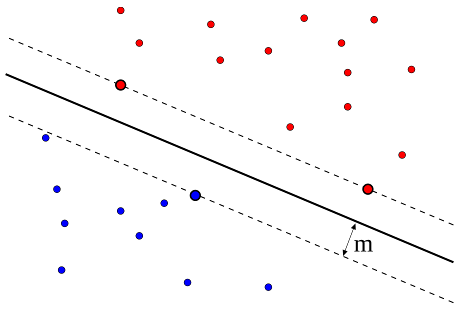
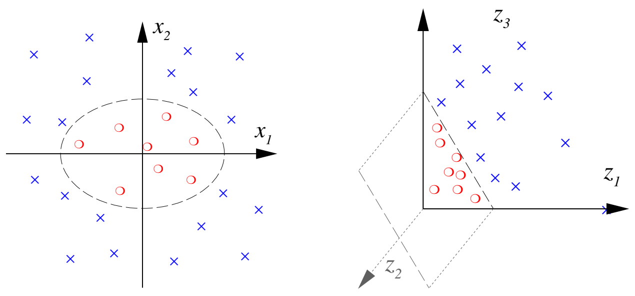
Support Vector Machine (SVM)

Extending the perceptron idea: use a **linear classifier with margin** and a **non-linear feature transformation**.



Nonlinear Transformation in Kernel Space

$$\Phi : \mathbb{R}^2 \to \mathbb{R}^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$$



Lagrangian Optimization Theory

Optimization under constraints (Primal Problem):

Given an optimization problem with domain $\Omega \subseteq \mathbb{R}^d$,

$$\begin{array}{rll} \text{minimize} & f(\mathbf{w}), & \mathbf{w} \in \Omega \\ \text{subject to} & g_i(\mathbf{w}) \le 0, & i = 1, \dots, k \\ & h_i(\mathbf{w}) = 0, & i = 1, \dots, m \end{array}$$

The **generalized Lagrangian function** is defined as

$$L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{w}) + \sum_{i=1}^{k} \alpha_i g_i(\mathbf{w}) + \sum_{i=1}^{m} \beta_i h_i(\mathbf{w})$$

Lagrangian Dual Problem (1797)

Definition (Langrangian Dual Problem):

The respective **Lagrangian dual problem** is given by

$$\begin{array}{rll} \text{maximize} & \theta(\boldsymbol{\alpha}, \boldsymbol{\beta}), & \\ \text{subject to} & \alpha_i \ge 0, & i = 1, \dots, k \end{array}$$

where $\quad \theta(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \inf_{\mathbf{w} \in \Omega} L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta})$

The value of the objective function at the optimal solution is called the **value of the problem**.

The **difference** between the values of the primal and the dual problems is known as the *duality gap*.

Upper Bound on Dual Costs

Theorem: Let $\mathbf{w} \in \Omega$ be a feasible solution of the primal problem of the previous definition and $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ a feasible solution of the respective dual problem. Then $f(\mathbf{w}) \ge \theta(\boldsymbol{\alpha}, \boldsymbol{\beta})$.

Proof:

$$\begin{aligned} \theta(\boldsymbol{\alpha}, \boldsymbol{\beta}) &= \inf_{\mathbf{u} \in \Omega} L(\mathbf{u}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \\ &\le L(\mathbf{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \\ &= f(\mathbf{w}) + \sum_{i=1}^{k} \underbrace{\alpha_i}_{\ge 0} \underbrace{g_i(\mathbf{w})}_{\le 0} + \sum_{j=1}^{m} \beta_j \underbrace{h_j(\mathbf{w})}_{=0} \quad \le f(\mathbf{w}) \end{aligned}$$

The feasibility of $\mathbf{w}$ implies $g_i(\mathbf{w}) \le 0$ and $h_i(\mathbf{w}) = 0$, while the feasibility of $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ implies $\alpha_i \ge 0$.

Duality Gap

Corollary: The value of the dual problem is upper bounded by the value of the primal problem,

$$\sup \{\theta(\boldsymbol{\alpha}, \boldsymbol{\beta}) : \boldsymbol{\alpha} \ge 0\} \quad \le \quad \inf \{f(\mathbf{w}) : \mathbf{g}(\mathbf{w}) \le 0, \mathbf{h}(\mathbf{w}) = 0\}$$

Theorem: The triple $(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ is a saddle point of the Lagrangian function for the primal problem, if and only if its components are optimal solutions of the primal and dual problems and if there is **no duality gap**, i.e., the primal and dual problems having the value

$$f(\mathbf{w}^*) = \theta(\boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$$

Strong Duality

Theorem: Given an optimization problem with convex objective function f and convex domain $\Omega \subseteq \mathbb{R}^d$,

$$\begin{array}{rll} \text{minimize} & f(\mathbf{w}), & \mathbf{w} \in \Omega \\ \text{subject to} & g_i(\mathbf{w}) \le 0, & i = 1, \dots, k \\ & h_i(\mathbf{w}) = 0, & i = 1, \dots, m \end{array}$$

where the g_i and h_i are affine functions, that is

$$\mathbf{h}(\mathbf{w}) = \mathbf{A}\mathbf{w} - \mathbf{b},$$

for some matrix $\mathbf{A}$ and vector $\mathbf{b}$, then *the duality gap is zero*.

(This case applies to SVMs!)

Remark: If the functions $g_i(\mathbf{w})$ are convex then strong duality holds provided some *constraint qualifications* are fulfilled (e.g. Slater condition).

Kuhn-Tucker Conditions (1951)

Theorem: Given an optimization problem with convex domain $\Omega \subseteq \mathbb{R}^d$,

$$\begin{array}{rll} \text{minimize} & f(\mathbf{w}), & \mathbf{w} \in \Omega \\ \text{subject to} & g_i(\mathbf{w}) \le 0, & i = 1, \dots, k \\ & h_i(\mathbf{w}) = 0, & i = 1, \dots, m \end{array}$$

with $f \in C^1$ convex and g_i, h_i affine, necessary and sufficient conditions for a normal point $\mathbf{w}^*$ to be an optimum are the existence of $\boldsymbol{\alpha}^*$, $\boldsymbol{\beta}^*$ such that

$$\frac{\partial L(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)}{\partial \mathbf{w}} = 0 \qquad \frac{\partial L(\mathbf{w}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)}{\partial \boldsymbol{\beta}} = 0$$

$$\alpha_i^* g_i(\mathbf{w}^*) = 0, \quad g_i(\mathbf{w}^*) \le 0, \quad \alpha_i^* \ge 0, \quad i = 1, \dots, k$$

Support Vector Machines (SVM)

Idea: linear classifier with margin and feature transformation.

