Principal Component Analysis

Lecture 11:

Guest Lecture from Dr. Jasmohan Bajaj,

Principal Component Analysis

ECE/CS 498 DS

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Announcements

- Guest Lecture today – Dr Jasmohan Bajaj
  - You will submit a brief summary of the key takeaways from the talk on Compass2G by the end of today's lecture
- Grad Students:
  - Initial grad project ideas due **Tonight (Feb 26) @ 11:59 PM**
    - Email the instructor and 4 grad TAs
    - Include all group members' names and NetIDs
  - Initial grad project discussions this week: **Today-Friday (Feb 26-28)**
    - Signup via: https://docs.google.com/spreadsheets/d/1Cd2RxSJWp8Im-K_sMkbuPRwxsTykOM3rdUzexSsYkko/edit?usp=sharing
    - All groups must sign up, and all group members must be present!
- MP2 Checkpoint 0.5, due **Mar 2 @ 11:59 PM** via Google Form
- HW 2 released, due **Mar 2 @ 11:59 PM on Compass2G**
  - Covers Bayesian networks and inferencing
- Midterm exam will take place on **Wed March 11th**

Dimensionality Reduction

- Can your data be explained with fewer dimensions?
  - Available data may have high dimensionality
  - Actual information of interest may be explained by a smaller number of dimensions/features

- Goal of dimensionality reduction is to explain the data with as few dimensions as possible while retaining the underlying "structure" in the data

- We use the terms "feature" and "dimension" interchangeably

- Several ways to reduce dimension of the data
  - Drop unimportant dimensions using e.g. domain knowledge
  - Take a (linear) combination of features*

Principal Components Analysis (PCA)

- Principal Components Analysis (PCA)
  - In PCA, "structure" refers to the variance in the data
  - Goal is to reduce dimensionality d (down to m) while explaining the most variance in the data so that with $m \ll d$, most of the data can be explained
  - The way we extract relevant features is by taking linear combinations of existing dimensions
  - Thus ***PCA is a statistical technique to analyze the relationships among a large number of variables and to explain these variables using smaller number of variables that we call its principal components***

- To define principal components
  - Center the data
  - Chose as the 1st direction, the direction of maximum variance in the data
  - 2nd direction is chosen to be perpendicular to the first , that explains the maximum remaining variance in the data
  - And so on (Keeping successive directions orthogonal)

PCA Example: Food Habits

- Average consumption of 17 different types of food was tracked in 4 different countries in the UK.
- Measurements are reported in grams per person per week
- **Do any of the countries seem to have unusual consumption patterns?**

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

http://setosa.io/ev/principal-component-analysis/

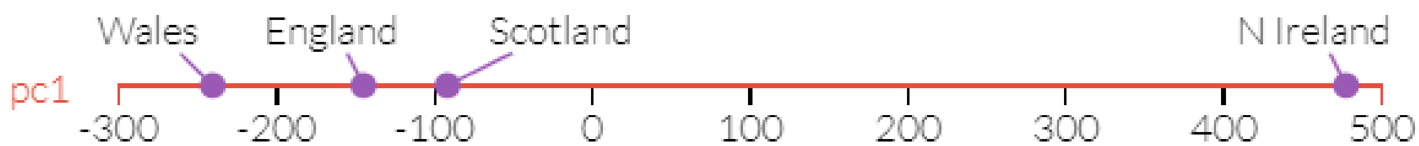
PCA Example: Food Habits

- In this setup, we have 17-dimensional data point $\boldsymbol{X} = (X_1, X_2, \dots, X_{17})$
  - E.g. X_1=Alcoholic Drinks, X_2=Beverages, … , X_{17}=Sugars
- PCA reduces the number of dimensions of the data points by projecting each point onto different axes called principal components
  - Each successive principal component explains the maximum remaining variance in the data set, and is orthogonal to the other components
  - Each projection is a linear combination of the original features
  - We refer to the projected points on the principal components as coordinates
  - In our example, the coordinate for the first principal component can be computed as

