Course 495: Advanced Statistical Machine Learning/Pattern Recognition

Deterministic Component Analysis

- Goal (Lecture): To present standard and modern Component Analysis (CA) techniques such as Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Graph/Neighbourhood based Component Analysis
- Goal (Tutorials): To provide the students the necessary mathematical tools for deeply understanding the CA techniques.

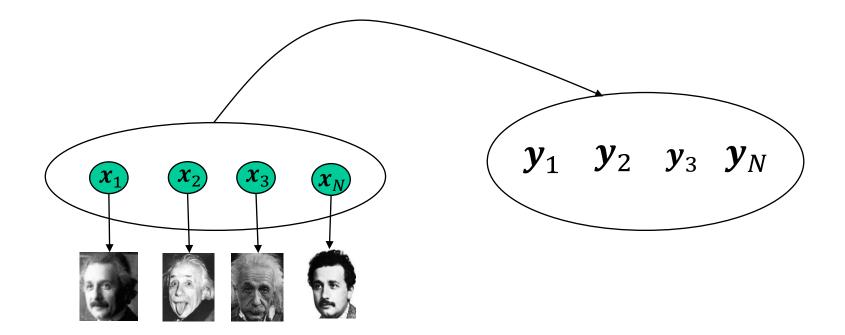
Materials

- Pattern Recognition & Machine Learning by C. Bishop Chapter 12
- Turk, Matthew, and Alex Pentland. "Eigenfaces for recognition." *Journal of cognitive neuroscience* 3.1 (1991): 71-86.
- Belhumeur, Peter N., João P. Hespanha, and David J. Kriegman. "Eigenfaces vs. fisherfaces: Recognition using class specific linear projection." *Pattern Analysis and Machine Intelligence, IEEE Transactions on* 19.7 (1997): 711-720.
- He, Xiaofei, et al. "Face recognition using laplacianfaces." *Pattern Analysis and Machine Intelligence, IEEE Transactions on* 27.3 (2005): 328-340.
- Belkin, Mikhail, and Partha Niyogi. "Laplacian eigenmaps for dimensionality reduction and data representation." *Neural computation* 15.6 (2003): 1373-1396.

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Deterministic Component Analysis

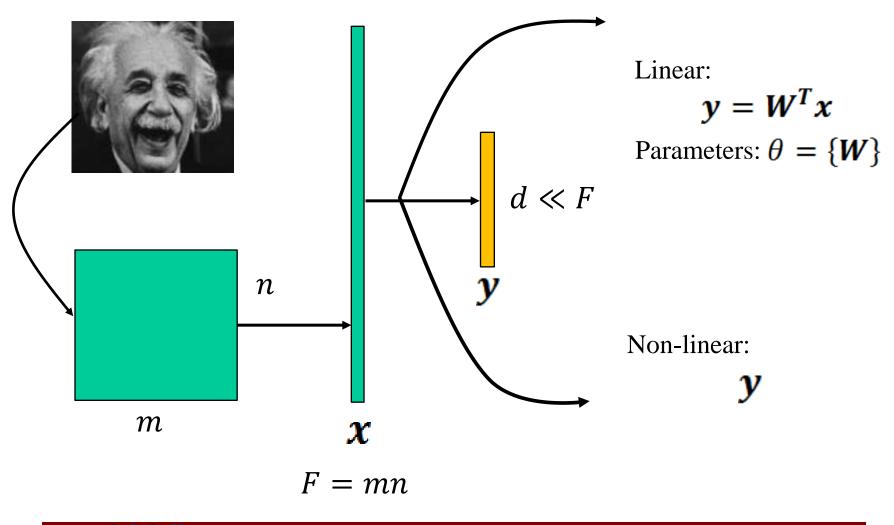
Problem: Given a population of data $\{x_1, \dots, x_N\} \in R^F$ (i.e. observations) find a latent space $\{y_1, \dots, y_N\} \in R^d$ (usually $d \ll F$) which is relevant to a task.



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Latent Variable Models



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- ✓ What are the properties of my latent space?
- ✓ How do I find it (linear, non-linear)?
- ✓ Which is the cost function?
- ✓ How do I solve the problem?