Transformation from original feature space to nonlinear feature space.

$$\mathbf{y}_i = \phi(\mathbf{x}_i) \quad \text{e.g. Polynomial, Radial Basis Function, ...}$$

$$\phi : \mathbb{R}^d \to \mathbb{R}^e \text{ with } d \ll e$$

$$z_i = \begin{cases} +1 \\ -1 \end{cases} \text{if } \mathbf{x}_i \text{ in class } \begin{cases} y_1 \\ y_2 \end{cases}$$

Training vectors should be linearly separable after mapping!

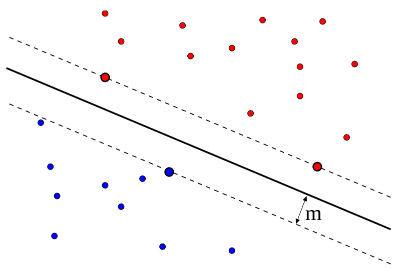
Linear discriminant function:

$$g(\mathbf{y}) = \mathbf{w}^\mathsf{T}\mathbf{y} + w_0$$

Support Vector Machine (SVM)

Find hyperplane that maximizes the **margin** m with

$$z_i\, g(\mathbf{y}_i) = z_i(\mathbf{w}^\mathsf{T}\mathbf{y} + w_0) \ge m \quad \text{for all } \mathbf{y}_i \in \mathcal{Y}$$



Vectors $\mathbf{y}_i$ with $z_i g(\mathbf{y}_i) = m$ are the **support vectors**.

Maximal Margin Classifier

Invariance: assume that the weight vector $\mathbf{w}$ is normalized ($\|\mathbf{w}\| = 1$) since a rescaling $(\mathbf{w}, w_0) \leftarrow (\lambda\mathbf{w}, \lambda w_0), m \leftarrow \lambda m$ does not change the problem.

Condition: $$z_i = \begin{cases} +1 & \mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0 \ge m \\ -1 & \mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0 \le -m \end{cases} \quad \forall i$$

Objective: maximize margin m s.t. joint condition $z_i\,(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) \ge m$ is met.

Learning problem: Find $\mathbf{w}$ with $||\mathbf{w}|| = 1$, such that the margin m is maximized.

$$\begin{array}{rl} \text{maximize} & m \\ \text{subject to} & \forall \mathbf{y}_i \in \mathcal{Y} : z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) \ge m \end{array}$$

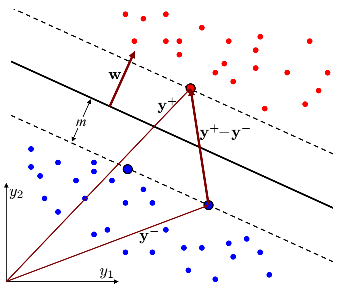
SVM Learning

What is the margin m?
Consider two points $\mathbf{y}^+, \mathbf{y}^-$ of class 1,2 which are located on both sides of the margin boundaries.

Transformation of objective:
rescaling $\mathbf{w} \leftarrow \frac{\mathbf{w}}{m}$, $w_0 \leftarrow \frac{w_0}{m}$ $\Rightarrow$

yields the constraints

$z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) \ge 1$



Margin:

$m = \frac{1}{2\|\mathbf{w}\|}(\mathbf{w}^\mathsf{T}\mathbf{y}^+ - \mathbf{w}^\mathsf{T}\mathbf{y}^-) = \frac{1}{\|\mathbf{w}\|}$

$m = \frac{1}{\|\mathbf{w}\|}$ follows from inserting $\pm(\mathbf{w}^\mathsf{T}\mathbf{y}^\pm + w_0) = 1$

$\Rightarrow$ maximizing the margin corresponds to minimizing the norm $||\mathbf{w}||$ for margin $m = 1$.

SVM Lagrangian

Minimize $||\mathbf{w}||$ for a given margin $m = 1$

$$\begin{array}{lrcl} \text{minimize} & \mathcal{T}(\mathbf{w}) & = & \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} \\ \text{subject to} & z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) & \geq & 1 \end{array}$$

Generalized Lagrange Function:

$$L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} - \sum_{i=1}^{n} \alpha_i \left[z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) - 1\right]$$

Functional and geometric margin: The problem formulation with margin $m = 1$ is called the *functional margin* setting; The original formulation refers to the *geometric margin*.

Stationarity of Lagrangian

Extremality condition:

$$\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i\leq n} \alpha_i z_i \mathbf{y}_i = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i\leq n} \alpha_i z_i \mathbf{y}_i$$

$$\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\alpha})}{\partial w_0} = -\sum_{i\leq n} \alpha_i z_i = 0$$

Resubstituting $\frac{\partial L}{\partial \mathbf{w}} = 0, \frac{\partial L}{\partial w_0} = 0$ into the Lagrangian function $L(\mathbf{w}, w_0, \boldsymbol{\alpha})$

$$\begin{aligned} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) &= \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} - \sum_{i\leq n} \alpha_i \left[z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) - 1\right] \\ &= \frac{1}{2}\sum_{i\leq n}\sum_{j\leq n} \alpha_i\alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j - \sum_{i\leq n}\sum_{j\leq n} \alpha_i\alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j + \sum_{i\leq n}\alpha_i \\ &= \sum_{i\leq n}\alpha_i - \frac{1}{2}\sum_{i\leq n}\sum_{j\leq n} \alpha_i\alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j \qquad \text{(note the scalar product!)} \end{aligned}$$

Dual Problem

The **Dual Problem** for support vector learning is

$$\begin{array}{ll} \text{maximize} & W(\boldsymbol{\alpha}) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i=1}^n \sum_{j=1}^n z_i z_j \alpha_i \alpha_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j \\ \text{subject to} & \forall i \; \alpha_i \geq 0 \quad \wedge \quad \sum_{i=1}^n z_i \alpha_i = 0 \end{array}$$

The optimal hyperplane $\mathbf{w}^*, w_0^*$ is given by

$$\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i^* z_i \mathbf{y}_i, \quad w_0^* = -\frac{1}{2}\left(\min_{i:z_i=1} \mathbf{w}^{*\mathsf{T}}\mathbf{y}_i + \max_{i:z_i=-1} \mathbf{w}^{*\mathsf{T}}\mathbf{y}_i\right)$$

where $\boldsymbol{\alpha}^*$ are the optimal Lagrange multipliers maximizing the Dual Problem.

