Unsupervised Learning: Dimensionality Reduction

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Outline

Overview

PCA

3 SNE & t-SNE

Unsupervised Learning

When the data we have does not have any labels, it is impossible for us to apply supervised learning.

E.g. The DNA or RNA data of virus is such an example.

Unsupervised learning is often performed as part of an pattern recognition.

In Week 1, the EDA (with numeric summary, visualisation and correlation relation as basic tools) is used to analyse each feature and each pair of features.

It is difficult to assess the results obtained from unsupervised learning methods \rightarrow no "indisputable" performance metric!

Unsupervised Learning

For an unlabelled $n \times p$ numeric data X, it may have the following patterns:

- n is much larger than p and the data is distributed along some subspace in $\mathbb{R}^p \to \text{dimension reduction}$
- n is small and p is large, the data are correlated and the features are linear combinations of fewer features → dimension reduction
- ullet Data are in closely-linked nonlinear distributed regions in high-dimensional feature space \to nonlinear dimension reduction
- Data are in "clusters" → clustering (next topic)

Dimensionality Reduction

Target: unlabelled data X with a set of **numeric** features X_1, \dots, X_p measured on n observations.

"Dimensionality reductions" are a class of unsupervised learning methods which try to **extract** essential "dimension" information of the data to "characterise" the data.

Some dimensionality reduction algorithms that are PCA (linear), SNE (nonlinear), t-SNE (non-parametric/nonlinear), Sammon mapping (nonlinear), Isomap (nonlinear), LLE (nonlinear), CCA (Canonical-Correlation Analysis, nonlinear), MVU (Maximum Variance Unfolding, nonlinear), Laplacian Eigenmaps (nonlinear), etc.

Dimensionality Reduction (cont)

The good news is that we need to study only PCA and t-SNE (t-Distributed Stochastic Neighbour Embedding) to effectively visualise data in lower dimensions.

The PCA tries to find a global structure and this can lead to local inconsistencies, i.e. far away point can become nearest neighbours.

The t-SNE tries to preserve local structure, i.e. the low dimensional neighbourhood "representation" should be the same as original neighbourhood.

Dimensionality Reduction in R

prcomp: PCA

cmdscale: Classical MDS

MASS::isoMDS: Nonmetric MDS

ica::icafast: ICA

Rtsne::Rtsne: t-SNE

- uwot::umap: Uniform Manifold Approximation and Projection
- ruta::autoencode: Autoencoders are neural networks that are trained to reconstruct their original inputs.
- phateR::phate: Potential of Heat-diffusion for Affinity-based Trajectory Embedding
- Rdimtools::do.fa: Factor Analysis
- Rdimtools::do.isomap, etc.

Dimensionality reduction functions from sklearn.decomposition:

- PCA([n_components, copy, ...]): Principal component analysis
- IncrementalPCA([n_components, ...]): Incremental PCA for large datasets.
- SparsePCA([n_components, ...]): Extract the set of sparse components that best reconstruct X.
- MiniBatchSparsePCA([...]): A variant of SparsePCA that is faster but less accurate.

Dimensionality Reduction in Python (cont) sklearn.decomposition (cont):

- KernelPCA([n_components, ...]): An extension of PCA which achieves non-linear dimensionality reduction through the use of kernels
- TruncatedSVD([n_components, ...]):
 Dimensionality reduction using truncated SVD (aka latent semantic analysis / LSA).
- SparseCoder(dictionary, *[, ...]) or sparse_encode(X, dictionary, *): It is an estimator that can be used to transform signals into sparse linear combination of atoms from a fixed, precomputed dictionary such as a discrete wavelet basis.

sklearn.decomposition (cont):

- DictionaryLearning([...]) or dict_learning(X, n_components, ...): It is a matrix factorisation problem that amounts to finding a (usually overcomplete) dictionary that will perform well at sparsely encoding the fitted data.
- dict_learning_online(X[, ...]): Solves a dictionary learning matrix factorisation problem online.
- MiniBatchDictionaryLearning([...]): A
 faster, but less accurate version of the dictionary
 learning algorithm that is better suited for large
 datasets.

sklearn.decomposition (cont):

- FactorAnalysis([n_components, ...]): It is similar to PCA but can model the variance in every direction of the input space independently (heteroscedastic noise)
- FastICA([n_components, ...]): a fast algorithm for Independent Component Analysis.
- NMF([n_components, init, ...]) or non_negative_factorization(X): Non-Negative Matrix Factorisation.
- LatentDirichletAllocation([...]): Latent Dirichlet Allocation with online variational Bayes algorithm.

