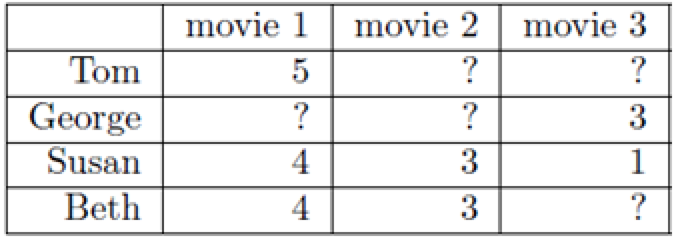
DATA8015 Math Foundation of Data Science

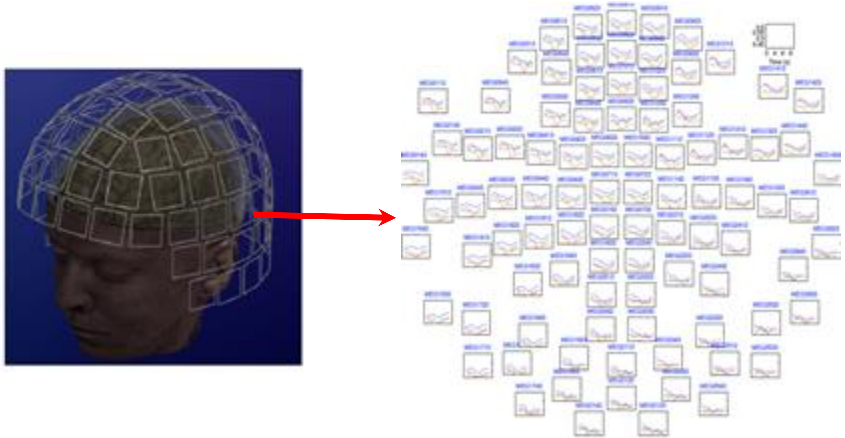
Principal Component Analysis

Dimensionality Reduction

- Vectors store features. Lots of features!
  - Document classification: thousands of words per doc
  - Netflix surveys: 480189 users x 17770 movies
  - MEG Brain Imaging: 120 locations x 500 time points x 20 objects



	movie 1	movie 2	movie 3
Tom	5	?	?
George	?	?	3
Susan	4	3	1
Beth	4	3	?



Dimensionality Reduction

Reduce dimensions

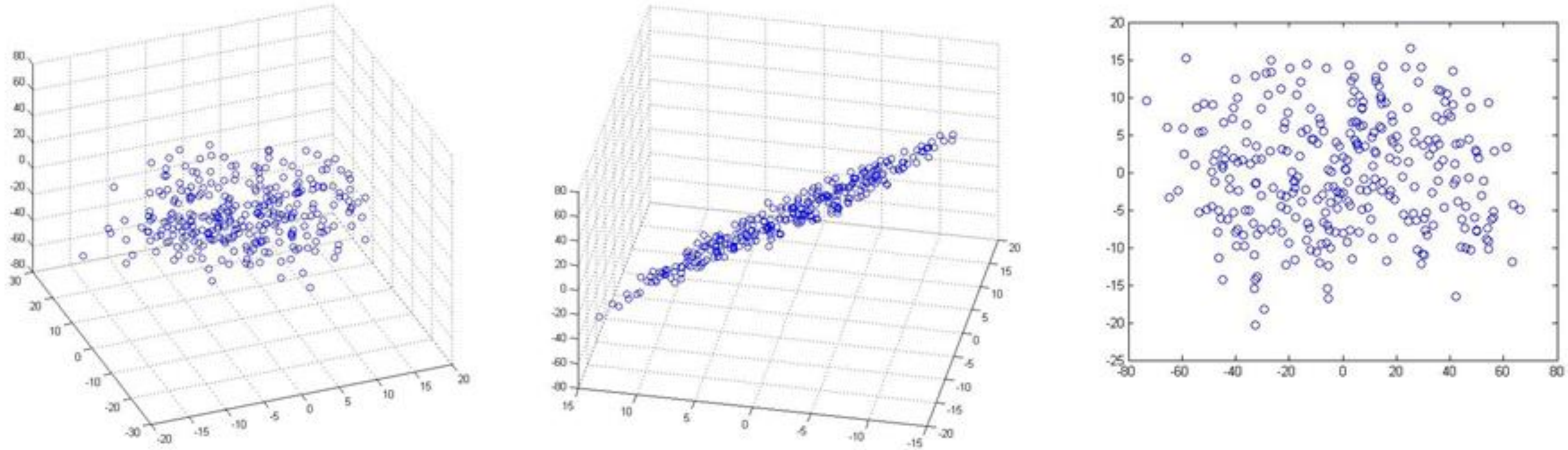
- Why?
  - Lots of features redundant
  - Storage & computation costs