Support Vectors

The **Kuhn-Tucker Conditions** for the maximal margin SVM are

$$\begin{array}{rcll} \alpha_i^*(z_i g^*(\mathbf{y}_i) - 1) & = & 0, & i = 1, \ldots, n \\ \alpha_i^* & \geq & 0, & i = 1, \ldots, n \\ z_i g^*(\mathbf{y}_i) - 1 & \geq & 0, & i = 1, \ldots, n \end{array}$$

The first one is known as the **Kuhn-Tucker complementary condition**. The conditions imply

$$\begin{array}{lll} z_i g^*(\mathbf{y}_i) = 1 \;\Rightarrow\; \alpha_i^* \geq 0 & & \text{Support Vectors (SV)} \\ z_i g^*(\mathbf{y}_i) \neq 1 \;\Rightarrow\; \alpha_i^* = 0 & & \text{Non Support Vectors} \end{array}$$

Optimal Decision Function

Sparsity:

$$\begin{aligned} g^*(\mathbf{y}) &= \mathbf{w}^{*\mathsf{T}}\mathbf{y} + w_0^* = \sum_{i=1}^{n} z_i \alpha_i^* \mathbf{y}_i^\mathsf{T}\mathbf{y} + w_0^* \\ &= \sum_{i\in\text{SV}} z_i \alpha_i^* \mathbf{y}_i^\mathsf{T}\mathbf{y} + w_0^* \end{aligned}$$

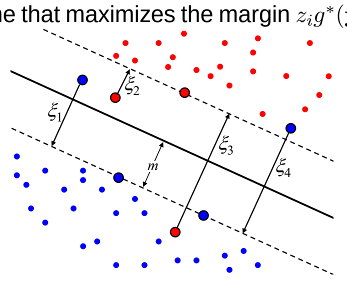
Remark: only few support vectors enter the sum to evaluate the decision function! $\Rightarrow$ efficiency and interpretability

Optimal margin: $\mathbf{w}^\mathsf{T}\mathbf{w} = \sum_{i\in\text{SV}} \alpha_i^*$

Soft Margin SVM

For each trainings vector $\mathbf{y}_i \in \mathcal{Y}$ a **slack variable** ξ_i is introduced to measure the violation of the margin constraint.

Find hyperplane that maximizes the margin $z_i g^*(\mathbf{y}_i) \geq m(1-\xi_i)$



Vectors $\mathbf{y}_i$ with $z_i g^*(\mathbf{y}_i) = m(1-\xi_i)$ are called **support vectors**.

Learning the Soft Margin SVM

Slack variables are penalized by L_1 norm.

$$\begin{array}{rrcl} \text{minimize} & \mathcal{T}(\mathbf{w},\boldsymbol{\xi}) & = & \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} + C\sum_{i=1}^n \xi_i \\ \text{subject to} & z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) & \geq & 1 - \xi_i \\ & \xi_i & \geq & 0 \end{array}$$

C controls the amount of constraint violations vs. margin maximization!

Lagrange function for soft margin SVM

$$\begin{aligned} L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} + C\sum_{i=1}^n \xi_i \\ &- \sum_{i=1}^n \alpha_i \left[z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) - 1 + \xi_i \right] - \sum_{i=1}^n \beta_i \xi_i \end{aligned}$$

Stationarity of Primal Problem

Differentiation:

$$\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^n \alpha_i z_i \mathbf{y}_i = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^n \alpha_i z_i \mathbf{y}_i$$

$$\frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \xi_i} = C - \alpha_i - \beta_i = 0 \qquad \frac{\partial L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial w_0} = -\sum_{i=1}^n \alpha_i z_i = 0$$

Resubstituting into the Lagrangian function $L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})$ yields

$$\begin{aligned} L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= \tfrac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} + C\textstyle\sum_{i=1}^n \xi_i \\ &- \textstyle\sum_{i=1}^n \alpha_i \left[z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) - 1 + \xi_i \right] - \textstyle\sum_{i=1}^n \beta_i \xi_i \end{aligned}$$

$$\begin{aligned} L(\mathbf{w}, w_0, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= \tfrac{1}{2}\textstyle\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j + C\sum_{i=1}^n \xi_i \\ &\quad - \textstyle\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j \\ &\quad + \textstyle\sum_{i=1}^n \alpha_i (1 - \xi_i) - \sum_{i=1}^n \beta_i \xi_i \\ &= \textstyle\sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j \\ &\quad + \textstyle\sum_{i=1}^n \underbrace{(C - \alpha_i - \beta_i)}_{=\frac{\partial L}{\partial \xi_i}=0} \xi_i \\ &= \textstyle\sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j z_i z_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j \end{aligned}$$

Constaints of the Dual Problem

The dual objective function is the same as for the maximal margin SVM. The only difference is the constraint

$$C - \alpha_i - \beta_i = 0$$

Together with $\beta_i \geq 0$ it implies

$$\alpha_i \leq C$$

The Kuhn-Tucker complementary conditions

$$\begin{array}{rcll} \alpha_i(z_i(\mathbf{w}^\mathsf{T}\mathbf{y}_i + w_0) - 1 + \xi_i) & = & 0, & i = 1, \ldots, n \\ \xi_i(\alpha_i - C) & = & 0, & i = 1, \ldots, n \end{array}$$

imply that nonzero slack variables can only occur when $\alpha_i = C$.

Dual Problem of Soft Margin SVM

The **Dual Problem** for support vector learning is

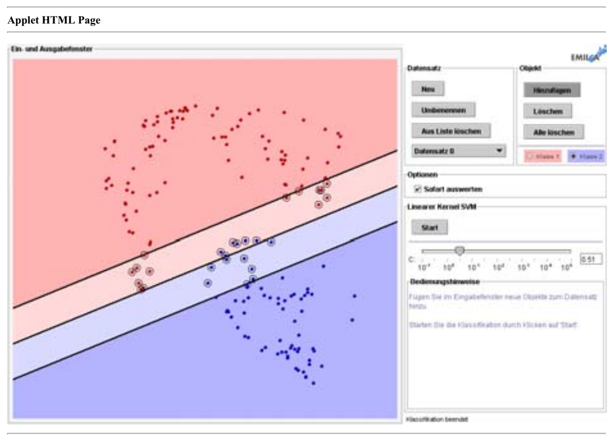
$$\begin{array}{rl} \text{maximize} & W(\boldsymbol{\alpha}) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i=1}^n \sum_{j=1}^n z_i z_j \alpha_i \alpha_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j \\ \text{subject to} & \sum_{j=1}^n z_j \alpha_j = 0 \ \wedge \ \forall i \ C \geq \alpha_i \geq 0 \end{array}$$

The optimal hyperplane $\mathbf{w}^*$ is given by

$$\mathbf{w}^* = \sum_{i=1}^n \alpha_i^* z_i \mathbf{y}_i$$

where $\boldsymbol{\alpha}^*$ are the optimal Lagrange multipliers maximizing the Dual Problem.

$\alpha_i^* > 0$ holds only for **support vectors**.



Fügen Sie im Eingabefenster neue Objekte zum Datensatz hinzu.

Starten Sie die Klassifikation durch Klicken auf Start.

