Principal Component Analysis and Linear Discriminant Analysis

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Table of Contents

Aims and Ideas

Aim: Classify data

Example: We measured 200 spectra of different materials. We want to now, which material contains which ingredients.

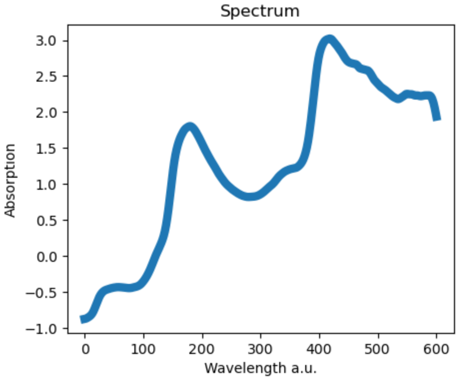

Figure: Example of measured spectra

Source: nirpyresearch

Aim: Classify data

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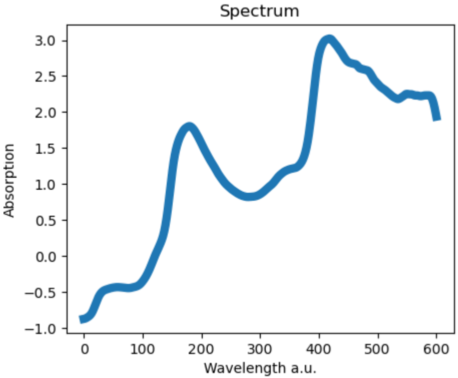
Strategy:

- reduce dimensions and get rid of noise



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Aim: Classify data

Example: We measured 200 spectra of different materials. We want to now, which material contains which ingredients.

Strategy:

- reduce dimensions and get rid of noise
- optimize distances
- only linear transformations

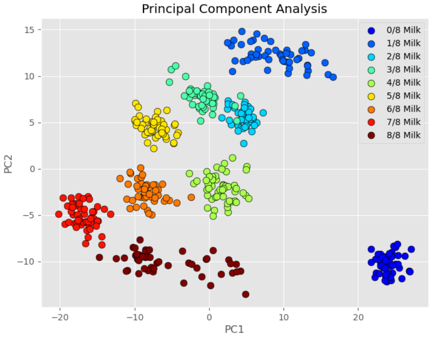

Figure: Reduced to two dimensions

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Aim: Classify data

Example: We measured 200 spectra of different materials. We want to now, which material contains which ingredients.

Strategy:

- reduce dimensions and get rid of noise
- optimize distances
- only linear transformations
- criteria for classification

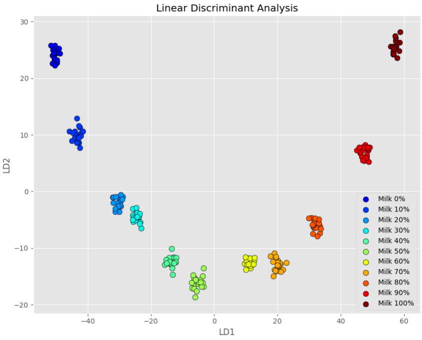
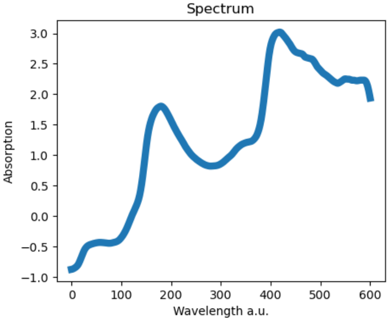


Figure: Easier to decide between classes

Source: nirpyresearch

Principal Component Analysis

Observations



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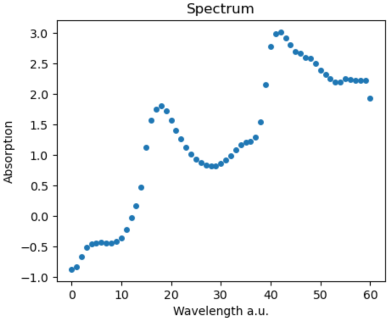

Typical spectrum

- high dimensional (every observed wavelength is new dimension)
- highly correlated (neighboring wavelengths have similar intensity)
- noisy
- few characteristic peaks

Decompose into few spectra (= change of basis, e.g. peaks)

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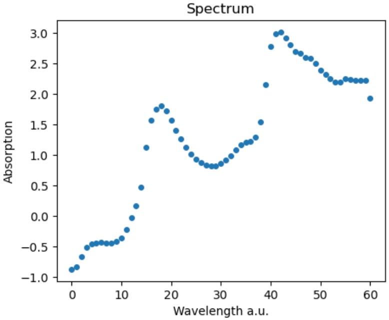