CreativeBlog

- Goal: take $x \in \mathbb{R}^d \to x \in \mathbb{R}^r,$ for $r \ll d$
  - But, minimize information loss

Dimensionality Reduction

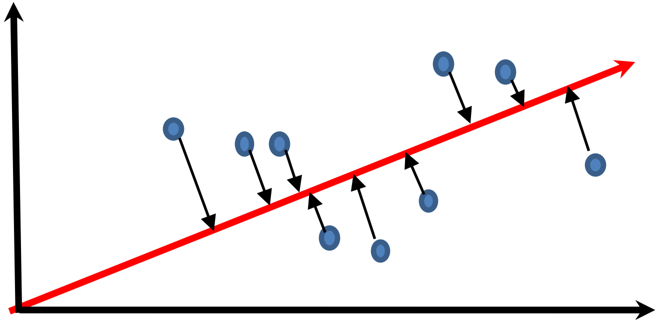
Examples: 3D to 2D



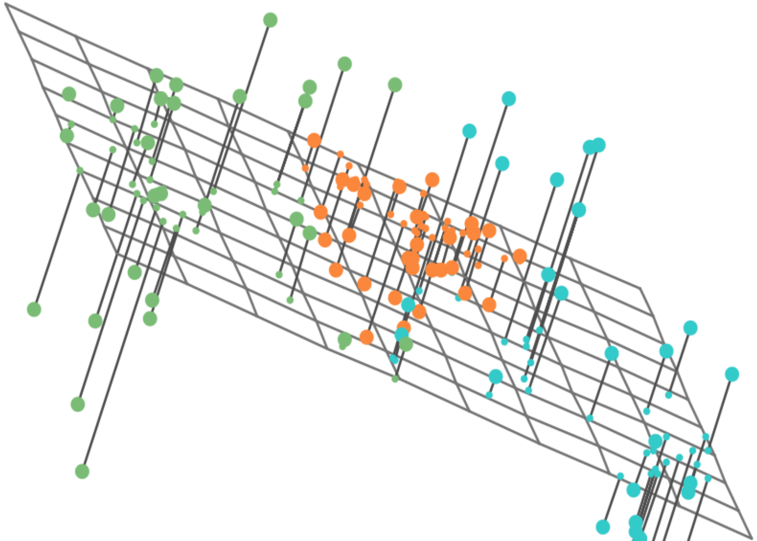
Andrew Ng

Principal Components Analysis (**PCA**)

- A type of dimensionality reduction approach
  - For when data is **approximately lower dimensional**



