CEE 616: Probabilistic Machine Learning

M5 Unsupervised Learning:
L5A: Principal Components Analysis

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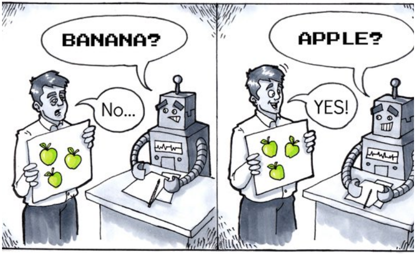
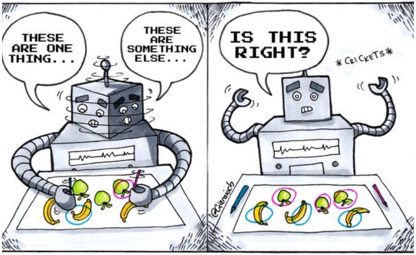
Outline

Unsupervised vs. supervised learning



Supervised Learning



Unsupervised Learning

- Supervised learning: given response y and p features measured on the same observations, predict y on the x_j
- Unsupervised learning: only p features; no given response; what then can we learn about the data?

Learning tools

Supervised

Goal: predict or infer a response (regression or classification)

- multiple linear regression
- logistic regression
- linear/quadratic discriminant analysis
- decision trees
- support vector machines

Unsupervised

Goal: exploration (e.g. grouping, pattern discovery, dimensional analysis)

- dimensionality reduction
- clustering

Dimensionality reductoin

Dimensionality reduction seeks to learn a suitable mapping from a high-dimensional feature space $\boldsymbol{x} \in \mathbb{R}^D$ to a low-dimensional **latent space** $\boldsymbol{z} \in \mathbb{R}^L$.

- **Parametric approach:** estimate $\boldsymbol{z} = f(\boldsymbol{x}; \boldsymbol{\theta})$
- **Nonparametric approach:** compute embedding $\boldsymbol{z}_n$ for each input $\boldsymbol{x}_n$
- Uses:
  - data pre-processing
  - model simplification
- Algorithms:
  - principal components analysis (PCA)
  - factor analysis (FA)
  - autoencoders

Principal components analysis (PCA)

PCA is a dimensionality reduction technique that seeks an L-dimensional basis that best captures the variance in a D-dimensional dataset

- The direction with the largest projected variance is the *first principal component*
- The orthogonal direction capturing the second largest projected variance is the *second principal component*
- The direction that maximizes the variance is that which also minimizes the mean squared error

Interpreting principal components

The first principal component of a design/feature matrix $\boldsymbol{X}$ can be considered as the "best-fit" (closest) line to all the datapoints.

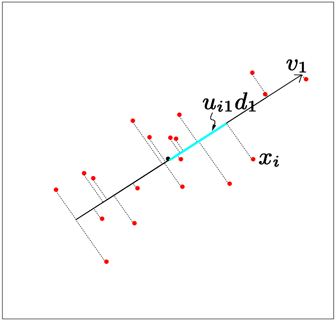


Figure: First principal component (PC) of a dataset. The PC minimizes the total squared distance from each point to its orthogonal projection onto the line

Interpreting principal components (cont.)

The first two principal components of a dataset span the [2D] plane closest to the data.

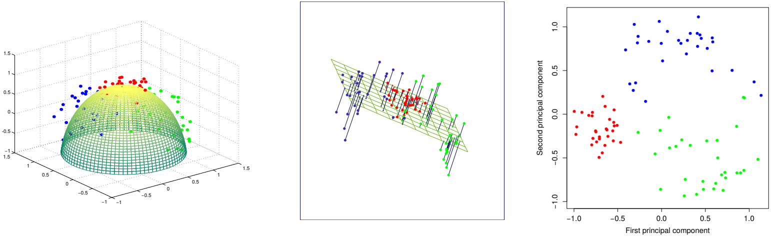


Figure: (L) Simulated dataset near surface of half-sphere. (C) Best 2-dimensional representationof data. (R) Projected points on the plane ($\boldsymbol{U}_2\boldsymbol{\Gamma}_2$)

Sample covariance matrix (review)