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A first example

- Let's assume that we want to find a descriptive latent space, i.e. best describes my population as a whole.
- How do I define it mathematically?
- Idea! This is a statistically machine learning course, isn't?
- Hence, I will try to preserve global statistical properties.

A first example

• What are the data statistics that can used to describe the variability of my observations?

• One such statistic is the variance of the population (how much the data deviate around a mean).

• Attempt: I want to find a low-dimensional latent space where the "majority" of variance is preserved (or in other words maximized).

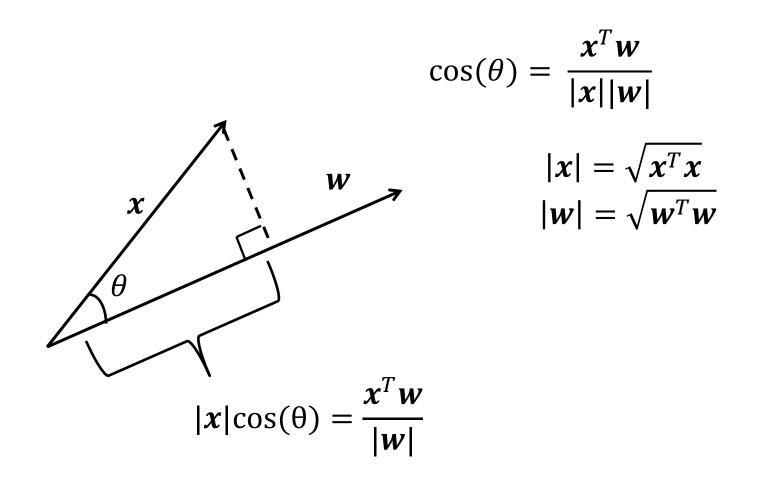
• Variance of the latent space $\{y_1, y_2, \dots, y_N\}$

$$\sigma_y^2 = \frac{1}{N} \sum_{i=1}^N (y_i - \mu_y)^2 \qquad \mu_y = \sum_{i=1}^N y_i$$

- •We want to find $\{y_1^o, \dots y_n^o\} = \underset{\{y_1,\dots,y_n\}}{\operatorname{argmax}} \sigma_y^2$
- •But we are missing something ... The way to do it.
- •Via a linear projection w

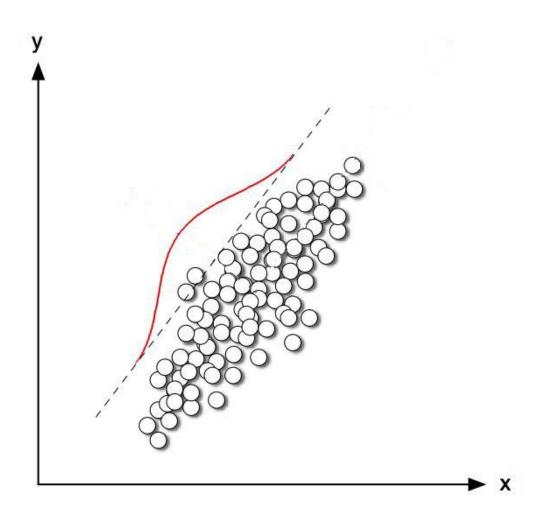
i.e.,
$$y_i = w^T x_i$$

PCA (geometric interpretation of projection)



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Assuming
$$y_i = w^T x_i$$
 latent space
 $\{y_1, ..., y_N\} = \{w^T x_1, ..., w^T x_N\}$
 $w_0 = \operatorname{argmax}_w \sigma^2 = \operatorname{argmax}_w \frac{1}{N} \sum (w^T x_i - w^T \mu)^2 \ \mu = \frac{1}{N} \sum_{i=1}^N x_i$
 $= \operatorname{argmax}_w \frac{1}{N} \sum (w^T (x_i - \mu))^2$
 $= \operatorname{argmax}_w \frac{1}{N} \sum w^T (x_i - \mu) \ (x_i - \mu)^T w$
 $= \operatorname{argmax}_w \frac{1}{N} w^T \left(\sum (x_i - \mu) \ (x_i - \mu)^T \right) w$
 $= \operatorname{argmax}_w w^T \mathbf{S}_t w$

