Machine Learning

Lecture 18: Principal Component Analysis (PCA)

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Context

Digital technologies, machine learning and AI are revolutionising the fields of medicine, research and public health.

1 PB = 1,000 TB

1. How can we make sense from this data?
2. Is it all useful data?
3. How can we make the data smaller, without losing much information?

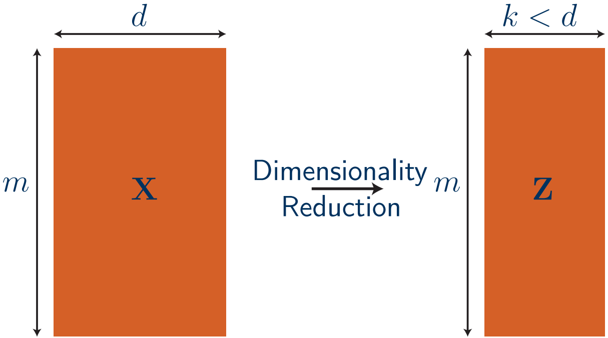
Learning Outcomes

1. Learn about the key motivation behind the use of the PCA method
2. Understand the geometrical explanation of the PCA method
3. Explain steps in one of the derivations of the PCA method
4. Apply the PCA method on a real dataset

References:

1. James *et al.*, *An Introduction to Statistical Learning*, Springer, 2013. (Sections 6.3, 6.7, and 10.2)
2. Bishop, *Pattern Recognition and Machine Learning*, Springer, 2008. (Section 12.1)

Dimensionality Reduction



Applications and Considerations

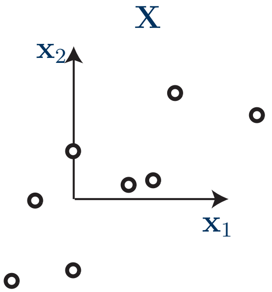
Applications of the PCA method (and many other dimensionality reduction methods)

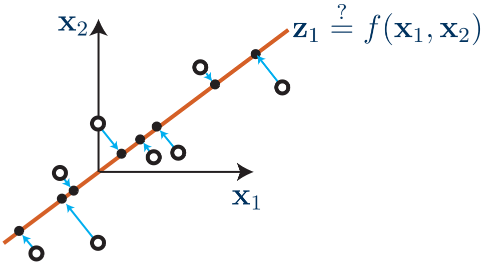
1. Visualisation
2. Exploration
3. Compression

Key considerations:

1. Reducing the number of columns ($d \to k$) by deletion is not meaningful.
2. Columns of $\mathbf{Z}$ are uncorrelated, *i.e.* minimal redundancy.
3. It is OK to make our variables *less interpretable*!

Principal Component Analysis





Notes

1. We are interested in finding projections of data points that are as similar to the original data points as possible, but which have a significantly lower intrinsic dimensionality.
2. Without loss of generality, we assume that the mean of data is zero.

Principal Component Analysis

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

$$\mathbf{Z}_{m\times k} = \mathbf{X}_{m\times d}\mathbf{U}_{d\times k}$$

$$\mathbf{Z} = [\mathbf{z}_1 \ \mathbf{z}_2 \ \cdots \ \mathbf{z}_k] \qquad \mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_d] \qquad \mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_k]$$

$$\mathbf{z}_1 = \mathbf{X}\mathbf{u}_1$$

Remarks

1. Principal components are a sequence of projections of the data, mutually uncorrelated and ordered in variance.
2. The columns $\mathbf{u}_{1\ldots k}$ of $\mathbf{U}$ are orthonormal, so that $\mathbf{u}_i^T\mathbf{u}_j = 0$ if and only if $i \neq j$ and $\mathbf{u}_i^T\mathbf{u}_i = 1$.

Key Different Perspectives to PCA

Three key approaches to PCA:

1. Maximum variance formulation (Hotelling 1933)
2. Minimum error formulation (Pearson 1901)
3. Probabilistic formulation (Tipping & Bishop 1997)

Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

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$$\mathbf{Z} = [\mathbf{z}_1 \ \mathbf{z}_2 \ \cdots \ \mathbf{z}_k] \qquad \mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_d] \qquad \mathrm{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_k]$$

$$\max_{\mathbf{u_1}} \mathrm{Var}[\mathbf{z}_1] = \max_{\mathbf{u_1}} \mathrm{Var}[\mathbf{X}\mathbf{u}_1]$$

Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

$$\mathbf{Z}_{m\times k} = \mathbf{X}_{m\times d}\mathbf{U}_{d\times k}$$

$$\mathbf{Z} = \begin{bmatrix}\mathbf{z}_1 & \mathbf{z}_2 & \cdots & \mathbf{z}_k\end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix}\mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_d\end{bmatrix} \qquad \mathbf{U} = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_k\end{bmatrix}$$

$$\max_{\mathbf{u_1}} \mathrm{Var}[\mathbf{z}_1] = \max_{\mathbf{u_1}} \mathrm{Var}[\mathbf{X}\mathbf{u}_1]$$

$$\max_{\mathbf{u_1}} \ \mathbf{z}_1^T\mathbf{z}_1 = \max_{\mathbf{u_1}} \ \mathbf{u}_1^T\mathbf{X}^T\mathbf{X}\mathbf{u}_1$$

$$= \max_{\mathbf{u}_1} \ \mathbf{u}_1^T\Sigma_{\mathbf{X}}\mathbf{u}_1 \qquad \Sigma_{\mathbf{X}} = \mathbf{X}^T\mathbf{X}\text{: } (\text{N} \times \text{covariance of } \mathbf{X})$$

Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

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$$\max_{\mathbf{u_1}} \mathrm{Var}[\mathbf{z}_1] = \max_{\mathbf{u_1}} \mathrm{Var}[\mathbf{X}\mathbf{u}_1]$$

$$\max_{\mathbf{u_1}} \ \mathbf{z}_1^T\mathbf{z}_1 = \max_{\mathbf{u_1}} \ \mathbf{u}_1^T\mathbf{X}^T\mathbf{X}\mathbf{u}_1$$

$$= \max_{\mathbf{u}_1} \ \mathbf{u}_1^T\Sigma_{\mathbf{X}}\mathbf{u}_1 \qquad \Sigma_{\mathbf{X}} = \mathbf{X}^T\mathbf{X}\text{: (N} \times \text{covariance of } \mathbf{X})$$

$$= \max_{\mathbf{u}_1} \ \mathbf{u}_1^T\Sigma_{\mathbf{X}}\mathbf{u}_1 \quad \text{s.t.} \quad \|\mathbf{u}_1\| = \mathbf{u}_1^T\mathbf{u}_1 = 1$$

Maximum Variance Formulation

Using the Lagrange multipliers method:

$$L(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T \Sigma_{\mathbf{X}} \mathbf{u}_1 - \lambda_1(\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

$$\frac{\partial L}{\partial \mathbf{u}_1} = 2\Sigma_{\mathbf{X}} \mathbf{u}_1 - 2\lambda_1 \mathbf{u}_1 = 0$$

Maximum Variance Formulation

Using the Lagrange multipliers method:

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$$\frac{\partial L}{\partial \mathbf{u}_1} = 2\Sigma_{\mathbf{X}} \mathbf{u}_1 - 2\lambda_1 \mathbf{u}_1 = 0$$

$\Sigma_{\mathbf{X}} \mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \quad \rightsquigarrow \quad \lambda_1$ and $\mathbf{u}_1$ are an eigenvalue-eigenvector pair of $\Sigma_{\mathbf{X}}$

Maximum Variance Formulation

Using the Lagrange multipliers method:

$$L(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T \Sigma_{\mathbf{X}} \mathbf{u}_1 - \lambda_1(\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

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$$\Sigma_{\mathbf{X}} \mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \quad \rightsquigarrow \quad$$ λ_1 and $\mathbf{u}_1$ are an eigenvalue-eigenvector pair of $\Sigma_{\mathbf{X}}$

$$\mathrm{Var}[\mathbf{z}_1] = \mathbf{u}_1^T \Sigma_{\mathbf{X}} \mathbf{u}_1 = \mathbf{u}_1^T \lambda_1 \mathbf{u}_1 = \lambda_1 \underbrace{\mathbf{u}_1^T \mathbf{u}_1}_{1} = \lambda_1$$

Maximum Variance Formulation

Using Lagrange multipliers:

$$L(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T \Sigma_{\mathbf{X}} \mathbf{u}_1 - \lambda_1(\mathbf{u}_1^T \mathbf{u}_1 - 1)$$

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$$\mathrm{Var}[\mathbf{z}_1] = \mathbf{u}_1^T \Sigma_{\mathbf{X}} \mathbf{u}_1 = \mathbf{u}_1^T \lambda_1 \mathbf{u}_1 = \lambda_1 \underbrace{\mathbf{u}_1^T \mathbf{u}_1}_{1} = \lambda_1$$

For $\Sigma_{\mathbf{X}}$ there are d eigenvalue-eigenvector pairs:

$$\begin{array}{ccccccccc} e_1 & > & e_2 & > & e_3 & > & \cdots & > & e_d \\ \mathbf{v}_1 & & \mathbf{v}_2 & & \mathbf{v}_3 & & \cdots & & \mathbf{v}_d \end{array}$$

Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

$$\mathbf{Z}_{m\times k} = \mathbf{X}_{m\times d}\mathbf{U}_{d\times k}$$

$$\mathbf{Z} = [\mathbf{z}_1 \ \mathbf{z}_2 \ \cdots \ \mathbf{z}_k] \qquad \mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_d] \qquad \mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_k]$$

The first principal direction $\mathbf{u}_1$ must be the eigenvector of $\Sigma_{\mathbf{X}}$ that corresponds to largest eigenvalue (e_1).

$$\mathbf{z}_1 = \mathbf{X}\mathbf{u}_1 \quad \rightarrow \quad \mathbf{z}_1 = \mathbf{X}\mathbf{v}_1$$

Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

$$\mathbf{Z}_{m\times k} = \mathbf{X}_{m\times d}\mathbf{U}_{d\times k}$$

$$\mathbf{Z} = \begin{bmatrix}\mathbf{z}_1 & \mathbf{z}_2 & \cdots & \mathbf{z}_k\end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix}\mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_d\end{bmatrix} \qquad \mathbf{U} = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_k\end{bmatrix}$$

The first principal direction $\mathbf{u}_1$ must be the eigenvector of $\Sigma_{\mathbf{X}}$ that corresponds to largest eigenvalue (e_1).

$$\mathbf{z}_1 = \mathbf{X}\mathbf{u}_1 \quad \rightarrow \quad \mathbf{z}_1 = \mathbf{X}\mathbf{v}_1$$

What about other principal components? $\quad \mathbf{z}_{2\ldots k} = \mathbf{X}\mathbf{u}_{2\ldots k} \stackrel{?}{=} \mathbf{X}\mathbf{v}_{2\ldots k}$

Each new principal direction $\mathbf{u}_i$ should:

- maximise $\mathrm{Var}[\mathbf{z}_i]$;
- be orthogonal to all other $\mathbf{u}_j$; extracting something new from $\mathbf{X}$.

Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

$$\mathbf{Z}_{m\times k} = \mathbf{X}_{m\times d}\mathbf{U}_{d\times k}$$

$$\mathbf{Z} = [\mathbf{z}_1 \ \mathbf{z}_2 \ \cdots \ \mathbf{z}_k] \qquad \mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \cdots \ \mathbf{x}_d] \qquad \mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_k]$$

For $\mathbf{z}_2$:

$$\mathbf{z}_2 = \mathbf{X}\mathbf{u}_2$$

$$\max_{\mathbf{u}_2} \ \mathrm{Var}[\mathbf{z}_2] = \max_{\mathbf{u}_2} \ \mathbf{u}_2^T \Sigma_{\mathbf{X}} \mathbf{u}_2$$

$$\text{s.t.} \quad \|\mathbf{u}_2\| = 1 \quad \& \quad \mathbf{u}_2^T \mathbf{u}_1 = 0$$

$$\mathbf{z}_2 = \mathbf{X}\mathbf{u}_2 \quad \rightarrow \quad \mathbf{z}_2 = \mathbf{X}\mathbf{v}_2$$

Because $\mathbf{u}_2$ must be the eigenvector of $\Sigma_{\mathbf{X}}$ that corresponds to second largest eigenvalue (e_2).

Summary - Maximum Variance Formulation

$$\mathbf{X}_{m\times d} \xrightarrow{PCA} \mathbf{Z}_{m\times k} \qquad (k < d)$$

$$\mathbf{Z}_{m\times k} = \mathbf{X}_{m\times d}\mathbf{U}_{d\times k} = \mathbf{X}_{m\times d}\mathbf{V}_{d\times k}$$

$$\mathbf{Z} = \begin{bmatrix}\mathbf{z}_1 & \mathbf{z}_2 & \cdots & \mathbf{z}_k\end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix}\mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_d\end{bmatrix} \qquad \mathbf{V} = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_k\end{bmatrix}$$

where columns of $\mathbf{V}_{d\times k}$ are the eigenvectors of $\Sigma_{\mathbf{X}} = \mathbf{X}^T\mathbf{X}$.