The sample covariance matrix is given by:

$$\widehat{\boldsymbol{\Sigma}} = E[(\boldsymbol{X} - \hat{\boldsymbol{\mu}})(\boldsymbol{X} - \hat{\boldsymbol{\mu}})^T] = \begin{pmatrix} \hat{\sigma}_1^2 & \hat{\sigma}_{12} & \cdots & \hat{\sigma}_{1D} \\ \hat{\sigma}_{21} & \hat{\sigma}_2^2 & \cdots & \hat{\sigma}_{2D} \\ \cdots & \cdots & \cdots & \cdots \\ \hat{\sigma}_{D1} & \hat{\sigma}_{D2} & \cdots & \hat{\sigma}_D^2 \end{pmatrix} \tag{1}$$

If $\boldsymbol{X}$ is mean centered, then we can write:

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{N}(\boldsymbol{X}^T\boldsymbol{X}) = \frac{1}{n} \begin{pmatrix} \boldsymbol{x}_1^T\boldsymbol{x}_1 & \boldsymbol{x}_1^T\boldsymbol{x}_2 & \cdots & \boldsymbol{x}_1^T\boldsymbol{x}_D \\ \boldsymbol{x}_2^T\boldsymbol{x}_1 & \boldsymbol{x}_2^T\boldsymbol{x}_2 & \cdots & \boldsymbol{x}_2^T\boldsymbol{x}_D \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{x}_D^T\boldsymbol{x}_1 & \boldsymbol{x}_D^T\boldsymbol{x}_2 & \cdots & \boldsymbol{x}_D^T\boldsymbol{x}_D \end{pmatrix} \tag{2}$$

The sample covariance matrix is given as the pairwise inner/dot products of the centered atrribute/feature vectors, normalized by the sample size N.

Projection of $\boldsymbol{X}$ onto first L basis vectors

The expression $\widetilde{\boldsymbol{x}}_j = \sum_{k=1}^{L} a_{jk}\boldsymbol{v}_k$ is a projection of $\boldsymbol{x}_j$ onto the first L basis vectors.

We derive a compact representation as follows:

$$\begin{aligned} \widetilde{\boldsymbol{x}}_j &= \boldsymbol{V}_L\boldsymbol{a}_L \\ \boldsymbol{a}_L &= \boldsymbol{V}_L^T\boldsymbol{x}_j \\ \implies \widetilde{\boldsymbol{x}}_j &= \boldsymbol{V}_L\boldsymbol{V}_L^T\boldsymbol{x}_j = \boldsymbol{P}_L\boldsymbol{x}_j \end{aligned}$$

where $\boldsymbol{P}_L = \boldsymbol{V}_L\boldsymbol{V}_L^T$ is the orthogonal **projection matrix** for the subspace spanned by the first L basis vectors.

- We can compute the error vector as the projection of $\boldsymbol{x}_j$ onto the subspace spanned by the remaining basis vectors:

$$\boldsymbol{\epsilon}_j = \sum_{k=L+1}^{D} a_{jk}\boldsymbol{v}_k = \boldsymbol{x}_j - \widetilde{\boldsymbol{x}}_j \tag{3}$$

Direction of max variance

We seek the unit vector $\boldsymbol{v}$ that maximizes the projected variance of the points.

If $\boldsymbol{X}$ is centered and $\boldsymbol{\Sigma}$ its covariance matrix, then the projection of X_j on $\boldsymbol{v}$ is:

$$X_j = \left(\frac{\boldsymbol{v}^T\boldsymbol{X}_j}{\boldsymbol{v}^T\boldsymbol{v}}\right)\boldsymbol{v} = (\boldsymbol{v}^T\boldsymbol{X}_j)\boldsymbol{v} = a_j\boldsymbol{v} \tag{4}$$

Across all points, the **projected variance** along $\boldsymbol{v}$ is:

$$\sigma_{\boldsymbol{v}}^2 = \frac{1}{n}\sum_{j=1}^{n}(a_j - \mu_{\boldsymbol{v}})^2 = \frac{1}{n}\sum_{j}\boldsymbol{v}^T(X_jX_j^T)\boldsymbol{v} = \boldsymbol{v}^T\boldsymbol{\Sigma}\boldsymbol{v} \tag{5}$$

The optimal basis that maximizes the projected variance $\sigma_{\boldsymbol{v}}^2$ subject to $\boldsymbol{v}^T\boldsymbol{v} = 1$ is:

$$\max_{\boldsymbol{v}} J(\boldsymbol{v}) = \boldsymbol{v}^T\boldsymbol{\Sigma}\boldsymbol{v} - \lambda(\boldsymbol{v}^T\boldsymbol{v} - 1) \tag{6}$$

Direction of max variance (cont.)