Dimensionality reduction functions from sklearn.manifold:

- MDS([n_components, metric, n_init, ...]):
 Multidimensional scaling seeks a low-dimensional
 representation of the data in which the distances
 respect well the distances in the original
 high-dimensional space.
- Isomap(*[, n_neighbors, ...]): Isometric Mapping Embedding, an extension of MDS or Kernel PCA.

sklearn.manifold (cont):

- LocallyLinearEmbedding(*[, ...]) or locally_linear_embedding(X, *, ...): A lower-dimensional projection of the data which preserves distances within local neighbourhoods.
- SpectralEmbedding([n_components, ...]) or spectral_embedding(adjacency, *[, ...]): Spectral embedding for non-linear dimensionality reduction using Laplacian Eigenmaps.
- TSNE([n_components, perplexity, ...]):
 T-distributed Stochastic Neighbor Embedding converts affinities of data points to probabilities.

Outline

Overview

PCA

3 SNE & t-SNE

PCA

Given unlabelled data X of shape $n \times p$.

Motivations:

- Some columns can be a constant (e.g. image data):
 Can we remove it?
- Some columns are "colinear".
 - Multicollinearity is a phenomenon in which two or more predictors in a multiple regression model are highly correlated;
 - Perfect multicolinearity: One column is a multiple of another column ⇒ covariance matrix has a determinant of 0;
 - ► Hight multicolinearity: covariance matrix has a determinant **close to 0**.



A major goal of PCA is to identify new predictors from the original predictors called 'factors' or 'latent variables' that are uncorrelated to each other by using the 'covariance matrix' of X.

Step 1: Shift the data to "column mean" / centre \bar{x} ,

$$x_{.j} \to x_{.j} - \overline{x}_j =: \widetilde{X}$$

Step 2 (necessary in real-world problem but not in test/exam): If scaling is necessary (due to large variations in the variances), transform the data:

$$s_{\cdot j} = \sqrt{\frac{\sum_{i=1}^{n} (x_{ij} - \overline{x}_{j})^{2}}{n-1}} \Rightarrow x_{\cdot j} \rightarrow \frac{x_{\cdot j} - \overline{x}_{j}}{s_{\cdot j}} =: \widetilde{X}$$

Step 3: Compute the **covariance matrix** of X:

$$\Sigma := \operatorname{Cov}(X) = \frac{1}{n-1} \widetilde{X}^T \widetilde{X}$$

The command in R is S = cov(X).

Step 4: Compute the eigenvalues and eigenvectors of Σ . According to year 1 linear algebra's "spectral theorem", Σ is nonnegative definite and can be diagonalised into $\Sigma = Q\Lambda Q^T$, where Q are formed from the eigenvectors and the diagonal matrix Λ are formed from the corresponding eigenvalues.

A matrix Σ is said to be *non-negative definite* if

$$x\Sigma x^{T} \geq 0$$
, $\forall x = (x_{1},...,x_{p})$, $x_{1}^{2} + ... + x_{p}^{2} = 1$.

Spectral Theorem: A non-negative definite matrix can be decomposed into

$$\Sigma = \lambda_1 \mathsf{v}_1 \mathsf{v}_1^\mathsf{T} + \dots + \lambda_q \mathsf{v}_q \mathsf{v}_q^\mathsf{T}, \quad q \le \min\{n, p\}. \tag{1}$$

Here, λ_i are the "eigenvalues" and v_i are the "eigenvectors". The eigenvectors are orthogonal to each other and $v_i^T v_i = 1$. Note that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_q$$
.



