CEE 616: Probabilistic Machine Learning

M5 Unsupervised Learning:
L5A: Principal Components Analysis

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College of Engineering

Thu, Nov 20, 2025

Outline

Unsupervised vs. supervised learning

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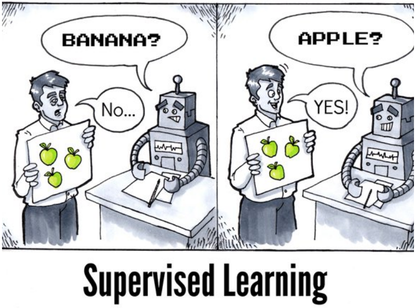

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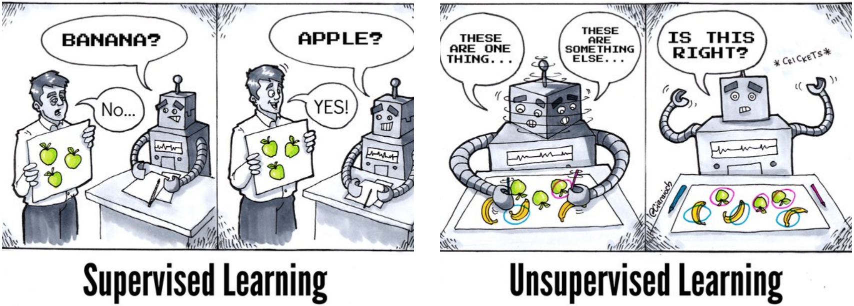

- Supervised learning: given response y and p features measured on the same observations, predict y on the x_j
- Unsupervised learning: only p features; no given response; what then can we learn about the data?

Learning tools

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Supervised

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

- multiple linear regression

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

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- clustering

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- The direction that maximizes the variance is that which also minimizes the mean squared error

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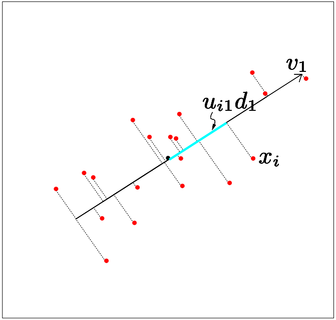

Figure: First principal component (PC) of a dataset. The PC minimizes the total squared distance from each point to its orthogonal projection onto the line

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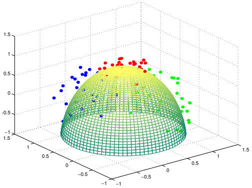

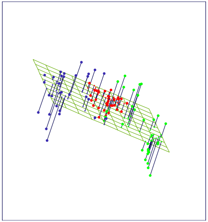

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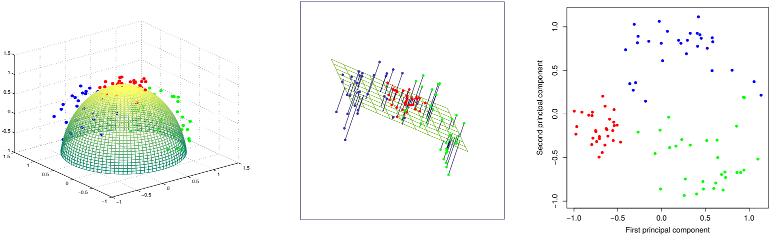

Figure: (L) Simulated dataset near surface of half-sphere. (C) Best 2-dimensional representationof data. (R) Projected points on the plane ($\boldsymbol{U}_2\boldsymbol{\Gamma}_2$)

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

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

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

$$\max_{\boldsymbol{v}} J(\boldsymbol{v}) =$$

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

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

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

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

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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:

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

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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

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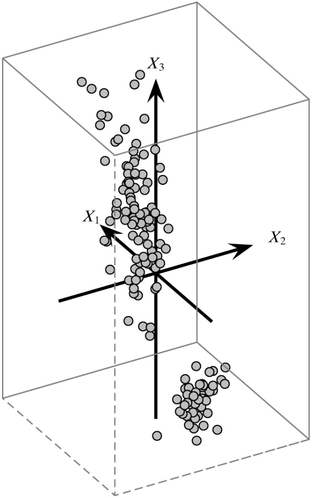

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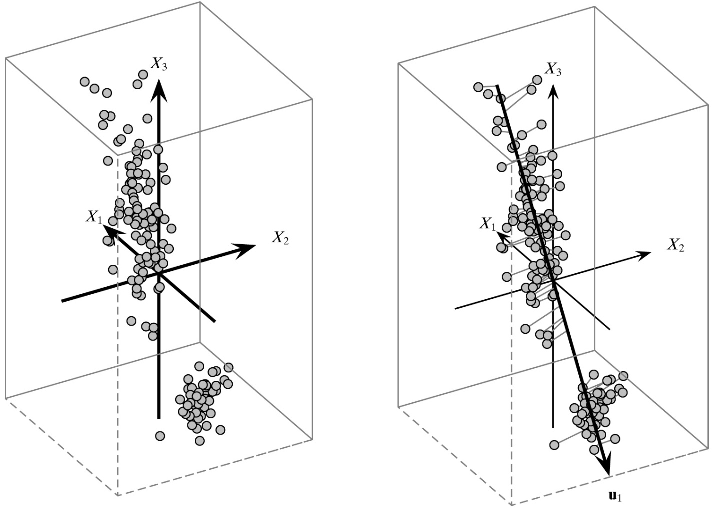