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$$\boldsymbol{w}_{o} = \operatorname{argmax}_{\boldsymbol{w}} \sigma^{2} = \operatorname{argmax}_{\boldsymbol{w}} \frac{1}{N} \boldsymbol{w}^{T} \, \mathbf{S}_{t} \boldsymbol{w} \ge 0$$

$$1 \sum_{\boldsymbol{w}} (\boldsymbol{w}_{v})^{T} \mathbf{S}_{t} \boldsymbol{w} \ge 0$$

$$S_t = \frac{1}{N} \sum (x_i - \mu) (x_i - \mu)^T$$

- There is a trivial solution of $w = \infty$
- We can avoid it by adding extra constraints (a fixed magnitude on $w (||w||^2 = w^T w = 1)$

$$\boldsymbol{w}_0 = \arg\max_{\boldsymbol{w}} \boldsymbol{w}^T \boldsymbol{S}_t \boldsymbol{w}$$

subject to (s.t.)
$$w^T w = 1$$

Formulate the Lagrangian

$$L(\boldsymbol{w}, \lambda) = \boldsymbol{w}^T \boldsymbol{S}_t \boldsymbol{w} - \lambda(\boldsymbol{w}^T \boldsymbol{w} - 1)$$
$$\frac{\partial \boldsymbol{w}^T \boldsymbol{S}_t \boldsymbol{w}}{\partial \boldsymbol{w}} = 2\boldsymbol{S}_t \boldsymbol{w} \qquad \frac{\partial \boldsymbol{w}^T \boldsymbol{w}}{\partial \boldsymbol{w}} = 2\boldsymbol{w}$$

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{0} \quad \Longrightarrow \quad \boldsymbol{S}_t \boldsymbol{w} = \lambda \boldsymbol{w}$$

\boldsymbol{w} is the largest eigenvector of \boldsymbol{S}_t

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$$S_t = \frac{1}{N} \sum (x_i - \mu) (x_i - \mu)^T = \frac{1}{N} X X^T$$
$$X = [x_1 - \mu, \dots, x_N - \mu]$$

 S_t is a symmetric matrix \Rightarrow all eigenvalues are real S_t is a positive semi-definite matrix, i.e.

 $\forall w \neq 0 \qquad w^T S_t w \ge 0 \quad (\text{all eigenvalues are non negative})$ $\operatorname{rank}(S_t) = \min(N - 1, F)$ $S_t = U \Lambda U^T \quad U^T U = I, U U^T = I$

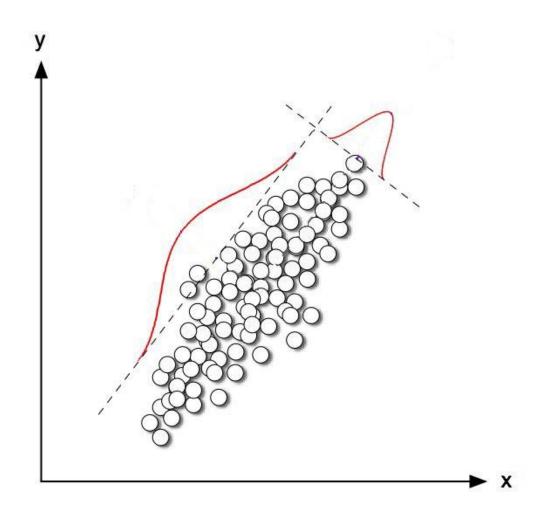
 \boldsymbol{x}_i

- How can we find a latent space with more than one dimensions?
- We need to find a set of projections $\{w_1, \dots, w_d\}$

$$\mathbf{y}_{i} = \begin{bmatrix} y_{i1} \\ \cdots \\ y_{id} \end{bmatrix} = \begin{bmatrix} \mathbf{w}_{1}^{T} \mathbf{x}_{i} \\ \cdots \\ \mathbf{w}_{d}^{T} \mathbf{x}_{i} \end{bmatrix} = \mathbf{W}^{T} \mathbf{x}_{i}$$
$$\mathbf{W} = [\mathbf{w}_{1}, \dots, \mathbf{w}_{d}]$$

