Introduction to Machine Learning in Geosciences GEO371/GEO398D.1

Dimensionality Reduction

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Content

https://www.cs.huji.ac.il/~shais/UnderstandingMachineLearning/understanding-machine-learning-theory-algorithms.pdf

Introduction

- Dimensionality reduction is the process of taking data in a high dimensional space and mapping it into a new space whose dimensionality is much smaller.
- This process is closely related to the concept of (lossy) compression in information theory.
- There are several reasons to reduce the dimensionality of the data.
- First, high dimensional data impose computational challenges.
- Moreover, in some situations high dimensionality might lead to poor generalization abilities of the learning algorithm.
- Finally, dimensionality reduction can be used for interpretability of the data, for finding meaningful structure of the data, and for illustration purposes.

Linear Transformation

- We apply linear transformation to the original data.
- The original data is $\mathbb{R}^d$ and we want to embed it into $\mathbb{R}^n$ $(n < d)$.
- We want to find a matrix $\mathbf{W} \in \mathbb{R}^{n,d}$ that induces the mapping $\mathbf{x} \mapsto \mathbf{Wx}$.
- A natural criterion for choosing $\mathbf{W}$ is in a way that will enable a reasonable recovery of the original $\mathbf{x}$.
- It is not hard to show that in general, exact recovery of $\mathbf{x}$ from $\mathbf{Wx}$ is impossible

PCA

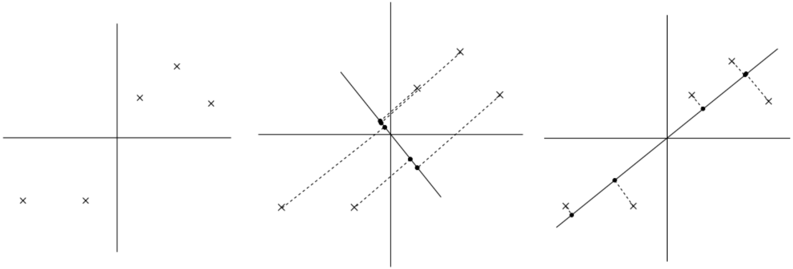
- Both the compression and the recovery are performed by linear transformations.
- The method finds the linear transformations for which the differences between the recovered vectors and the original vectors are minimal in the least squared sense.

Lower dimension Projections

- Obtain a new feature vector by transforming the original features $x_1, x_2, ..., x_n$
- New features are linear combinaIons of old ones
- Unsupervised Setting!

PCA

Which projection is better?



From notes by Andrew Ng

Using a new basis for the data

- Project a point into a (lower dimensional) space:
  - **point**: $\mathbf{x} = (x_1,\ldots,x_n)$
  - **select a basis** – set of unit (length 1) basis vectors $(\mathbf{u}_1,\ldots,\mathbf{u}_k)$
    - we consider orthonormal basis:
      - $\mathbf{u}_j \bullet \mathbf{u}_j = 1$, and $\mathbf{u}_j \bullet \mathbf{u}_l = 0$ for $j \neq l$
  - **select a center** – $\bar{\mathbf{x}}$, defines offset of space
  - **best coordinates** in lower dimensional space defined by dot-products: $(z_1,\ldots,z_k)$, $z_j^i = (\mathbf{x}^i - \bar{\mathbf{x}}) \bullet \mathbf{u}_j$

$$\boxed{\hat{\mathbf{x}}^i = \bar{\mathbf{x}} + \sum_{j=1}^{k} z_j^i \mathbf{u}_j}$$

David Sontag, New York

PCA

- Assume we want to reduce the dimensionality of a number of data points $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N$ to 1 by projecting onto a unit vector $\mathbf{u}$, and we want to keep the squared error small:

$$\textit{minimize} \quad \sum_{n=1}^{N} ||\mathbf{x}_N - (\mathbf{u}^T \mathbf{x}_N)\mathbf{u}||.$$

This optimization problem can be turned into the equivalent problem

$$\textit{maximize} \quad \mathbf{u}^T \mathbf{C} \mathbf{u}$$

PCA

Maximize variance of projection

Let $x^{(i)}$ be the ith data point minus the mean.

Choose unit-length u to maximize:

$$\frac{1}{m}\sum_{i=1}^{m}({x^{(i)}}^T u)^2 = \frac{1}{m}\sum_{i=1}^{m} u^T x^{(i)} {x^{(i)}}^T u$$

$$= u^T \left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)} {x^{(i)}}^T \right) u.$$

Covariance matrix Σ

Let ||u||=1 and maximize. Using the method of Lagrange multipliers, can show that the solution is given by the principal eigenvector of the covariance matrix! **(shown on board)**

