dots x^{n-1}\}$
  - mean $\mu = \frac{1}{n} \sum_j x^j$
  - variance $\mathrm{var}(x) = \sigma^2 = \frac{1}{n} \sum_j (x^j - \mu)^2$

Covariance

- covariance between 2 variables x_0 and x_1 :
  - measure of the linear relationship between two random variables
  - $\text{covar}(x_0, x_1) = \text{E}[(x_0 - \mu_0)(x_1 - \mu_1)] = \frac{1}{n}\sum_j (x_0^j - \mu_0)(x_1^j - \mu_1)$

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- Example of linearly correlated variables : $x_1^j = \lambda x_0^j$
  - $\text{covar}(x_0, x_1) = \sum_j (x_0^j - \overline{x_0})(x_1^j - \overline{x_1}) = \lambda\, \text{var}(x_0)$
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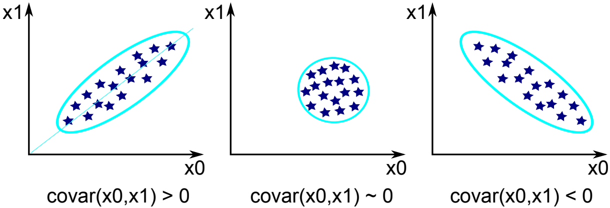
    - high value : means correlation between the 2 variables
- Example of non correlated variables : $E[x_0 * x_1] = E[x_0] * E[x_1]$
  - thus $\text{covar}(x_0, x_1) = 0$



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- variances :

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- mean of samples : $\boldsymbol{\mu} = 0.5\,[x_0^0 + x_0^1, x_1^0 + x_1^1]$
- variances :
  - $\mathrm{var}(x_0) = \mathrm{covar}(x_0, x_0) = \sigma_0^2 = \frac{1}{n}\sum_j (x_0^j - \mu_0)^2$
  - $\mathrm{var}(x_1) = \mathrm{covar}(x_1, x_1) = \sigma_1^2 = \frac{1}{n}\sum_j (x_1^j - \mu_1)^2$
- covariance matrix :

$$\Sigma = \begin{pmatrix} \sigma_0^2 & \mathrm{covar}(x_0, x_1) \\ \mathrm{covar}(x_0, x_1) & \sigma_1^2 \end{pmatrix}$$

- variance : $\mathrm{var}(\boldsymbol{x}) = \mathrm{tr}(\Sigma) = \sigma_0^2 + \sigma_1^2$

Variance-covariance matrix

- original variables of dimension $p \geq 2$: $\mathbf{X^j} = [x_0^j \dots x_{p-1}^j]$
- variance-covariance matrix : symmetric matrix of dim $p \times p$:

$$\Sigma = \begin{pmatrix} \mathrm{var}(x_0) & \mathrm{covar}(x_0, x_1) & \dots & \mathrm{covar}(x_0, x_{p-1}) \\ \mathrm{covar}(x_0, x_1) & \mathrm{var}(x_1) & \dots & \mathrm{covar}(x_0, x_{p-1}) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{covar}(x_0, x_{p-1p}) & \mathrm{covar}(x_1, x_{p-1}) & \dots & \mathrm{var}(x_{p-1}) \end{pmatrix}$$

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Outline

PCA (1901 Karl Pearson, 1936 H. Hotelling)

- Unsupervised
- Analysis of variance-covariance matrix
- Reducing the dimension of data
- Visualisation of data of the reduced dimension is 2 or 3
- Interpretation : dependance between variables
- PCA : often as pre-processing

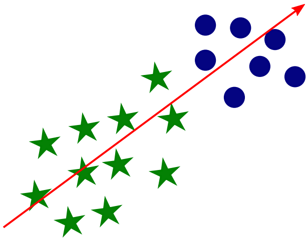
Explained variance

$$\Sigma = \begin{pmatrix} \text{var}(x_0) & \text{covar}(x_0, x_1) & \dots & \text{covar}(x_0, x_{p-1}) \\ \text{covar}(x_0, x_1) & \text{var}(x_1) & \dots & \text{covar}(x_0, x_{p-1}) \\ \vdots & \vdots & \ddots & \vdots \\ \text{covar}(x_0, x_{p-1p}) & \text{covar}(x_1, x_{p-1}) & \dots & \text{var}(x_{p-1}) \end{pmatrix}$$

- variance $= \mathrm{tr}(\Sigma) = \sum_i \sigma_i^2$
  - symmetric squared matrix : diagonalization is possible !
  - there exists a basis of orthogonal vectors where the covariance matrix is diagonal
    - these vectors are eigenvectors of Σ
    - elements on the diagonal are eigenvalues
    - variance $= \sum_k \lambda_k$
- Idea of PCA
  - diagonalisation of Σ
    - order eigenvalues by decreasing order
  - if 0 is a eigenvalue : the corresponding dimensions can be removed
  - the lower eigenvalues do not contribute a lot to the variance