Klassifikation beendet

Linear Programming Support Vector Machines

Idea: Minimize an estimate of the number of positive multipliers $\sum_{i=1}^n \alpha_i$ which improves bounds on the generalization error.

The **Lagrangian** for the LP-SVM is

$$\begin{array}{rl} \text{minimize} & W(\boldsymbol{\alpha},\xi) = \sum_{i=1}^n \alpha_i + C\sum_{i=1}^n \xi_i \\ \text{subject to} & z_i\left[\sum_{j=1}^n \alpha_j \mathbf{y}_i^\mathsf{T}\mathbf{y}_j + w_0\right] \geq 1-\xi_i, \\ & \alpha_i \geq 0,\ \xi_i \geq 0,\ 1 \leq i \leq n \end{array}$$

Advantage: efficient LP solver can be used.

Disadvantage: theory is not as well understood as for standard SVMs.

Non–Linear SVMs

Feature extraction by non linear transformation $\mathbf{y} = \phi(\mathbf{x})$

Problem:

$$\mathbf{y}_i^\mathsf{T}\mathbf{y}_j = \phi^\mathsf{T}(\mathbf{x}_i)\phi(\mathbf{x}_j)$$

is the inner product in a high dimensional space.

A **kernel function** is defined by

$$\forall \mathbf{x},\mathbf{z} \in \Omega: \quad K(\mathbf{x},\mathbf{z}) = \phi^\mathsf{T}(\mathbf{x})\phi(\mathbf{z})$$

Using the kernel function the discriminant function becomes

$$g(\mathbf{x}) = \sum_{i=1}^n \alpha_i z_i \underbrace{K(\mathbf{x}_i,\mathbf{x})}_{\text{replaces } \mathbf{y}_i^\mathsf{T}\mathbf{y}}$$

Characterization of Kernels

For any symmetric matrix $K(\mathbf{x}_i,\mathbf{x}_j)|_{i,j=1}^n$ (Gram matrix) there exists an eigenvector decomposition

$$K = V\Lambda V^\mathsf{T}.$$

V: orthogonal matrix of eigenvectors $(v_{ti})|_{i=1}^n$
Λ: diagonal matrix of eigenvalues λ_t

Assume all eigenvalues are nonnegative and consider mapping

$$\phi: \mathbf{x}_i \to \left(\sqrt{\lambda_t}v_{ti}\right)_{t=1}^n \in \mathbb{R}^n, i = 1,\ldots,n$$

Then it follows

$$\phi^\mathsf{T}(\mathbf{x}_i)\phi(\mathbf{x}_j) = \sum_{t=1}^n \lambda_t v_{ti}v_{tj} = \left(V\Lambda V^\mathsf{T}\right)_{ij} = K_{ij} = K(\mathbf{x}_i,\mathbf{x}_j)$$

Positivity of Kernels

Theorem: Let Ω be a finite input space with $K(\mathbf{x},\mathbf{z})$ a symmetric function on Ω. Then $K(\mathbf{x},\mathbf{z})$ is a kernel function if and only if the matrix

$$K = (K(\mathbf{x}_i,\mathbf{x}_j))_{i,j=1}^n$$

is *positive semi-definite* (has only non-negative eigenvalues).

Extension to infinite dimensional Hilbert Spaces:

$$<\phi(\mathbf{x}),\phi(\mathbf{z})> = \sum_{i=1}^\infty \lambda_i\phi_i(\mathbf{x})\phi_i(\mathbf{z})$$

Mercer's Theorem

Theorem (Mercer): Let Ω be a compact subset of $\mathbb{R}^n$. Suppose K is a continuous symmetric function such that the integral operator $T_K: L_2(X) \to L_2(X)$,

$$(T_K f)(\cdot) = \int_\Omega K(\cdot,\mathbf{x})f(\mathbf{x})d\mathbf{x},$$

is positive, that is $\int_{\Omega\times\Omega} K(\mathbf{x},\mathbf{z})f(\mathbf{x})f(\mathbf{z})d\mathbf{x}d\mathbf{z} > 0 \quad \forall f \in L_2(\Omega)$
Then we can expand $K(\mathbf{x},\mathbf{z})$ in a uniformly convergent series in terms of T_K's eigen-functions $\phi_j \in L_2(\Omega)$, with $||\phi_j||_{L_2} = 1$ and $\lambda_j > 0$.

Possible Kernels

Remark: Each kernel function, that hold Mercer's conditions describes an inner product in a high dimensional space. The kernel function replaces the inner product.

Possible Kernels:

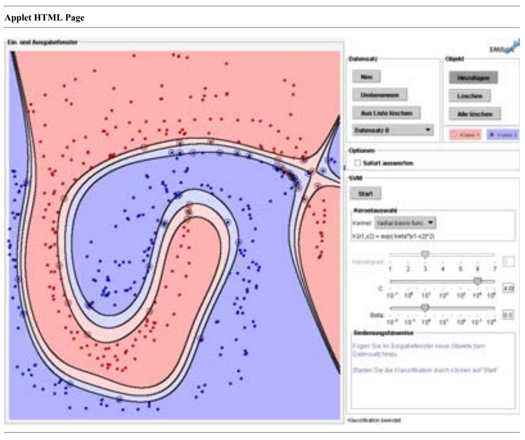
$$\begin{array}{llcll} a) & K(\mathbf{x},\mathbf{z}) & = & \exp\left(-\frac{||\mathbf{x}-\mathbf{z}||^2}{2\sigma^2}\right) & \text{(RBF Kernel)} \\ b) & K(\mathbf{x},\mathbf{z}) & = & \tanh\kappa\mathbf{x}\mathbf{z} - b & \text{(Sigmoid Kernel)} \\ c) & K(\mathbf{x},\mathbf{z}) & = & (\mathbf{x}\mathbf{z})^d & \text{(Polynomial Kernel)} \\ & K(\mathbf{x},\mathbf{z}) & = & (\mathbf{x}\mathbf{z}+1)^d & \\ d) & K(\mathbf{x},\mathbf{z}) & : & \text{string kernels for sequences} & \end{array}$$

Kernel Engineering

Kernel composition rules: Let K_1, K_2 be kernels over $\Omega \times \Omega, \Omega \subseteq \mathbb{R}^d$, $a \in \mathbb{R}^+, f(.)$ a real-vealued function $\phi : \Omega \to \mathbb{R}^e$ with K_3 a kernel over $\mathbb{R}^e \times \mathbb{R}^e$.

