THE UNIVERSITY OF TEXAS AT AUSTIN
Department of Statistics and Data Sciences
College of Natural Sciences

SDS 385: Stat Models for Big Data

Lecture 12: PCA and LDA

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Principal Component Analysis

- Goal: Find the direction of the most variance.
- Say X is the data matrix
- The average is $\bar{\boldsymbol{x}} = \frac{\sum_{i=1}^{n} \boldsymbol{x}_i}{n}$
- Let $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i - \bar{\boldsymbol{x}}$

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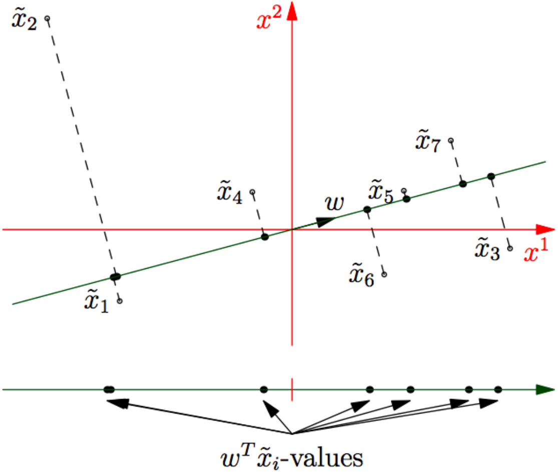
- Let $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i - \bar{\boldsymbol{x}}$
- The sample variance of $(\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_n)$ *along a direction* w is give by:

$$\frac{1}{n} \sum_{i=1}^{n} (\tilde{\boldsymbol{x}}_i^T w)^2$$

- What is the sample variance of $(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$ *along a direction* $\boldsymbol{w}$?

Principal Component Analysis



First component

- So the first PC direction is:

$$\boldsymbol{w}_1 = \arg \max_{\|\boldsymbol{w}\|=1} \frac{1}{n} \sum_{i=1}^{n} (\tilde{\boldsymbol{x}}_i^T \boldsymbol{w})^2$$

- And the first PC component of $\tilde{\boldsymbol{x}}_i$ is $\tilde{\boldsymbol{x}}_i^T \boldsymbol{w}_1$

First component

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$$\boldsymbol{w}_k = \arg \max_{\substack{\|\boldsymbol{w}\|=1 \\ \boldsymbol{w} \perp \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{k-1}}} \frac{1}{n} \sum_{i=1}^{n} (\tilde{\boldsymbol{x}}_i^T \boldsymbol{w})^2$$

- And the k^{th} PC component of $\tilde{\boldsymbol{x}}_i$ is $\tilde{\boldsymbol{x}}_i^T \boldsymbol{w}_k$
- Note that $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_k$ form an orthogonal basis.

Simple algorithm

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- This is the first eigenvector of $S = \tilde{X}^T \tilde{X}$

Eigenvector and eigenvalues

- Any square symmetrix matrix S has real eigenvalues
- The i^{th} eigenvalue,vector pair satisfy $S\boldsymbol{w}_i = \lambda_i \boldsymbol{w}_i$
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- The eigenvectors are orthogonal to each other, and normalized to have length 1.
- In matrix terms, we can write:

$$S = U\Sigma U^T, \text{ where}$$

  - columns of U are the orgonal eigenvectors, and
  - Σ is a diagonal matrix with eigenvalues on the diagonal
- The larger the magnitude of the eigenvalue, more important the eigenvector

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- Its the scalar multiple of the sample covariance matrix

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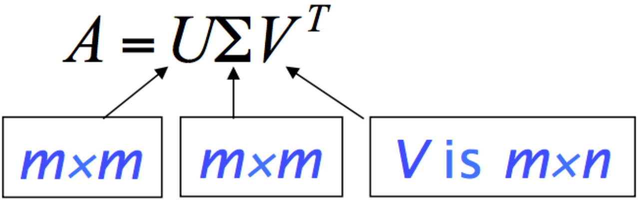
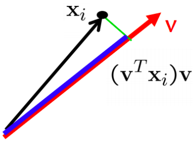
- So, all you have to do is to calculate eigenvectors of the covariance matrix.
- But, do I even need to do that?
- The right singular vectors of $\tilde{X}$ is just fine.
- How many PC's? (more of a dissertaiton question)

Singular value decomposition



- The columns of U are orthogonal eigenvectos of AA^T
- The columns of V are orthogonal eigenvectos of A^TA
- A^TA and AA^T have the same eigenvalues

Second interpretation



- Minimum reconstruction error:

$$(\boldsymbol{x}_i - (\boldsymbol{x}_i^T \boldsymbol{w})\boldsymbol{w})^T (\boldsymbol{x}_i - (\boldsymbol{x}_i^T \boldsymbol{w})\boldsymbol{w}) = \boldsymbol{x}_i^T \boldsymbol{x}_i - (\boldsymbol{x}_i^T \boldsymbol{w})^2$$

- So, the first PC direction gives the direction projecting on which has the **minimum reconstruction error**.

