Dimensionality Reduction

Machine Learning 10-601B

Seyoung Kim

Text document retrieval/labelling

- Represent each document by a high-dimensional vector in the space of words

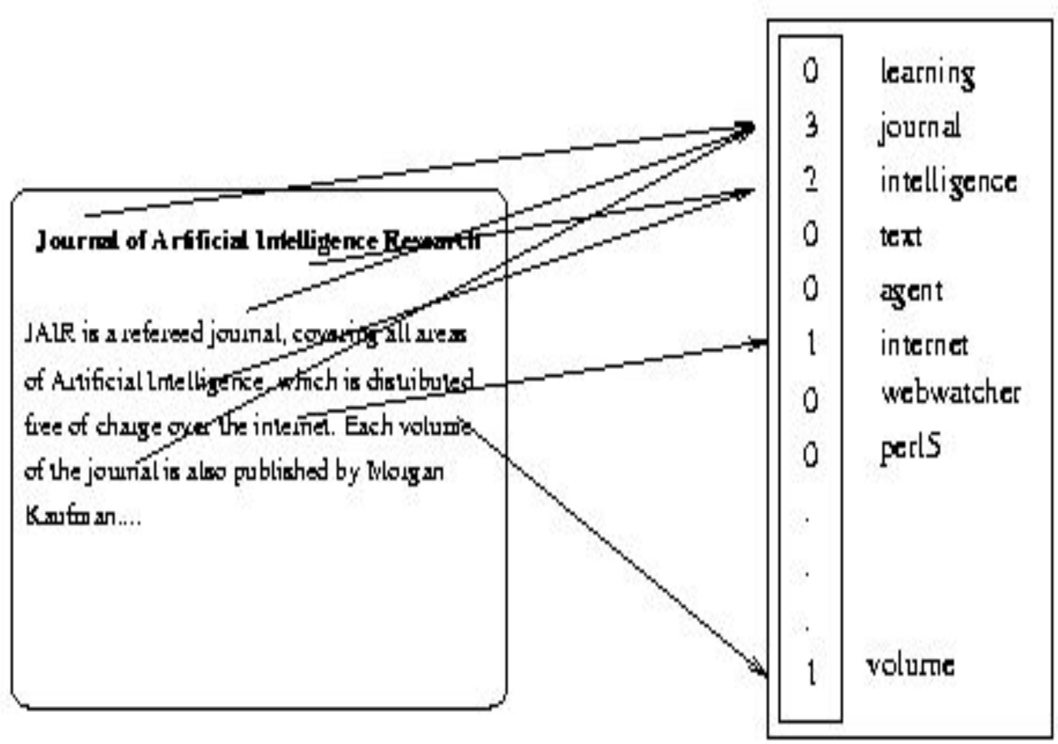


Image retrieval/labelling

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

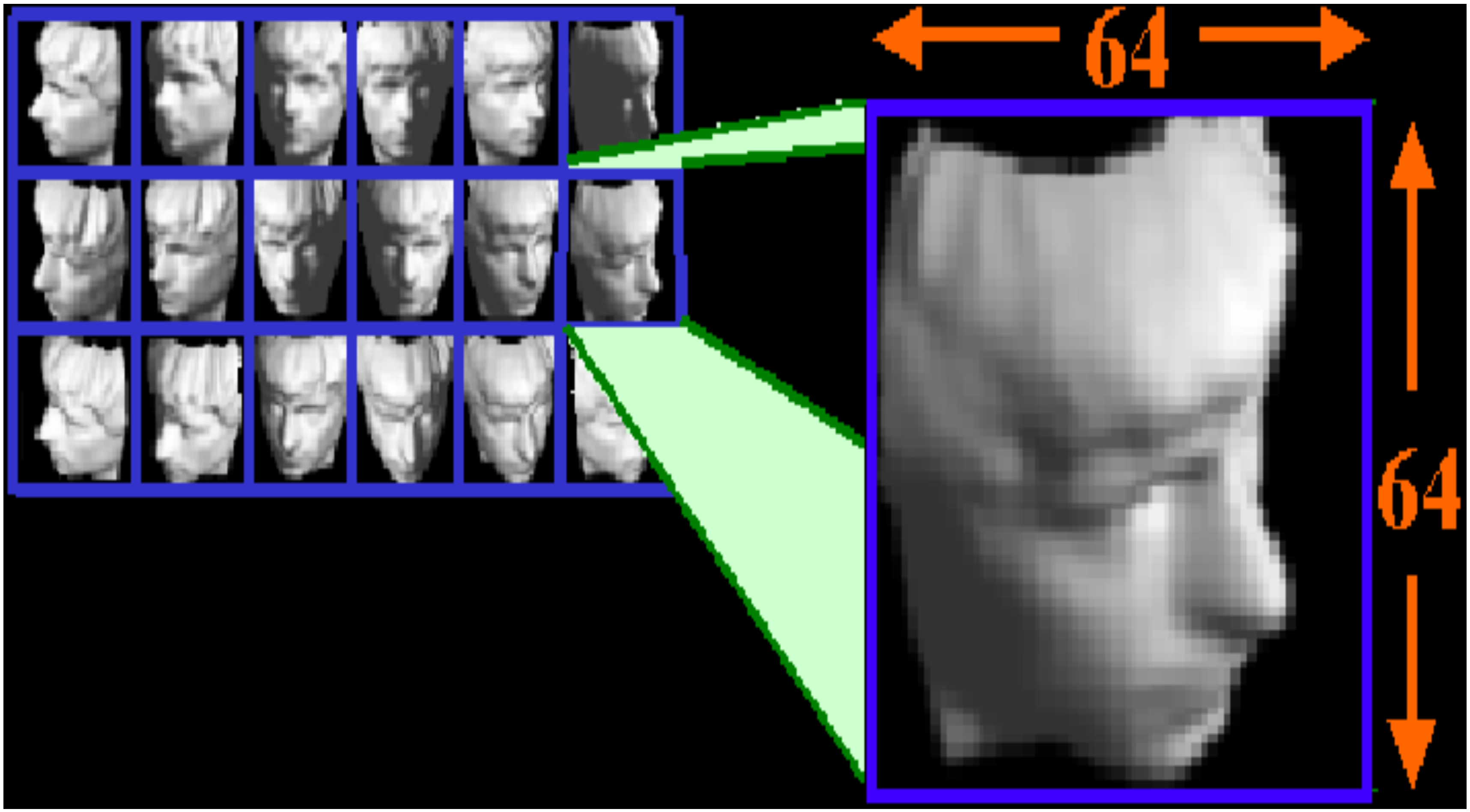
Dimensionality Bottlenecks

- Data dimension
  - Input variables X: High
    - 1-5M lexicon token in text documents
    - 1024^2 pixels of a projected image on a IR camera sensor
    - N^2 expansion factor to account for all pairwise correlations