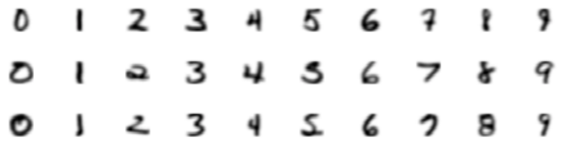
Then the following functions are kernels:

1. $K(\mathbf{x}, \mathbf{z}) = K_1(\mathbf{x}, \mathbf{z}) + K_2(\mathbf{x}, \mathbf{z})$,
2. $K(\mathbf{x}, \mathbf{z}) = aK_1(\mathbf{x}, \mathbf{z})$,
3. $K(\mathbf{x}, \mathbf{z}) = K_1(\mathbf{x}, \mathbf{z})K_2(\mathbf{x}, \mathbf{z})$,
4. $K(\mathbf{x}, \mathbf{z}) = f(\mathbf{x})f(\mathbf{z})$,
5. $K(\mathbf{x}, \mathbf{z}) = K_3(\phi(\mathbf{x}), \phi(\mathbf{z}))$,
6. $K(\mathbf{x}, \mathbf{z}) = p(K_1(\mathbf{x}, \mathbf{z}))$, ($p(x)$ is a polynomial with positive coefficients)
7. $K(\mathbf{x}, \mathbf{z}) = \exp(K_1(\mathbf{x}, \mathbf{z}))$,



Example: Hand Written Digit Recognition

- 7291 training images und 2007 test images (16x16 pixel, 256 gray values)



Classification method	test error
human classification	2.7 %
perceptron	5.9 %
support vector machines	4.0 %

SVMs for Secondary Structure Prediction

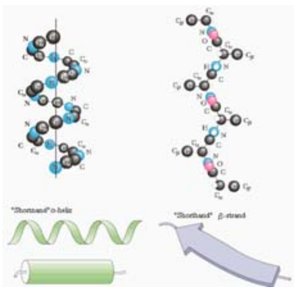
Proteins are represented in “zeroth order” by the percentage of amino-acids in the polypeptide chain; $\rightsquigarrow$ “vectorial” representation in $\mathbb{R}^{20}$

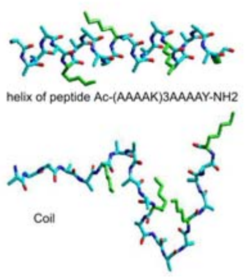
Protein structure problem: **sequence** as primary structure, **local motives** as secondary structure, **protein folds** as ternary structure.

SVM classification typically use the *RBF* kernel

$$k(\mathbf{x}, \mathbf{y}) = \exp\left(-\gamma \|\mathbf{x} - \mathbf{y}\|^2\right)$$

Secondary structure prediction as a multiclass problem: Detect classes *helix (H)*, *sheet (E)* and *coil (C)*





Accuracy measure: $Q_3 = \%$ of correct 3-state symbols, i.e.

$$Q_3 = \frac{\#\text{correctly predicted residues}}{\text{total \# of residues}} \cdot 100$$

Practical Problem: How to apply SVMs for $k > 2$ classes?

Linear Discriminants and the Multicategory Case

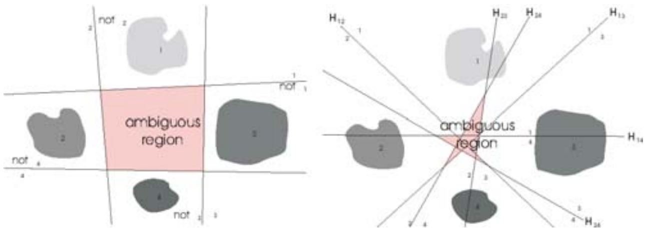
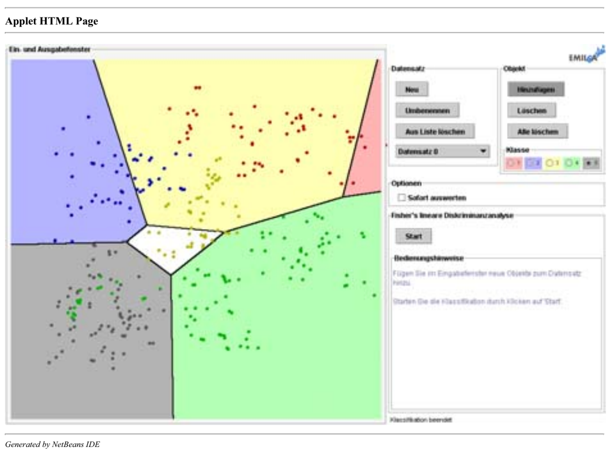


FIGURE 5.3. Linear decision boundaries for a four-class problem. The Top figure shows ω_i/not ω_i dichotomies while the bottom figure shows ω_i/ω_j dichotomies and the corresponding decision boundaries H_{ij}. The pink regions have ambiguous category assignments. From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*.

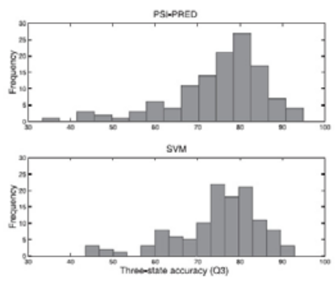
Idea: it is often preferable to reformulate the multiclass problem as $(k-1)$ “*class* α – *not class* α” dichotomies or $k(k-1)/2$ “*class* α *or* β” dichotomies.

Problem: some areas in feature space are ambiguously classified.



Experimental Results

- *PHD* (by B. Rost *et al.*, Neural Network based approach) – 72-74% Q_3
- *Psi-pred* (by D. T. Jones *et al.*, Neural Network based approach) – 76-78% Q_3
- The extensive study by *Ward* et al. (Bioinformatics, 2003) with different SVM realization reports results 73-77% Q_3
- Two-layer classification strategy with position-specific scoring scheme (*Guo* et al., Proteins, 2004)). Accuracy ranges from 78% – 80%.



Histogram of Q_3 scores for 121 test proteins (Ward *et al.*, Bioinformatics 19:13, 2003)

Machine Learning on Audio Data

Project with the company Phonak (Stäfa), producer of hearing aids.

Task: Given an accoustic environment, find appropriate control settings for the hearing aid:

- Speech understanding in silent and noisy environments
- Natural hearing of music and sounds in nature
- Comfortable setting for noisy environments

Classification of Audio Data

Current setting: Four sound classes are defined corresponding to the basic hearing goals:

$\longrightarrow$ *Speech*
$\longrightarrow$ *Speech in Noise*
$\longrightarrow$ *Music*
$\longrightarrow$ *Noise*

Goal: Let the hearing instrument autonomously decide which environment you are in!

Question: Are the four sound classes supported by sound statistics?

