Foundations of Machine Learning
AI2000 and AI5000

FoML-28
PCA

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భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
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Data-driven Intelligence
& Learning Lab

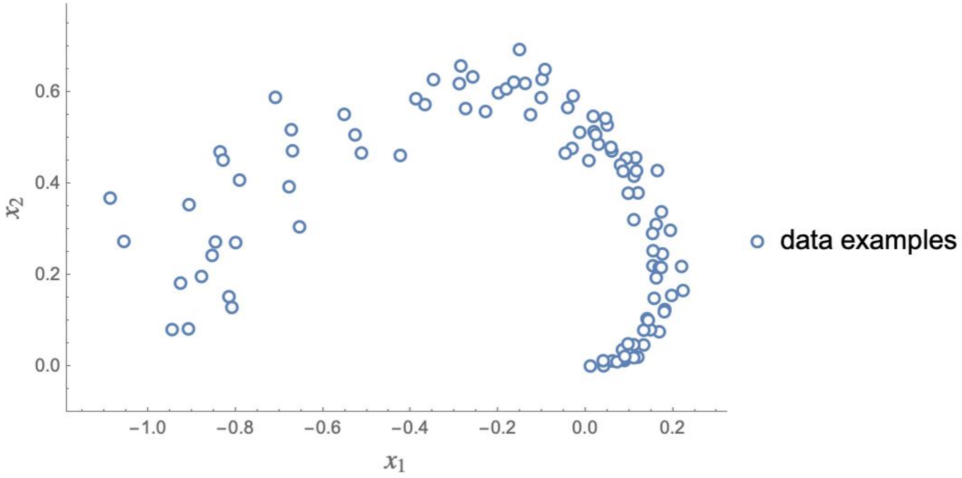
So far in FoML

- Intro to ML and Probability refresher
- MLE, MAP, and fully Bayesian treatment
- Supervised learning
  a. Linear Regression with basis functions
  b. Bias-Variance Decomposition
  c. Decision Theory - three broad classification strategies
  d. Neural Networks
- Unsupervised learning
  a. K-Means, Hierarchical, and GMM for clustering

For today

- PCA - Principal Component Analysis (Pearson, 1901) & (Hotelling, 1933)

Manifold coordinates as Latent variables



$$\{x_1,\ x_2\} = \{t\cos(3\ t),\ t\sin(3\ t)\}$$

Figure credits

Example - facial image data

- Possible degrees of freedom
  - Skull size
  - Skin color
  - Eye color
  - Facial attributes
  - Horizontal orientation
  - Vertical orientation
  - Mood (e.g., happy)
  - etc.

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Latent subspace will be a nonlinear transformation of image data

PCA

- Linear latent subspaces

What is PCA?

- Tool to summarize a large set of variables (dimensions) with a smaller set

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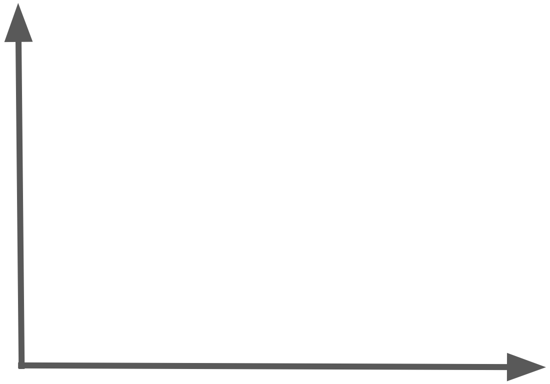
What is PCA?

- Smaller set need not be a subset of original variables!
    - Rather, combinations of original variables
- They may not mean the same as originals
    - lost interpretability!
- New variables are independent of each other!

What is PCA?