Step 5 (optional): Construct the principal components:

$$PC_1 = e_{11}\tilde{X}_1 + e_{12}\tilde{X}_2 + \cdots + e_{1q}\tilde{X}_q, \ PC_2 = e_{21}\tilde{X}_1 + e_{22}\tilde{X}_2 + \cdots + e_{2q}\tilde{X}_q, \ dots \ PC_q = e_{q1}\tilde{X}_1 + e_{q2}\tilde{X}_2 + \cdots + e_{qq}\tilde{X}_q.$$

where $v_i = (e_{i1}, e_{i2}, ..., e_{iq})$.

Example 11.1.1

Given an unlabelled data with 15 observations and feature columns (but tabulate in horizontal form to save space). Find all the principal components.

	1	2	3	4	5	6	7	8
$\overline{X_1}$	8.095	6.91	4.119	4.4	4.65	2.329	9 8.27	72 4.595
X_2	4.104	5.272	4.063	5.366	5.238	3 4.71	1 2.4	6 0.581
X_3	2.351	-2.827	-3.786	-0.261	-1.09	6 -1.45	6 -1.7	27 -1.292
	9	10	11	12	13	14	15	_
$\overline{X_1}$	8.071	6.403	4.136	7.283	2.744	4.939	4.924	_
X_2	5.883	3.624	3.514	-1.301	3.584	3.024	2.754	
X_3	0.938	2.949	2.918	-0.738	3.866	-0.803	5.154	_

Example 11.1.1 (cont)

Solution: It is possible for us to find the principal components using linear algebra. First, let us, calculate the column means:

$$\overline{x}_{.j} = (5.45800, 3.52513, 0.27933)$$

and shift X to the "centre", i.e. $X = x_{.j} - \overline{x}_{.j}$:

	1	2	3	4	5	6	7	8
X_1	2.637	1.452	-1.339	-1.058	-0.808	-3.129	2.814	-0.863
X_2	0.578867	1.746867	0.537867	1.840867	1.712867	1.185867	-1.065133	-2.944133
X ₃	2.071667	-3.106333	-4.065333	-0.540333	-1.375333	-1.735333	-2.006333	-1.571333
	9	10	11	12	13	14	15	
X_1	2.613	0.945	-1.322	1.825	-2.714	-0.519	-0.534	
X_2	2.357867	0.098867	-0.011133	-4.826133	0.058867	-0.501133	-0.771133	
X ₃	0.658667	2.669667	2.638667	-1.017333	3.586667	-1.082333	4.874667	

Example 11.1.1 (cont)

The covariance matrix of X is

$$\mathsf{Cov}(X) = \frac{1}{15 - 1} \widetilde{X}^T \widetilde{X} = \begin{bmatrix} 3.700046 & -0.441594 & -0.261248 \\ -0.441594 & 3.63697 & -0.097637 \\ -0.261248 & -0.097637 & 6.82242 \end{bmatrix}$$

We need to find the eigenvalues of Cov(X). This can be done using university linear algebra (determinant, r.e.f)

$$\lambda_i = 6.845301, 4.105652, 3.208484$$

Using R: eigen(S).



Example 11.1.1 (cont)

The corresponding eigenvectors are the **weighted vectors**

$$v_1 = \begin{bmatrix} -0.080068 \\ -0.019308 \\ 0.996602 \end{bmatrix}, \quad v_2 = \begin{bmatrix} 0.722438 \\ -0.689991 \\ 0.044673 \end{bmatrix}, \quad v_3 = \begin{bmatrix} 0.686784 \\ 0.723560 \\ 0.069195 \end{bmatrix}$$

The first, second and third principal components of X are:

$$PC_1 = -0.080068X_1 - 0.019308X_2 + 0.996602X_3$$

 $PC_2 = 0.722438X_1 - 0.689991X_2 + 0.044673X_3$
 $PC_3 = 0.686784X_1 + 0.723560X_2 + 0.069195X_3$

PCA in Python

pca = sklearn.decomposition.PCA(); pca.fit(X)

PCA in R

```
pca = prcomp(x, retx=TRUE, center=TRUE, scale=FALSE, tol=NULL, rank=NULL, ...) pca$center: \overline{x}_{.j} pca$sdev: \sqrt{\lambda_i} pca$sdev: [v_1, v_2, \cdots] pca$x: [\widetilde{X}v_1, \widetilde{X}v_2, \cdots] pca$scale: \sqrt{\frac{\sum_i (x_{ij} - \overline{x}_{.j})^2}{n-1}}
```

Final Exam Jan 2019, Q1(c); Need to use "linear algebra" You are given the following information:

- The data set consists of 3000 observations and 2 predictors, X_1 and X_2 .
- The covariance matrix, C of X_1 and X_2 is

$$C = \begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix}$$

Final Exam Jan 2019, Q1(c) cont.