Features from Audio Data

Feature set: Common features are

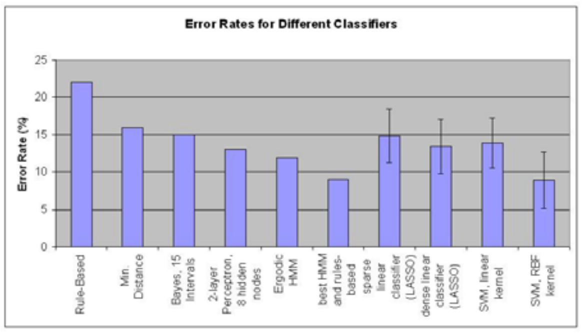
- distribution of the spectrum
- tonality
- rhythm
- estimated signal to noise ratio (SNR)
- ... and others

Strong computational constraints in the hearing aid!

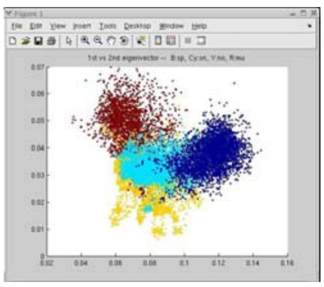
- Very little computational power and memory is available.
- Delay must not exceed a few ten miliseconds

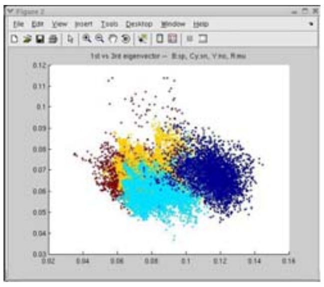
$\longrightarrow$ Complex features can only be approximated.

Classification Quality for different Classifiers



Linear Discriminant Analysis

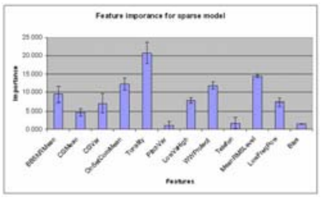


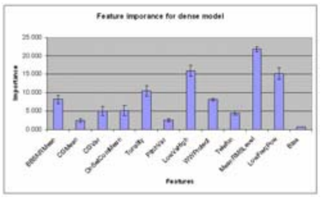


- Speech and most music files can be clearly separated.
- Speech in noise and noise are substantially overlapping.

Feature importance

Relative feature importance for a sparse and a dense linear model:





- All of the currently used features are used ...
- ... but not all features have the same importance.

Machine Learning: Topic Chart

- **Core problems of pattern recognition**
- **Bayesian decision theory**
- **Perceptrons and Support vector machines**
- ***Data clustering***
- **Dimension reduction**

Supervised vs. Unsupervised learning

Training data: A sample from the data source with the correct classification/regression solution already assigned.

Supervised learning = Learning based on training data.

Two steps:

1. Training step: Learn classifier/regressor from training data.
2. Prediction step: Assign class labels/functional values to test data.

Perceptron, LDA, *SVMs*, linear/ridge/kernel ridge regression are all supervised methods.

Unsupervised learning: Learning without training data.

Unsupervised learning

Examples:

- Data clustering. (Some authors do not distinguish between clustering and unsupervised learning.)
- Dimension reduction techniques.

Data clustering: Divide input data into groups of similar points.
$\rightarrow$ Roughly the unsupervised counterpart to classification.

Note the difference:

- Supervised case: Fit model to each class of training points, then use models to classify test points.
- Clustering: Simultaneous inference of group structure and model.

Grouping or Clustering: the k-Means Problem

Given are d-dimensional sample vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$

Define ...

- ... assignment vector $c \in \{1, \ldots, k\}^n$
- ... prototypes $\mathbf{y}_\nu \in \mathcal{Y} \subset \mathbb{R}^d$ $(\nu \in \{1, \ldots, k\})$

Problem: Find c and $\mathbf{y}_\nu$ such that the clustering costs are minimized ($c_i := c(\mathbf{x}_i)$)

$$R^{\text{km}}(c, \mathcal{Y}) = \sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{y}_{c_i}||^2$$

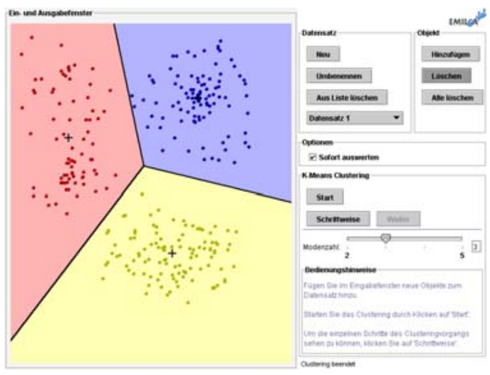
Mixed combinatorial and continuous optimization problem

k-Means Algorithm

1. **Choose** k sample objects randomly as prototypes, i.e., select $\mathcal{Y} = \{\mathbf{x}_1, \dots, \mathbf{x}_k\}$
2. **Iterate**:
   - Keep prototypes $\mathbf{y}_{c_i}$ fixed and assign sample vectors $\mathbf{x}_i$ to nearest prototype
   $$c_i = \arg \min_{\nu \in \{1,\dots,k\}} ||\mathbf{x}_i - \mathbf{y}_{c_i}||^2$$
   - Keep assignments c_i fixed and estimate prototypes
   $$\mathbf{y}_\nu = \frac{1}{n_\nu} \sum_{i:c_i=\nu} \mathbf{x}_i \quad \text{with} \quad n_\nu = |\{i : c_i = \nu\}|$$

Clustering of Vector Data

Applet HTML Page



Fügen Sie im Eingabefenster neue Objekte zum Datensatz hinzu.

Starten Sie das Clustering durch Klicken auf 'Start'.

Um die einzelnen Schritte des Clusteringvorgangs sehen zu können, klicken Sie auf 'Schrittweise'.

Clustering beendet

Generated by NetBeans IDE

Mixture models

Def.: A *finite mixture model* is a probability density of the form

$$p(x) = \sum_{j=1}^{l} c_j p_j(x)$$

where the p_j are probability densities on a common domain Ω, $c_j \geq 0$ constants and $\sum_j c_j = 1$.

Remarks:

- p is a density on Ω.
- If all components are parametric models, then so is p.
- Most common: Gaussian mixture, $p_j(x) := g(x|\mu_j, \sigma_j)$.

Mixture models: Interpretation

Recall: Addition on probabilities $\leftrightarrow$ logical OR.

Represented data source:

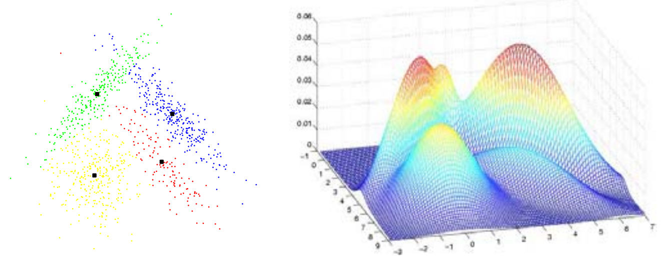
- Source = set of component sources (modeled by the p_j)
- Each data value is drawn from exactly one component source.
- c_j: Probability of draw from p_j.