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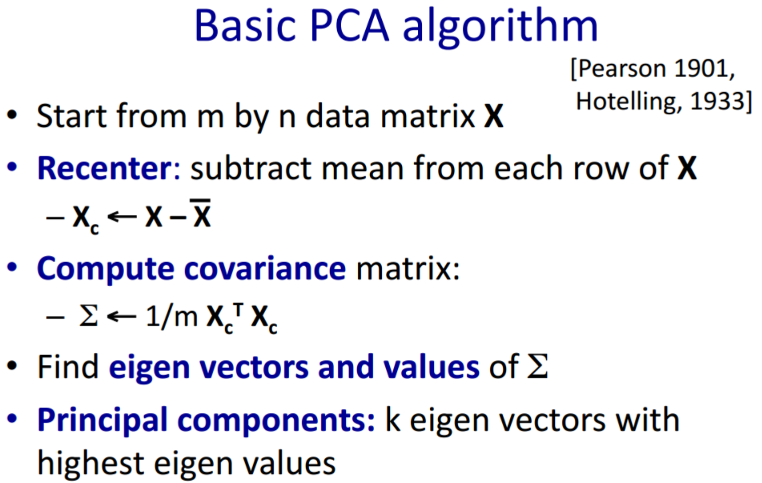
PCA



Basic PCA algorithm

[Pearson 1901, Hotelling, 1933]

- Start from m by n data matrix **X**
- **Recenter**: subtract mean from each row of **X**
  - $\mathbf{X}_c \leftarrow \mathbf{X} - \overline{\mathbf{X}}$
- **Compute covariance** matrix:
  - $\Sigma \leftarrow 1/m \, \mathbf{X}_c^T \mathbf{X}_c$
- Find **eigen vectors and values** of Σ
- **Principal components:** k eigen vectors with highest eigen values

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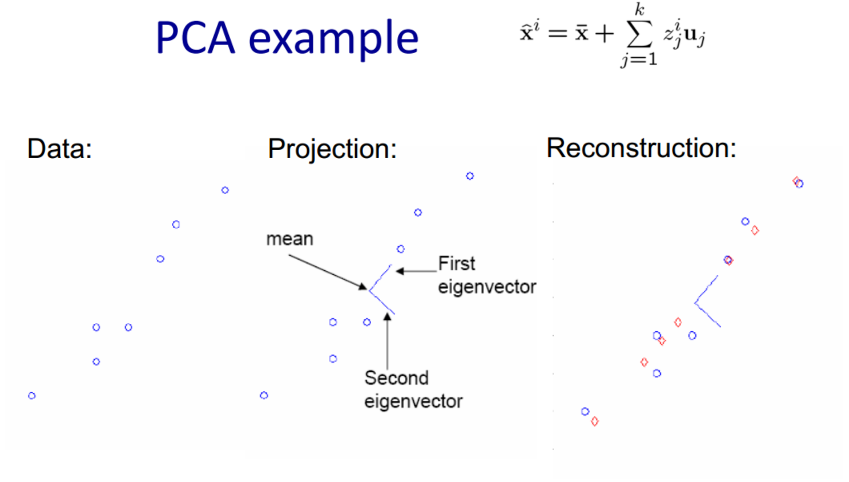
PCA



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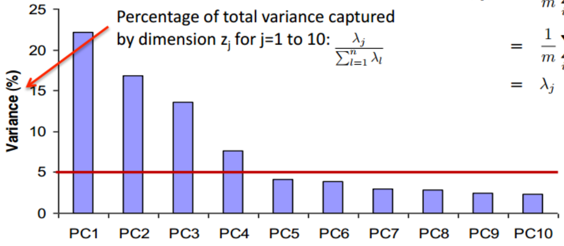
Dimensionality reduction with PCA

In high-dimensional problem, data usually lies near a linear subspace, as noise introduces small variability

Only keep data projections onto principal components with **large** eigenvalues

Can *ignore* the components of lesser significance.

$$\begin{aligned}\mathrm{var}(z_j) &= \frac{1}{m}\sum_{i=1}^{m}(z_j^i)^2 \\ &= \frac{1}{m}\sum_{i=1}^{m}(x^i \cdot u_j)^2 \\ &= \lambda_j\end{aligned}$$

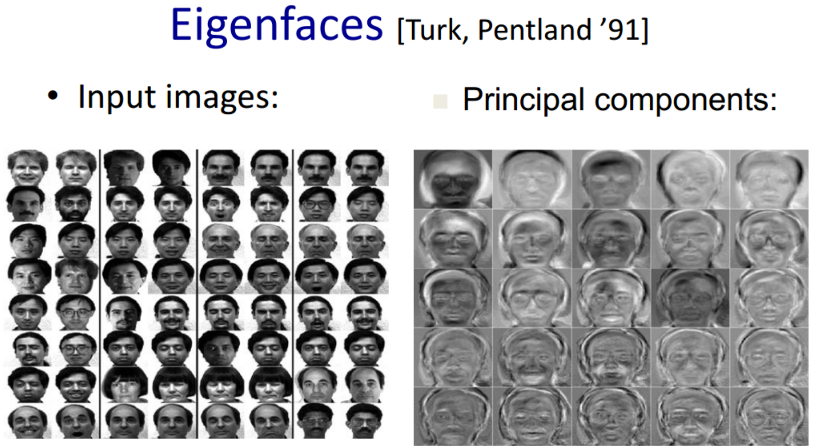


You might lose some information, but if the eigenvalues are small, you don't lose much