- Ompute the eigenvalues, λ_1 and λ_2 . For each of the eigenvalues computed, find the eigenvectors, v_1 and v_2 . (7 marks)
- First principal component, PC1 is the linear combination of predictors that has the maximum variance among all principal components. Based on your answer in (i), write the equation of first principal component for this data set. (2 marks)

Solution:

(i) Eigenvalues:

$$|C - \lambda I| = \begin{vmatrix} 2.0 - \lambda & 0.8 \\ 0.8 & 0.6 - \lambda \end{vmatrix}$$
$$= \lambda^2 - 2.6\lambda + 0.56 = 0$$
$$\Rightarrow x = 0.236985, 2.363015$$

[2 marks]

Solution (cont):

Eigenvectors:

 $\lambda = 0.236985$:

$$\begin{bmatrix} 2.0 - 0.236985 & 0.8 \\ 0.8 & 0.6 - 0.236985 \end{bmatrix} v_1 = 0 \Rightarrow$$

$$\mbox{v_1} = \frac{1}{\sqrt{0.8^2 + (-1.763015)^2}} \begin{bmatrix} 0.8 \\ -1.763015 \end{bmatrix} = \begin{bmatrix} 0.413216 \\ -0.910633 \end{bmatrix} \label{eq:v1}$$
 [2.5 marks]

 $\lambda = 2.363015$:

$$\begin{bmatrix} 2.0 - 2.363015 & 0.8 \\ 0.8 & 0.6 - 2.363015 \end{bmatrix} v_2 = 0$$

$$\Rightarrow v_2 = \frac{1}{\sqrt{0.8^2 + (-(-0.363015))^2}} \begin{bmatrix} 0.8 \\ -(-0.363015) \end{bmatrix}$$

$$= \begin{bmatrix} 0.910633 \\ 0.413217 \end{bmatrix}$$
 [2.5 marks]

(ii) PC1 is the linear combination of predictors with highest eigenvalue $\lambda_1 = 2.363015$, i.e.

$$PC_1 = 0.910633X_1 + 0.413217X_2.$$



A little bit more theory: Let $Y = \frac{1}{\sqrt{n-1}}\tilde{X}$ and $\lambda_i = \sigma_i^2$. From (1), we have

$$Y^TY = \sigma_1^2 \mathbf{v}_1 \mathbf{v}_1^T + \dots + \sigma_q^2 \mathbf{v}_q \mathbf{v}_q^T$$

Since $v_i^T v_j = 0$ for $i \neq j$, $v_i^T v_i = 1$, we have

$$Y^{T}Yv_{i} = (\sigma_{1}^{2}v_{1}v_{1}^{T} + \dots + \sigma_{q}^{2}v_{q}v_{q}^{T})v_{i} = \sigma_{i}^{2}v_{i}$$
$$\Rightarrow Y^{T}(\frac{1}{\sigma_{i}}Yv_{i}) = \sigma_{i}v_{i}.$$

Let $u_i = \frac{1}{\sigma_i} Y v_i$ and $U = [u_1, ..., u_q]$. Putting left and right column vectors into matrix form, we have

$$Y^TU = VS$$
, $V = [v_1, ..., v_q]$, $S = diag(\sigma_1, ..., \sigma_q)$.

From which we obtain the singular value decomposition (SVD):

$$Y^T = VSU^T \Rightarrow Y = USV^T$$
.

Note that $S^T = S$, U is related to pca\$x, V is related to pca\$rotation and σ_i is pca\$sdev mentioned earlier in Example 11.1.1.