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Maximize the variance in each dimension

$$W_o = \arg \max_{W} \frac{1}{N} \sum_{k=1}^{d} \sum_{i=1}^{N} (y_{ik} - \mu_{ik})^2$$
$$= \arg \max_{W} \frac{1}{N} \sum_{k=1}^{d} \sum_{i=1}^{N} w_k^T (x_i - \mu_i) (x_i - \mu_i)^T w_k$$
$$= \arg \max_{W} \sum_{k=1}^{d} w_k^T S_t w_k = \arg \max_{W} \operatorname{tr}[W^T S_t W]$$

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$$W_{o} = \arg \max_{W} \operatorname{tr}[W^{T}S_{t}W]$$

s.t. $W^{T}W = I$
Lagrangian $L(W, \Lambda) = \operatorname{tr}[W^{T}S_{t}W] \operatorname{-tr}[\Lambda(W^{T}W - I)]$
 $\frac{\partial \operatorname{tr}[W^{T}S_{t}W]}{\partial W} = 2S_{t}W$ $\frac{\partial \operatorname{tr}[\Lambda(W^{T}W - I)]}{\partial W} = 2W\Lambda$
 $\frac{\partial L(W, \Lambda)}{\partial W}$

$$\frac{\partial L(W, \Lambda)}{\partial W} = 0 \qquad S_t W = W\Lambda \quad \text{Does it ring a bell?}$$

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• Hence, W has as columns the d eigenvectors of S_t that correspond to its d largest nonzero eigenvalues

 $W = U_d$

$$tr[\boldsymbol{W}^T \boldsymbol{S}_t \boldsymbol{W}] = tr[\boldsymbol{W}^T \boldsymbol{U} \boldsymbol{\Lambda} \boldsymbol{U}^T \boldsymbol{W}] = tr[\boldsymbol{\Lambda}_d]$$

Example: \boldsymbol{U} be 5x5 and \boldsymbol{W} be a 5x3

$$\boldsymbol{W}^{T}\boldsymbol{U} = \begin{bmatrix} u_{1}.u_{1} & u_{1}.u_{2} & u_{1}.u_{3} & u_{1}.u_{4} & u_{1}.u_{5} \\ u_{2}.u_{1} & u_{2}.u_{2} & u_{2}.u_{3} & u_{2}.u_{4} & u_{2}.u_{5} \\ u_{3}.u_{1} & u_{3}.u_{2} & u_{3}.u_{3} & u_{3}.u_{4} & u_{3}.u_{5} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

Hence the maximum is

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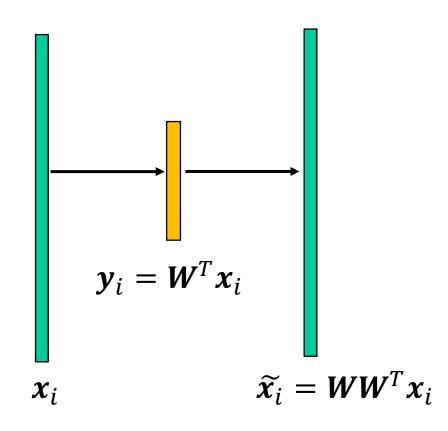
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$$\operatorname{tr}[\mathbf{\Lambda}_d] = \sum_{i=1}^d \lambda_d$$

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PCA (another perspective)

• We want to find a set of bases *W* that best reconstructs the data after projection



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PCA (another perspective)

Let us assume for simplicity centred data (zero mean)

• Reconstructed data $\widetilde{X} = WY = W^TWX$

$$W_{0} = \arg\min_{W} \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{F} (x_{ij} - \widetilde{x_{ij}})^{2}$$
$$= \arg\min_{W} ||X - WW^{T}X||^{2}_{F} (1)$$

s.t.W'W = I

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PCA (another perspective)