Slide from Aarti Singh

David

PCA



Eigenfaces [Turk, Pentland '91]

- Input images:
- Principal components:

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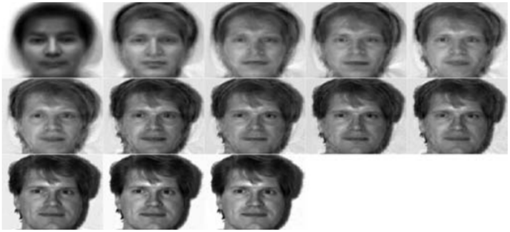
PCA

Eigenfaces reconstruction

- Each image corresponds to adding together (weighted versions of) the principal components:



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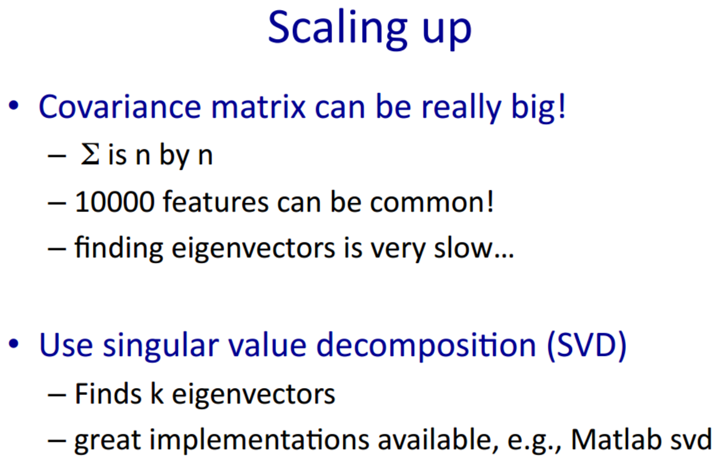

Scaling up

- Covariance matrix can be really big!
  - Σ is n by n
  - 10000 features can be common!
  - finding eigenvectors is very slow…
- Use singular value decomposition (SVD)
  - Finds k eigenvectors
  - great implementations available, e.g., Matlab svd

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SVD

- Write $\mathbf{X} = \mathbf{Z}\,\mathbf{S}\,\mathbf{U}^T$
  - $\mathbf{X} \leftarrow$ data matrix, one row per datapoint
  - $\mathbf{S} \leftarrow$ singular value matrix, diagonal matrix with entries σ_i
    - Relationship between singular values of **X** and eigenvalues of Σ given by $\lambda_i = \sigma_i^2/m$
  - $\mathbf{Z} \leftarrow$ weight matrix, one row per datapoint
    - **Z** times **S** gives coordinate of x_i in eigenspace
  - $\mathbf{U}^T \leftarrow$ singular vector matrix
    - In our setting, each row is eigenvector $\mathbf{u}_j$

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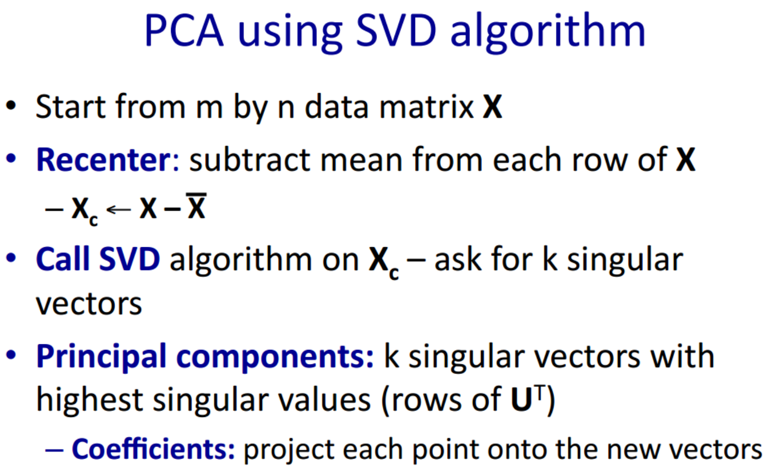
Linear Discriminant Analysis - LDA



PCA using SVD algorithm

- Start from m by n data matrix $\mathbf{X}$
- **Recenter**: subtract mean from each row of $\mathbf{X}$
  - $\mathbf{X_c} \leftarrow \mathbf{X} - \overline{\mathbf{X}}$
- **Call SVD** algorithm on $\mathbf{X_c}$ – ask for k singular vectors
- **Principal components:** k singular vectors with highest singular values (rows of $\mathbf{U}^T$)
  - **Coefficients:** project each point onto the new vectors

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PCA

SUMMARY

- In PCA, the main idea to re-express the available dataset to extract the relevant information by reducing the redundancy and minimize the noise.
- We didn't care about whether this dataset represent features from one or more classes, i.e. the discrimination power was not taken into consideration while we were talking about PCA .
- In PCA, we had a dataset matrix $\mathbf{X}$ with dimensions *mxn*, where columns represent different data samples.
- We first started by subtracting the mean to have a zero mean dataset, then we computed the covariance matrix $\mathbf{S} = \mathbf{X}\mathbf{X}^T$.
- Eigen values and eigen vectors were then computed for $\mathbf{S}$. Hence the new basis vectors are those eigen vectors with highest eigen values, where the number of those vectors was our choice.