Low rank approximation

- Take the centered data matrix $\tilde{X}$ with SVD

$$\tilde{X} = USV^T$$

- Project on the top k PC's $W \in \mathbb{R}^{p \times k}$

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- So $W = \arg \min_{\text{rank}(B)=k, B \in \mathbb{R}^{n \times p}} \|\tilde{X} - B\|_F^2$ and the reconstruction error is $\sum_{i=k+1}^{p} \sigma_i^2$

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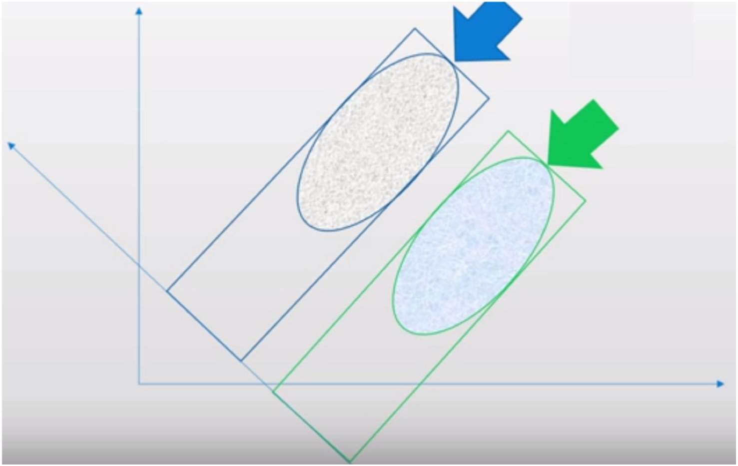
- This explains why you want to take large k to reduce approx. error.

Linear Discriminant Analysis

- PCA did not have class information
- LDA does take that into account.
- We will do it for two classes.



LDA

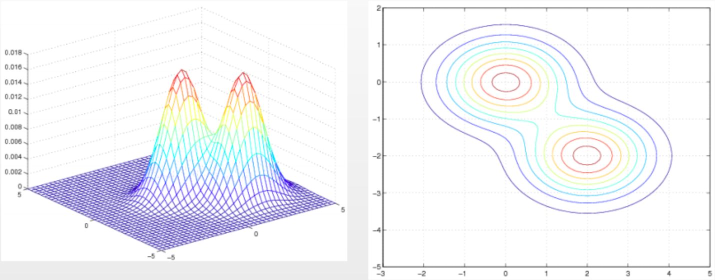
- Assume that the data is coming from a mixture of two Gaussians with parameters $(\mu_k, \Sigma_k), k \in \{1, 2\}$

LDA

- Assume that the data is coming from a mixture of two Gaussians with parameters $(\mu_k, \Sigma_k), k \in \{1, 2\}$
- Recall the density of a multivariate gausssian

$$f(x) = \frac{1}{(2\pi)^{p/2}|\Sigma_k|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)\right)$$

A pretty picture



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$$\begin{aligned} \arg\max_k P(y = k|\boldsymbol{x}, \Theta) &= \arg\max_k \frac{P(\boldsymbol{x}|y = k, \Theta)P(y = k)}{P(\boldsymbol{x})} \\ &= \arg\max_k P(\boldsymbol{x}|y = k, \Theta)P(y = k) \end{aligned}$$

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- So decision rule for class 1 is

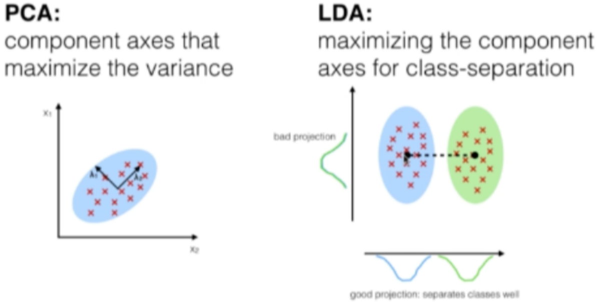
$$\begin{aligned}&-\frac{1}{2}\log|\Sigma_1|^{1/2} - \frac{1}{2}(x-\mu_1)^T\Sigma_1^{-1}(x-\mu_1) + \log\pi_1 \\ &> -\frac{1}{2}\log|\Sigma_2|^{1/2} - \frac{1}{2}(x-\mu_2)^T\Sigma_2^{-1}(x-\mu_2) + \log\pi_2\end{aligned}$$

- For $\Sigma_1 \neq \Sigma_2$, this is a quadratic function.