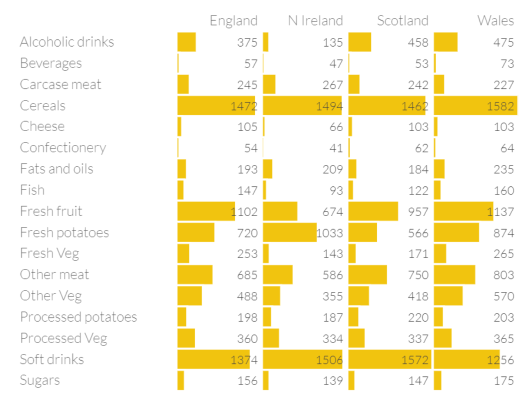
$$
\begin{aligned}
&-0.46X_1 - 0.026X_2 + 0.048X_3 - 0.048X_4 - 0.057X_5 - 0.030X_6 \\
&- 0.0052X_7 - 0.084X_8 - 0.63X_9 + 0.40X_{10} - 0.15X_{11} - 0.26X_{12} \\
&- 0.24X_{13} - 0.027X_{14} - 0.036X_{15} + 0.23X_{16} - 0.038X_{17}
\end{aligned}
$$

PCA Example: Food Habits

- We project each sample (17-D datapoint) onto the first principal component and plot the projections



- From this plot, we can see that N Ireland's food habits are notably different from those of the other UK countries.
  - This wasn't as apparent from examining the raw data
  - Upon closer examination, N Ireland on average consumes more fresh potatoes and less fresh fruits, cheese, fish and alcoholic drinks
  - Geographically, this makes sense since N Ireland is the only of these countries that lies on a separate island from Great Britain



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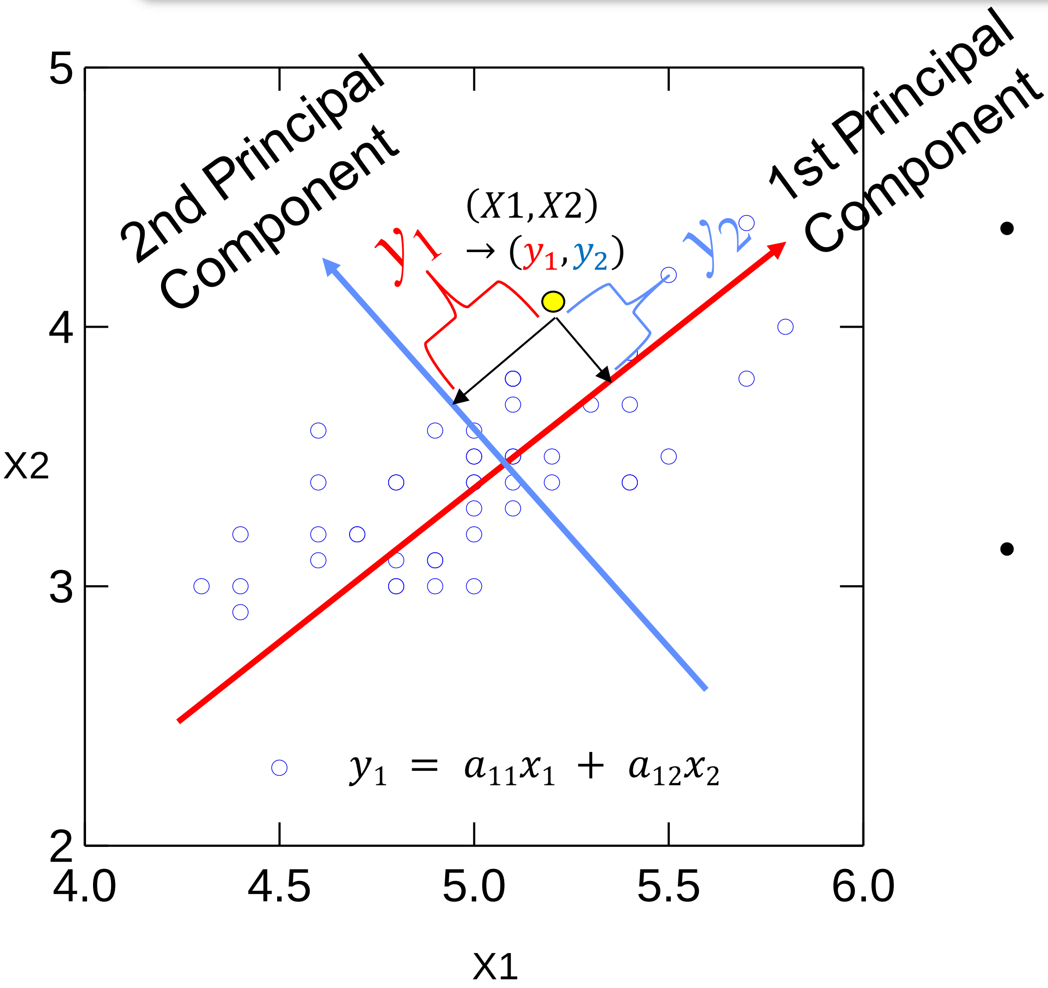
PCA: Dimensionality Reduction Method