Linear Discriminant Analysis - LDA

The objective of LDA is to perform dimensionality reduction while preserving as much of the class discriminatory information as possible

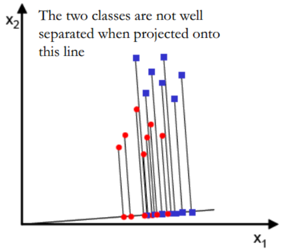
Linear Discriminant Analysis - LDA

- Consider a pattern classification problem, where we have C-classes, e.g. seabass, tuna, salmon …
- Each class has $\mathbf{N}_i$ *m*-dimensional samples, where *i* = *1,2, …, C.*
- Hence we have a set of *m*-dimensional samples $\{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^{Ni}\}$ belong to class $\boldsymbol{\omega}_i$.
- Stacking these samples from different classes into one big fat matrix **X** such that each column represents one sample.
- **We seek to obtain a transformation of X to Y through projecting the samples in X onto a hyperplane with dimension *C-1*.**
- **Let's see what does this mean?**

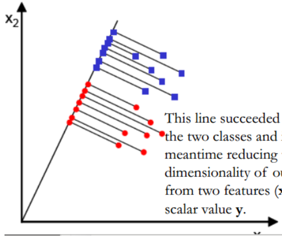
http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf

Linear Discriminant Analysis - LDA

LDA … Two Classes



The two classes are not well separated when projected onto this line



This line succeeded in separating the two classes and in the meantime reducing the dimensionality of our problem from two features $(\mathbf{x}_1,\mathbf{x}_2)$ to only a scalar value **y**.

- Assume we have *m*-dimensional samples $\{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^N\}$, N_1 of which belong to $\boldsymbol{\omega}_1$ and N_2 belong to $\boldsymbol{\omega}_2$.
- We seek to obtain a scalar **y** by projecting the samples **x** onto a line (C-1 space, C = 2).

$$y = w^T x \quad where \quad x = \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_m \end{bmatrix} \quad and \quad w = \begin{bmatrix} w_1 \\ \cdot \\ \cdot \\ w_m \end{bmatrix}$$

  – where **w** is the projection vectors used to project **x** to **y**.

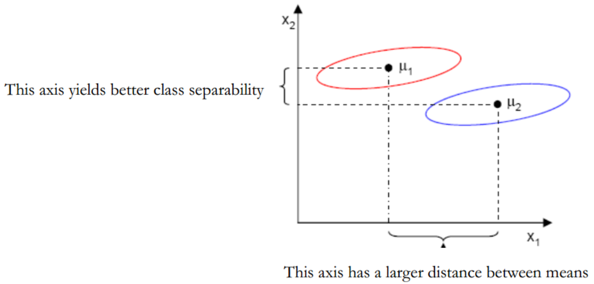
- **Of all the possible lines we would like to select the one that maximizes the separability of the scalars.**

http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf

Linear Discriminant Analysis - LDA

LDA … Two Classes

- However, the distance between the projected means is not a very good measure since it does not take into account the standard deviation within the classes.


x2
μ1
μ2
x1
This axis yields better class separability
This axis has a larger distance between means

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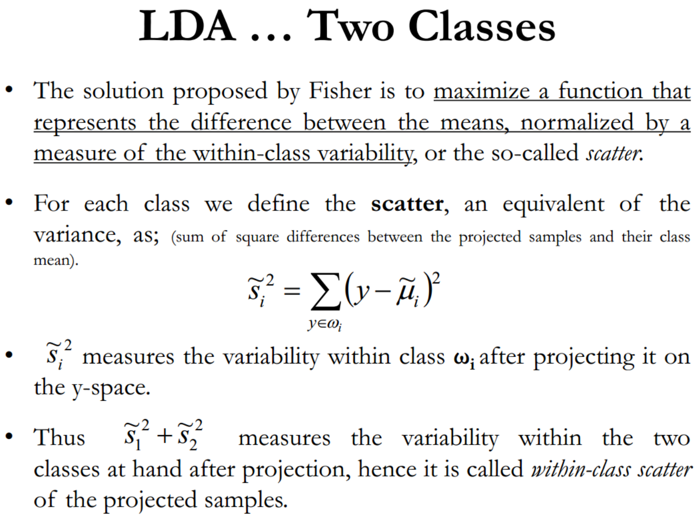
Linear Discriminant Analysis - LDA



LDA … Two Classes

- The solution proposed by Fisher is to maximize a function that represents the difference between the means, normalized by a measure of the within-class variability, or the so-called *scatter*.
- For each class we define the **scatter**, an equivalent of the variance, as; (sum of square differences between the projected samples and their class mean).

$$\tilde{s}_i^2 = \sum_{y \in \omega_i} (y - \tilde{\mu}_i)^2$$

- $\tilde{s}_i^2$ measures the variability within class $\boldsymbol{\omega_i}$ after projecting it on the y-space.
- Thus $\tilde{s}_1^2 + \tilde{s}_2^2$ measures the variability within the two classes at hand after projection, hence it is called *within-class scatter* of the projected samples.