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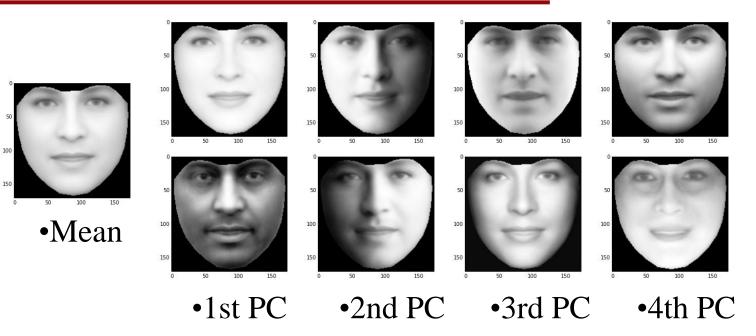
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$$\begin{aligned} \left\| X - WW^{T}X \right\|_{F}^{2} \\ &= \operatorname{tr} \left[\left(X - WW^{T}X \right)^{T} \left(X - WW^{T}X \right) \right] \\ &= \operatorname{tr} \left[X^{T}X - X^{T}WW^{T}X - X^{T}WW^{T}X + X^{T}WW^{T}WW^{T}X \right] \\ &= \operatorname{tr} \left[X^{T}X \right] - \operatorname{tr} \left[X^{T}WW^{T}X \right] \\ & \text{constant} \\ &\min(1) \Rightarrow \max_{W} \operatorname{tr} \left[W^{T}XX^{T}W \right] \end{aligned}$$

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PCA (applications)

•TEXTURE



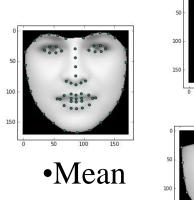


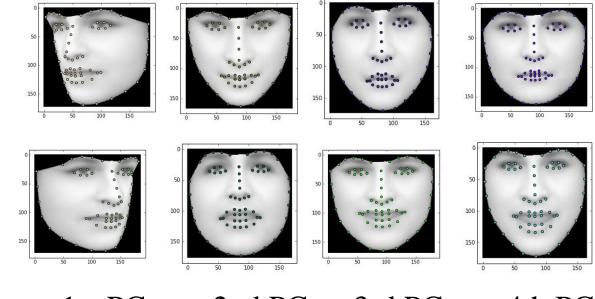


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PCA (applications)

•SHAPE



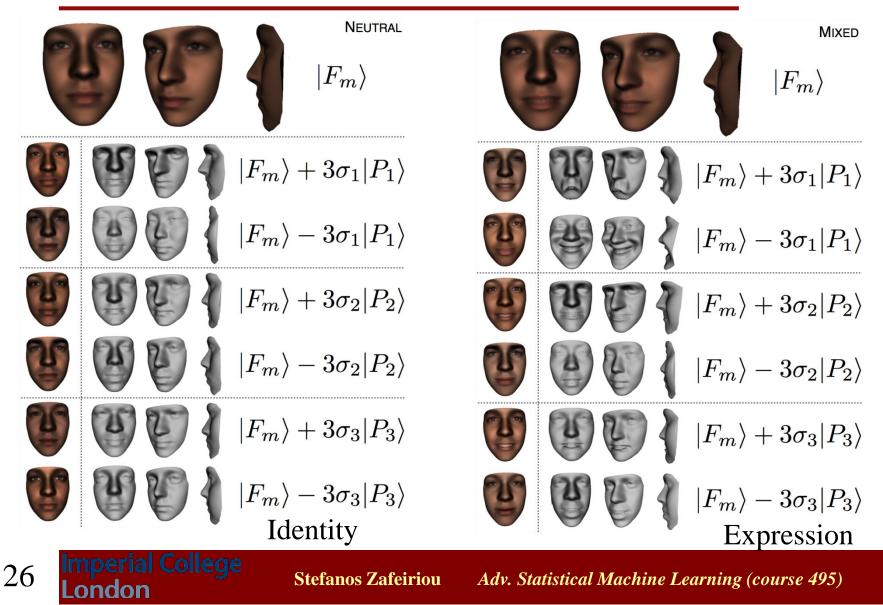


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PCA (applications)



