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 $\bar{\boldsymbol{x}} = \dfrac{\sum_{i=1}^{n} \boldsymbol{x}_i}{n}$
- Let $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i - \bar{\boldsymbol{x}}$

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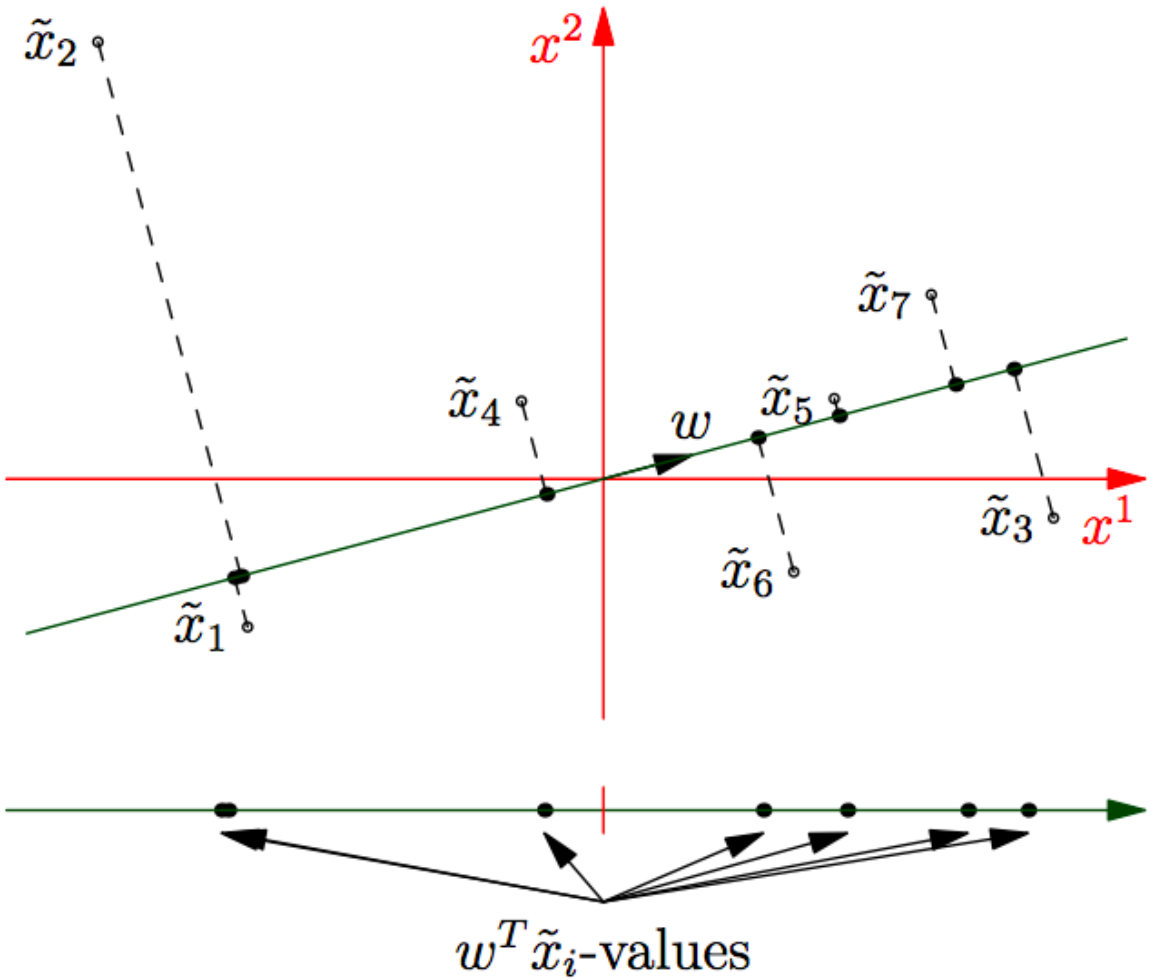
- Let $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i - \bar{\boldsymbol{x}}$
- The sample variance of $(\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_n)$ *along a direction* w is give by:

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

- 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

- So the k^{th} PC direction is:

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

- 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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Eigenvector and eigenvalues