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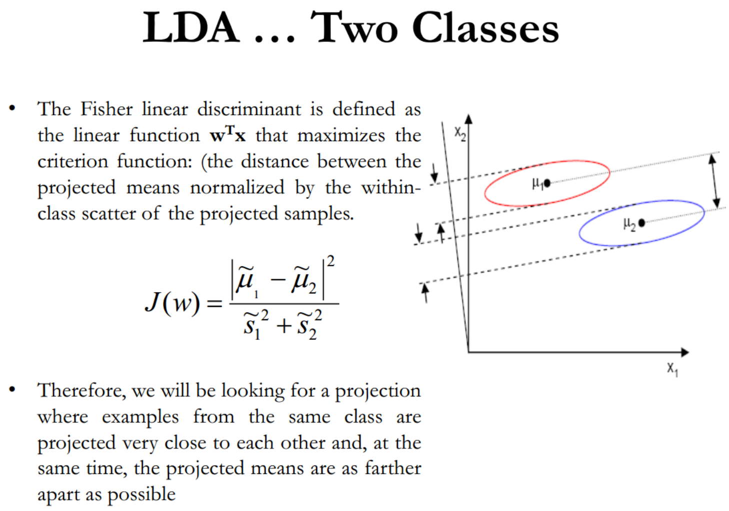
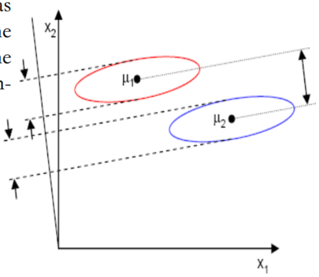
Linear Discriminant Analysis - LDA



LDA … Two Classes

- The Fisher linear discriminant is defined as the linear function $\mathbf{w}^T\mathbf{x}$ that maximizes the criterion function: (the distance between the projected means normalized by the within-class scatter of the projected samples.

$$J(w) = \frac{\left|\tilde{\mu}_1 - \tilde{\mu}_2\right|^2}{\tilde{s}_1^2 + \tilde{s}_2^2}$$



- Therefore, we will be looking for a projection where examples from the same class are projected very close to each other and, at the same time, the projected means are as farther apart as possible

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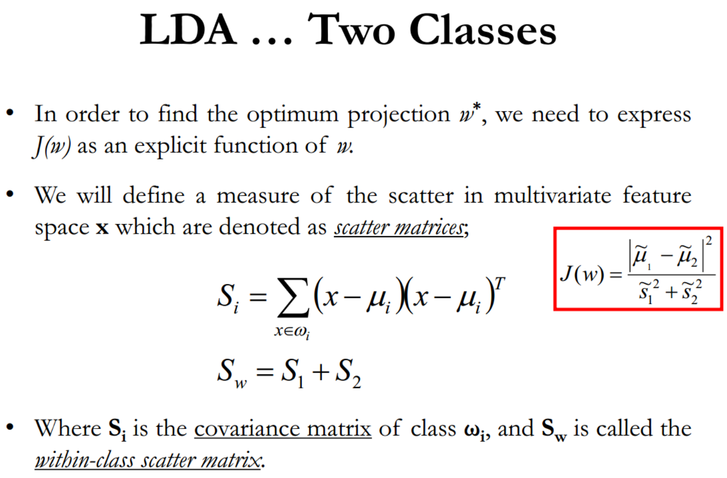
Linear Discriminant Analysis - LDA



LDA … Two Classes

- In order to find the optimum projection w^*, we need to express $J(w)$ as an explicit function of w.
- We will define a measure of the scatter in multivariate feature space **x** which are denoted as <u>*scatter matrices*</u>;

$$S_i = \sum_{x \in \omega_i} (x - \mu_i)(x - \mu_i)^T$$

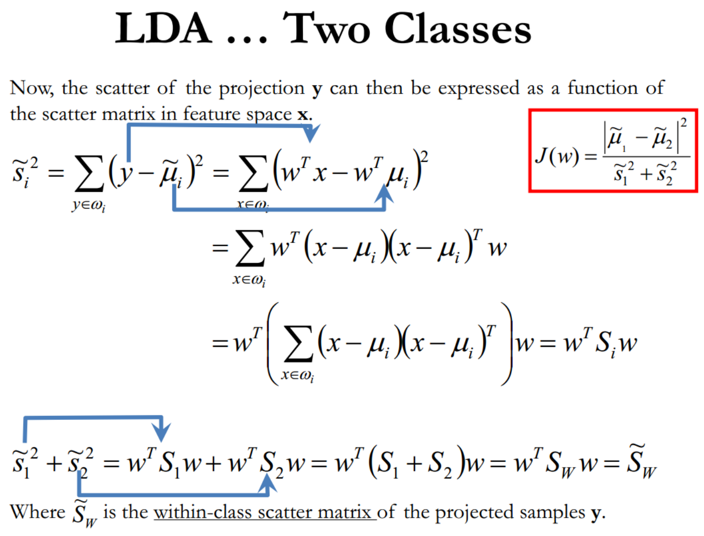
$$S_w = S_1 + S_2$$

$$\boxed{J(w) = \frac{\left|\tilde{\mu}_1 - \tilde{\mu}_2\right|^2}{\tilde{s}_1^2 + \tilde{s}_2^2}}$$

- Where $\mathbf{S_i}$ is the <u>covariance matrix</u> of class $\boldsymbol{\omega_i}$, and $\mathbf{S_w}$ is called the <u>*within-class scatter matrix*</u>.