- What is a good feature?
  - Simplify the explanation of the input
  - Reduce dimensionality
- Why pick the direction that maximizes variability?

Principal Component Analysis

- From p random vectors (features in the dataset) $X = [X_1, X_2, \dots, X_p]$
- Produce p new variables: $y_1, y_2, \dots, y_p$:

$$\left.\begin{aligned} y_1 &= a_{11}x_1 + a_{12}x_2 + \dots + a_{1p}x_p \\ y_2 &= a_{21}x_1 + a_{22}x_2 + \dots + a_{2p}x_p \\ &\dots \\ y_p &= a_{p1}x_1 + a_{p2}x_2 + \dots + a_{pp}x_p \end{aligned}\right\}$$

- y_j's are **principal components**
- $a_{j1}, a_{j2}, \dots, a_{jp}$ are **regression coefficients**
- There are no intercepts (since we centered data)

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \dots & a_{pp} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix}$$

$$\Rightarrow \boldsymbol{Y} = \boldsymbol{A}\boldsymbol{X}$$

- y_j's are **uncorrelated** (orthogonal) - covariance among each pair of the principal axes is zero
- y_1 explains as much of original variance in data set, y_2 explains as much of the remaining variance, and so on

PCA Applications

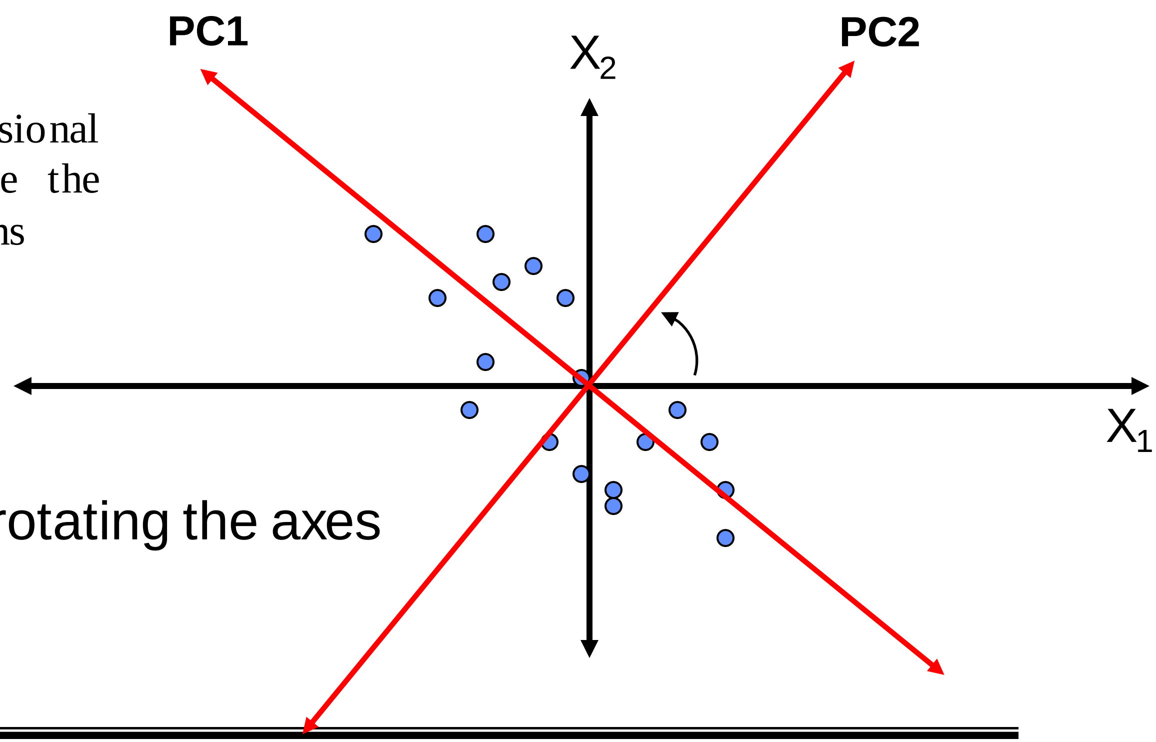
- Uses:
  - Data Visualization
  - Data Reduction
  - Data Classification
  - Trend Analysis
  - Factor Analysis
  - Noise Reduction
  - Regression
  - Clustering