    - 1,000,000 genetic variants in a human's genome

- Information dimension: Low
  - Number of free parameters describing probability densities
    - Unsupervised learning p(X)
    - Supervised learning p(Y|X): the prediction of Y depends on "information dimension" of X

Intuition: how does your brain store these pictures?

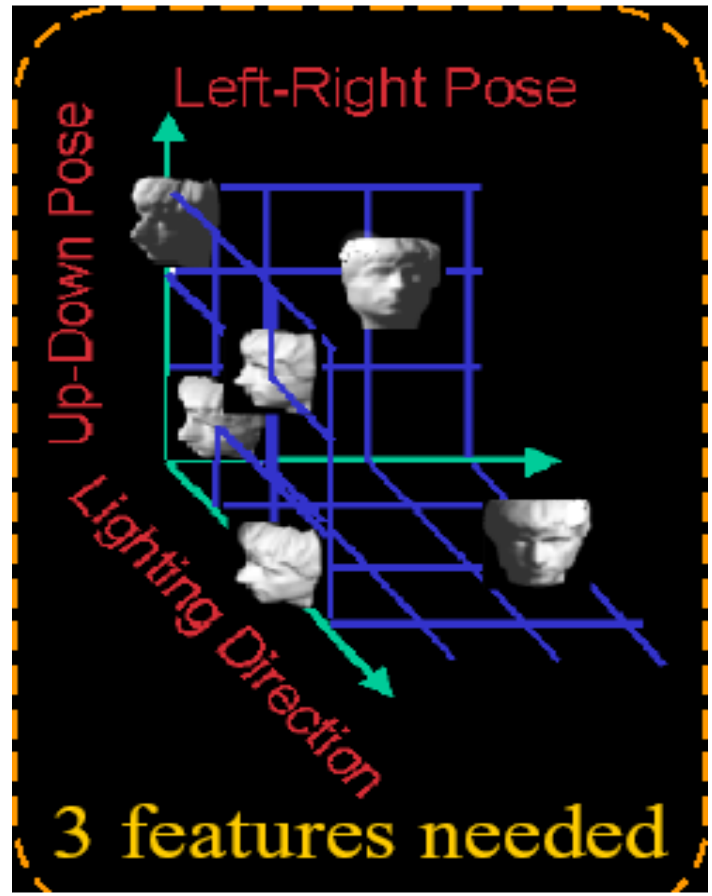
Brain Representation



Brain Representation

- Every pixel?
- Or perceptually meaningful structure?
  - Up-down pose
  - Left-right pose
  - Lighting direction