`http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf`

Linear Discriminant Analysis - LDA



LDA … Two Classes

- Now, the scatter of the projection **y** can then be expressed as a function of the scatter matrix in feature space **x**.

$$\tilde{s}_i^2 = \sum_{y \in \omega_i} (y - \tilde{\mu}_i)^2 = \sum_{x \in \omega_i} \left(w^T x - w^T \mu_i\right)^2$$

$$= \sum_{x \in \omega_i} w^T (x - \mu_i)(x - \mu_i)^T w$$

$$= w^T \left(\sum_{x \in \omega_i} (x - \mu_i)(x - \mu_i)^T \right) w = w^T S_i w$$

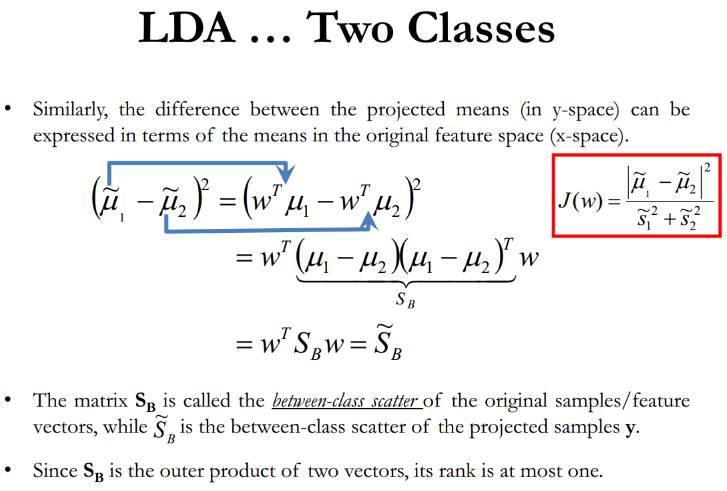
$$\boxed{J(w) = \frac{\left|\tilde{\mu}_1 - \tilde{\mu}_2\right|^2}{\tilde{s}_1^2 + \tilde{s}_2^2}}$$

$$\tilde{s}_1^2 + \tilde{s}_2^2 = w^T S_1 w + w^T S_2 w = w^T (S_1 + S_2) w = w^T S_W w = \tilde{S}_W$$

Where $\tilde{S}_W$ is the within-class scatter matrix of the projected samples **y**.

http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf

Linear Discriminant Analysis - LDA



LDA … Two Classes

- Similarly, the difference between the projected means (in y-space) can be expressed in terms of the means in the original feature space (x-space).

$$\left(\tilde{\mu}_1 - \tilde{\mu}_2\right)^2 = \left(w^T\mu_1 - w^T\mu_2\right)^2$$

$$= w^T \underbrace{\left(\mu_1 - \mu_2\right)\left(\mu_1 - \mu_2\right)^T}_{S_B} w$$

$$= w^T S_B w = \tilde{S}_B$$

$$\boxed{J(w) = \frac{\left|\tilde{\mu}_1 - \tilde{\mu}_2\right|^2}{\tilde{s}_1^2 + \tilde{s}_2^2}}$$

- The matrix $\mathbf{S_B}$ is called the *between-class scatter* of the original samples/feature vectors, while $\tilde{S}_B$ is the between-class scatter of the projected samples **y**.
- Since $\mathbf{S_B}$ is the outer product of two vectors, its rank is at most one.

http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf

Linear Discriminant Analysis - LDA

LDA … Two Classes

- We can finally express the Fisher criterion in terms of $\mathbf{S_W}$ and $\mathbf{S_B}$ as:

$$\boxed{J(w) = \frac{\left|\tilde{\mu}_1 - \tilde{\mu}_2\right|^2}{\tilde{s}_1^{\,2} + \tilde{s}_2^{\,2}} = \frac{w^T S_B w}{w^T S_W w}}$$

- Hence ***J(w)*** **is a measure of the difference between class means (encoded in the between-class scatter matrix) normalized by a measure of the within-class scatter matrix.**

http://www.sci.utah.edu/~shireen/pdfs/tutorials/Elhabian_LDA09.pdf

Linear Discriminant Analysis - LDA

LDA … Two Classes

- To find the maximum of *J(w)*, we differentiate and equate to zero.

$$\frac{d}{dw}J(w) = \frac{d}{dw}\left(\frac{w^T S_B w}{w^T S_W w}\right) = 0$$

$$\Rightarrow \left(w^T S_W w\right)\frac{d}{dw}\left(w^T S_B w\right) - \left(w^T S_B w\right)\frac{d}{dw}\left(w^T S_W w\right) = 0$$

$$\Rightarrow \left(w^T S_W w\right) 2 S_B w - \left(w^T S_B w\right) 2 S_W w = 0$$