The proportion of variation explained by the kth principal component is defined to be the eigenvalue, λ_k for that component divided by the sum of the eigenvalues. In other words, the kth principal component explains the following proportion of the total variation, which denote as proportion of variance, PVE_k , explained by PC_k :

$$PVE_k = \frac{\lambda_k}{\lambda_1 + \lambda_2 + \dots + \lambda_p}, \quad k = 1, \dots, p.$$
 (2)

A related quantity is the proportion of variation explained by the first k principal components is the cumulative proportion of variance explained until PC_k :

$$CPVE_k = \frac{\lambda_1 + \dots + \lambda_k}{\lambda_1 + \lambda_2 + \dots + \lambda_p}, \quad k = 1, 2, \dots, p.$$
 (3)

In another word, $CPVE_k$ is the cumulation of PVE_s .

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If the proportion of variation explained by the first k principal components is large, then not much information is lost by considering only the first k principal components. In general, we only retain the first k principal components and balance the two conflicting desires:

- To obtain the simplest possible interpretation, we want k to be as small as possible.
- To avoid loss of information, we want

 $CPVE_k \approx 1.$

How many principal components should we use? One of the methods to determine the number of principal components is to look at a scree plot (https://en.wikipedia.org/wiki/Scree_plot). With the eigenvalues ordered from largest to the smallest, a scree plot is the plot of "principal component" λ_k against k. The number of components is determined at the point beyond which the remaining eigenvalues are all relatively small and of comparable size.

Example 11.1.3

The dataset (https://www.openml.org/d/509) from the guide "Places Rated Almanac", by Richard Boyer and David Savageau, copyrighted and published by Rand McNally, uses nine rating criteria: (1) Climate and Terrain, (2) Housing, (3) Health Care & Environment, (4) Crime, (5) Transportation, (6) Education, (7) The Arts, (8) Recreation, (9) Economics.

Note that within the dataset, except for housing and crime, the higher the score the better. For housing and crime, the lower the score the better. Where some communities might rate better in the arts, other communities might rate better in other areas such as having a lower crime rate and good educational opportunities.

Example 11.1.3 (cont.)

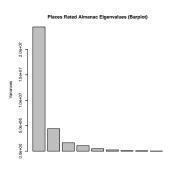
Suppose that principal component analysis has been implemented and the eigenvalues of each principal component are shown in the table below.

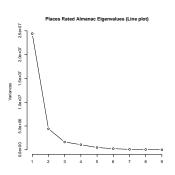
k	1	2	3	4	5	6
$\overline{\lambda_k}$	24413669	4408005	1638040	1076356	478338.3	240851.8
k	7	8	9			
λ_k	92809.94	66995.9	10962.63			

Compute the proportion of variance explained by each component and the cumulative proportion respectively. After that, construct a scree plot and determine the number of principal components to be considered.

Example 11.1.3 (cont.)

There are two ways to represent "scree plot", one using "bar chart", the other using "line plot".





Example 11.1.4

The correlations between the principal components and the original variables for Example 11.1.3 are shown in the table below.

Variable	PC1	PC2	PC3	
Climate	0.00642	-0.01546	0.00669	
Housing	0.26914	-0.93721	0.08264	
Health	0.17832	0.02054	-0.02776	
Crime	0.02813	0.01090	-0.03761	
Transportation	0.14930	-0.01876	-0.97153	
Education	0.02519	0.00140	-0.04151	
Arts	0.93086	0.28226	0.15103	
Recreation	0.06982	-0.10385	-0.14957	
Economy	0.02513	-0.17336	-0.01274	

Example 11.1.4 (cont)

Solution:

First Principal Component - PC1

The first principal component is **strongly correlated** with the original variable Arts. It increases with all features, in particular, Arts. Based on the correlation of 0.93086, the first principal component is primarily a measure of the Arts and it has $0.93086 \times PVE_1 = 70\%$ influence. It would follow that communities with high values tend to have a lot of arts available, in terms of museums, fine arts, public radio stations, public television stations, universities offering degrees in the arts, symphony orchestras, theatres, opera companies, dance companies, public libraries etc. Whereas communities with small values would have very few of these types of opportunities.

Example 11.1.4 (cont)

Second Principal Component - PC2

The second principal component decreases with the feature Housing and increases with the feature Arts. This component can be viewed as a measure of things utility bills, property taxes, mortgage payments related to Housing have 12.7% $(0.93721 \times PVE_2)$ significance.