- Examples:
  - How many unique "sub-sets" are in the sample?
  - How are they similar / different?
  - What are the underlying factors that influence the samples?
  - Which time / temporal trends are (anti)correlated?
  - Which measurements are needed to differentiate?
  - How to best present what is "interesting"?
  - Which "sub-set" does this new sample rightfully belong?

Trick: Rotate Coordinate Axes

Suppose we have a population measured on p random variables $X_1,\ldots,X_p$. Note that these random variables are represented on a p-axes Cartesian coordinate system. Our goal is to develop a new set of p axes (linear combinations of the original p axes) in the directions of greatest variability:

PCA derives the best possible k dimensional ($k < p$) representation to minimize the Euclidean distances among observations



This is accomplished by rotating the axes

Principal Component Analysis (eigenvalues and eigenvectors)

- Let M be either the correlation or covariance matrix of the original data
  - We will discuss later whether correlation or covariance matrix should be used for a dataset

- The **First Principal Component** $(a_{11},a_{12},...,a_{1p})$ is the eigenvector corresponding to the largest eigenvalue of M
  - The direction is specified by the normalized eigenvector
  - The magnitude is specified by the largest eigenvalue of M – **this reflects how much variance in the data is explained by this principal component**

- The **Second Principal Component** $(a_{21},a_{22},...,a_{2p})$ is the eigenvector corresponding to the second-largest eigenvalue of M

…

- The **pth Principal Component** $(a_{p1},a_{p2},...,a_{pp})$ is the eigenvector corresponding to the pth-largest eigenvalue of M

The Algebra of PCA: Covariance Matrix

- First step is to calculate the variance-covariance among every pair of the *p* features/dimensions in the dataset of n observations

$$S = Covariance\ (X) = \frac{1}{n}(X - \bar{x})^T (X - \bar{x})$$

- Square, symmetric matrix
- Diagonals are the variances, off-diagonals are the covariances

	X_1	X_2
X_1	6.6707	3.4170
X_2	3.4170	6.2384

Variance-covariance Matrix

Trace (sum of diagonals): 12.9091

- Sum of the diagonals of the variance-covariance matrix is called the trace and it represents the total variance in the data

The Algebra of PCA

Finding the principal components and their explained variance involves eigen analysis of the covariance or correlation matrix (S)

$$\boldsymbol{Sa} = \boldsymbol{\lambda a}$$

Covariance Matrix

eigenvalue eigenvector

- First eigenvector (corresponding to largest eigenvalue) is the first principal component
- Second eigenvector (corresponding to the second largest eigenvalue) is the second principal component
- And so…
- An eigenvalue divided by the trace of S defines the percent of variance in the data explained by the principal component corresponding to that eigenvalue

The Algebra of PCA: Eigenvalues

- Eigenvalues (latent roots) of S are solutions (λ) to the characteristic equation

$$\left|\mathbf{S} - \boldsymbol{\lambda}\mathbf{I}\right| = \mathbf{0} \Rightarrow \begin{vmatrix} s_{11} - \lambda & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} - \lambda & \cdots & s_{2p} \\ \vdots & \ddots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} - \lambda \end{vmatrix} = 0$$