Taking the derivative of $J(\boldsymbol{v})$ w.r.t. $\boldsymbol{v}$ and setting to zero, we obtain:

$$\begin{aligned}\frac{\partial(\boldsymbol{v}^T\boldsymbol{\Sigma}\boldsymbol{v} - \alpha(\boldsymbol{v}^T\boldsymbol{v} - 1))}{\partial \boldsymbol{v}} &= \mathbf{0} \\ \Longrightarrow 2\boldsymbol{\Sigma}\boldsymbol{v} - 2\lambda\boldsymbol{v} &= \mathbf{0} \\ \boldsymbol{\Sigma}\boldsymbol{v} &= \lambda\boldsymbol{v}\end{aligned}$$

Thus λ is an eigenvalue of $\boldsymbol{\Sigma}$ and $\boldsymbol{v}$ the eigenvector.

Recall that the projected variance is given by $\sigma_{\boldsymbol{v}}^2 = \boldsymbol{v}^T\boldsymbol{\Sigma}\boldsymbol{v}$. Thus:

$$\sigma_{\boldsymbol{v}}^2 = \boldsymbol{v}^T\lambda\boldsymbol{v} = \lambda \tag{7}$$

To maximize $\sigma_{\boldsymbol{v}}^2$ we set λ to the largest eigenvalue λ_1 of $\boldsymbol{\Sigma}$; $\boldsymbol{v}_1$ indicates the direction of max variance (first principal component).

Iris dataset: first principal component

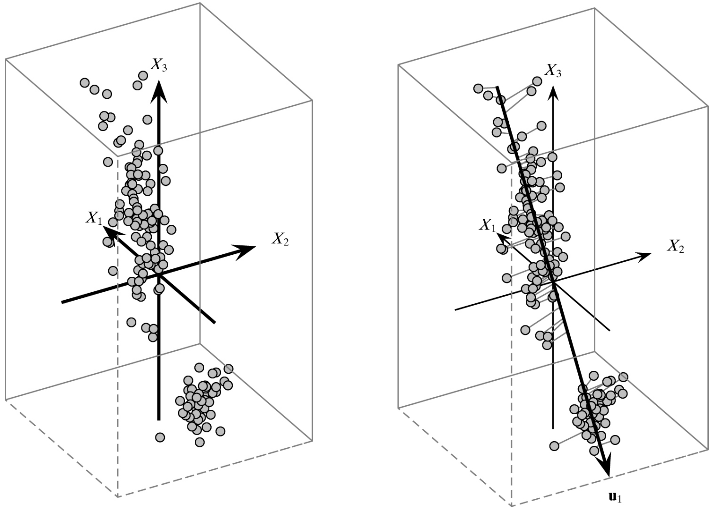


Figure: (Left) Iris dataset showing original basis: sepal length (X_1), sepal width (X_2) and petal length (X_3). (Right) First principal component $\boldsymbol{u}_1$ superimposed

Two dimensions

If we solve a similar optimization problem for two basis vectors $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$, we obtain the first and second principal components whose total projected variance is $\lambda_1 + \lambda_2$.

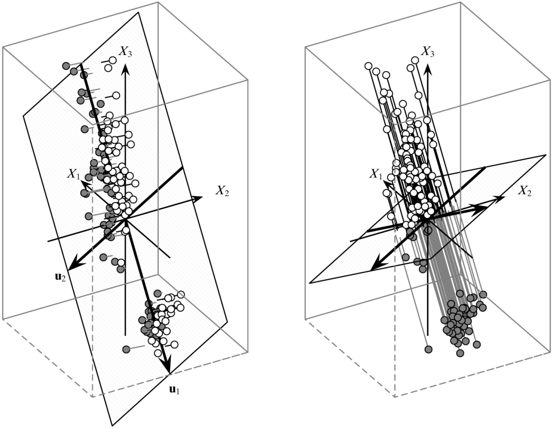


Figure: (Left) Optimal two-dimensional basis for Iris data. (Right) Non-optimal basis

Singular value decomposition (SVD)

Recall the singular value decomposition of $\boldsymbol{X}$:

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^T \tag{8}$$

where:

- $\boldsymbol{X}$ is an $N \times D$ data matrix, whose entries have been centered ($x_{nj} \leftarrow x_{nj} - \overline{x}_j$)
- $\boldsymbol{U}$ is an $N \times D$ orthogonal[1] matrix. The columns of $\boldsymbol{U}$ are called *left singular vectors*
- $\boldsymbol{S}$ is a $D \times D$ diagonal matrix (whose elements are called *singular values*)
- $\boldsymbol{V}$ is an $D \times D$ orthogonal[2] matrix. The columns of $\boldsymbol{V}$ are called *right singular vectors*
- The columns of $\boldsymbol{US}$ are called the **principal components** of $\boldsymbol{X}$.

[1] i.e. $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$ and $\boldsymbol{U}^T = \boldsymbol{U}^{-1}$

[2] i.e. $\boldsymbol{V}^T\boldsymbol{V} = \boldsymbol{I}$ and $\boldsymbol{V}^T = \boldsymbol{V}^{-1}$

SVD (cont.)

$$\overbrace{\begin{pmatrix} x_{11} & \cdots & x_{1D} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{ND} \end{pmatrix}}^{\boldsymbol{X}} = \overbrace{\begin{pmatrix} u_{11} & \cdots & u_{1D} \\ \vdots & \ddots & \vdots \\ u_{N1} & \cdots & u_{ND} \end{pmatrix}}^{\boldsymbol{U}\text{: eigenvectors of } \boldsymbol{X}\boldsymbol{X}^T} \overbrace{\begin{pmatrix} \sqrt{\lambda_1} & \cdots & 0 \\ 0 & \ddots & 0 \\ 0 & \cdots & \sqrt{\lambda_D} \end{pmatrix}}^{\substack{\boldsymbol{S}\text{: } \sqrt{\text{eigenvalues}} \text{ of } \boldsymbol{X}\boldsymbol{X}^T \\ \text{also singular values of } \boldsymbol{X}}} \overbrace{\begin{pmatrix} v_{11} & \cdots & v_{1D} \\ \vdots & \ddots & \vdots \\ v_{D1} & \cdots & v_{DD} \end{pmatrix}}^{\boldsymbol{V}\text{: eigenvectors of } \boldsymbol{X}^T\boldsymbol{X}} \tag{9}$$

- The columns $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_D$ are the left singular vectors of $\boldsymbol{X}$
- The columns $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_D$ are the right singular vectors of $\boldsymbol{X}$
- The elements $\sqrt{\lambda_1} \geq \ldots \geq \sqrt{\lambda_D} = 0$ are the singular values of $\boldsymbol{X}$
- $\lambda_1 \geq \ldots \geq \lambda_D = 0$ are the eigenvalues of $\boldsymbol{X}\boldsymbol{X}^T$ and also of $\boldsymbol{X}^T\boldsymbol{X}$

PCA via SVD

- In the SVD framework, this means we find the best number L of principal components $\boldsymbol{u}_k s_k$, where $k = 1, \dots, L, L+1, \dots, D$.[3]
- The transformed (reduced) dataset is given by:

$$\boldsymbol{Z} = \boldsymbol{U}_L \boldsymbol{S}_L = \boldsymbol{X}\boldsymbol{V}_L \tag{10}$$

  where $\boldsymbol{Z} \in \mathbb{R}^{N \times L}$ is the **score matrix** and $\boldsymbol{U}_L$, $\boldsymbol{S}_L$ and $\boldsymbol{V}_L$ are the L-truncated matrix components of the SVD of $\boldsymbol{X}$

  - $\boldsymbol{V}_L$ is also referred to as the **weight matrix** W
- The data matrix $\boldsymbol{X}$ can be approximately recovered from the transformation by:

$$\widetilde{\boldsymbol{X}} = \boldsymbol{Z}\boldsymbol{V}_L^T \tag{11}$$

  where $\boldsymbol{V}_L^T \in \mathbb{R}^{L \times D}$ (**loadings matrix**) is the transpose of the first L columns of $\boldsymbol{V}$
- Thus, PCA is considered the L-truncated SVD approximation of $\boldsymbol{X}$:

$$\widetilde{\boldsymbol{X}} = \boldsymbol{U}_L \boldsymbol{S}_L \boldsymbol{V}_L^\top \tag{12}$$

[3] Note that $s_k = \sqrt{\lambda_k}$ in our notation.