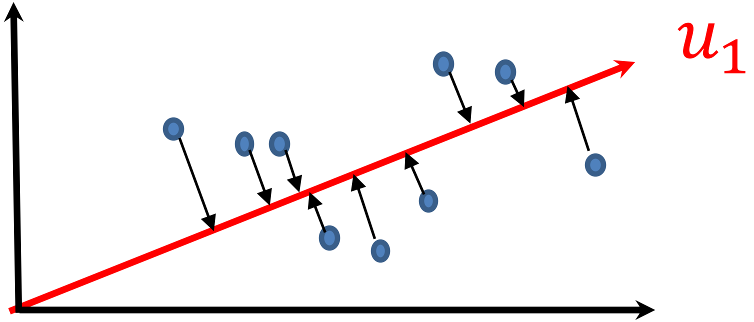
2D
↓
1D

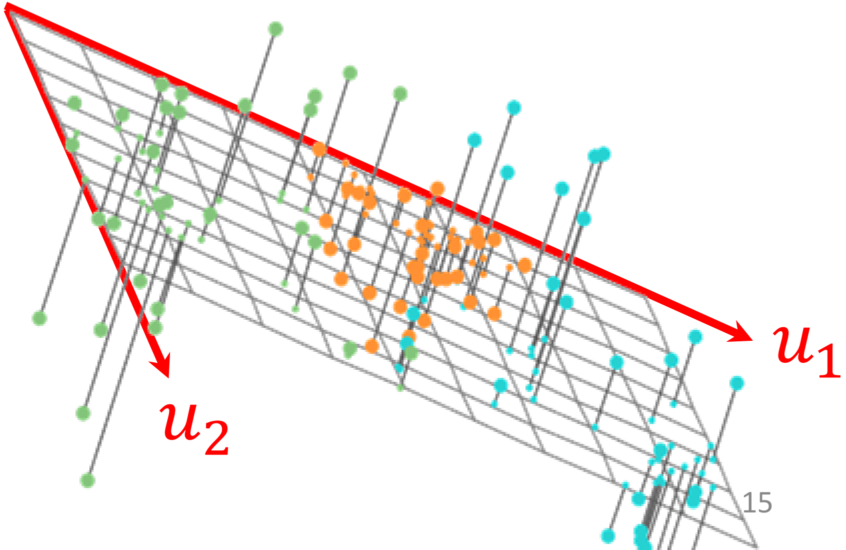


3D
↓
2D

Principal Components Analysis (**PCA**)

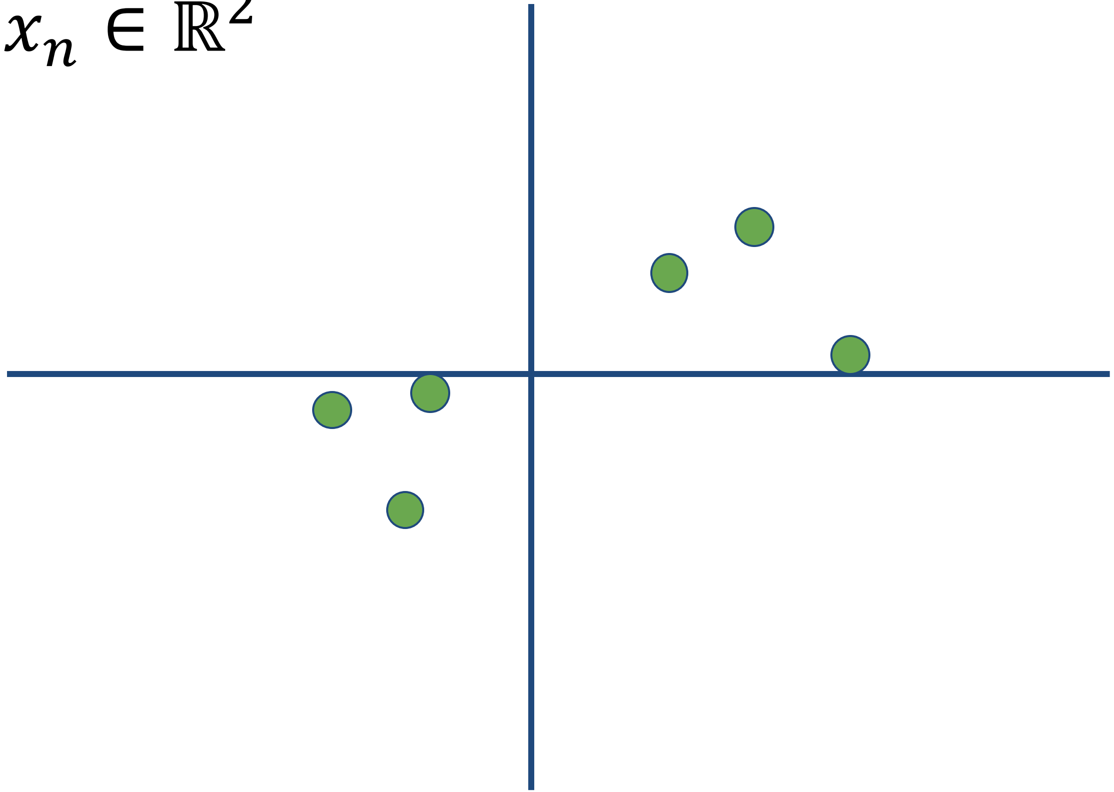
- Find **axes** $u_1, u_2, \dots, u_r \in \mathbb{R}^d$ of a subspace
  - Will project to this subspace
- Want to preserve data
  - minimize projection error
- These vectors are the **principal components**