- the eigenvalues, $\lambda_1, \lambda_2, \ldots \lambda_p$ are the variances of the coordinates on each principal component axis
- the sum of all *p* eigenvalues equals the trace of S (the sum of the variances of the original variables)

The Algebra of PCA: Eigenvalues

- Computing the eigenvalues of the covariance matrix

$$S = \begin{bmatrix} 6.6707 & 3.4170 \\ 3.4170 & 6.2384 \end{bmatrix}$$

Trace = 12.9091

$$|\mathbf{S} - \lambda\mathbf{I}| = \mathbf{0} \quad \Rightarrow \quad \left| \begin{bmatrix} 6.6707 & 3.4170 \\ 3.4170 & 6.2384 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \right| = 0$$

$$\Rightarrow \quad \begin{vmatrix} 6.6707 - \lambda & 3.4170 \\ 3.4170 & 6.2384 - \lambda \end{vmatrix} = 0$$

$$\Rightarrow \quad (6.6707 - \lambda)(6.2384 - \lambda) - 3.4170 * 3.4170 = 0$$

$$\Rightarrow \quad \lambda^2 - 12.9091\lambda + 29.934 = 0$$

$$\Rightarrow \quad \boldsymbol{\lambda_1 = 9.8783, \lambda_2 = 3.0308}$$

Note: $\lambda_1 + \lambda_2 = 12.9091$

- **After selecting $k < p$ components, the total variance in the dataset is not equal to the trace of the Covariance matrix**

The Algebra of PCA: Eigenvectors

- Each **eigenvector** consists of *p* values which represent the "contribution" of each variable to the **principal component** axis
- Eigenvectors are uncorrelated (orthogonal)
  - their dot product $a_i^T a_j = 0$ if $i \neq j$
- Eigenvectors can be obtained using the following equation

$$\boldsymbol{S a_i = \lambda_i a_i}$$

for all $i \in \{1,2, \ldots, p\}$

The Algebra of PCA: Eigenvectors

Computing the eigenvectors of the covariance matrix S using the calculated eigenvalues:

$$S = \begin{bmatrix} 6.6707 & 3.4170 \\ 3.4170 & 6.2384 \end{bmatrix}$$

$$\lambda_1 = 9.8783 \quad \lambda_2 = 3.0308$$

Let us look at the first eigenvector:

$$Sa_1 = \lambda_1 a_1 \qquad \Rightarrow \qquad (S - \lambda_1 I)a_1 = 0$$

$$\Rightarrow \begin{bmatrix} 6.6707 - 9.8783 & 3.4170 \\ 3.4170 & 6.2384 - 9.8783 \end{bmatrix} \begin{bmatrix} a_{11} \\ a_{12} \end{bmatrix} = 0$$

$$\Rightarrow \begin{bmatrix} -3.2076 & 3.4170 \\ 3.4170 & -3.6399 \end{bmatrix} \begin{bmatrix} a_{11} \\ a_{12} \end{bmatrix} = 0 \quad \Rightarrow \quad \begin{matrix} -3.2076a_{11} + 3.4170a_{12} = 0 \text{ (Eq2)} \\ 3.4170a_{11} - 3.6399a_{12} = 0 \text{ (Eq1)} \end{matrix}$$

Solving Eq1 and Eq2 simultaneously, we get: $a_{11} = 1.0653, a_{12} = 1$

Similarly, can solve for a_2. Eigenvectors are: $\boldsymbol{a_1} = \frac{1}{\sqrt{1.0653^2+1^2}} \begin{bmatrix} \mathbf{1.0653} \\ \mathbf{1} \end{bmatrix}, \boldsymbol{a_2} = \frac{1}{\sqrt{0.9387^2+1^2}} \begin{bmatrix} \mathbf{-0.9387} \\ \mathbf{1} \end{bmatrix}$

The Algebra of PCA: Eigenvectors

- Eigenvectors are uncorrelated (orthogonal)
  - their dot product $a_i^T a_j = 0$ if $i \neq j$

- From the example, we get

	Eigenvectors $\downarrow$ $\boldsymbol{a_1}$	$\downarrow$ $\boldsymbol{a_2}$
$\boldsymbol{X_1}$	1.0653	-0.9387
$\boldsymbol{X_2}$	1	1

