Linear models: SVM, PCA

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Recap

Lecture 3:
Logistic Regression

- Linear classification
  - margin
  - loss functions
- Logistic regression
  - sigmoid derivation
  - Maximum Likelihood Estimation (MLE)
  - logistic loss
  - probability calibration
- Multiclass aggregation strategies
  - One vs Rest
  - One vs One
- Metrics in classification
  - Accuracy, Balanced accuracy
  - Precision, Recall, F-score
  - ROC curve, PR curve, AUC
  - Confusion matrix

Outline

- Support Vector Machine (SVM)
  - History
  - Motivation
  - Solution for separable design
  - Inseparable design, soft margin
  - Kernels
- Dimensionality reduction and PCA
  - Problem statement
  - Eckart–Young theorem
  - Equivalent definitions

Maximum Likelihood Estimation

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Maximum Likelihood Estimation

What are reasons behind defining “best” linear estimator?

Maximize probability of particular parameter to explain given data

$$L(\theta|X, Y) = P(X, Y|\theta)$$

assuming i.i.d. observations

$$P(X, Y|\theta) = \Pi_{i=1}^{n} P(x^i, y^i|\theta)$$

$$\log L(\theta|X, Y) = \sum_{i=1}^{n} \log P(x^i, y^i|\theta)$$

Support Vector Machine

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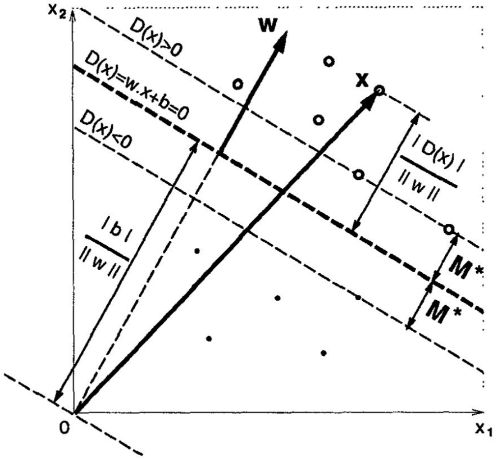
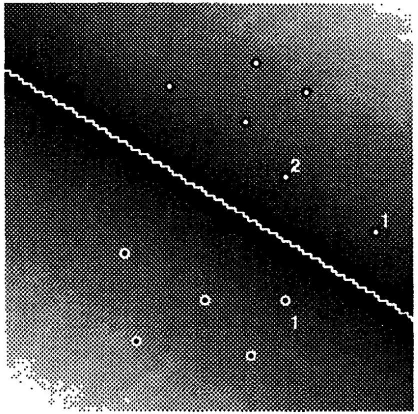
Support Vector Machine

1. History
2. Motivation
3. Solution for separable design
4. Inseparable design, soft margin
5. Kernels
    a. Kernel definition (Hilbert spaces, inner product, positive semidefiniteness)
    b. Kernels properties (addition, infinite sums)
    c. Types of kernels (poly, exponential, gaussian)
6. Current state

History



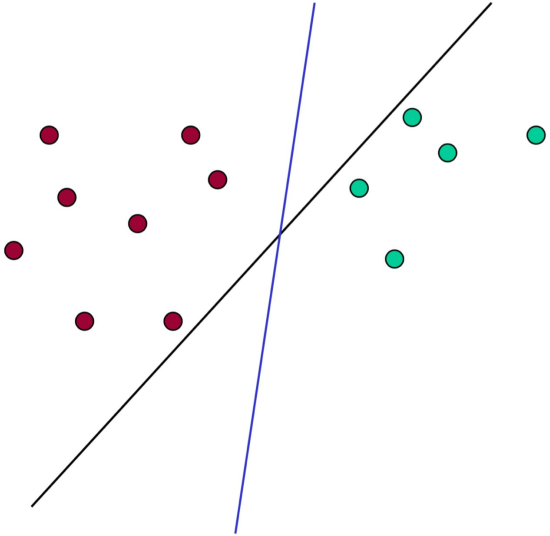


1963: SVM introduced by Soviet mathematicians
Vladimir Vapnik and Alexey Chervonenkis