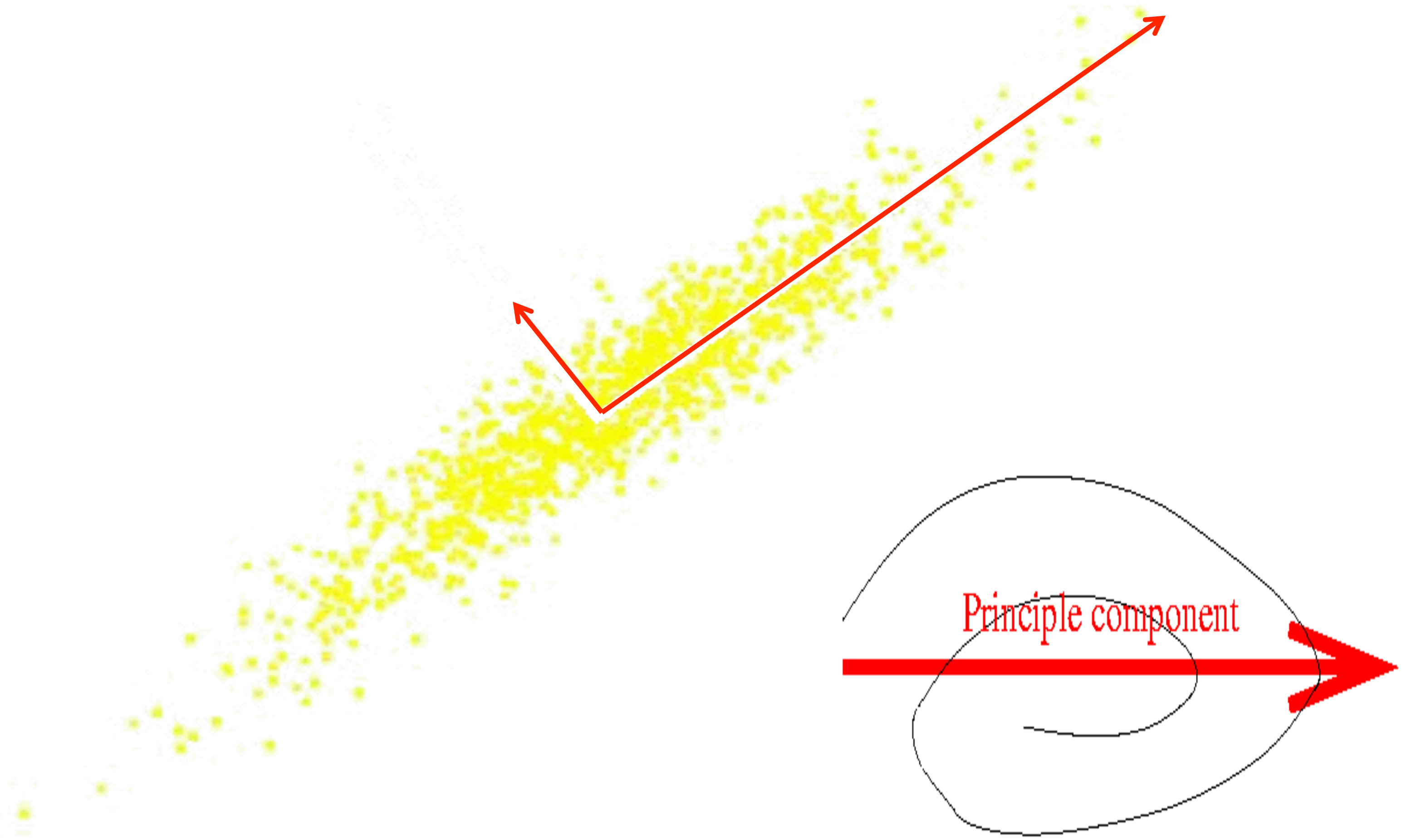
  So, your brain successfully reduced the high-dimensional inputs to an intrinsically 3-dimensional manifold!