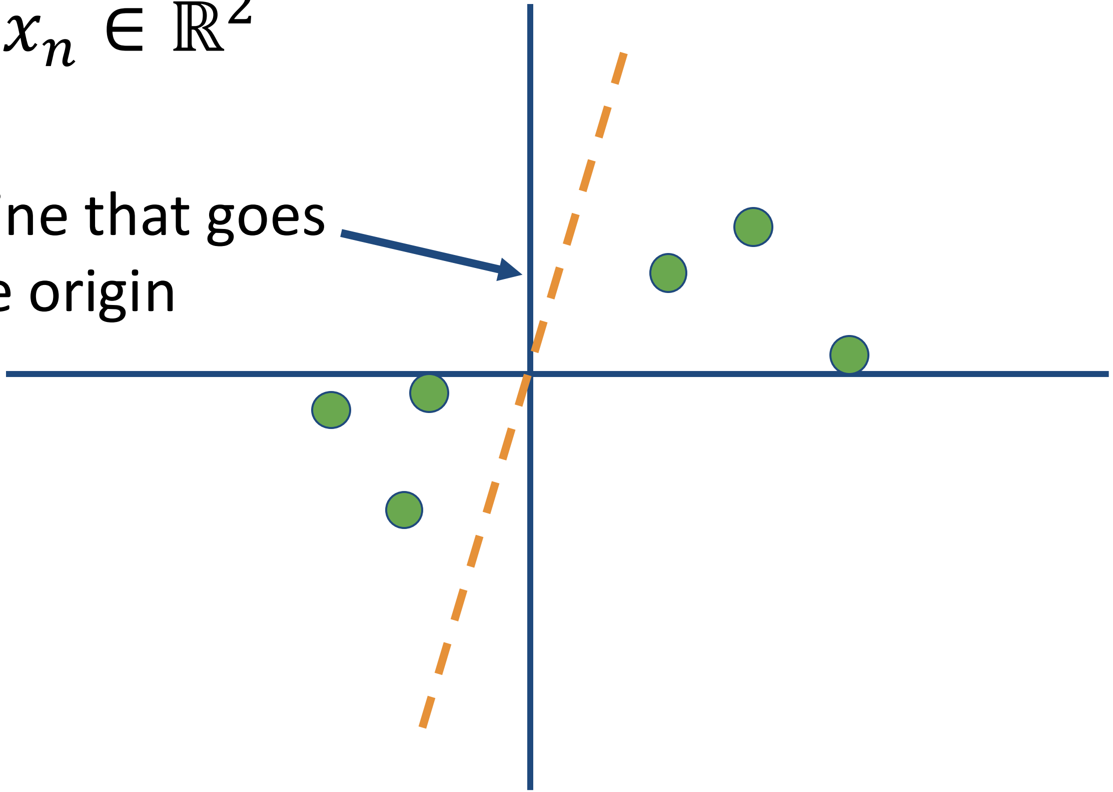
Projection: An Example

$x_1, x_2, \ldots, x_n \in \mathbb{R}^2$



Projection: An Example

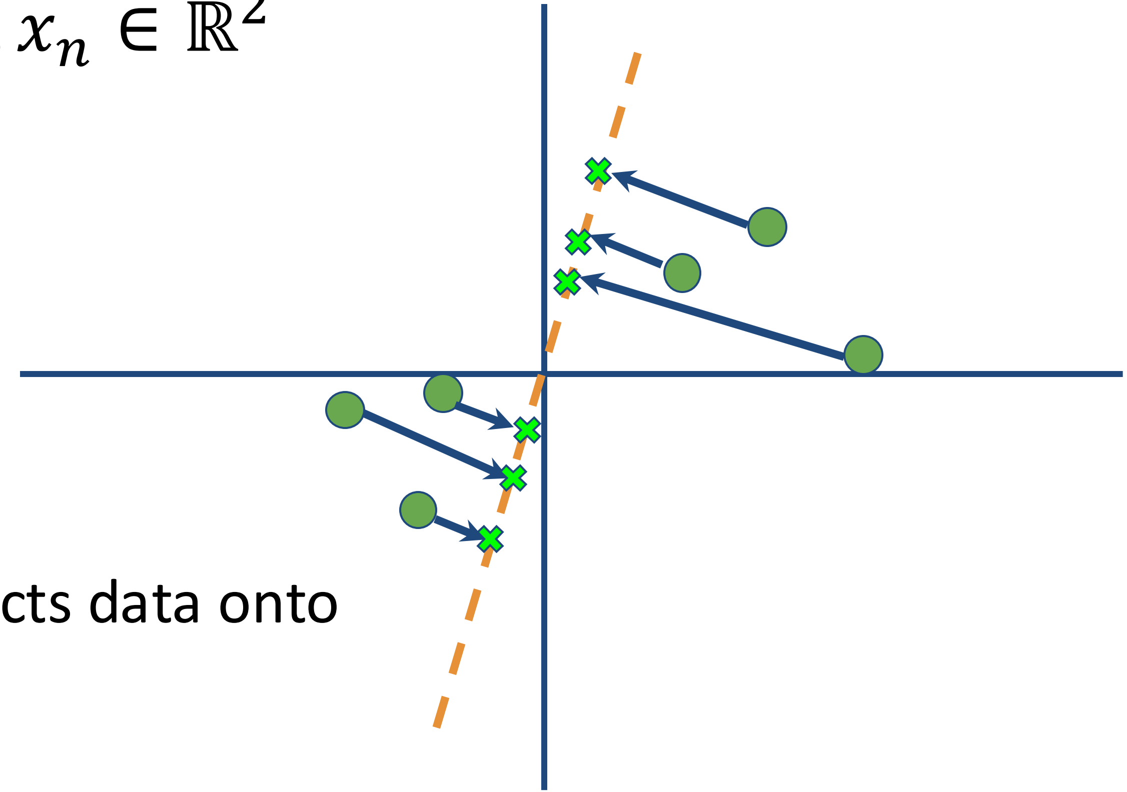