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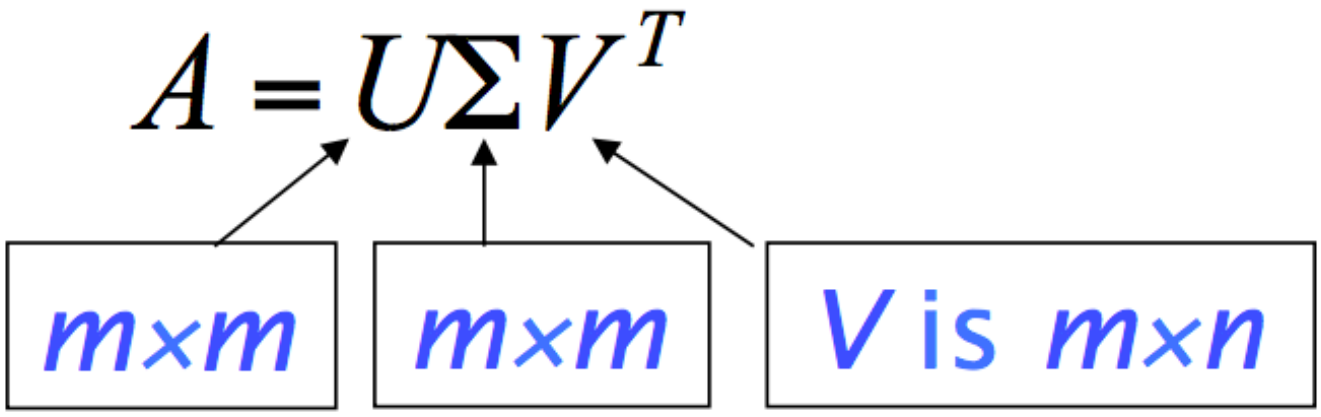
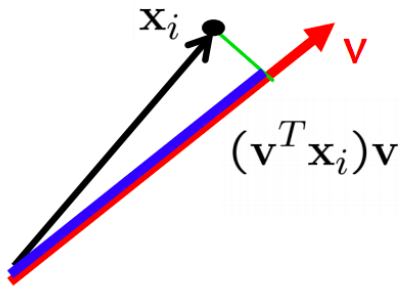
- So, all you have to do is to calculate eigenvectors of the covariance matrix.
- But, do I even need to do that?
- The right singular vectors of $\tilde{X}$ is just fine.
- How many PC's? (more of a dissertaiton question)

Singular value decomposition



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

Second interpretation



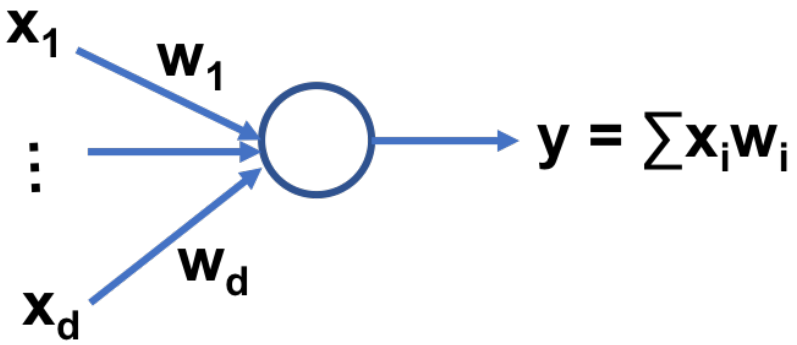
- Minimum reconstruction error:

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

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

Online PCA - Oja's algorithm

- Erikki Oja wrote a seminar paper in 1982 about a simple neural network model.
- He was inspired by the Hebbian principle (1949, "The organization of behavior", Donald Hebb) which claims that the synaptic energy increases from presynaptic cells stimulating post-synaptic cells.



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- For each data-point, you do:

$$w_{t+1} \leftarrow w_t + \eta_t (x_i^T w_t) x_t$$

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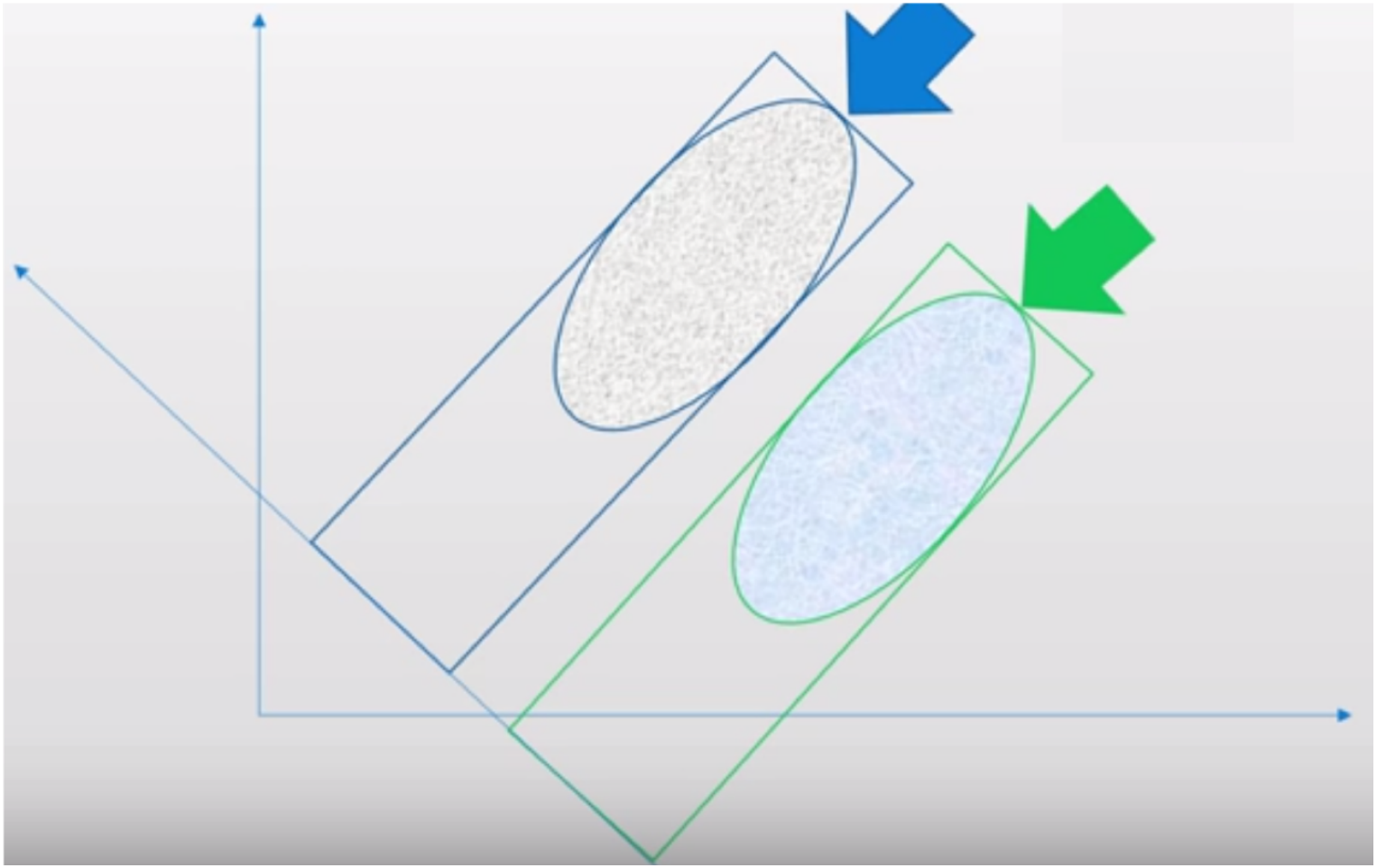
- Note that here, you do not need to construct the covariance matrix explicitly, which is extremely useful, when d is much larger than n, i.e. in high dimensional settings.
- Step size η can be set as $\log n/n$ or $\eta_t \propto 1/t$
- Sharp error bounds show that the final solution converges to the principal component and the error has weak dependence on dimensionality d