Example 11.1.4 (cont)

Third Principal Component - PC3

The third principal component decreases mainly with increasing Transportation and increases slightly with increasing Arts. This suggests that places with bad transportation has 4.9% ($0.97153 \times PVE_3$) significance.

Final Exam May 2019, Q1(c)

An investigation is carried out to examine the eating habit of citizens in each state in Malaysia. A total of 8 types of food had been investigated — the average consumption of each type of food (grams) per person per week in each state in Malaysia was recorded. The 8 types of food are listed below:

- $x_1 = \mathsf{Fish}$
- $x_2 = Meat$
- $x_3 = Grain$
- $x_4 = Dairy$

- $x_5 = \text{Beans}$
- $x_6 = Egg$
- x_7 = Vegetables
- $x_8 = Fruit$

Final Exam May 2019, Q1(c) cont
For advanced analysis on the eating habit, the analyst would like to reduce the dimension of the data.
Therefore, principal component analysis has been performed. Eigenvalues computed from the principal component analysis are

$$\lambda = [0.0342, 0.6432, 2.3664, 0.5869, 1.1894, 0.0032, 5.6379, 0.0179]^T$$

Final Exam May 2019, Q1(c) cont

- State the variance explained by each principal component. With a targeted cumulative proportion of variance explained (CPVE) of 85%, state the number of principal components to be considered. (4 marks)
- Given that the eigenvector for PC1 is

```
e_1 = \begin{bmatrix} 0.174 & -0.626 & -0.146 & 0.667 & -0.249 & 0.743 & 0.598 & 0.484 \end{bmatrix}.
```

Interpret the principal component results with respect to the types of food. You should provide explanation on which types of food are the most and the least contributed to PC1, as well as the correlation between PC1 and that variable. (5 marks)

Solution: (i)

Variance explained = eigenvalue (Highest for PC1 in descending order)

PC	λ	PVE	CPVE
1	5.6379	0.5380	0.5380
2	2.3664	0.2258	0.7638
3	1.1894	0.1135	0.8773
4	0.6432	0.0614	0.9387
5	0.5869	0.0560	0.9947
6	0.0342	0.0033	0.9980
7	0.0179	0.0017	0.9997
8	0.0032	0.0003	1.0000
Total	10.4791		
1.65) (5.65)			

With targeted CPVE of 85%, 3 principal components (PC1, PC2 and PC3), with CPVE of 87.73%, should be considered.

Solution: (ii)

The correlation between PC1 and variables are shown below:

	T (F)		
Variable, <i>x_i</i>	Type of Food	e_{1i}	
	Fish	0.174	
	Meat	-0.626	
X ₃	Grain	-0.146	
X ₄	Dairy	0.667	
X ₅	Beans	-0.249	
	Egg	0.743	
X ₇	Vegetables	0.598	
X ₈	Fruit	0.484	

Solution: (ii)

Egg is the most contributed to PC1 as it has the highest absolute in the eigenvalues which is 0.743. Egg is positively correlated with PC1 since it has a positive value. This means that PC1 will be higher if the egg consumption increases.

Grain is the least contributed to PC1 as it has the lowest absolute in the eigenvalues which is -0.146. Grain is negatively correlated with PC1 since it has a negative value. This means that PC1 will be lower if the grain consumption increases.

A biplot is a 2D "scatter plot" of PC_1 and PC_2 In the above, we required that n > p. However, for the case of n < p, we just need to transpose the data X and all the decomposition can be carried out.

For the case n < p, it corresponds to data that are collected on a large number of variables from a single population.

There would be too many pairwise correlations between the variables to consider, i.e. there are $\binom{p}{2} = \frac{p(p-1)}{2}$ correlations or scatter plots to be examined. E.g. when p=10, there are 45 scatter plots!

A *biplot* is a 2D "scatter plot" of the first and the second principle components. In the above, we required that n > p. However, for the case of $n \le p$, we just need to transpose the data X and all the decomposition can be carried out.

For the case $n \leq p$, it corresponds to data that are collected on a **large number of variables** from a single population. With a large number of variables, the dispersion matrix may be too large to study and interpret properly. There would be too many pairwise correlations between the variables to consider, i.e. there are $\binom{p}{2} = \frac{p(p-1)}{2}$ correlations or scatter plots to be examined. For example, when p=10, there are 45 scatter plots! Hence, graphical displays may also not be particularly helpful when the data set is very large.