1992: kernel trick (Vapnik, Boser, Guyon)

1995: soft margin (Vapnik, Cortes)

Motivation



Linear separable case

Many separating hyperplanes exist

Maximize width

Margin

$$y \in \{1, -1\}$$

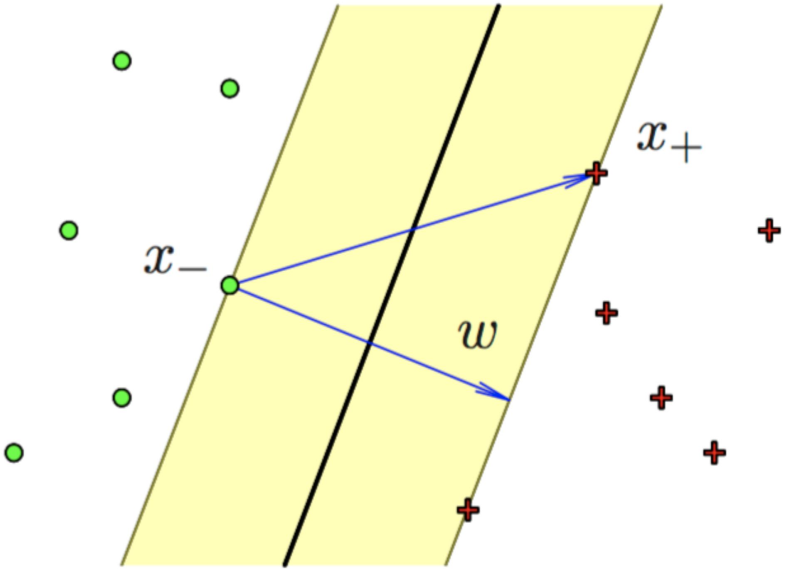
$$y_i = 1 : w^T x_i - c > 0$$

$$y_i = -1 : w^T x_i - c < 0$$

$$c_+(w) = \min_{y_i=1}(w^T x_i)$$

$$c_-(w) = \max_{y_i=-1}(w^T x_i)$$

$$\rho(w) = \frac{c_+(w) - c_-(w)}{2}$$



$$\rho\left(\frac{w_0}{||w_0||}\right) = \frac{1}{||w_0||}$$

Optimization problem

$$y_i = 1 : w^T x_i - c > 0$$

$$y_i = -1 : w^T x_i - c < 0$$

$$M_i = y_i \cdot (w^T x_i - c)$$

$$\rho(w) = \frac{1}{||w||} \to \max_{w,c}$$

$$s.t.\ y_i(w^T x_i - c) \geq 1$$

Convex problem!

$$L(w, c, \alpha) = \frac{1}{2} w^T w - \sum_i \alpha_i (y_i(w^T x_i - c) - 1)$$

Many of them are zeros

Hinge loss

$$L(w, c, \alpha) = \frac{1}{2} w^T w - \sum_i \alpha_i (y_i (w^T x_i - c) - 1)$$