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

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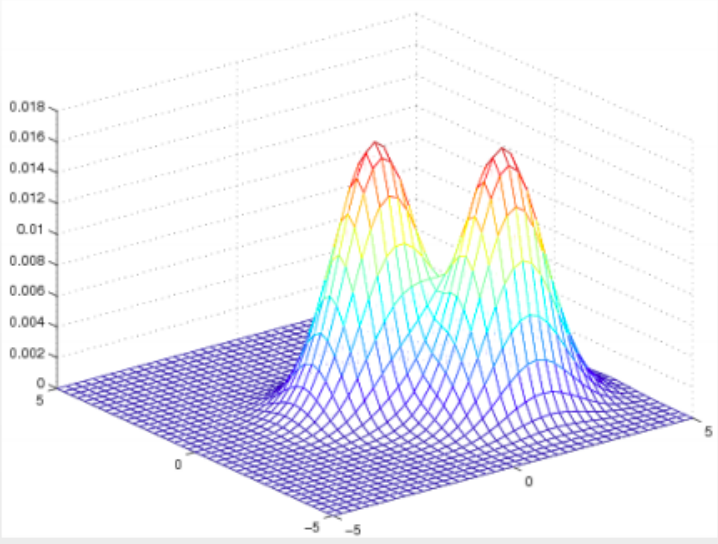
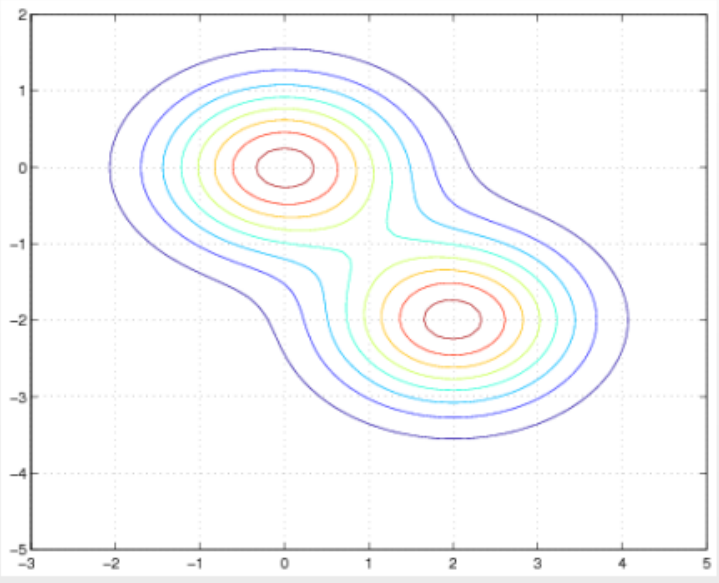
- Recall the density of a multivariate gausssian

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

A pretty picture





LDA

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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

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

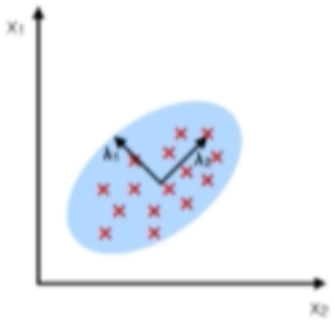
- For $\Sigma_1 \neq \Sigma_2$, this is a quadratic function.

LDA

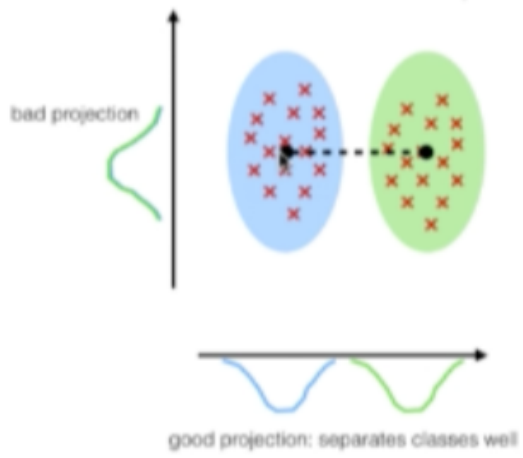
- LDA assumes that $\Sigma_1 = \Sigma_2$
- So now we get a linear decision boundary

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

PCA:
component axes that maximize the variance



LDA:
maximizing the component axes for class-separation



Estimation

- Class proportion

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- 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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- Why not use QDA?

Multiple classes

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- Transform datapoint x to $\tilde{x} := D^{-1/2}U^Tx$
- Mean becomes: $\tilde{\mu}_j := D^{-1/2}U^T\hat{\mu}_j$

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- Remember Mahanobis distance?

$$(x-\hat{\mu}_j)^T\hat{\Sigma}^{-1}(x-\hat{\mu}_j) = (\tilde{x}-\tilde{\mu}_j)^T(\tilde{x}-\tilde{\mu}_j)$$

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- After this "whitening", the decision rule becomes very simple:
  - Assign x to class j such that $(\tilde{x}-\tilde{\mu}_j)^T(\tilde{x}-\tilde{\mu}_j) - \log\hat{\pi}_j$

LDA algorithm

- Estimate parameters by $\hat{\pi}_j$, $\hat{\mu}_j$, $\hat{\Sigma}$
- Compute eigendecomposition of $\hat{\Sigma} = UDU^T$
- Transform the means to $\tilde{\mu}_j$
- For a datapoint x, compute the whitened point $\tilde{x}$
- Now assign to class j that minimizes $\frac{1}{2}\text{dist}(\tilde{x}, \tilde{\mu}_j)^2 - \log \hat{\pi}_j$

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  - Just $K - 1$

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- So the LDA decision rule will be unchanged if we project into the subspace spanned by the centers.

Acknowledgment

- Some pictures are borrowed from Brett Bernstein's notes from NYU and Jia Li's notes from PSU
- Some slides are borrowed from Ryan Tibshirani's notes
- Elements of statistical learning, HTF