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Prerequisites for PCA

- Standardize (0 mean and unit variance)
- Correlated data

Mathematical formulation

Let v^1, v^2 be two instances (e.g. spectra) and *mean-free*. Recall, the correlation of both vectors is given by the scalar product:

$$\langle v^1, v^2 \rangle = \sum_{i=1}^{n} v_i^1 v_i^2 \tag{1}$$

Input: m instances with n attributes each
See the data as an $m \times n$-matrix A
The covariance matrix is

$$Cov(A, A) = A^T \cdot A = \begin{pmatrix} \langle v^1, v^1 \rangle & \langle v^1, v^2 \rangle & \dots & \langle v^1, v^n \rangle \\ \langle v^2, v^1 \rangle & \langle v^2, v^2 \rangle & \dots & \langle v^2, v^n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle v^n, v^1 \rangle & \langle v^n, v^2 \rangle & \dots & \langle v^n, v^n \rangle \end{pmatrix} \tag{2}$$

Mathematical formulation II

$$Cov(A,A) = A^T \cdot A = \begin{pmatrix} \langle v^1, v^1 \rangle & \langle v^1, v^2 \rangle & \dots & \langle v^1, v^n \rangle \\ \langle v^2, v^1 \rangle & \langle v^2, v^2 \rangle & \dots & \langle v^2, v^n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle v^n, v^1 \rangle & \langle v^n, v^2 \rangle & \dots & \langle v^n, v^n \rangle \end{pmatrix} \tag{3}$$

- Compute Eigenvalues and Eigenvectors of $A^T A$ (or SVD from A)
- Eigenvectors are called principal components (PCs)
- Eigenvalues are the relevance of the PC

Usage: Dimensional reduction

Take only take first few PCs

- contain most of the information
- PCs are linear independent and uncorrelated
- first Eigenvalues are easy to compute (Power Method, QR)
- unimportant PCs contain mostly noise

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Unsupervised learning

Example

1. Standardize data for every wavelength(mean 0, variance 1)
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3. Look at variance ratio (take up to 80%) e.g. PC1: 70%, PC2: 10%, PC3: 6%, PC4: 2%,...
4. Plot PCs against each other

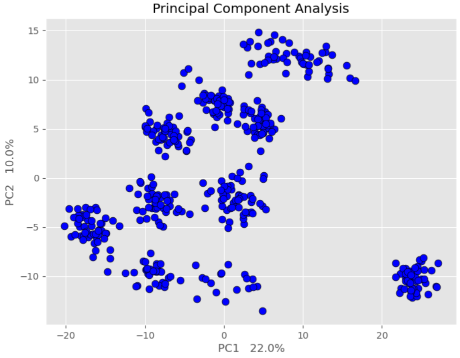

Figure: PC1 vs PC2

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Maybe additional data can help.

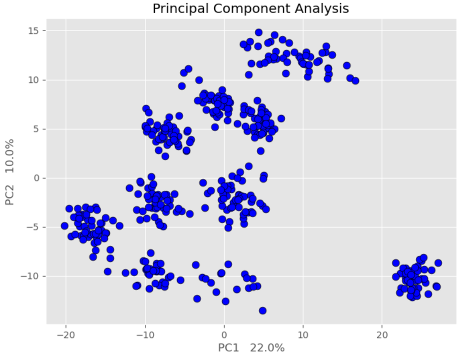

Figure: PC1 vs PC2

Linear Discriminant Analysis

Overview LDA

Linear Discriminant Analysis (**LDA**):

- classifier (sorts unknown data into known classes)
- LDA is a supervised method
- maximizes between-class variance
- minimizes within-class variance
- finds a decision boundary

Prerequisites for LDA

- data is linearly independent Gaussian distributed

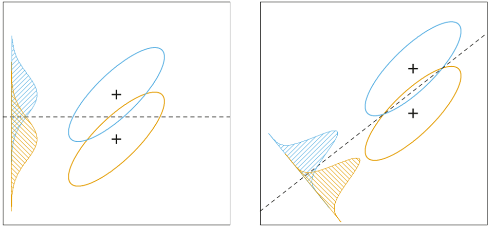

Figure: Idea of LDA

Mathematical formulation

Given N instances $v_i \in \mathbb{R}^d$, separated into K classes $C_1, \ldots, C_K$. Define mean vector for each class C_i, $m_i = \frac{1}{|C_i|} \sum_{v \in C_i} v \in \mathbb{R}^d$ and the overall mean, $m = \frac{1}{N} \sum_{i=0}^{N} v_i \in \mathbb{R}^d$

- Between-class variance (to maximize):

$$S_B = \sum_{i=1}^{K} |C_i|(m_i - m)(m_i - m)^T \in \mathbb{R}^{d \times d}$$

- Within-class variance (to minimize):

$$S_W = \sum_{k=1}^{K} \sum_{x_i \in C_k} (x_i - m_k)(x_i - m_k)^T \in \mathbb{R}^{d \times d}$$

Mathematical formulation II

$$S_B = \sum_{i=1}^{K} |C_i|(m_i - m)(m_i - m)^T \qquad S_W = \sum_{k=1}^{k} \sum_{x_i \in C_k} (x_i - m_k)(x_i - m_k)^T \tag{4}$$