LDA

- LDA assumes that $\Sigma_1 = \Sigma_2$
- So now we get a linear decision boundary

$$x^T \Sigma^{-1}(\mu_1 - \mu_2) > \frac{\mu_1 + \mu_2}{2} \Sigma^{-1}(\mu_1 - \mu_2) - \log \frac{\pi_1}{\pi_2}$$



Estimation

- Class proportion

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- Class mean
$$\hat{\mu}_k = \frac{\sum_{y_i=k} x_i}{n}.$$

- Common class covariance matrix
$$\hat{\Sigma} = \frac{\sum_{k=1}^{K} \sum_{y_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T}{n - K}.$$

Multiple classes

- For datapoint x whose class you want to predict, for each class $k \in \{1, \ldots, K\}$, compute the **linear discriminant function** $\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k$ *with estimated parameters*

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- Assign x to class that maximixes this function.
- Why not use QDA?

Multiple classes

Note that LDA equivalently minimizes over $j = 1, \ldots K$,

$$\frac{1}{2}(x - \hat{\mu}_j)^T \hat{\Sigma}^{-1}(x - \hat{\mu}_j) - \log \hat{\pi}_j$$

It helps to factorize $\hat{\Sigma}$ (i.e., compute its eigendecomposition):

$$\hat{\Sigma} = UDU^T$$

where $U \in \mathbb{R}^{p \times p}$ has orthonormal columns (and rows), and $D = \mathrm{diag}(d_1, \ldots d_p)$ with $d_j \geq 0$ for each j. Then we have $\hat{\Sigma}^{-1} = UD^{-1}U^T$, and

$$(x - \hat{\mu}_j)^T \hat{\Sigma}^{-1}(x - \hat{\mu}_j) = \| \underbrace{D^{-1/2}U^T x}_{\tilde{x}} - \underbrace{D^{-1/2}U^T \hat{\mu}_j}_{\tilde{\mu}_j} \|_2^2$$

This is just the squared distance between $\tilde{x}$ and $\tilde{\mu}_j$

Multiple classes

Hence the LDA procedure can be described as:

1. Compute the sample estimates $\hat{\pi}_j, \hat{\mu}_j, \hat{\Sigma}$
2. Factor $\hat{\Sigma}$, as in $\hat{\Sigma} = UDU^T$
3. Transform the class centroids $\tilde{\mu}_j = D^{-1/2}U^T\hat{\mu}_j$
4. Given any point $x \in \mathbb{R}^p$, transform to $\tilde{x} = D^{-1/2}U^T x \in \mathbb{R}^p$, and then classify according to the nearest centroid in the transformed space, adjusting for class proportions—this is the class j for which $\frac{1}{2}\|\tilde{x} - \tilde{\mu}_j\|_2^2 - \log \hat{\pi}_j$ is smallest

What is this transformation doing? Think about applying it to the observations:

$$\tilde{x}_i = D^{-1/2}U^T x_i, \quad i = 1, \ldots n$$

This is basically sphering the data points, because if we think of $x \in \mathbb{R}^p$ were a random variable with covariance matrix $\hat{\Sigma}$, then

$$\mathrm{Cov}(D^{-1/2}U^T x) = D^{-1/2}U^T\hat{\Sigma}UD^{-1/2} = I$$

Multiple classes

LDA compares the quantity $\frac{1}{2}\|\tilde{x} - \tilde{\mu}_j\|_2^2 - \log \hat{\pi}_j$ across the classes $j = 1, \ldots K$. Consider the affine subspace $M \subseteq \mathbb{R}^p$ spanned by the transformed centroids $\tilde{\mu}_1, \ldots \tilde{\mu}_K$, which has dimension $K - 1$

For any $\tilde{x} \in \mathbb{R}^p$, we can decompose $\tilde{x} = P_M\tilde{x} + P_{M^\perp}\tilde{x}$, so

$$\begin{aligned}\|\tilde{x} - \tilde{\mu}_j\|_2^2 &= \|\underbrace{P_M\tilde{x} - \tilde{\mu}_j}_{\in M} + \underbrace{P_{M^\perp}\tilde{x}}_{\in M^\perp}\|_2^2 \\ &= \|P_M\tilde{x} - \tilde{\mu}_j\|_2^2 + \|P_{M^\perp}\tilde{x}\|_2^2\end{aligned}$$

The second term doesn't depend on j

What this is telling us: the LDA classification rule is unchanged if we project the points to be classified onto M, since the distances orthogonal to M don't matter

Acknowledgment

- Some pictures are borrowed from Brett Bernstein's notes from NYU and Jia Li's notes from PSU
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