$$L^{\text{hinge}} = (1 - M)_+$$

$$L(w, c, \alpha) = \frac{1}{2} ||w||_2^2 + \sum_i \alpha_i L_i^{\text{hinge}}$$

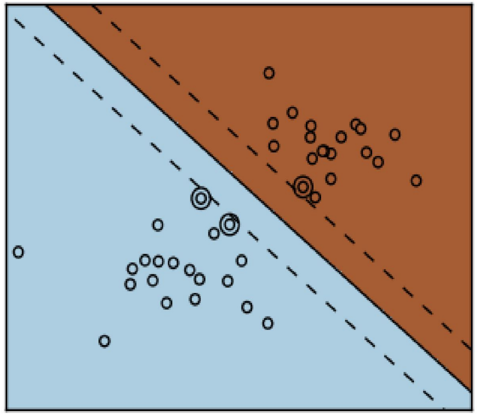
Inseparable case

Let our model mistake, but penalize that mistakes

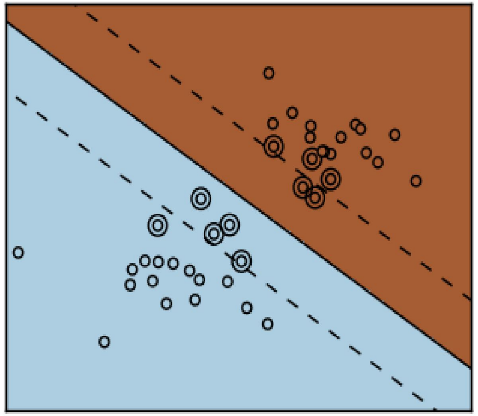
Implemented via margin slack variables

$$\begin{cases} \frac{1}{2}\langle w, w\rangle + C\sum_{i=1}^{\ell}\xi_i \to \min\limits_{w,w_0,\xi}; \\ y_i\big(\langle w, x_i\rangle - w_0\big) \geqslant 1 - \xi_i, \quad i = 1,\dots,\ell; \\ \xi_i \geqslant 0, \quad i = 1,\dots,\ell. \end{cases}$$

Big C



Small C



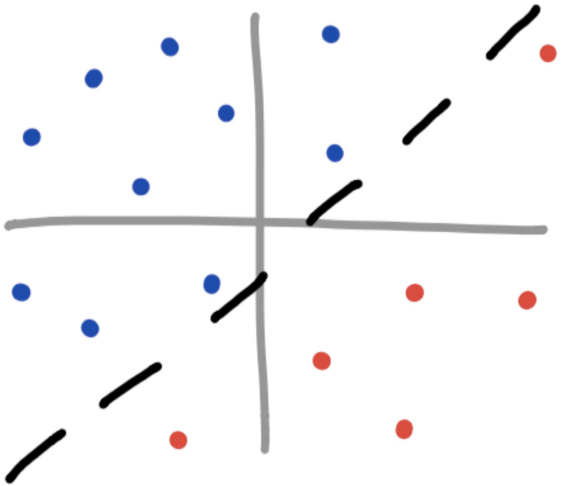
Kernel trick

$$y_i = 1 : w^T x_i - c > 0$$
$$y_i = -1 : w^T x_i - c < 0$$

$$\begin{matrix} x \mapsto \phi(x) \\ w \mapsto \phi(w) \end{matrix} \implies < w, x > \mapsto < \phi(w), \phi(x) >$$