- PCA: Unsupervised approach good for compression of data and data reconstruction. Good statistical prior.
- PCA: Not explicitly defined for classification problems (i.e., in case that data come with labels)
- How do we define a latent space it this case? (i.e., that helps in data classification)

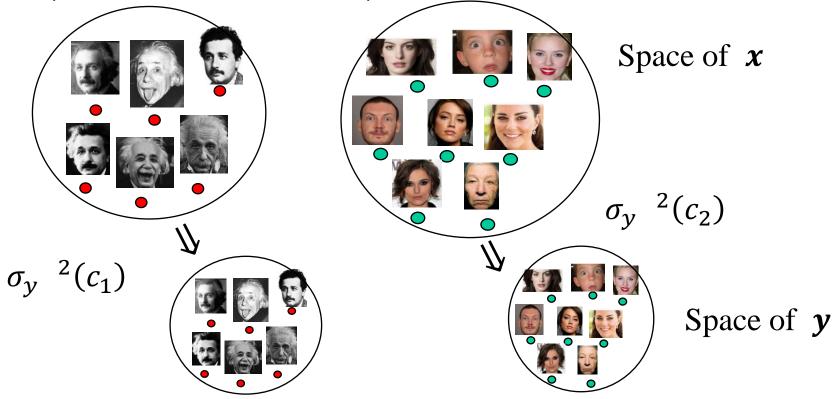
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- We need to properly define statistical properties which may help us in classification.
- Intuition: We want to find a space in which

(a) the data consisting each class look more like each other, while

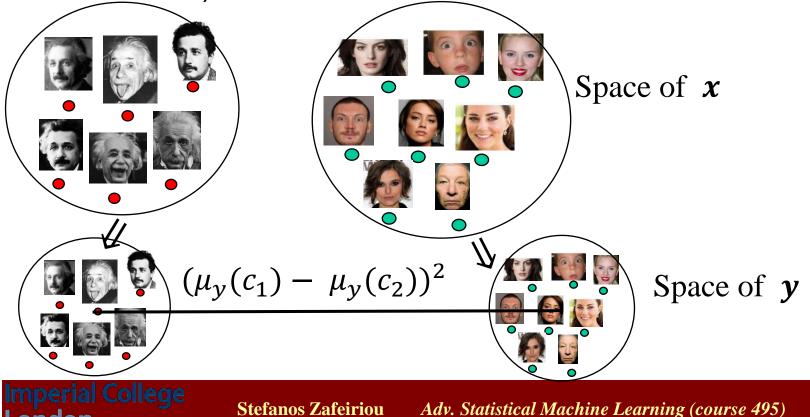
(b) the data of separate classes look more dissimilar.

 How do I make my data in each class look more similar? Minimize the variability in each class (minimize the variance)



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 How do I make the data between classes look dissimilar? I move the data from different classes further away from each other (increase the distance between their means).



A bit more formally. I want a latent space *y* such that:

$$\sigma_y^2(c_1) + \sigma_y^2(c_2)$$
 is minimum

$$(\mu_y(c_1) - \mu_y(c_2))^2$$
 is maximum

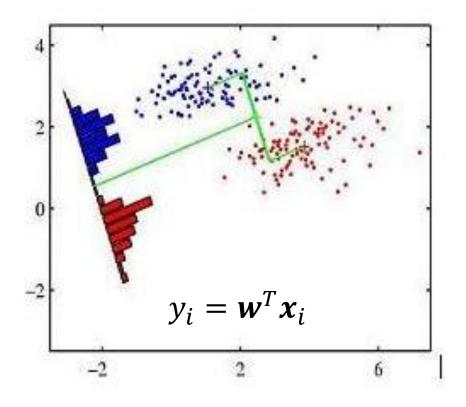
How do I combine them together?

minimize
$$\frac{\sigma_y^2(c_1) + \sigma_y^2(c_2)}{(\mu_y(c_1) - \mu_y(c_2))^2}$$

Or maximize
$$\frac{(\mu_y(c_1) - \mu_y(c_2))^2}{\sigma_y^2(c_1) + \sigma_y^2(c_2)}$$

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How can I find my latent space?