An example - Public Health in Scotland

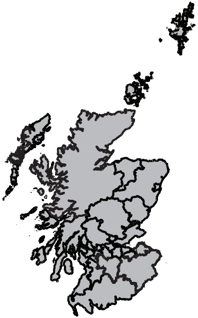
Source: Scottish Public Health Observatory (ScotPHO)
Region: All 32 Councils in Scotland
Year: 2019

Data: Six indicators were extracted

1) Active travel to school
2) Alcohol-related hospital admissions
3) Drug-related deaths
4) Attempted murder & serious assault
5) Drug crimes recorded
6) Smoking quit attempts

Labels: Employment deprivation level

Low v.s. **High**



ScotPHO

An example - Public Health in Scotland

Data Exploration

1) Active travel to school
2) Alcohol-related hospital admissions
3) Drug-related deaths
4) Attempted murder & serious assault
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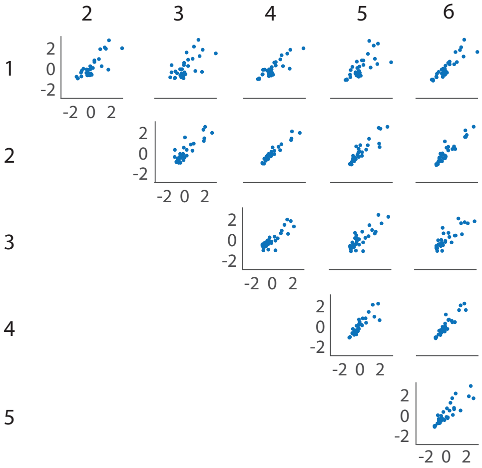
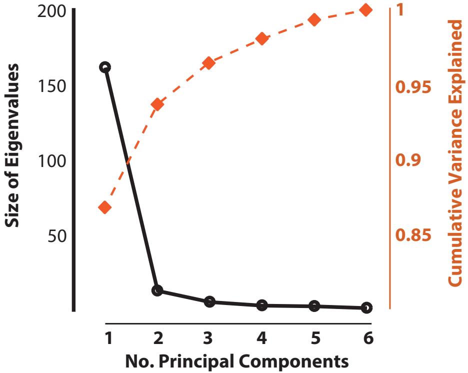
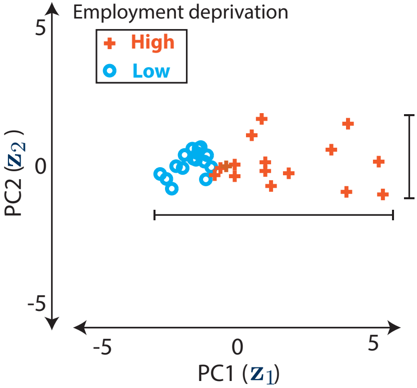
6) Smoking quit attempts



An example - Public Health in Scotland

PCA Results:





Cumulative variance explained $= \frac{\sum_{i=1}^{k} e_i}{\sum_{i=1}^{d} e_i}$

where e_i is the i^{th} eigenvalue

PCA - Bad Applications

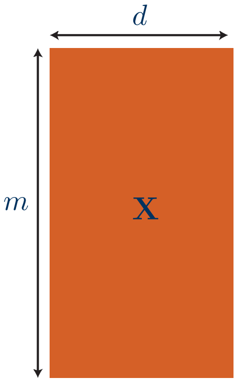
1. Doing PCA to avoid overfitting is a bad idea. Instead use regularisation.
2. Doing PCA to for dimensionality reduction before classification is also a bad idea. Instead use a method called, linear discriminant analysis (LDA).

PCA Implementation

There are three (potentially four) implementations for the PCA methods. For the centred design matrix $\mathbf{X}_{m\times d}$ with the covariance matrix $\mathbf{\Sigma}_{\mathbf{X}} = \frac{1}{m}\mathbf{X}^T\mathbf{X}$

1. Eigenvector decomposition of $\mathbf{\Sigma}_{\mathbf{X}}$ - computational cost $\mathcal{O}(d^3)$
2. Singular value decomposition of $\mathbf{\Sigma}_{\mathbf{X}}$ - computational cost $\mathcal{O}(d^3)$
3. Singular value decomposition of $\mathbf{X}$ - computational cost $\mathcal{O}(md^2)$
   - Prove it as practice.
   - Start with the singular value decomposition of $\mathbf{X}$, that is $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}_{\mathbf{X}}\mathbf{V}^T$
4. Eigenvector decomposition of Gram matrix $K = \mathbf{X}\mathbf{X}^T$ - computational cost $\mathcal{O}(d^3)$

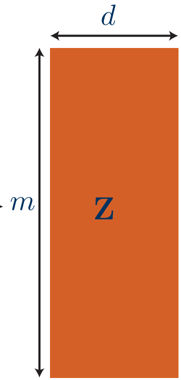
PCA - Summary



A measure of how variables are associated with each another (**Covariance matrix**, $\Sigma_{\mathbf{X}}$).

The directions in which our data is dispersed (**Eigenvectors** of $\Sigma_{\mathbf{X}}$).

The relative importance of these different directions (**Eigenvalues** of $\Sigma_{\mathbf{X}}$).



PCA linearly combines our variables and allows us to drop projections that are less informative.