PCA via SVD (cont.)

Since $\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{V}_L$, we can also recover $\boldsymbol{X}$ by:

$$\widetilde{\boldsymbol{X}} = \boldsymbol{Z}\boldsymbol{V}_L^T = \boldsymbol{X}\boldsymbol{V}_L\boldsymbol{V}_L^T \tag{13}$$

The matrix $\boldsymbol{V}_L\boldsymbol{V}_L^T$ is called the **projection matrix**.

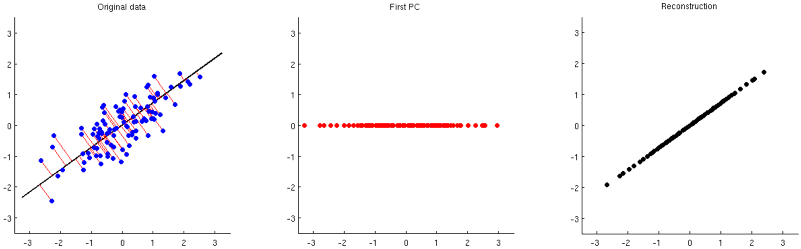


Figure: 1D projection of dataset onto first PC and reconstruction

- When $L = D$, then $\boldsymbol{V}_L\boldsymbol{V}_L^T = \boldsymbol{I}_D$ ($D \times D$ identity matrix) and $\boldsymbol{X}$ is recovered exactly
- A great illustration can be found **here**.

Proportion of variance explained

The total variance present in the dataset (mean-centered) is given by:

$$\sum_{j=1}^{D} \mathbb{V}(\boldsymbol{x}_j) = \sum_{j=1}^{D} \lambda_j \tag{14}$$

That is, the eigenvalues of the covariance matrix $\boldsymbol{X}^T\boldsymbol{X}$ sum up to the total variance. Since $\boldsymbol{X}^T\boldsymbol{X}$ is positive semidefinite, its eigenvalues are non-negative:

$$\lambda_1 \geq \lambda_2 \cdots \lambda_L \geq \lambda_{L+1} \cdots \geq \lambda_D \geq 0 \tag{15}$$

The total projected variance in the L-dimensional subspace is given by:

$$\mathbb{V}(\widetilde{\boldsymbol{X}}) = \sum_{j=1}^{L} \lambda_j \tag{16}$$

The **proportion of variance explained** by the jth PC is then given by:

$$PVE = \frac{\lambda_j}{\sum_{j=1}^{D} \lambda_j} \tag{17}$$

- $\sqrt{\lambda_j}$ are the diagonal (non-zero) elements of the singular value matrix $\boldsymbol{S}$

Selecting the “best” L-dimensional approximation

For a given number of dimensions L, the cumulative PVE is given by:

$$CVPE_L = \frac{\sum_{j=1}^{L} \lambda_j}{\sum_{j'=1}^{D} \lambda_{j'}} \tag{18}$$

We choose M (number of PCs) such that the CVPE is greater than a reasonably large threshold:

$$\begin{aligned} L^* &= \min L & (19) \\ \text{s.t.} \quad & CVPE_L \geq \tau & (20) \end{aligned}$$

where τ is the desired threshold (e.g. 0.9)

- This can also be visualized using a **scree plot**

Dimensionality reduction for regression

- Previous methods to control variance:
  - Subset selection
  - Coefficient shrinkage
- All used original predictors in dataset $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_D$.
- We can also improve a fit by training a model on a transformation of the input space: $\boldsymbol{z}_1, \boldsymbol{z}_2, \ldots, \boldsymbol{z}_L$:

$$\boldsymbol{z}_j = \sum_{j=1}^{L} \boldsymbol{X} v_j, \quad L < D \tag{21}$$

  - if $L << D$, variance of coefficients can be signficantly reduced
  - The estimation problem is thus reduced from estimating $D+1$ coefficients to $L+1$ coefficients
- Consider **principal components analysis (PCA)** as an approach for regression
  - In selecting the number of principal components as regressors, we can use cross-validation to choose the L which gives the lowest error estimate.

Principal components regression (PCR)

Let the columns $\boldsymbol{z}_k$ be the linear combinations (principal components) of the original inputs X_j (or $\boldsymbol{x}_j$).