Dividing by $2w^T S_W w$:

$$\Rightarrow \left(\frac{w^T S_W w}{w^T S_W w}\right) S_B w - \left(\frac{w^T S_B w}{w^T S_W w}\right) S_W w = 0$$

$$\Rightarrow S_B w - J(w) S_W w = 0$$

$$\Rightarrow S_W^{-1} S_B w - J(w) w = 0$$

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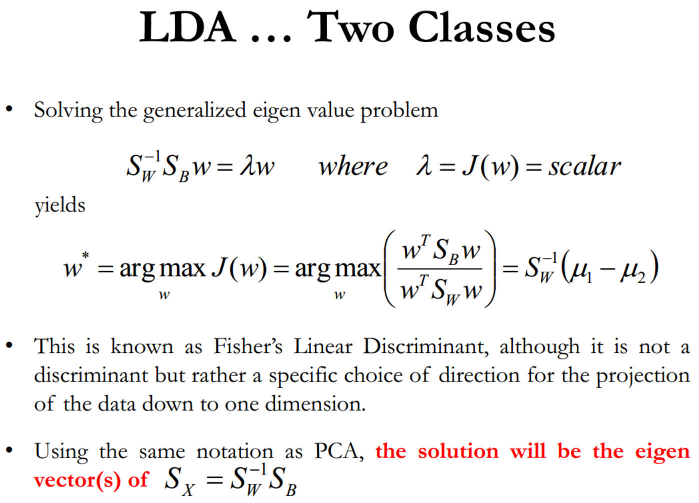
Linear Discriminant Analysis - LDA



LDA … Two Classes

- Solving the generalized eigen value problem

$$S_W^{-1} S_B w = \lambda w \qquad where \quad \lambda = J(w) = scalar$$

yields

$$w^* = \arg\max_w J(w) = \arg\max_w \left(\frac{w^T S_B w}{w^T S_W w} \right) = S_W^{-1}(\mu_1 - \mu_2)$$

- This is known as Fisher's Linear Discriminant, although it is not a discriminant but rather a specific choice of direction for the projection of the data down to one dimension.

- Using the same notation as PCA, **the solution will be the eigen vector(s) of** $S_X = S_W^{-1} S_B$

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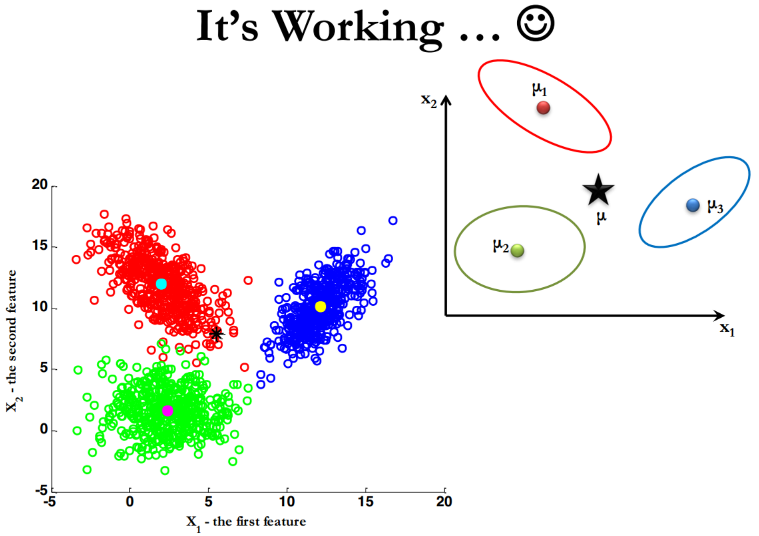
Linear Discriminant Analysis - LDA



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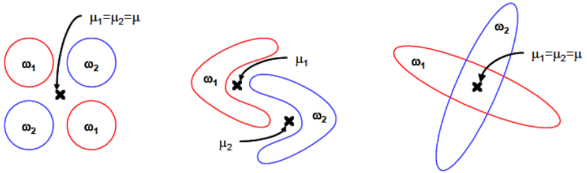
Linear Discriminant Analysis - LDA

Limitations of LDA ☹

- **LDA produces at most C-1 feature projections**
  - If the classification error estimates establish that more features are needed, some other method must be employed to provide those additional features
- **LDA is a parametric method since it assumes unimodal Gaussian likelihoods**
  - If the distributions are significantly non-Gaussian, the LDA projections will not be able to preserve any complex structure of the data, which may be needed for classification.