Principal Component Analysis

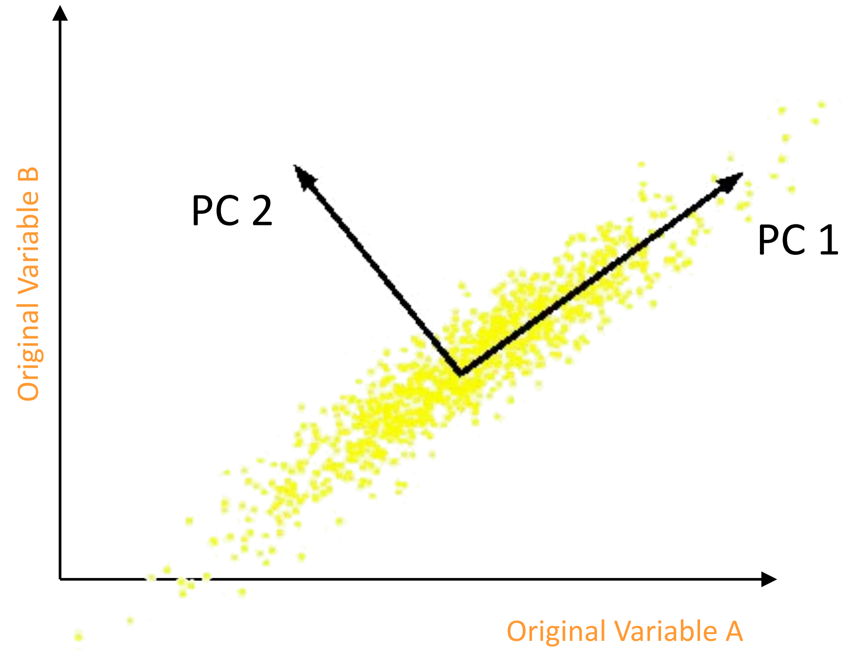
- Areas of variance in data are where items can be best discriminated and key underlying phenomena are observed 差异最大的方向
- If two items or dimensions are highly correlated or dependent
  - They are likely to represent highly related phenomena 合并差异小的方向
  - We want to combine related variables, and focus on uncorrelated or independent ones, especially those along which the observations have high variance
- We look for the phenomena underlying the observed covariance/co-dependence in a set of variables
- These phenomena are called "principal components"

An example:



Principal Component Analysis

- The new variables/dimensions
  - Are uncorrelated with one another
    - Orthogonal in original dimension space
  - Capture as much of the original variance in the data as possible
  - Are called Principal Components
  - Are linear combinations of the original ones



- Orthogonal directions of greatest variance in data

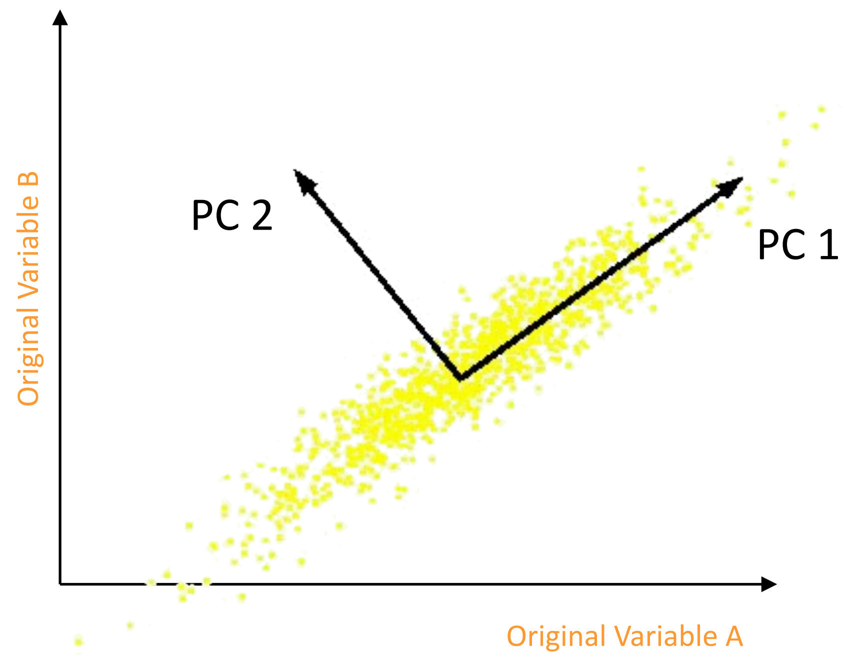
- Projections along PC1 discriminate the data most along any one axis