$x_1, x_2, \ldots, x_n \in \mathbb{R}^2$



A random line that goes through the origin

Projection: An Example

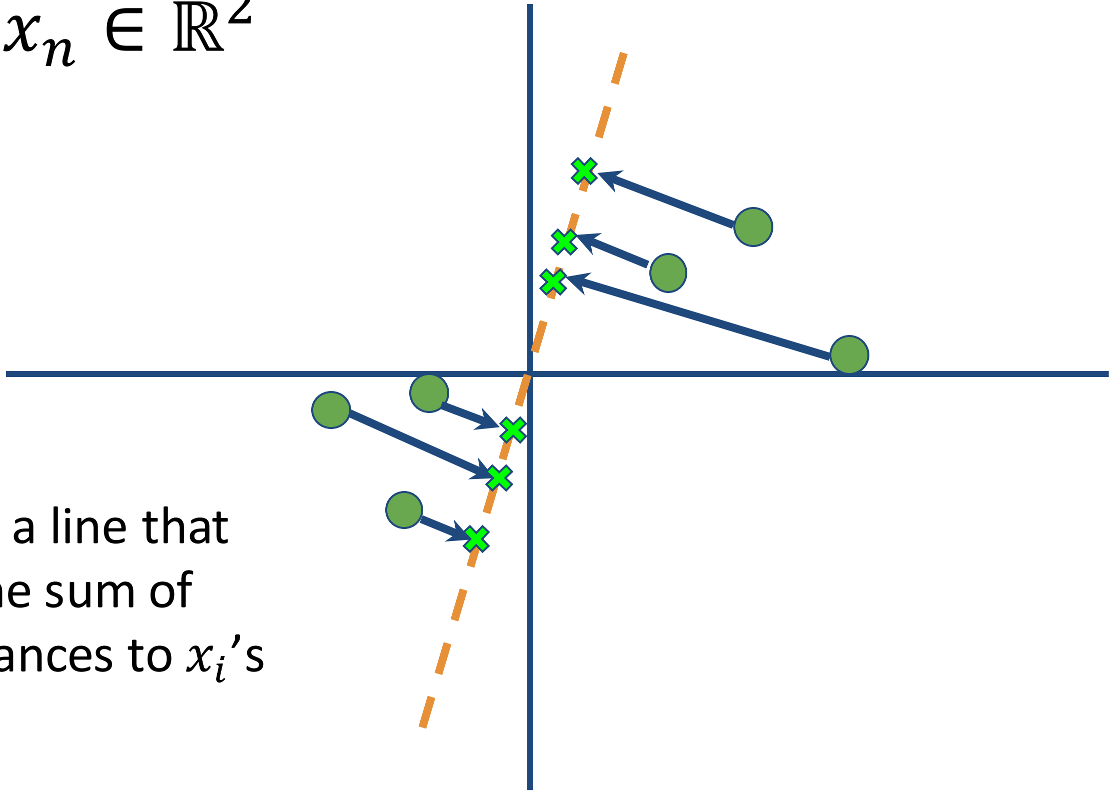
$x_1, x_2, \ldots, x_n \in \mathbb{R}^2$