- Checking for orthogonality:

$$a_1^T a_2 = 1.0653 * (-0.9387) + 1 = 0$$

The Algebra of PCA

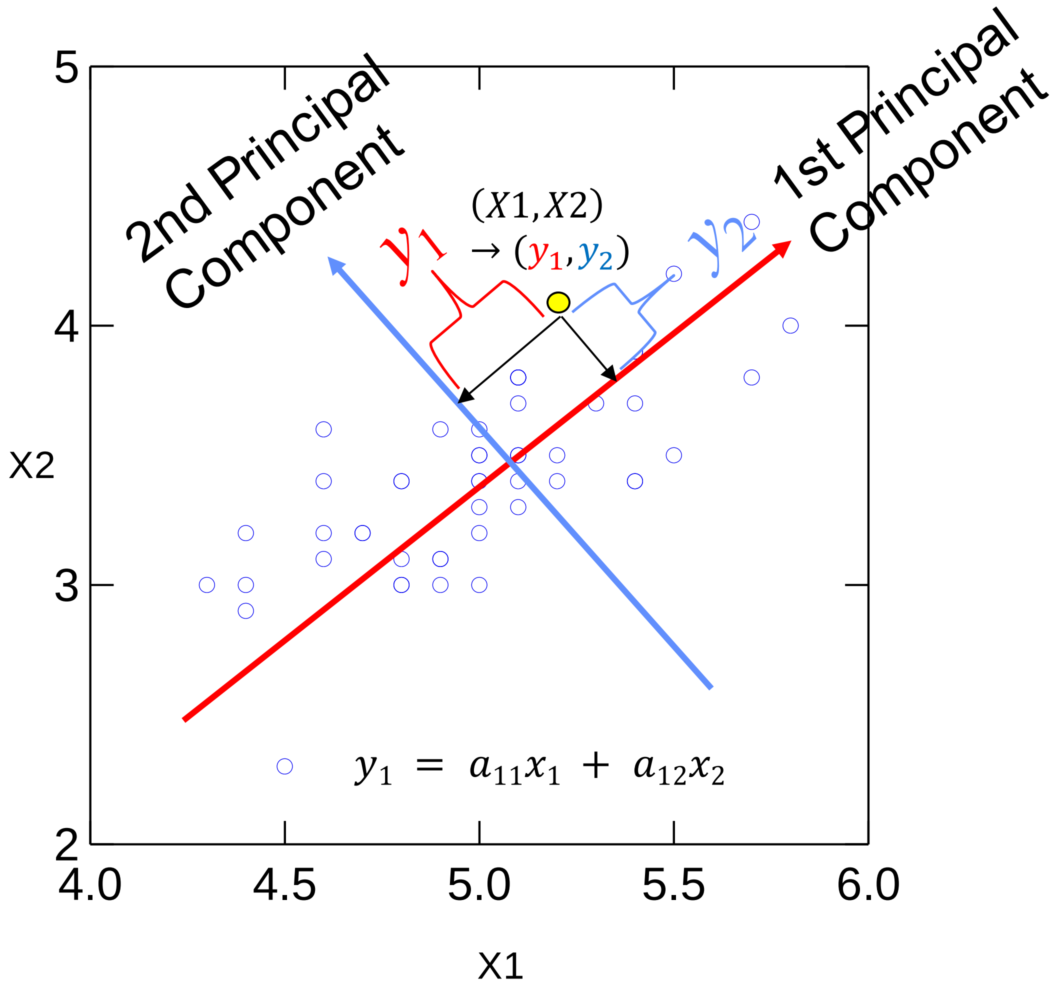
- Coordinates of each observation on the j^{th} principal axis, known as the **scores** on PC j, are computed as

$$y_j = a_{j1}x_1 + a_{j2}x_2 + \dots + a_{jk}x_k$$

$$E.g, \qquad y_1 = 1.0653x_1 + 1x_2$$

- variance of the scores on each PC axis is equal to the corresponding eigenvalue for that axis
- the eigenvalue represents the variance displayed ("explained" or "extracted") by the kth axis
- the sum of the first k eigenvalues is the variance explained by the k-dimensional ordination.