Principal Component Analysis

- First principal component is the direction of greatest variability (covariance) in the data

- Second is the next orthogonal (uncorrelated) direction of greatest variability
  – So first remove all the variability along the first component, and then find the next direction of greatest variability

- And so on …



Eigen/diagonal Decomposition

- Let $\mathbf{S} \in \mathbb{R}^{m \times m}$ be a **square** matrix

- **Theorem**: Exists an **eigen decomposition**

$$\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1}$$

diagonal

Unique for distinct eigen-values

(cf. matrix diagonalization theorem)

- Columns of ***U*** are **eigenvectors** of ***S*** U是S的特征向量组成的矩阵

- Diagonal elements of $\mathbf{\Lambda}$ are **eigenvalues** of $\mathbf{S}$ λ是S的特征值组成的矩阵

$$\mathbf{\Lambda} = \text{diag}(\lambda_1, \ldots, \lambda_m), \quad \lambda_i \geq \lambda_{i+1}$$

Eigenvalues & Eigenvectors

- For symmetric matrices, eigenvectors for distinct eigenvalues are **orthogonal**

$$Sv_1 = \lambda_1 v_1,\ Sv_2 = \lambda_2 v_2, \text{ and } \lambda_1 \neq \lambda_2 \Rightarrow v_1 \bullet v_2 = 0$$

- All eigenvalues of a real symmetric matrix are **real**.

$$\text{if } |S - \lambda I| = 0 \text{ and } \mathrm{S} = \mathrm{S}^{\mathrm{T}} \Rightarrow \lambda \in \Re$$

- All eigenvalues of a positive semidefinite matrix are **non-negative**

$$\forall w \in \Re^n, w^T S w \geq 0, \text{ then if } \mathrm{Sv} = \lambda \mathrm{v} \Rightarrow \lambda \geq 0$$

Computing the Components

- Projection of vector **x** onto an axis (dimension) **u** is $\mathbf{u}^T\mathbf{x}$
- Assume **X** is a normalized *n*x*p* data matrix for *n* samples and *p* features. Direction of greatest variability is that in which the average square of the projection is greatest:

Maximize $\quad (1/n)\, \mathbf{u}^T\mathbf{X}^T\mathbf{X}\mathbf{u}$

s.t $\quad \mathbf{u}^T\mathbf{u} = 1$

Computing the Components

- Projection of vector $\mathbf{x}$ onto an axis (dimension) $\mathbf{u}$ is $\mathbf{u}^T\mathbf{x}$
- Assume $\mathbf{X}$ is a normalized *n*x*p* data matrix for *n* samples and *p* features. Direction of greatest variability is that in which the average square of the projection is greatest:

Maximize $(1/n)\, \mathbf{u}^T\mathbf{X}^T\mathbf{X}\mathbf{u}$

s.t $\mathbf{u}^T\mathbf{u} = 1$

Construct Langrangian $(1/n)\, \mathbf{u}^T\mathbf{X}^T\mathbf{X}\mathbf{u} + \lambda(1-\mathbf{u}^T\mathbf{u})$

Vector of partial derivatives set to zero

$$1/n\, \mathbf{X}^T\mathbf{X}\mathbf{u} - \lambda\mathbf{u} = 0$$

Computing the Components

- Projection of vector $\mathbf{x}$ onto an axis (dimension) $\mathbf{u}$ is $\mathbf{u}^T\mathbf{x}$
- Assume $\mathbf{X}$ is a normalized *nxp* data matrix for *n* samples and *p* features. Direction of greatest variability is that in which the average square of the projection is greatest:

Maximize $\quad \mathbf{(1/n)\ u^T X^T X u}$

s.t $\quad \mathbf{u}^T\mathbf{u} = 1$

Construct Langrangian $(1/n)\ \mathbf{u}^T\mathbf{X}^T\mathbf{X}\mathbf{u} + \lambda(1-\mathbf{u}^T\mathbf{u})$

Vector of partial derivatives set to zero

$$\mathbf{1/n\ X^T X u} - \lambda\mathbf{u} = 0$$

or equivalently $\mathbf{Su} - \lambda\mathbf{u} = 0$ (S $=\mathbf{1/n\ X^T X}$: covariance matrix)