Geometrical interpretation

- original variables : $x_1, x_2, .., x_p$
- principal components : $c_1, c_2, ...c_k, ..., c_q$ with $q \leq p$
- $c_k = \sum_j a_{jk} x_j$ with :
  - c_k and c_j not correlated
  - maximum variance and
  - decreasing importance



Principal component

- eigenvalues, ordered - eigenvectors
- $tr(\mathbf{\Sigma}) = \sigma^2 = \sum_{i=1}^{n} \lambda_i$
- each eigenvalue participates to the global variance

Examples : variance explained

- PCA on Iris dataset :
  - if we perform the PCA on dimension 4 (not very useful) :

```
from sklearn import datasets
from sklearn.decomposition import PCA
X, y = datasets.load_iris(return_X_y=True)
pca4 = PCA(n_components=4)
pca4.fit(X)
X4 = pca4.transform(X)
print("explained variance : ", pca4.explained_variance_ratio_)
```

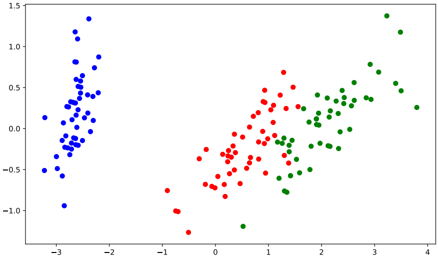
```
explained variance :  [0.92461872 0.05306648 0.01710261 0.00521218]
```

  - with 4 components : 100% of the variance is explained
  - with 3 components : 99.5%
  - with 2 components : 97.8%

Examples : plot the Iris dataset on 2d

```
# PCA transformation
pca2 = PCA(n\_components=2)
pca2.fit(X)
X2 = pca2.transform(X)

#plot
colors = ['b', 'r', 'g']
col = [colors[c] for c in y]
plt.figure(figsize=(10, 6))
plt.scatter(X2[:, 0], X2[:, 1], c=col, marker="o")
```



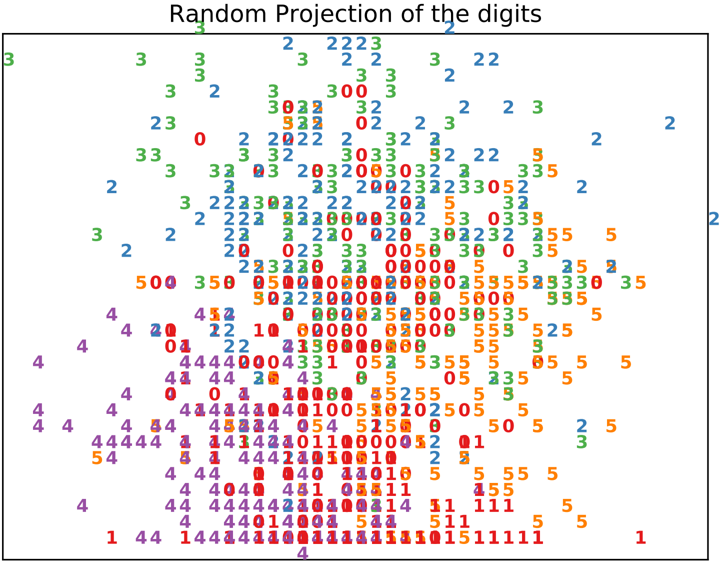
Links to codes

- PCA on Iris dataset :
  - from dimension 4 to dimension 3 for visualisation (https://scikit-learn.org/stable/auto_examples/decomposition/plot_pca_iris.html)
  - from dimension 4 to dimension 2 (https://scikit-learn.org/stable/auto_examples/decomposition/plot_pca_vs_lda.html)
  - explained variance ratio (first two components) : [0.92461872 0.05306648]

Practice (part 1)

- With the digit dataset
  - Find the smallest dimension after PCA such that 95% of the variance is explained.
    - hint : `numpy.cumsum` and `numpy.where`
  - What is the proportion of explained variance in dimension 2 ?
  - Plot the digits after a PCA in 2D. Compare with the previous approach.