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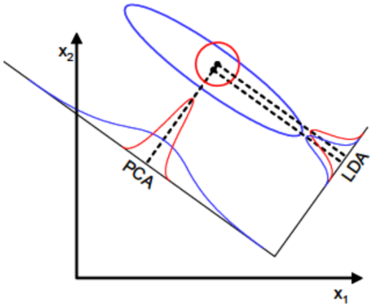
Linear Discriminant Analysis - LDA

Limitations of LDA ☹

- LDA will fail when the discriminatory information is not in the mean but rather in the variance of the data



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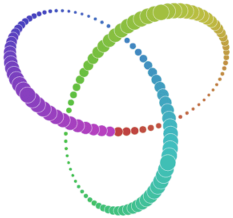
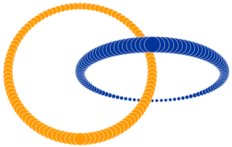
t-SNE

Motivation

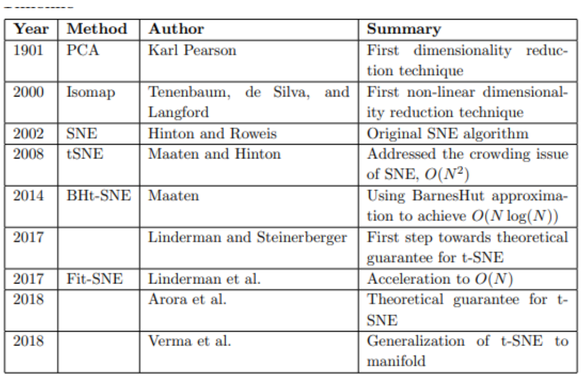
- t-SNE : t-distributed Stochastic Neighbor Embedding
- allows us to separate data that cannot be separated by any straight line!





https://erdem.pl/2020/04/t-sne-clearly-explained

t-SNE



Year	Method	Author	Summary
1901	PCA	Karl Pearson	First dimensionality reduction technique
2000	Isomap	Tenenbaum, de Silva, and Langford	First non-linear dimensionality reduction technique
2002	SNE	Hinton and Roweis	Original SNE algorithm
2008	tSNE	Maaten and Hinton	Addressed the crowding issue of SNE, $O(N^2)$
2014	BHt-SNE	Maaten	Using BarnesHut approximation to achieve $O(N\log(N))$
2017		Linderman and Steinerberger	First step towards theoretical guarantee for t-SNE
2017	Fit-SNE	Linderman et al.	Acceleration to $O(N)$
2018		Arora et al.	Theoretical guarantee for t-SNE
2018		Verma et al.	Generalization of t-SNE to manifold

http://www.cs.columbia.edu/~verma/classes/uml/lec/uml_lec8_tsne.pdf

t-SNE

- PCA is a linear dimension reduction technique that seeks to maximize variance and preserves large pairwise distances. In other words, things that are different end up far apart. This can lead to poor visualization especially when dealing with non-linear manifold structures. Think of a manifold structure as any geometric shape like: cylinder, ball, curve, etc.
- t-SNE differs from PCA by preserving only small pairwise distances or local similarities whereas PCA is concerned with preserving large pairwise distances to maximize variance.
- The t-SNE algorithm calculates a similarity measure between pairs of instances in the high dimensional space and in the low dimensional space. It then tries to optimize these two similarity measures using a cost function.

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t-SNE

- measure similarities between points in the high dimensional space.
    - For each data point (xi) we'll center a Gaussian distribution over that point.
    - Then we measure the density of all points (xj) under that Gaussian distribution.
    - Then renormalize for all points. This gives us a set of probabilities (Pij) for all points. Those probabilities are proportional to the similarities. All that means is, if data points x1 and x2 have equal values under this gaussian circle then their proportions and similarities are equal and hence you have local similarities in the structure of this high-dimensional space.
    - The Gaussian distribution or circle can be manipulated using what's called perplexity, which influences the variance of the distribution (circle size) and essentially the number of nearest neighbors.

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t-SNE

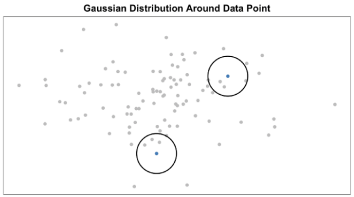

Figure 2 — Measuring pairwise similarities in the high-dimensional space

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t-SNE

- measure similarities between points in the high dimensional space.
  - instead of using a Gaussian distribution you use a Student t-distribution with one degree of freedom, which is also known as the Cauchy distribution.
  - This gives us a second set of probabilities (Qij) in the low dimensional space.
  - As you can see the Student t-distribution has heavier tails than the normal distribution.
  - The heavy tails allow for better modeling of far apart distances.

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t-SNE

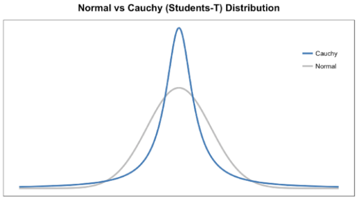

Figure 3 — Normal vs Student t-distribution

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t-SNE

- The last step is that we want these set of probabilities from the low-dimensional space (Qij) to reflect those of the high dimensional space (Pij) as best as possible.
- We want the two map structures to be similar. We measure the difference between the probability distributions of the two-dimensional spaces using Kullback-Liebler divergence (KL). It is an asymmetrical approach that efficiently compares large Pij and Qij values.
- Finally, we use gradient descent to minimize our KL cost function.

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Summary

Compressed Sensing

Encoder