In PCR, we regress the response $\boldsymbol{y}$ onto the subspace spanned by $\boldsymbol{z}_k = \boldsymbol{X} v_k$, where $L \leq D$ and $\boldsymbol{z}_k$ are the principal components of $\boldsymbol{X}$:

$$\hat{\boldsymbol{y}}_{(L)}^{pcr} = \overline{y}\mathbf{1} + \sum_{j=1}^{L} \hat{\theta}_j \boldsymbol{z}_j \tag{22}$$

The coordinates of $\widetilde{\boldsymbol{x}}_j$ in the new L-dimensional basis are then given by:

$$\boldsymbol{z}_j = \boldsymbol{V}_L^T \boldsymbol{x}_j \tag{23}$$

and the estimates are:

$$\hat{\theta}_j = \frac{\boldsymbol{z}_j^T \boldsymbol{y}}{\boldsymbol{z}_j^T \boldsymbol{z}_j} \tag{24}$$

We can then express the solution in terms of PCR coefficients of $\boldsymbol{x}_j$:

$$\hat{\boldsymbol{y}}_{(L)}^{pcr} = \overline{y}\mathbf{1} + \boldsymbol{X}\hat{\boldsymbol{w}}^{pcr} \tag{25}$$

Partial least squares regression

This is a supervised and iterative form of PCR in which the construction of $\boldsymbol{z}_j$ is informed by the correlation of each $\boldsymbol{x}_j$ with $\boldsymbol{y}$.

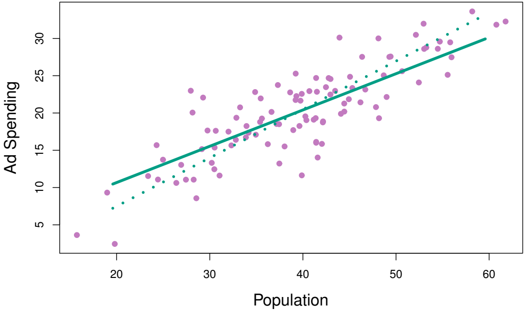


Figure: An example showing the first PLS direction (solid line) and first PCR direction (dotted line)

Summary of PCA steps

- Perform singular value decomposition of $N \times D$ data matrix $\boldsymbol{X}$:

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^T \tag{26}$$

- Determine the number of principal components M to extract/retain using the cumulative proportion of variance explained:

$$CVPE_L = \frac{\sum_{j=1}^{L} \lambda_j}{\sum_{j'=1}^{D} \lambda_{j'}} \tag{27}$$

- Get loadings matrix $\boldsymbol{V}_L^T$ by truncating $\boldsymbol{V}^T$
- Find score matrix $\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{V}_L = \boldsymbol{X}\boldsymbol{W}$ (transformed data into reduced subspace). Use $\boldsymbol{Z}$ for regression, clustering, etc
- Approximation of original data matrix can be obtained via:

$$\widetilde{\boldsymbol{X}} = \boldsymbol{Z}\boldsymbol{V}_L^T = \boldsymbol{Z}\boldsymbol{W}^\top \tag{28}$$

Outlook

Key points

- PCA is a technique used for reducing the dimensionality of a dataset and exploring underlying patterns in the variables
- PCA identifies a low-dimensional subspace that captures the largest fraction of the input data variance
- Standardizing (mean centering and scaling by standard deviation) is desired to ensure that variances are not dominated by features on a larger scale

Reading

- **PMLI** 20.1
- **ESL** 14.5 (note that in the book $\boldsymbol{D}$ corresponds to the $\boldsymbol{S}$ used in this lecture)
- **PMLCE** 10.2

Ridge estimates

Recall the ridge regression estimate:

$$\hat{\boldsymbol{w}}^R = (\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y} \tag{29}$$

The **singular value decomposition** of $\boldsymbol{X}$ can yield important insights into the nature of the solution:

$$\boldsymbol{X} = \boldsymbol{UDV}^T \tag{30}$$

where $\boldsymbol{U}_{N\times D}$ and $\boldsymbol{V}_{D\times D}$ are orthogonal matrices. Recall that an orthogonal matrix is one whose columns/rows are orthogonal unit vectors (i.e. all rows and columns have only one non-zero element: ±1); $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$