The Algebra of PCA



The covariance matrix on *p* principal axes has a simple form:

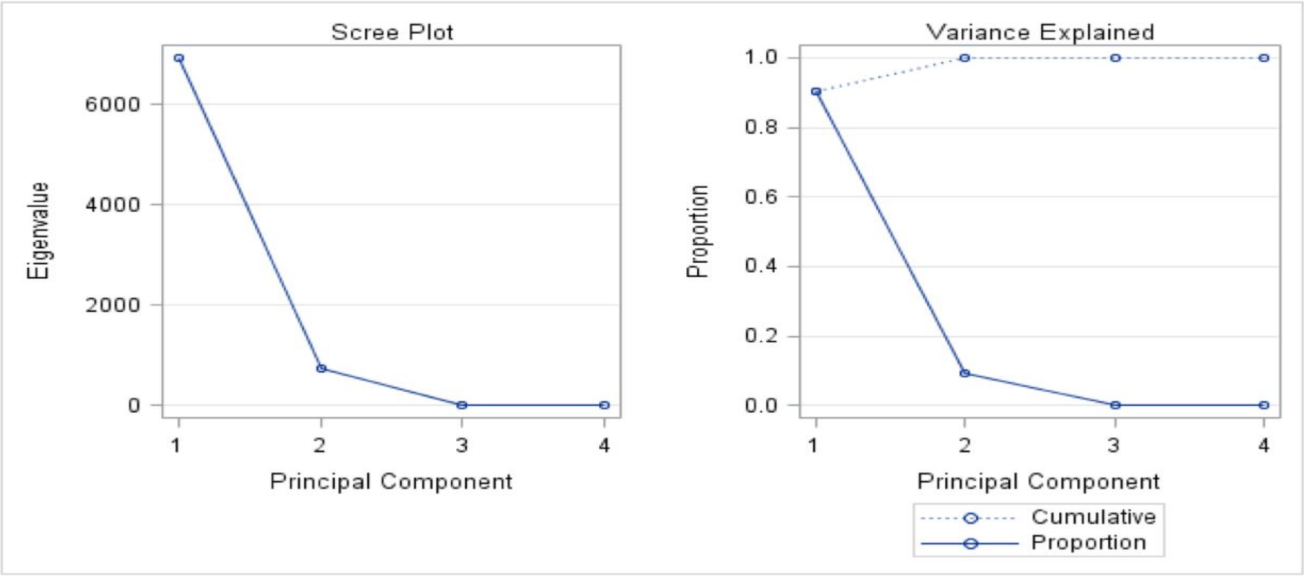
- all off-diagonal values are zero (the principal axes are uncorrelated)
- the diagonal values are the eigenvalues.

	PC_1	PC_2
PC_1	9.8783	0.0000
PC_2	0.0000	3.0308

Variance-covariance Matrix of the PC axes

Number of Dimensions

- If input was p-dimensions, how many dimensions do we keep
  - No solid answer, heuristics exists
- Look at Eigen values
  - They show variance of each component at some point they will be small



The Algebra of PCA: Covariance/Correlation Matrix

- PCA can be found using the covariance matrix OR the correlation matrix
- ***Covariance Matrix:***
  - Variables must be in same units
  - Emphasizes variables with most variance
  - **Using covariance's among variables only makes sense if they are measured in the same units**
- ***Correlation Matrix:***
  - Variables are standardized (mean 0.0, SD 1.0)
  - Variables can be in different units
  - All variables have same impact on analysis