As $\mathbf{u} \neq \mathbf{0}$ then $\mathbf{u}$ must be an eigenvector of S with eigenvalue λ

Computing the Components

- Projection of vector **x** onto an axis (dimension) **u** is $\mathbf{u}^T\mathbf{x}$
- Assume **X** is a normalized *n*x*p* data matrix for *n* samples and *p* features. Direction of greatest variability is that in which the average square of the projection is greatest:

Maximize $\quad (1/n)\, \mathbf{u}^T\mathbf{X}^T\mathbf{X}\mathbf{u}$

s.t $\quad \mathbf{u}^T\mathbf{u} = 1$

Construct Langrangian $(1/n)\, \mathbf{u}^T\mathbf{X}^T\mathbf{X}\mathbf{u} - \lambda\mathbf{u}^T\mathbf{u}$

Vector of partial derivatives set to zero

$$1/n\ \mathbf{X}^T\mathbf{X}\mathbf{u} - \lambda\mathbf{u} = 0$$

or equivalently $\mathbf{S}\mathbf{u} - \lambda\mathbf{u} = 0$ ($S = 1/n\ \mathbf{X}^T\mathbf{X}$: covariance matrix)

As $\mathbf{u} \neq \mathbf{0}$ then **u** must be an eigenvector of S with eigenvalue λ

- λ is the principal eigenvalue of the **covariance matrix S**
- The eigenvalue denotes the amount of variability captured along that dimension

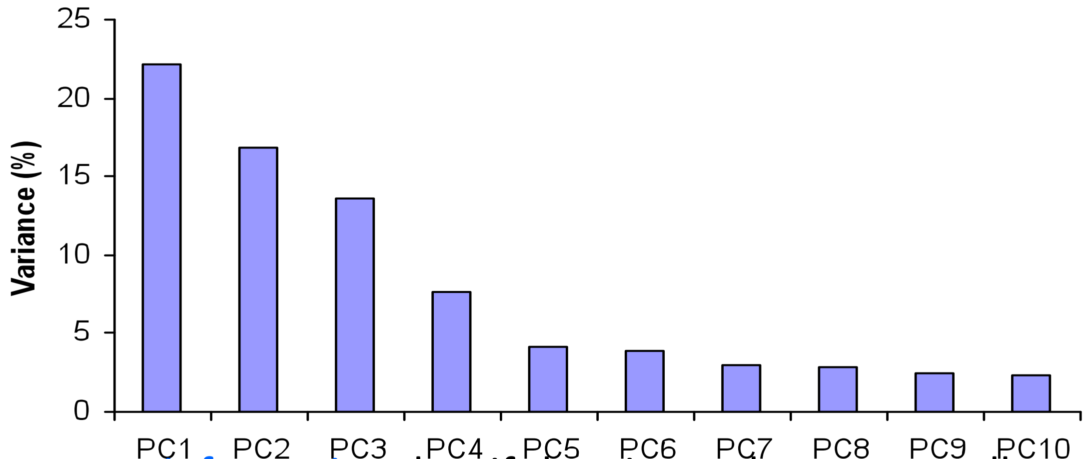
PCs, Variance and Least-Squares

- The first PC retains the greatest amount of variation in the sample
- The k^{th} PC retains the kth greatest fraction of the variation in the sample
- The k^{th} largest eigenvalue of the covariance matrix C is the variance in the sample along the k^{th} PC
- The least-squares view: PCs are a series of linear least squares fits to a sample, each orthogonal to all previous ones (Bishop 12.1.2)

How Many PCs?

- For p original dimensions, sample covariance matrix is pxp, and has up to p eigenvectors. So p PCs.
- Where does dimensionality reduction come from?

  Can *ignore* the components of lesser significance.



You do lose some information, but if the eigenvalues are small, you don't lose much

- p dimensions in original data
- Calculate p eigenvectors and eigenvalues
- choose only the first q eigenvectors, based on their eigenvalues
- final data set has only q dimensions

Applying PCA to Images

- 361 x 261 pixels, 83781 dimensional data

Reconstructing the Images from 4 PCs

- The principal components are also images

Reconstructing the Images from 4 PCs

Summary:

- Principle
  - Linear projection method to reduce the number of parameters
  - Transfer a set of correlated variables into a new set of uncorrelated variables
  - Map the data into a space of lower dimensionality
  - Form of unsupervised learning
- Properties
  - It can be viewed as a rotation of the existing axes to new positions in the space defined by original variables
  - New axes are orthogonal and represent the directions with maximum variability