$\boldsymbol{D}$ is a $D \times D$ diagonal matrix; $d_j \geq 0$

$$\begin{aligned}\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{w}}^{OLS} &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ &= \boldsymbol{USDV}^T(\boldsymbol{VDU}^T\boldsymbol{USV}^T)^{-1}\boldsymbol{VSU}^T\boldsymbol{y} \\ &= \boldsymbol{U}(\boldsymbol{S}^2)^{-1}\boldsymbol{S}^2\boldsymbol{U}^T\boldsymbol{y} \\ &= \boldsymbol{UU}^T\boldsymbol{y}\end{aligned}$$

Ridge estimate decomposition

We can then write the ridge solutions as:

$$\begin{aligned}\boldsymbol{X}\hat{\boldsymbol{w}}^R &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X}+\lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y}\\ &= \boldsymbol{US}(\boldsymbol{S}^2+\lambda\boldsymbol{I})^{-1}\boldsymbol{SU}^T\boldsymbol{y}\\ &= \sum_{j=1}^{p}\boldsymbol{u}_j\frac{d_j^2}{d_j^2+\lambda}\boldsymbol{u}_j^T\boldsymbol{y}\end{aligned}$$

where $\boldsymbol{u}_j$ are the columns of $\boldsymbol{U}$.

Thus, we see that ridge regression shrinks the coordinates of $\boldsymbol{y}$ in the basis $\boldsymbol{U}$ by $\frac{d_j^2}{d_j^2+\lambda}$.

- As d_j decreases, the term $\frac{d_j^2}{d_j^2+\lambda}$ increases.
- Thus, more shrinkage is applied to the coordinates whose basis vectors correspond to smaller d_j.

Principal components

Keeping in mind that $\boldsymbol{X}$ is a centered matrix, then the sample covariance matrix is given by:

$$\boldsymbol{S} = \frac{\boldsymbol{X}^T\boldsymbol{X}}{N} \tag{31}$$

Substituting $\boldsymbol{X}$ with its SVD we obtain:

$$\boldsymbol{X}^T\boldsymbol{X} = (\boldsymbol{UDV}^T)^T\boldsymbol{UDV}^T = \boldsymbol{VDU}^T\boldsymbol{UDV}^T = \boldsymbol{VD}^2\boldsymbol{V}^T \tag{32}$$

- The columns $\boldsymbol{v}_j$ of $\boldsymbol{V}$ are the **eigenvectors** of $\boldsymbol{X}$ (or **principal components**).
- The expression $\boldsymbol{VD}^2\boldsymbol{V}^T$ is called the **eigendecomposition** of $\boldsymbol{S}$.

First principal component

Given the eigen decomposition:

$$\boldsymbol{X}^T\boldsymbol{X} = \boldsymbol{V}\boldsymbol{S}^2\boldsymbol{V}^T \tag{33}$$

The first principal component[4] of $\boldsymbol{X}$ satisfies the property:

$$\mathbb{V}(\boldsymbol{z}_1) = \mathbb{V}(\boldsymbol{X}\boldsymbol{v}_1) = \frac{s_1^2}{N} = \frac{\lambda_1}{N} \tag{34}$$

- The variable $\boldsymbol{z}_1$ is the **first principal component** of $\boldsymbol{X}$:

  $$\boldsymbol{z}_1 = \boldsymbol{X} v_1 = \boldsymbol{u}_1 s_1 \tag{35}$$

  where the vector $\boldsymbol{u}_1$ is the normalized first principal component.
- The last principal component has minimum variance.
- Since this corresponds to the lowest s_k, this corresponds to the direction shrunk the most by the ridge regression

[4] Also known as Karhunen-Loeve direction

Principal components — 2 dimensions

Ridge regression projects $\boldsymbol{y}$ onto the principal components, shrinking the coefficient of the low-variance component more than the high-variance component.

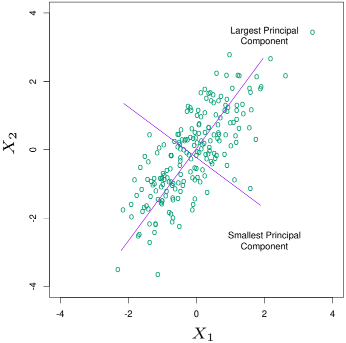


Figure: Principal components of a two-dimensional input dataset. The largest principal component (PC) maximizes the variance of the projected data. The smallest PC minimizes that variance.

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