$$r_{ij} = \frac{C_{ij}}{\sqrt{V_i V_j}}$$

Covariance of variables *i* and *j*

Correlation between variables *i* and *j*

Variance of variable *j*

	X_1	X_2
X_1	6.6707	3.4170
X_2	3.4170	6.2384

Variance-covariance Matrix

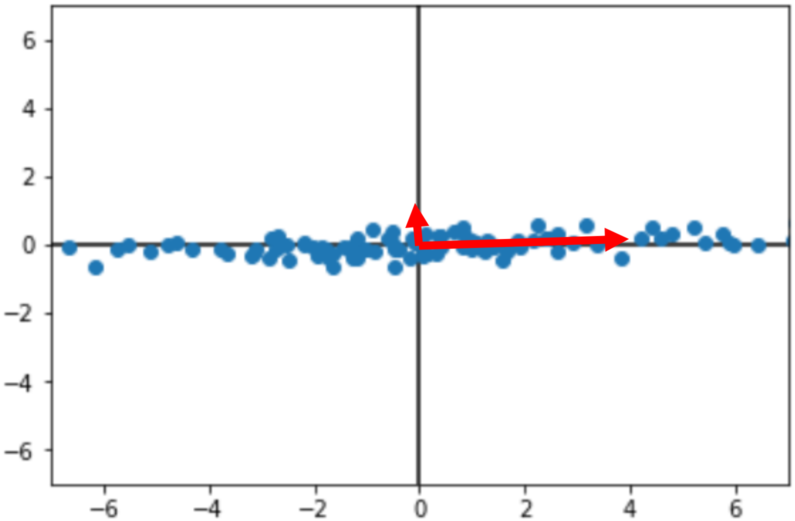
	X_1	X_2
X_1	1.0000	0.5297
X_2	0.5297	1.0000

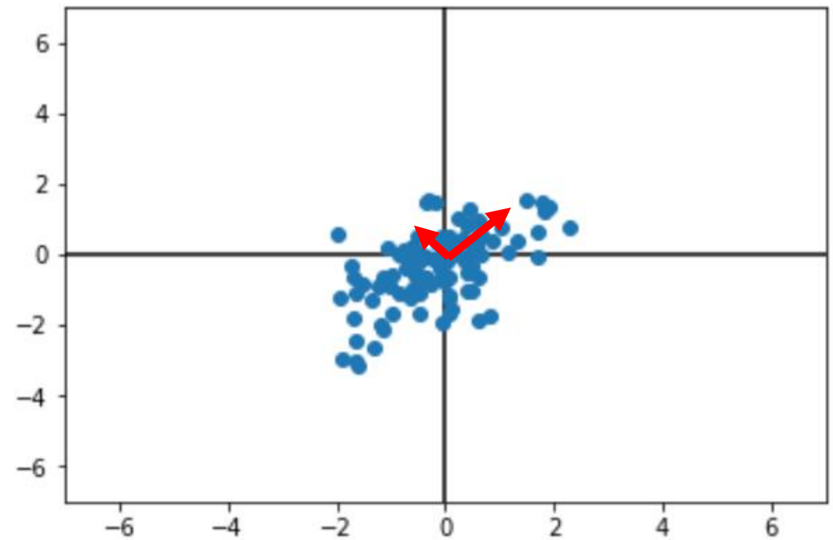
Correlation Matrix

Trace (sum of diagonals): 12.9091

Trace (sum of diagonals): 2.0

The Algebra of PCA: Covariance/Correlation Matrix





$$\begin{bmatrix} 10 & 0.5 \\ 0.5 & 0.1 \end{bmatrix}$$

Covariance matrix

$$\begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$

Correlation matrix

- If variance of features is not on comparable scale, then principal components have high contribution from features with large variance

PCA with Correlation Matrix

- Compute correlation matrix from covariance matrix:

$$\boldsymbol{r_{ij}} = \frac{\boldsymbol{C_{ij}}}{\sqrt{\boldsymbol{V_i V_j}}}$$

Correlation between variables *i* and *j*

Covariance of variables *i* and *j*

Variance of variable *j*

- Solve eigenvalue equation: $\boldsymbol{S_{cor} a = \lambda a}$

Correlation Matrix

- Compute eigenvalues by solving: $|\boldsymbol{S_{cor} - \lambda I}| = \boldsymbol{0}$

- Compute eigenvectors (principal components) by solving the following for each eigenvalue λ_i: $(\boldsymbol{S_{cor} - \lambda_i I})\boldsymbol{a_i} = \boldsymbol{0}$

- Principal components may be different for correlation matrix and covariance matrix

Additional Resources

- Textbook “The Elements of Statistical Learning” , Section 14.5 Principal Components, Curves and Surfaces
- Roweis, Sam T. "EM algorithms for PCA and SPCA." *Advances in neural information processing systems*. 1998.