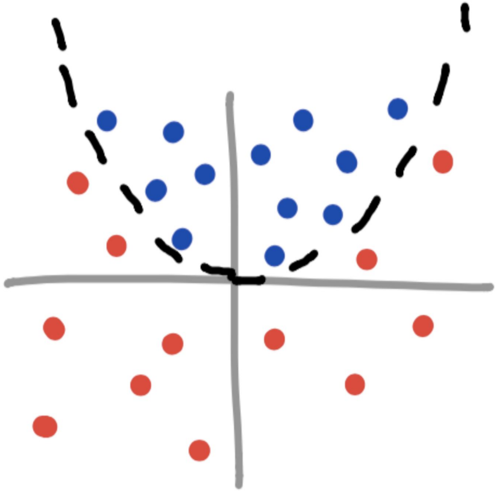
$$K(w, x) = < \phi(w), \phi(x) >$$

Kernel types



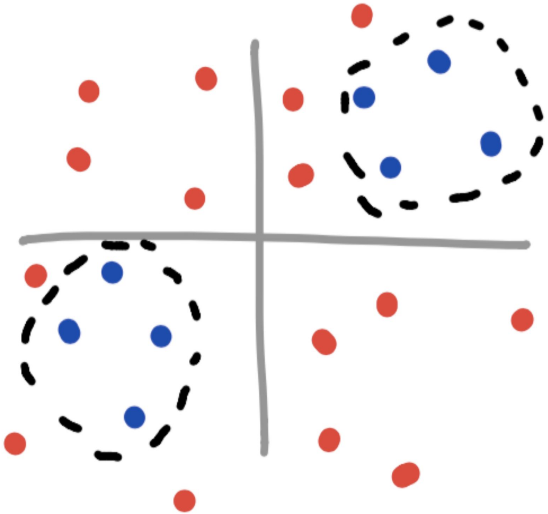
$K(w,x) = \langle w,x \rangle$

Linear



$K(w,x) = (\gamma \langle w,x \rangle + r)^d$

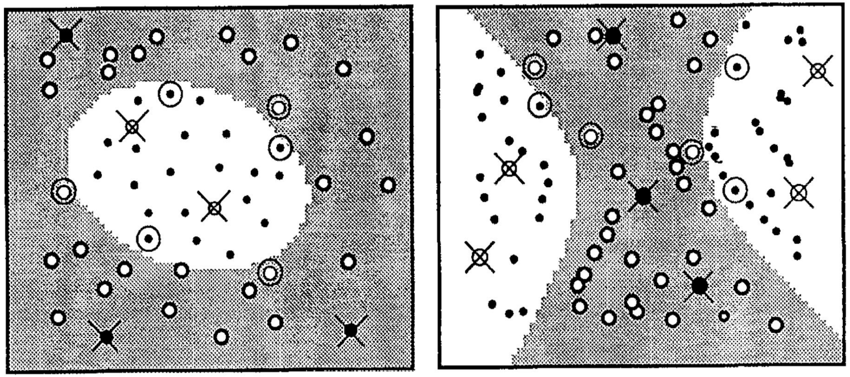
Polynomial



$K(w,x) = e^{-\gamma \|w-x\|^2}$

Gaussian
radial basis function

Current state



Principal Component Analysis

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Principal Component Analysis

$$x_1, \ldots, x_n \to g_1, \ldots, g_k, k \leq n$$

$$U : UU^T = I, G = XU$$

$$\hat{X} = GU^T \approx X$$

$$||GU^T - X|| \to \min_{G,U} \ s.t. \ rank(G) \leq k$$

Singular value decomposition

$$||GU^T - X|| \to \min_{G,U} \; s.t.\; rank(G) \leq k$$

$$X = V\Sigma U^T : ||GU^T - V\Sigma U^T||_2 = ||G - V\Sigma||_2$$

$$G = V\Sigma' : ||V\Sigma' - V\Sigma||_2 = ||\Sigma' - \Sigma||_2$$

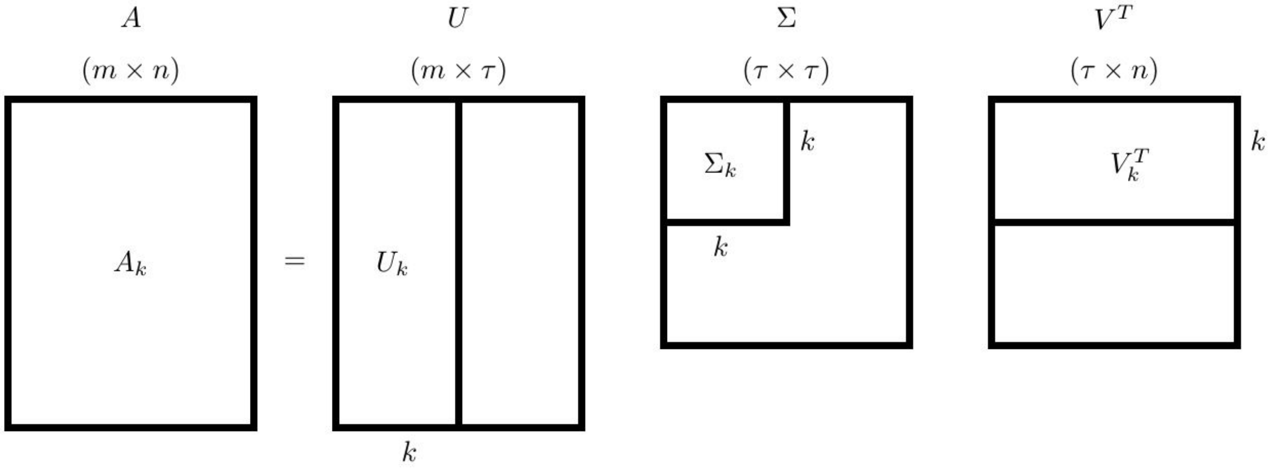
$$||A||_2 = \sigma_{max}(A) : ||\Sigma' - \Sigma||_2 = \sigma_k(\Sigma) = \sigma_k(X)$$