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$$\sigma_{y}^{2}(c_{1}) = \frac{1}{N_{c_{1}}} \sum_{x_{i} \in c_{1}} (y_{i} - \mu_{y}(c_{1}))^{2} \qquad \mu(c_{1}) = \frac{1}{N_{c_{1}}} \sum_{x_{i} \in c_{1}} x_{i}$$
$$= \frac{1}{N_{c_{1}}} \sum_{x_{i} \in c_{1}} (w^{T}(x_{i} - \mu(c_{1})))^{2}$$
$$= \frac{1}{N_{c_{1}}} \sum_{x_{i} \in c_{1}} w^{T}(x_{i} - \mu(c_{1}))(x_{i} - \mu(c_{1}))^{T} w$$
$$= w^{T} \frac{1}{N_{c_{1}}} \sum_{x_{i} \in c_{1}} (x_{i} - \mu(c_{1}))(x_{i} - \mu(c_{1}))^{T} w$$
$$= w^{T} S_{1} w$$

$$\sigma_y^{2}(c_2) = \boldsymbol{w}^T \boldsymbol{S}_2 \boldsymbol{w}$$

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$$\sigma_y^{2}(c_1) + \sigma_y^{2}(c_2) = w^T (S_1 + S_2) w$$

 S_w within class scatter matrix

$$(\mu_{y}(c_{1}) - \mu_{y}(c_{2}))^{2} = \boldsymbol{w}^{T}(\boldsymbol{\mu}(c_{1}) - \boldsymbol{\mu}(c_{2}))(\boldsymbol{\mu}(c_{1}) - \boldsymbol{\mu}(c_{2}))^{T}\boldsymbol{w}$$

 S_b between class scatter matrix

$$\frac{(\mu_y(c_1) - \mu_y(c_2))^2}{\sigma_y^{2}(c_1) + \sigma_y^{2}(c_2)} = \frac{w^T S_b w}{w^T S_w w}$$

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 $\max \boldsymbol{w}^T \boldsymbol{S}_b \boldsymbol{w}$ s.t. $\boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w} = 1$

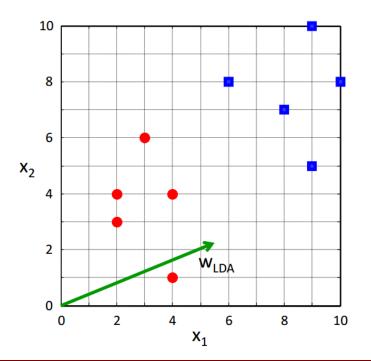
Lagrangian:
$$L(\boldsymbol{w}, \lambda) = \boldsymbol{w}^T \boldsymbol{S}_b \boldsymbol{w} - \lambda(\boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w} - 1)$$

$$\frac{\partial \boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w}}{\partial \boldsymbol{w}} = 2\boldsymbol{S}_w \boldsymbol{w} \qquad \frac{\partial \boldsymbol{w}^T \boldsymbol{S}_b \boldsymbol{w}}{\partial \boldsymbol{w}} = 2\boldsymbol{S}_b \boldsymbol{w}$$
$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{0} \implies \qquad \lambda \boldsymbol{S}_w \boldsymbol{w} = \boldsymbol{S}_b \boldsymbol{w}$$

w is the largest eigenvector of $S_w^{-1}S_b$ $w \propto S_w^{-1}(\mu(c_1) - \mu(c_2))$

Compute the LDA projection for the following 2D dataset

$$\begin{split} c_1 &= \{(4,1), (2,4), (2,3), (3,6), (4,4)\} \\ c_2 &= \{(9,10), (6,8), (9,5), (8,7), (10,8)\} \end{split}$$



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Solution (by hand)

•The class statistics are $S_1 = \begin{bmatrix} 0.8 & -0.4 \\ -0.4 & 2.64 \end{bmatrix}$ $S_2 = \begin{bmatrix} 1.84 & -0.04 \\ -0.04 & 2.64 \end{bmatrix}$