PCA projects data onto this line

Projection: An Example

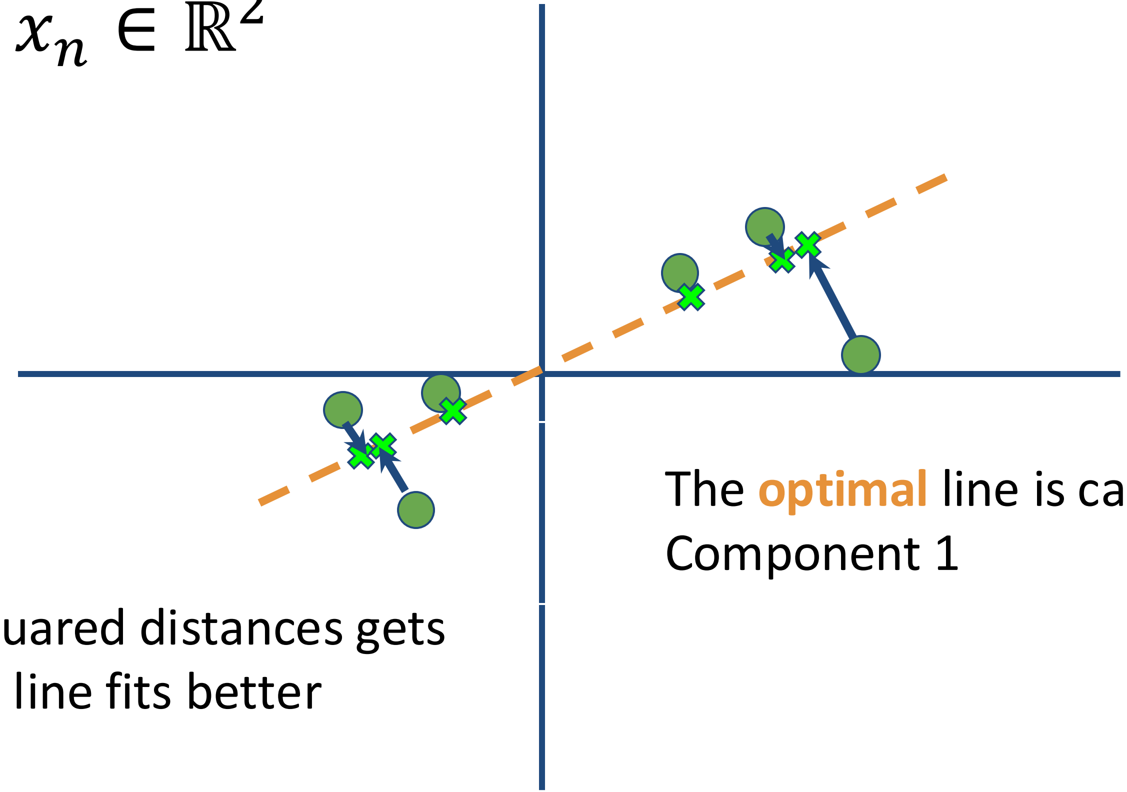
$x_1, x_2, \ldots, x_n \in \mathbb{R}^2$