Eckart–Young–Mirsky theorem

Singular value decomposition

$$||GU^T - X|| \to \min_{G,U} \; s.t. \; rank(G) \leq k$$

$$X = V\Sigma U^T \qquad \sigma_k(\Sigma) = \sigma_k(X)$$



Eckart–Young–Mirsky theorem

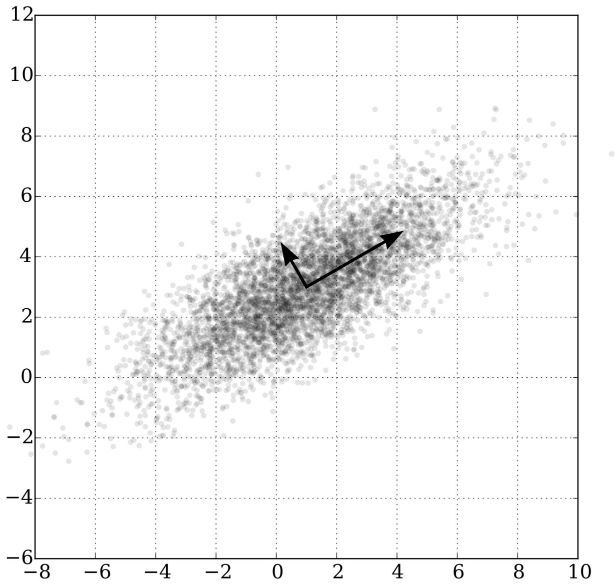
Another approach

Residual variance maximization

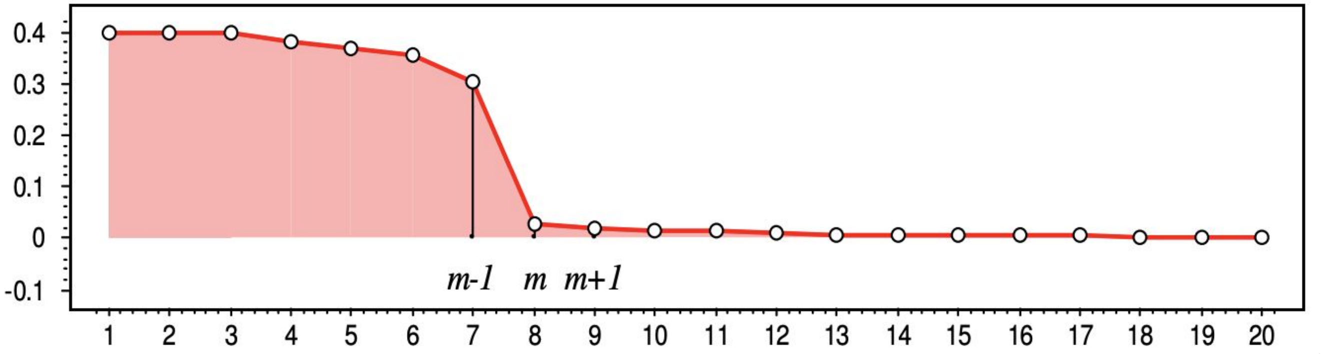
Take new basis vectors greedy

Same result for G and U

Always normalize data before PCA!!!



Dimensionality reduction



Get rid of low-variance components

$$E_m = \frac{\|GU^\intercal - F\|^2}{\|F\|^2} = \frac{\lambda_{m+1} + \cdots + \lambda_n}{\lambda_1 + \cdots + \lambda_n} \leqslant \varepsilon.$$

Dimensionality reduction

Let’s walk through space…

Dimensionality reduction

16 components

Dimensionality reduction

50 components

Dimensionality reduction

250 components

Revise

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Next time

- Decision trees and thresholds

Thanks for attention!

Questions?

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