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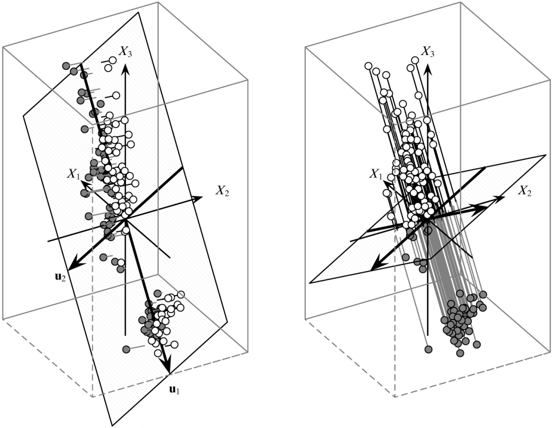

Figure: (Left) Optimal two-dimensional basis for Iris data. (Right) Non-optimal basis

Singular value decomposition (SVD)

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

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

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SVD (cont.)

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\tag{9}
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SVD (cont.)

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PCA via SVD

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

PCA via SVD

- In the SVD framework, this means we find the best number L of principal components $\boldsymbol{u}_k s_k$, where $k = 1, \ldots, L, L+1, \ldots, D$.[3]

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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 $\boldsymbol{X}$

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where $\boldsymbol{V}_L^T \in \mathbb{R}^{L \times D}$ (**loadings matrix**) is the transpose of the first L columns of $\boldsymbol{V}$

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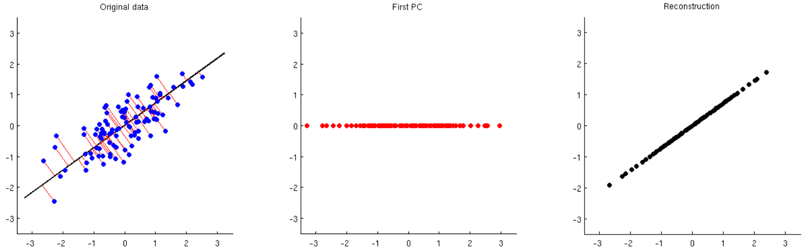

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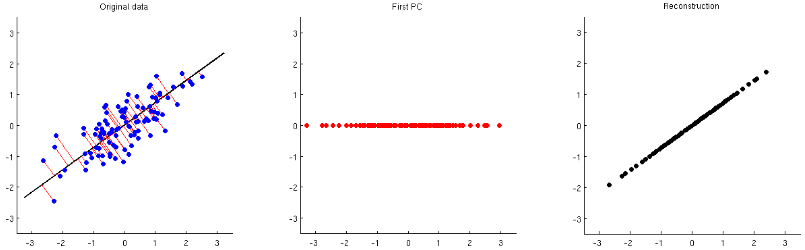

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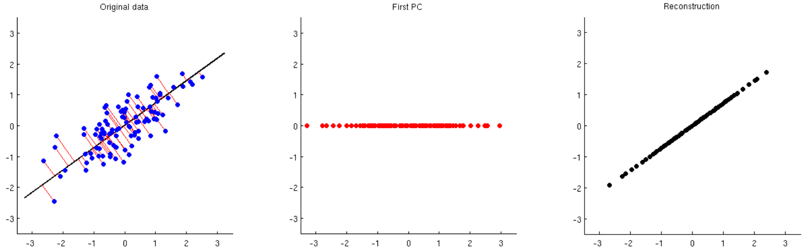

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- A great illustration can be found **here**.

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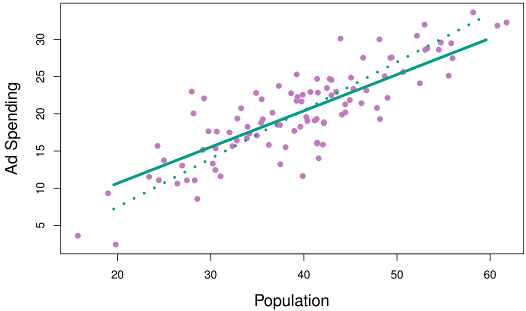

Figure: An example showing the first PLS direction (solid line) and first PCR direction (dotted line)

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Ridge estimates

Recall the ridge regression estimate:

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

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

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T \tag{30}$$

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; $d_j \geq 0$

$$\begin{aligned}\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{w}}^{OLS} &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ &= \boldsymbol{U}\boldsymbol{S}\boldsymbol{D}\boldsymbol{V}^T(\boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^T)^{-1}\boldsymbol{V}\boldsymbol{S}\boldsymbol{U}^T\boldsymbol{y} \\ &= \boldsymbol{U}(\boldsymbol{S}^2)^{-1}\boldsymbol{S}^2\boldsymbol{U}^T\boldsymbol{y} \\ &= \boldsymbol{U}\boldsymbol{U}^T\boldsymbol{y}\end{aligned}$$

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

Ridge estimate decomposition

We can then write the ridge solutions as:

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

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:

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

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- Since this corresponds to the lowest s_k, this corresponds to the direction shrunk the most by the ridge regression

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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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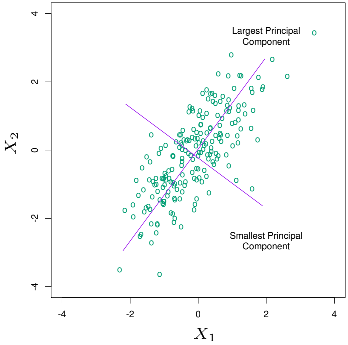

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