Goal: finding a line that **minimizes** the sum of squared distances to x_i's

Projection: An Example

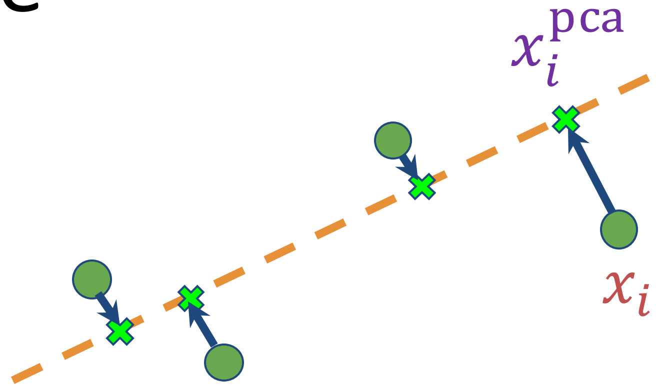
$x_1, x_2, \ldots, x_n \in \mathbb{R}^2$



The **optimal** line is called Principal Component 1

The sum of squared distances gets smaller as the line fits better

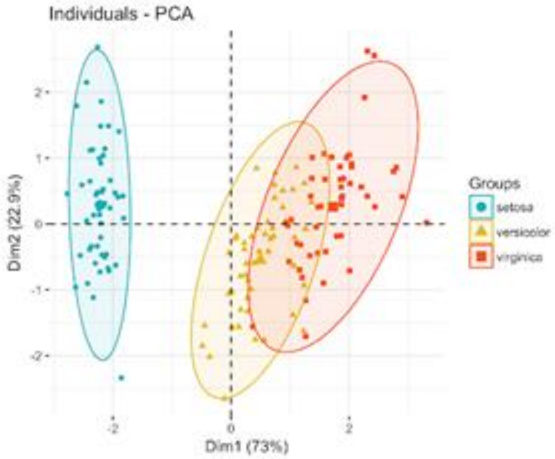
PCA Procedure



- **Inputs:** data $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$
  - **Centered data with** $\frac{1}{n}\sum_{i=1}^{n} x_i = 0$
- **Output:**
  principal components $u_1, \ldots, u_r \in \mathbb{R}^d$
  - Can show: they are top **eigenvectors** of $S = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^\top$ (covariance matrix)
  - Each x_i projected to $x_i^{\mathrm{pca}} = \sum_{j=1}^{m} u_j (u_j^\top x_i)$

Many Variations

- PCA, Kernel PCA, ICA, CCA
  - Extract structure from high dimensional dataset
- Uses:
  - **Visualization**
  - Efficiency
  - Noise removal
  - Downstream machine learning use



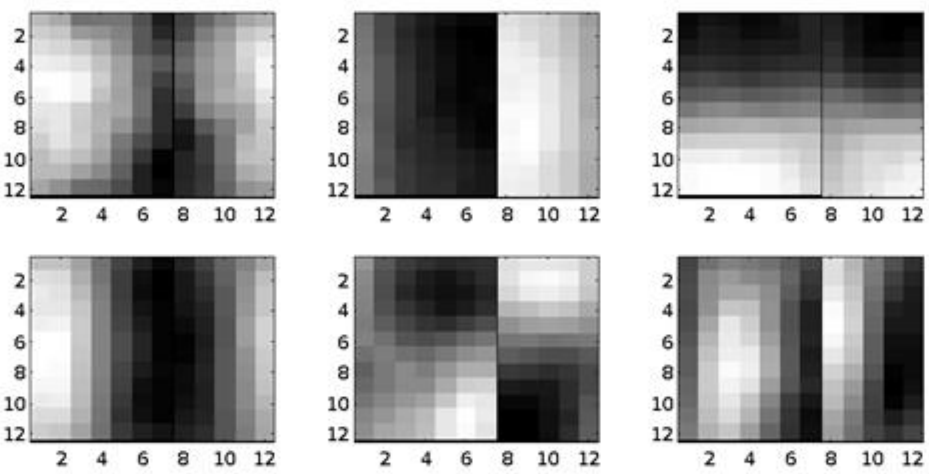
STHDA

Application: Image Compression

- Start with image; divide into 12x12 patches
  - That is, 144-D vector
  - **Original image:**