- Gives the directions along which the data are highly 'variable'
  - Projects linearly such that the variance in the projected space is maximal



PCA

- Data $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$ $\mathbf{x}_i \in \mathbb{R}^D$

- Aim: project data onto M dimensional space (M < D) maximizing the variance of the projected data

PCA

- Mean $\bar{\mathbf{x}} =$

- Covariance $\mathbf{S} =$

1D representation using PCA

- Project data onto a direction where most of the variance is preserved
- Projecting onto $\mathbf{u}_1$ gives a scalar → 1D representation

$$\mathbf{z}_i = \mathbf{u}_1{}^T \mathbf{x}_i$$

1D representation using PCA

- Direction of u_1 is important → consider unit vector in that direction

$$||\mathbf{u}_1||_2 = 1$$

1D representation using PCA

- Consider the variance in the new subspace

$$\mathrm{Var}[\mathbf{z}] =$$

1D representation using PCA

- Let's find the direction (u_1) that maximizes the variance in z_i

$$\arg\max_{\mathbf{u}_1} \quad \mathbf{u}_1{}^T \mathbf{S} \mathbf{u}_1 \quad \text{such that} \quad \mathbf{u}_1^T \mathbf{u} = 1$$

PCA via maximum variance

- Repeat the procedure for the next M-1 orthogonal vectors
  - Maximize the variance by projecting onto a direction orthogonal to the found ones
  - These are the next M-1 eigenvectors of the covariance matrix (S)

PCA - Eigen decomposition

- For the symmetric PSD matrix $\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$
- Eigenvectors are orthonormal (contained in U)
- Eigenvalues are non-negative (contained in $\mathbf{\Lambda}$)

PCA - Eigen decomposition

- Variance is Tr(S)

$$\mathbf{S} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$$

PCA - some notes

PCA - Scaling the features

- Sensitive to the scales of the features/variables
  - Features with greater range dominate the process of finding the PCs
- Perform standardization to prevent this

PCA - Proportion of the Variance Explained

- How much of the information is lost by projecting onto PCs?

PCA - Proportion of the Variance Explained

- Total variance

$$\sum_{j=1}^{p} \mathrm{Var}(X_j) = \sum_{j=1}^{p} \frac{1}{n} \sum_{i=1}^{n} x_{ij}^2$$

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- Variance explained by the 'm'th PC

$$\frac{1}{n} \sum_{i=1}^{n} z_{im}^2$$

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- Variance explained by the ‘m’th PC

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PVE of the ‘m’th PC =

PCA - How many PCs to consider?

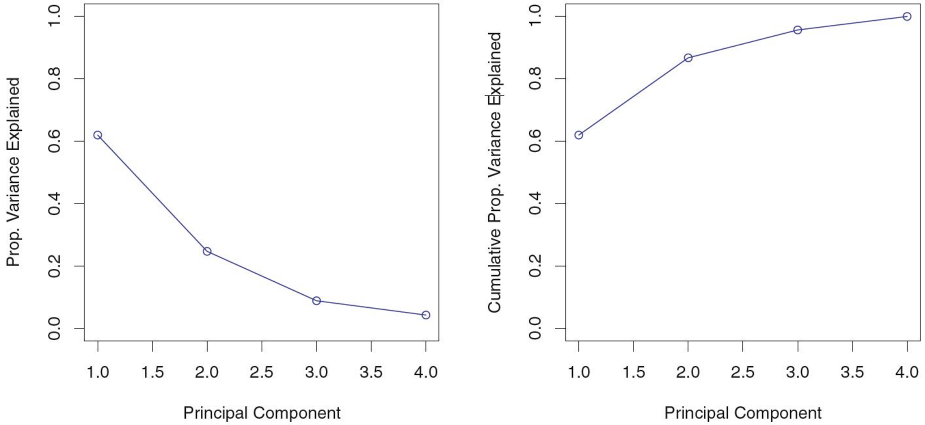
- For an n X p data matrix
  - min(n-1, p) PCs are possible
  - Why?

PCA - How many PCs to consider?

- For an n X p data matrix
  - min(n-1, p) PCs are possible
- Not all of them may be interesting

PCA - How many PCs to consider?

- Generally, we want the ‘smallest’ number of them → good understanding of the data
- → scree plot & elbow



PCA

- Doesn't discard the redundant variables
  - Finds new variables (linear combinations of the 'p' variables) that summarize the data well
  - The 'best' variables (among the all possible linear combinations)
  - Resulting new features are uncorrelated (covariance matrix will be diagonal)

Applications of PCA

- Dimensionality reduction → tackles curse of dimensionality
- Less compute requirement
- Less prone to overfitting
- Useful preprocessing

Next

- PCA continued