Example 11.1.7
Consider the "EATING IN THE UK" from http:
//setosa.io/ev/principal-component-analysis/.
This is a 17-dimension example. The table below is the average consumption of 17 types of food in grams per person per week for every country in the UK.

Example 11.1.7 (cont)

	England	Wales	Scotland	N.Ireland
Cheese	105	103	103	66
Carcass meat	245	227	242	267
Other meat	685	803	750	586
Fish	147	160	122	93
Fresh potatoes	720	874	566	1033
Processed potatoes	198	203	220	187
Fats and oils	193	235	184	209
Sugars	156	175	147	139
Fresh Veg	253	265	171	143
Other Veg	488	570	418	355
Processed Veg	360	365	337	334
Fresh fruit	1102	1137	957	674
Cereals	1472	1582	1462	1494
Beverages	57	73	53	47
Soft drinks	1374	1256	1572	1506
Alcoholic drinks	375	475	458	135
Confectionery	54	64	62	41

Example 11.1.7 (cont) The PVEs and CPVEs are given as a summary to PCA:

```
        Importance of components:

        PC1
        PC2
        PC3
        PC4

        Standard deviation
        324.1502
        212.7478
        73.87622
        4.189e-14

        Proportion of Variance
        0.6744
        0.2905
        0.03503
        0.000e+00

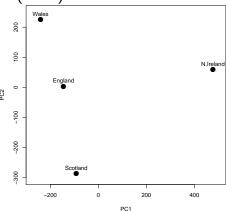
        Cumulative Proportion
        0.6744
        0.9650
        1.00000
        1.000e+00
```

Example 11.1.7 (cont)

A script to compute the above values and produce a biplot is listed below.

```
# From https://bioboot.github.io/bggn213_f17/class-material/UK_food_r
  x = read.csv("UK foods.csv")
  rownames(x) = x[,1]
  x = x[,-1]
                     # Remove first column
  ### Print x as a nice table (an alternative is R's View() function)
  #knitr::kable(x, caption="The full UK foods data table")
  pca = prcomp(t(x))
8
  print(pca$sdev^2)
  print(summary(pca))
  plot(pca$x[,1], pca$x[,2], xlab="PC1", ylab="PC2", xlim=c(-270,500),
0
    ylim=c(-300,250), pch=16, cex=2)
  text(pca$x[,1], pca$x[,2]+19, colnames(x))
  # biplot(pca)
```

Example 11.1.7 (cont)



Example 11.1.7 (cont)

From the biplot, we detect that Northern Ireland is a major outlier. Once we go back and look at the data in the table, this makes sense: the Northern Irish eat way more grams of fresh potatoes and way fewer of fresh fruits, cheese, fish and alcoholic drinks. It's a good sign that structure we've visualised reflects a major fact of real-world geography: Northern Ireland is the only of the four countries not on the island of Great Britain.

PCA has been very successful in a lot of dimensional reduction tasks. For example latent semantic analysis uses PCA, population structure in the genetic data from different geographical locations can be inferred using PCA etc.

Despite it's popularity, PCA has some obvious shortcomings, most notably is the assumption that data lie on a linear subspace. If the data lie along a curled plane, e.g. a swiss roll embedded in 3D Euclidean space, PCA wouldn't be able to find the 2-dimensional representation even though the data is obviously 2d.

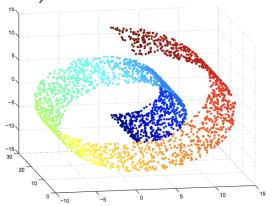


Figure 1: A curled plane: the swiss roll.

Generated using Rdimtools::aux.gensamples(500, dname="swiss")

Outline

Overview

PCA

SNE & t-SNE

SNE and t-SNE

PCA is a linear algorithm and it cannot "project" the nonlinear relationship between features to low dimensional space well. On the other hand, SNE (Stochastic Neighbour Embedding) and t-SNE (t-Distributed SNE) use probability distributions with random walk on neighbourhood graphs to identify and try to preserve the "nonlinear" structure of the data.