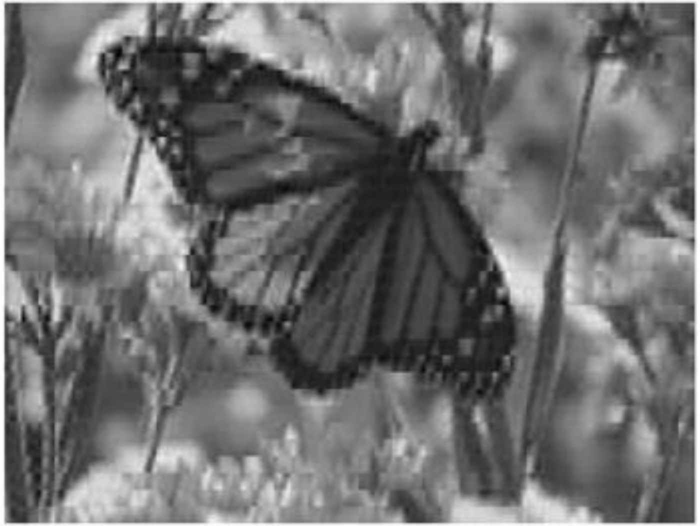
Application: Image Compression

- 6 principal components (as an image)



Application: Image Compression

- Project to 6D

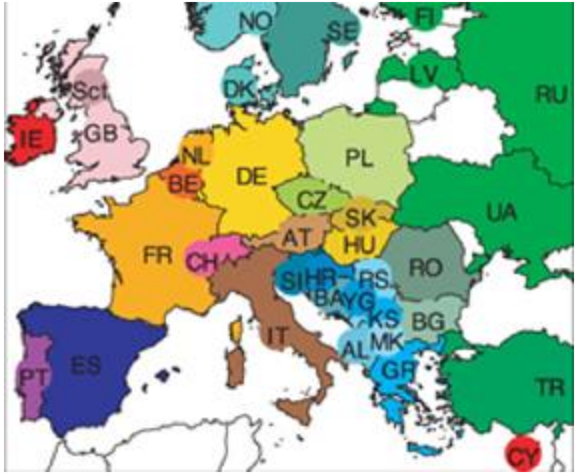


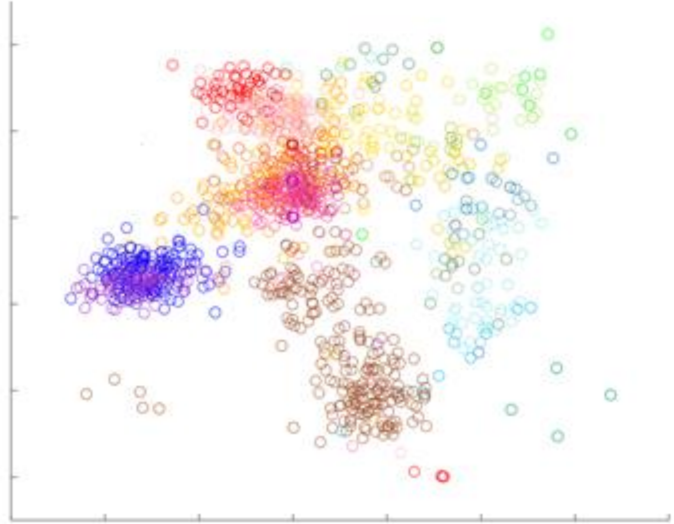
Compressed

Original

Application: Exploratory Data Analysis

- [**Novembre et al. ’08**]: Take top two singular vectors of people x SNP matrix (POPRES)





“Genes Mirror Geography in Europe”