Find transformation $W : \mathbb{R}^d \to \mathbb{R}^l$ $(l \leq d)$ to maximize

$$\mathcal{L}(W, \lambda) = W^T S_B W - \lambda(W^T S_W W - 1) \tag{5}$$

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$$\frac{\partial \mathcal{L}}{\partial W} = 2S_B W - 2\lambda S_W W = 0 \quad \Rightarrow \quad S_B W = \lambda S_W W \tag{6}$$

Decision Boundary

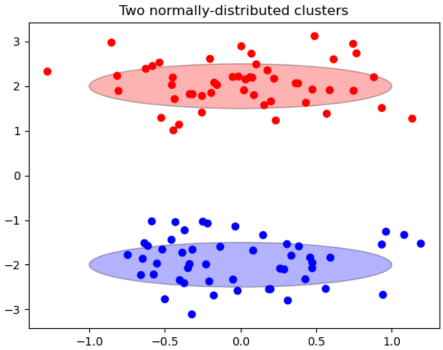
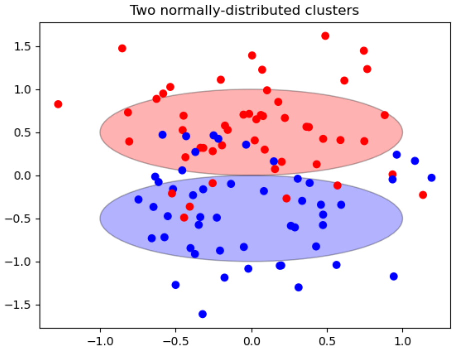


Figure: Where to place decision boundary?

Decision Boundary



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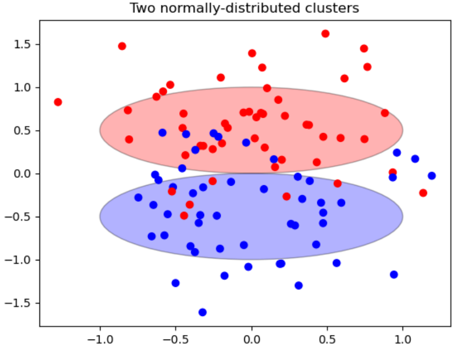


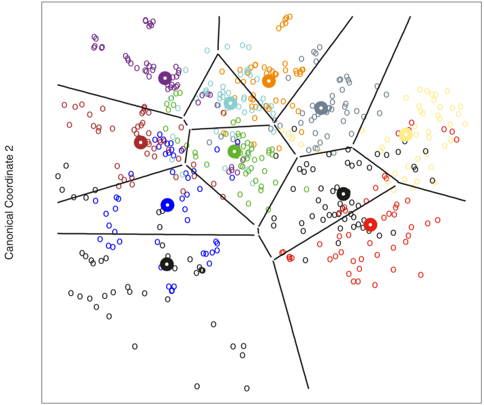
Figure: Where to place decision boundary?

- W gives a new coordinate system
- set decision boundary in 2d, s.t.

$$\frac{\#Upper}{\#Lower} = \frac{|C_1|}{|C_2|}$$

Decision Boundary

Classification in Reduced Subspace



- W gives a new coordinate system
- set decision boundary in 2d, s.t.

$$\frac{\#Upper}{\#Lower} = \frac{|C_1|}{|C_2|}$$

- Do this in 2d successively,

PCA vs LDA

Comparison PCA vs LDA

	PCA	**LDA**
Input	correlated	linearly independent
Output	linearly independent	classes
Purpose	dimensional reduction	classification
learning	unsupervised	supervised

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similar applications because

- classes and PCs are correlated
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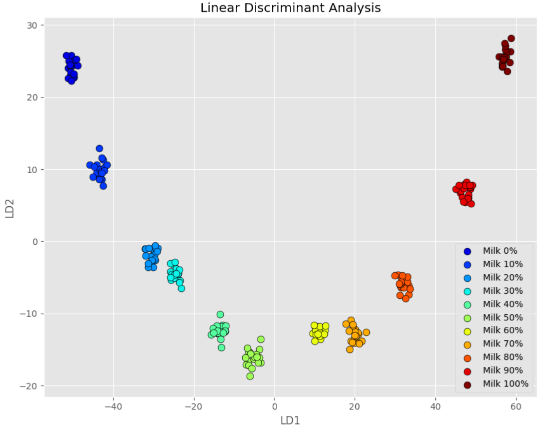
Best: PCA *and* LDA

Questions


Linear Discriminant Analysis
LD2
LD1
30
20
10
0
−10
−20
−40
−20
0
20
40
60
Milk 0%
Milk 10%
Milk 20%
Milk 30%
Milk 40%
Milk 50%
Milk 60%
Milk 70%
Milk 80%
Milk 90%
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