Outline


Random Projection of the digits

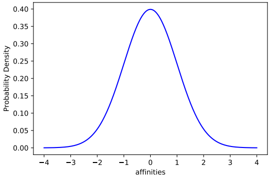
Idea of t-SNE (Maaten-Hinton 2008)

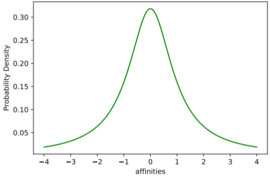
https://www.jmlr.org/papers/volume9/vandermaaten08a/vandermaaten08a.pdf

- Build map in which distances between points reflect similarities in the data
  - typical map dimension : 2 or 3
  - preserving local structures
  - t-SNE : try to avoid all points collapsing
- Non linear dimension reduction
  - converts affinities of data points to probabilities represented by Gaussian joint probabilities
  - affinities in the embedded space are represented by Student's **t**-distributions (heavy tailed)
  - minimisation of Kullback-Leibler divergence of the two distributions (gradient descent) : moves points in the embedded space
- Exact algorithm of t-SNE is computationally expensive (huge compared to PCA)
- Stochastic algorithm : multiple restarts with different seeds can yield different results

Conversions of affinities

- Why a Gaussian distribution ?
  - In the original space, we want to capture close elements and do no care of distant elements
- Why a Student's t-distribution ?
  - In the embedded space, the samples are initially randomly projected. We need to be able to capture them even if they are initially projected far away.

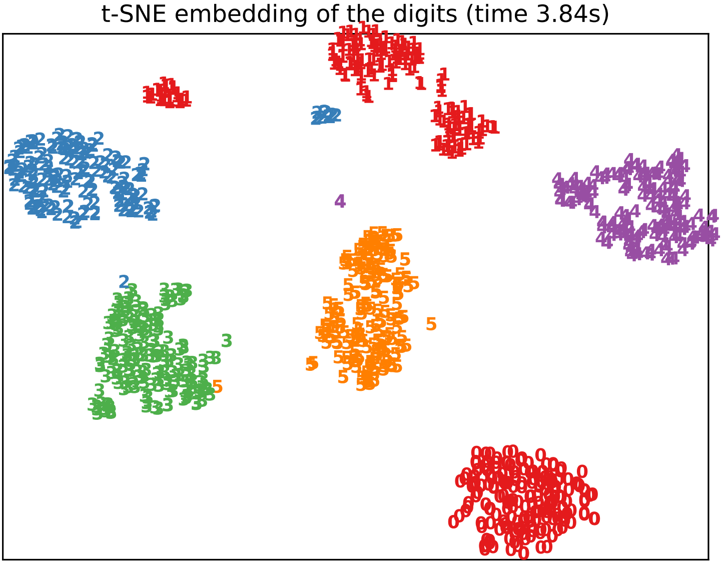




Iterative algorithm

- random initialisation of samples in the embedded space
- iterative minimisation of the KL divergence :
  - compute the distances between embedded points
  - use the t-distribution to transform these values + normalisation
  - compute the gradient of KL and move the samples points in the embedded space

Example using the digit dataset

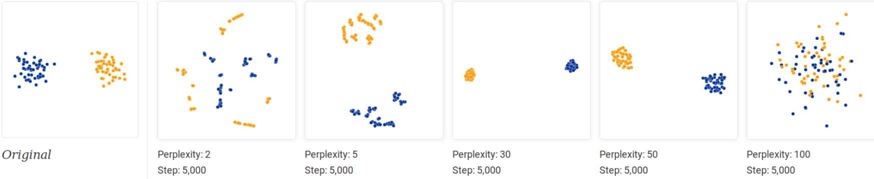


Short intro to t-SNE

https://www.youtube.com/watch?v=NEaUSP4YerM

Parameters of t-SNE

- Perplexity (usually between 5 and 50). Illustration from `https://distill.pub/2016/misread-tsne/`



- Early exaggeration factor : optimization in two steps :
  - exaggeration phase : joint probabilities in the original space are artificially multiplied by a factor
  - final optimization
  - *Controls how tight natural clusters in the original space are in the embedded space and how much space will be between them. For larger values, the space between natural clusters will be larger in the embedded space. Again, the choice of this parameter is not very critical. [from the documentation]*
- Learning rate ϵ : not too small, not too large.
- Maximum number of iterations : 5000 ?

Barnes-Hut t-SNE

- approximation of t-SNE, more scalable.
  - many of the pairwise interactions between points are similar
- Another parameter : angle :
  - tradeoff between performance and accuracy
  - usual range : from 0.2 to 0.8
    - larger angles imply that we can approximate larger regions by a single point, leading to better speed but less accurate results.
- Limitations :
  - target dimension less than 3. Mostly 2.
  - only for dense dataset (for sparse dataset use exact t-SNE)

Code for visualisation in 2D using t-SNE

```
from sklearn import manifold
tsne = manifold.TSNE(n_components=2, init='pca', random_state=0)
X_tsne = tsne.fit_transform(X)
```

Practice (part2)

- Compare PCA and tSNE for the visualisation in 2D of the digit dataset
  - compare the speed of transformation
  - compare the plots and play with the parameters
- With a dimension reduction to 2D, plot the results of a classification with a decision tree from last week
  - colors will represent the truth classes
  - shapes will represent the predicted classes