Application to clustering: Natural model if...

1. each data point belongs to exactly one group.
2. we have some idea what the group densities look like.

Gaussian mixture model

$$p(x|\boldsymbol{\mu}, \boldsymbol{\sigma}) = \sum_{j=1}^{l} c_j g(x|\mu_j, \sigma_j)$$



Parametric mixtures: Inference

Inference: How can we estimate the model parameters c_j, μ_j, σ_j?

We refer to the source information (i.e.,which component was a data point drawn from) as *assignments*.

Problem:

- Parameters can be estimated by ML *if assignments are known*.
- Assignments can be estimated from model if parameters are known.

Idea: Iterative approach.

Expectation-Maximization algorithm

Estimate Gaussian mixture from data values $x_1, \dots, x_n$.

Approach: Regard class assignments as random variables.

Notation: Assignment variables $M_{ij} := \begin{cases} 1 & x_i \text{ drawn from } p_j \\ 0 & \text{otherwise} \end{cases}$

Algorithm: Iterates two steps:

- **E-step:** Estimate expected values for M_{ij} from current model configuration.
- **M-step:** Estimate model parameters from current assignment probabilities $\mathsf{E}[M_{ij}]$.

This will require some more explanation.

Gaussian mixture: E-step

Current model parameters: $\tilde{\boldsymbol{\theta}} = (\tilde{\mathbf{c}}, \tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\sigma}})$ (from last M-step)

Compute expectations:

$$\begin{aligned} \mathsf{E}\left[M_{ij} \middle| \mathbf{x}, \tilde{\boldsymbol{\theta}}\right] &= \Pr\{x_i \text{ was drawn from } p_j\} \\ &= \frac{c_j p(x_i|\tilde{\theta}_j)}{\sum_{k=1}^{l} c_k p(x_i|\tilde{\theta}_k)} = \frac{c_j g\left(x_i|\tilde{\mu}_j, \tilde{\sigma}_j\right)}{\sum_{k=1}^{l} c_k g\left(x_i|\tilde{\mu}_k, \tilde{\sigma}_k\right)} \end{aligned}$$

Jargon: The binary assignments ("hard assignments") are *relaxed* to values $\mathsf{E}[M_{ij}] \in [0,1]$ ("soft assignments").

Gaussian mixture: M-step

Task: Estimate model parameters given assignments.

Easy for hard assignments:

- Select all x_i with $M_{ij} = 1$.
- Perform ML estimation on this data subset.

Can we do it for soft assignments? The log-likelihood is

$$l_{\mathbf{M}}(\theta) = \sum_{i=1}^{n} \log\left(\sum_{j=1}^{l} M_{ij} c_j g\left(x_i|\mu_j, \sigma_j\right)\right)$$

Technical problem: We want to substitute expected values for M_{ij}. We can apply an expectation to $l_{\mathbf{M}}$, but how do we get it into the log?

Gaussian mixture: M-step

Trick: (This is a true classic.)

$$\sum_{i=1}^{n} \log\left(\sum_{j=1}^{l} M_{ij} c_j g\left(x_i|\mu_j, \sigma_j\right)\right) = \sum_{i=1}^{n}\sum_{j=1}^{l} M_{ij} \log\left(c_j g\left(x_i|\mu_j, \sigma_j\right)\right)$$

Explanation: For all i, $M_{ij_0} = 1$ for exactly one j_0. So:

$$\log\left(\sum_{j=1}^{l} M_{ij} f_j\right) = \log\left(f_{j_0}\right) = M_{ij_0} \log\left(f_{j_0}\right) = \sum_{j} M_{ij} \log\left(f_j\right)$$

Note: This introduces an error, because it is only valid for hard assignments. We relax assignments, and relaxation differs inside and outside logarithm.

Gaussian mixture: M-step

Expected log-likelihood:

$$\begin{aligned} \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\theta}}\left[l(\theta)\right] &= \mathsf{E}\left[\sum_{i=1}^{n}\sum_{j=1}^{l} M_{ij} \log\left(c_j g\left(x_i|\mu_j, \sigma_j\right)\right)\right] \\ &= \sum_{i=1}^{n}\sum_{j=1}^{l} \mathsf{E}[M_{ij}] \log\left(c_j g\left(x_i|\mu_j, \sigma_j\right)\right) \\ &= \underbrace{\sum_{i,j} \mathsf{E}[M_{ij}] \log\left(c_j\right)}_{1} + \underbrace{\sum_{i,j} \mathsf{E}[M_{ij}] \log\left(g\left(x_i|\mu_j, \sigma_j\right)\right)}_{2} \end{aligned}$$

- Substitute E-step results for $\mathsf{E}[M_{ij}]$.
- Maximize (1) and (2) separately w. r. t. c_j and μ_j, σ_j.

Gaussian mixture: M-step

Maximizing (1):

$$c_j := \frac{1}{n} \sum_{i} \mathsf{E}[M_{ij}]$$

Maximizing (2): For 1D Gaussian model, analytic maximization gives

$$\begin{aligned} \tilde{\mu}_j &= \frac{\sum_{i=1}^{n} x_i \mathsf{E}[M_{ij}]}{\sum_{i=1}^{n} \mathsf{E}[M_{ij}]} \\ \tilde{\sigma}_j^2 &= \frac{\sum_{i=1}^{n} \left(x_i - \tilde{\mu}_j\right)^2 \mathsf{E}[M_{ij}]}{\sum_{i=1}^{n} \mathsf{E}[M_{ij}]} \end{aligned}$$

$\rightarrow$ weighted form of the standard ML estimators.

EM algorithm: Summary

Notation: $Q(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) := \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\theta}}\left[l_{\mathbf{M}}(\theta)\right]$

EM algorithm:

- **E-step:**
  1. Substitute current parameter estimates $\tilde{\boldsymbol{\theta}}$ into model.
  2. Estimate expectations $\mathsf{E}\left[M_{ij}\right]$.
  3. Substitute estimates into log-likelihood. This gives Q as function of $\boldsymbol{\theta}$.
- **M-step:**
  Parameter estimation: Maximize $Q(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}})$ w. r. t. $\boldsymbol{\theta}$.

Observation: This does not seem to be limited to a specific model (like Gaussian mixtures). Can it be generalized?

EM: General case

When can EM be applied?
If we can define hidden variables $\mathbf{M}$ such that

- The joint density $p(\mathbf{x}, \mathbf{M}|\boldsymbol{\theta})$ is known.
- Expected values of the hidden variables can be estimated from a given model configuration.
- Given estimates for the hidden variables, ML estimation is possible.

When do we want to apply EM for ML estimation? If . . .