SNE converts the high-dimensional Euclidean distances between data points into conditional probabilities that represent similarities, i.e.

$$\mathbb{P}(X = x_j | X = x_i) = \frac{\exp(-\frac{\|x_i - x_j\|^2}{2\sigma_i^2})}{\sum_{k \neq i} \exp(-\frac{\|x_i - x_k\|^2}{2\sigma_i^2})} =: p_{j|i}$$

where σ_i is the variance of the Gaussian that is centred on the data point x_i .

Assume that the "projected" high-dimensional points x_i and x_j to a low-dimension "space" is y_i and y_j respectively. The conditional probability of y_i and y_j is

$$\mathbb{P}(Y = y_j | Y = y_i) = \frac{\exp(-\|y_i - y_j\|^2)}{\sum_{k \neq i} \exp(-\|y_i - y_k\|^2)} =: q_{j|i}.$$
(4)

Note that, we define

$$\mathbb{P}(Y = y_i | Y = y_i) = 0, \text{ for all } i$$

since we only want to model pair-wise similarity.

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To measure the minimisation of sum of difference of conditional probability, SNE minimises the sum of *Kullback-Leibler divergences* (mentioned in the Entropy Section) overall data points using a gradient descent method:

$$C = \sum_{i} \sum_{j} p_{j|i} \ln \frac{p_{j|i}}{q_{j|i}}.$$
 (5)

In other words, the SNE cost function (5) focuses on retaining the local structure of the data in the map (for reasonable values of the variance of the Gaussian in the high-dimensional space, σ_i).

t-SNE tries to minimise symmetric version of the SNE cost function:

$$C = \sum_{i} \sum_{j} p_{ij} \ln \frac{p_{ij}}{q_{ij}}, \ p_{ij} := \frac{p_{j|i} + p_{i|j}}{2n}, \ q_{ij} := \frac{q_{j|i} + q_{i|j}}{2n}$$

and employs a heavy-tailed distribution in the low-dimensional space:

$$\mathbb{P}(\mathsf{Y} = \mathsf{y}_{j}|\mathsf{Y} = \mathsf{y}_{i}) = \frac{(1 + \|\mathsf{y}_{i} - \mathsf{y}_{j}\|^{2})^{-1}}{\sum_{k \neq i} (1 + \|\mathsf{y}_{i} - \mathsf{y}_{k}\|^{2})^{-1}} =: q_{j|i}$$
(6)

to alleviate both the crowding problem & the optimisation problems of SNE.

In R, t-SNE is implemented in tsne::tsne and Rtsne::Rtsne (based on C++, much faster). In Python, t-SNE is implemented as sklearn.manifold.TSNE. Therefore many other manifold unsupervised learning methods in sklearn.manifold which are not explored, such as Isomap, LocallyLinearEmbedding (contain a lot of variance: method='standard', 'hessian', 'modified' or 'ltsa'), SpectralEmbedding, MDS (multi-dimensional scaling), etc.

Example 11.2.1: An R script to compare PCA and t-SNE on the MNIST data is listed below.

```
# https://www.analyticsvidhya.com/blog/2017/01/t-sne-implementation-r
library(Rtsne) # Uses Barnes-Hut-TSNE algorithm instead of the slower
train = read.csv("mnist_train.csv")
X = train[.-1]
train$label = as.factor(train$label)
colours = rainbow(length(unique(train$label)))
names(colours) = unique(train$label)
# https://www.youtube.com/watch?v=xPBO-MMxIoQ[R Tutorial: PCA and t-S
pca = prcomp(train[,-1], rank=2) # project data to first two PCs only
plot(pca$x[,1:2], pch=as.character(train$label),
                   col=colours[train$label], main="Biplot")
# Takes a long time to calculate: dim(X) = 10000 \times 784
tsne = Rtsne(X, dims=2, perplexity=30, verbose=TRUE, max_iter=500)
time.taken = system.time(Rtsne(X, dims=2, perplexity=30,
                               verbose=TRUE, max iter=500))
plot(tsne$Y, t='n', main="tsne")
text(tsne$Y, labels=train$label, col=colours[train$label])
```

6

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0

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