•The within and between class scatter are

$$\boldsymbol{\mu}_1 = [3.0 \ 3.6]^T \qquad \boldsymbol{\mu}_2 = [8.4 \ 7.6]^T$$

$$S_b = \begin{bmatrix} 29.16 & 21.6 \\ 21.6 & 16.0 \end{bmatrix}$$
 $S_w = \begin{bmatrix} 2.64 & -0.44 \\ -0.44 & 5.28 \end{bmatrix}$

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The LDA projection is then obtained as the solution of the generalized eigenvalue problem

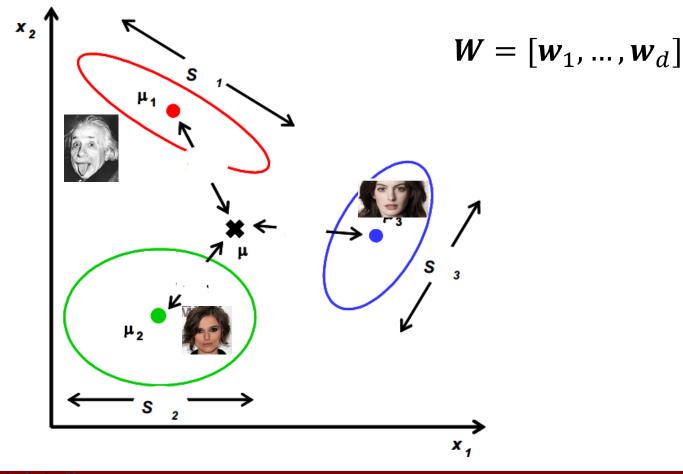
$$S_w^{-1}S_bw = \lambda w \rightarrow \left|S_w^{-1}S_b - \lambda I\right| = 0 \rightarrow \begin{vmatrix} 11.89 - \lambda & 8.81 \\ 5.08 & 3.76 - \lambda \end{vmatrix} = 0 \rightarrow \lambda = 15.65$$

$$\begin{bmatrix} 11.89 & 8.81 \\ 5.08 & 3.76 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = 15.65 \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \rightarrow \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0.91 \\ 0.39 \end{bmatrix}$$

Or directly by

$$w^* = S_W^{-1}(\mu_1 - \mu_2) = [-0.91 \ -0.39]^T$$

LDA (Multiclass & Multidimensional case)



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LDA (Multiclass & Multidimensional case)

Within-class scatter matrix

$$S_{w} = \sum_{j=1}^{C} S_{j} = \sum_{j=1}^{C} \frac{1}{N_{c_{j}}} \sum_{x_{i} \in c_{j}} (x_{i} - \mu(c_{j}))(x_{i} - \mu(c_{j}))^{T}$$

Between-class scatter matrix

$$\boldsymbol{S}_{b} = \sum_{j=1}^{c} (\boldsymbol{\mu}(c_{j}) - \boldsymbol{\mu}) (\boldsymbol{\mu}(c_{j}) - \boldsymbol{\mu})^{\mathrm{T}}$$

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 $\max \operatorname{tr}[\boldsymbol{W}^{\mathrm{T}}\boldsymbol{S}_{b}\boldsymbol{W}] \text{ s.t. } \boldsymbol{W}^{\mathrm{T}}\boldsymbol{S}_{w}\boldsymbol{W} = \mathbf{I}$

Lagranging: $L(W, \Lambda) = tr[w^T S_b w] - tr[\Lambda(W^T S_w W - I)]$

$$\frac{\partial \operatorname{tr}[\mathbf{W}^T \mathbf{S}_b \mathbf{W}]}{\partial W} = 2\mathbf{S}_b W \quad \frac{\partial \operatorname{tr}[\mathbf{\Lambda}(\mathbf{W}^T \mathbf{S}_w \mathbf{W} - \mathbf{I})]}{\partial W} = 2\mathbf{S}_w W \Lambda$$
$$\frac{\partial \operatorname{L}(W, \Lambda)}{\partial W} = \mathbf{0} \quad \Rightarrow \quad \mathbf{S}_b W = \mathbf{S}_w W \Lambda$$
the eigenvectors of $\mathbf{S}_w^{-1} \mathbf{S}_b$ that correspond to the largest eigenvalues

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