- . . . ML is hard for $p(\mathbf{x}|\boldsymbol{\theta})$
- . . . ML is easy for $p(\mathbf{x}, \mathbf{M}|\boldsymbol{\theta})$ when we know $\mathbf{M}$.
- . . . we can efficiently compute expectations for $\mathbf{M}$.

The two log-likelihoods

The density of the augmented data $(\mathbf{x}, \mathbf{M})$ is:

$$p(\mathbf{x}, \mathbf{M}|\boldsymbol{\theta}) = p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})\, p(\mathbf{x}|\boldsymbol{\theta})$$

This means we deal with two different log-likelihoods:

- The one we are actually interested in:

$$l(\boldsymbol{\theta}) = \log\left(p(\mathbf{x}|\boldsymbol{\theta})\right)$$

- The one including the hidden variables:

$$l_{\mathbf{M}}(\boldsymbol{\theta}) = \log\left(p(\mathbf{x}, \mathbf{M}|\boldsymbol{\theta})\right)$$

$l(\boldsymbol{\theta})$ is constant w. r. t. the expectation $\mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}[\,.\,]$ in the algorithm. $l_{\mathbf{M}}(\boldsymbol{\theta})$ is dependent on hidden variables $\mathbf{M}$.

Proof of Convergence

What we want to show: $l(\boldsymbol{\theta}) > l(\tilde{\boldsymbol{\theta}})$.

Rewrite $l(\boldsymbol{\theta})$ using definition of conditional prob.:

$$\begin{aligned} l(\boldsymbol{\theta}) = \log\left(p(\mathbf{x}|\boldsymbol{\theta})\right) &= \log\left(\frac{p(\mathbf{x}, \mathbf{M}|\boldsymbol{\theta})}{p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})}\right) \\ &= l_{\mathbf{M}}(\boldsymbol{\theta}) - \log\left(p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})\right) \end{aligned}$$

Apply the expectation:

$$\begin{aligned} \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[l(\boldsymbol{\theta})\right] &= \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[l_{\mathbf{M}}(\boldsymbol{\theta})\right] - \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})\right)\right] \\ \Leftrightarrow \quad l(\boldsymbol{\theta}) &= Q(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) - \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})\right)\right] \end{aligned}$$

Proof of convergence

We want to show that this is larger than

$$l(\tilde{\boldsymbol{\theta}}) = Q(\tilde{\boldsymbol{\theta}}, \tilde{\boldsymbol{\theta}}) - \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p\left(\mathbf{M}|\mathbf{x}, \tilde{\boldsymbol{\theta}}\right)\right)\right]$$

First term Q: Two possibilities,

1. Q is already maximal (algorithm converged).
2. Otherwise: $Q(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) > Q(\tilde{\boldsymbol{\theta}}, \tilde{\boldsymbol{\theta}})$.

For the second term holds:

$$\mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p\left(\mathbf{M}|\mathbf{x}, \tilde{\boldsymbol{\theta}}\right)\right)\right] \geq \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})\right)\right] \qquad (*)$$

Proof of convergence

Summary:

$$\begin{aligned} l(\boldsymbol{\theta}) &= Q(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}) - \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p(\mathbf{M}|\mathbf{x}, \boldsymbol{\theta})\right)\right] \\ &> Q(\tilde{\boldsymbol{\theta}}, \tilde{\boldsymbol{\theta}}) - \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p\left(\mathbf{M}|\mathbf{x}, \tilde{\boldsymbol{\theta}}\right)\right)\right] \\ &= l(\tilde{\boldsymbol{\theta}}) \end{aligned}$$

We're done, except for $(*)$.

Proof of $(*)$: Use *Jensen's inequality*: If f is a convex function then $\mathsf{E}\left[f(X)\right] \geq f\left(\mathsf{E}[X]\right)$ for any RV X. The log function is concave, so $\mathsf{E}\left[\log(X)\right] \leq \log\left(\mathsf{E}[X]\right)$.

Abbreviate $p := p\left(\mathbf{M}|\mathbf{x},\boldsymbol{\theta}\right)$ and $\tilde{p} := p\left(\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}\right)$.

$$\begin{aligned}
\mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(p\right)\right] &= \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\frac{p}{\tilde{p}}\cdot\tilde{p}\right)\right] \\
&= \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\frac{p}{\tilde{p}}\right)\right] + \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\tilde{p}\right)\right] \\
&\leq \log\left(\mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\frac{p}{\tilde{p}}\right]\right) + \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\tilde{p}\right)\right] \\
&= \log\left(\sum\tilde{p}\cdot\frac{p}{\tilde{p}}\right) + \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\tilde{p}\right)\right] \\
&= \log(\underbrace{\sum p}_{=1}) + \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\tilde{p}\right)\right] \\
&= \mathsf{E}_{\mathbf{M}|\mathbf{x},\tilde{\boldsymbol{\theta}}}\left[\log\left(\tilde{p}\right)\right] \qquad \square
\end{aligned}$$

Convergence results

Theoretical convergence guarantees:

- What we have shown above: The log-likelihood increases with each iteration. This does not imply convergence to local maximum.
- For sufficiently regular log-likelihoods, the algorithm always converges to a *local* maximum of the log-likelihood.

What can go wrong: Like any gradient-type algorithm, it can get stuck in a saddle point or even a local minimum. Note:

- This is a *scale problem*. It happens when the gradient step is too large to resolve a local maximum and oversteps.
- Can be prevented by requiring regularity conditions.
- Only happens for numerical M-step.

Convergence in practice

Hard to analyze:

- Cost function (log-likelihood) changes between steps.
- Influence of hidden variables is not entirely understood.

Local minima/saddle points: Convergence to these points is a theoretical possibility, but usually not a practical problem.

Worst problem: Initialization. EM results tend to be highly dependent on initial values.

Common strategy: Initialize with random values. Rerun algorithm several times and choose solution which has the largest likelihood.

k-Means algorithm

Simplify Gaussian mixture model EM:

1. Assume that all Gaussians have the same variance.
2. Use hard assignments instead of expectations.

Resulting algorithm: Alternate steps

1. For each class, choose all assigned data values and average them. ($\rightarrow$ ML estimation of Gaussian mean for hard assignments.)
2. Assign each value to class under which its probability of occurrence is largest.

Hence the name: For k classes, algorithm iteratively adjust means (= class averages).

Some history

EM: Introduced by Dempster, Laird and Rubin in 1977. Previously known as Baum-Welch algorithm for Hidden Markov Models.

k-Means: Also known as Lloyd-Max-Algorithm in vector quantization. In 1973, Bezdek introduced a 'fuzzy' version of k-Means which comes very close to EM for mixture models.

EM convergence: Dempster, Laird and Rubin proved a theorem stating that EM always converges to a local maximum, but their proof was wrong. In 1983, Wu gave a number of regularity conditions sufficient to ensure convergence to a local maximum.