Machine Learning Linear Classification

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Linear Classification

Let $\mathcal{X}=\mathbb{R}^d$ be the input space, then the classifier $f:\mathbb{R}^d \to \{-1,1\}$ has the form

$$f(x) = \operatorname{sign}(\langle w, x \rangle + b) = \begin{cases} 1 & \text{if } \langle w, x \rangle + b > 0, \\ -1 & \text{if } \langle w, x \rangle + b \leq 0. \end{cases}$$

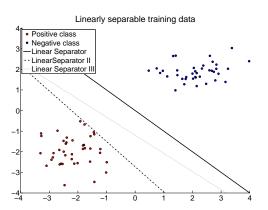
Separation of the input space \mathbb{R}^d into two half spaces.

A training set $T = (X_i, Y_i)_{i=1}^n$ is **linearly separable** if there exists a weight vector w and an offset b such that,

$$Y_i f(X_i) = Y_i (\langle w, X_i \rangle + b) > 0, \quad \forall i = 1, \ldots, n,$$

 \Rightarrow There exists a **hyperplane** $\{x \in \mathbb{R}^d \mid \langle w, x \rangle + b = 0\}$ which separates the sets $X_+ = \{X_i \in T \mid Y_i = 1\}$ and $X_- = \{X_i \in T \mid Y_i = -1\}$.

Linear Classification II



A training sample of a two-class problem in \mathbb{R}^2 . The two classes are linearly separable and three different decision hyperplanes are shown which separate the two classes.

Linear Classification III

No distinction between the original input space $\mathcal{X} = \mathbb{R}^d$ and a possibly larger **feature space**, where we use basis functions/feature maps ϕ_i

$$x \in \mathbb{R}^d \longrightarrow (\phi_1(x), \ldots, \phi_D(x)),$$

to the feature space \mathbb{R}^D .

Functions are linear in the parameters but not necessarily linear in the input space!

Linear Classification III

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Definition

Let $g: \mathcal{X} \to \mathbb{R}$ be a function and f(x) = sign(g(x)) be the resulting classifier with output in $\mathcal{Y} = \{-1, 1\}$, then we call the set

$$\{x \in \mathcal{X} \mid g(x) = 0\},\$$

the **decision boundary** of the classifier f.

Linear Classification IV

Three linear methods:

- Linear Discriminant Analysis,
- Logistic Regression,
- Support Vector Machines.

All three methods construct a **linear** classifier but all three have different **objectives**.

Linear Discriminant Analysis (LDA)

Properties and Motivation:

- often also called Fisher Discriminant Analysis named after its inventor Ronald A. Fisher, the "father" of parametric statistics.
- In **linear** classification the data x enters the classifier only via the inner product $\langle w, x \rangle$ with the weight vector.
 - ▶ Projection of the feature space \mathbb{R}^D onto the line $L = \{\alpha w \mid \alpha \in \mathbb{R}\}$,
 - Classification of the data by thresholding.

What is the best projection in the sense that it optimally separates the data ?

LDA II

Definitions:

• The class **centroids** m_+ and m_- of the positive and negative class are defined as:

$$m_{+} = \frac{1}{n_{+}} \sum_{\{i \mid Y_{i}=1\}} X_{i}, \qquad m_{-} = \frac{1}{n_{-}} \sum_{\{i \mid Y_{i}=-1\}} X_{i},$$

where $n_+ = |\{i \mid Y_i = 1\}|$ and $n_- = |\{i \mid Y_i = -1\}|$.

 The within-class covariances of the projections of the positive and negative class are given by

$$\sigma_{w,+}^{2} = \sum_{\{i \mid Y_{i}=1\}} \left(\langle w, X_{i} \rangle - \langle w, m_{+} \rangle \right)^{2},$$

$$\sigma_{w,-}^{2} = \sum_{\{i \mid Y_{i}=-1\}} \left(\langle w, X_{i} \rangle - \langle w, m_{-} \rangle \right)^{2}.$$

LDA III

Criterion:

- Large Distance of the projected class centroids $\langle w, m_+ \rangle$ and $\langle w, m_- \rangle$,
 - Small variances around the projected class centroids.
- The Fisher criterion is defined as

$$J(w) = \frac{\langle w, m_+ - m_- \rangle^2}{\sigma_{w,+}^2 + \sigma_{w,-}^2}.$$

LDA IV

Fisher criterion in matrix formulation:

The **between-class covariance** matrix C_B is defined as

$$C_B = (m_+ - m_-)(m_+ - m_-)^T$$

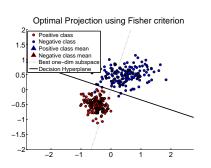
and the total within-class covariance matrix C_W as

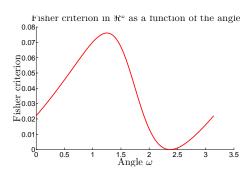
$$C_W = \sum_{\{i \mid Y_i = 1\}} (X_i - m_+)(X_i - m_+)^T + \sum_{\{i \mid Y_i = -1\}} (X_i - m_-)(X_i - m_-)^T.$$

Then the **Fisher criterion** J(w) can be written as

$$J(w) = \frac{\langle w, C_B w \rangle}{\langle w, C_W w \rangle}.$$

LDA V





Left: Projection w optimizing the Fisher criterion and the optimal projection line $\{\alpha w + \frac{1}{2}(m_+ + m_-) \mid \alpha \in \mathbb{R}\}$. **Right:** The Fisher criterion as a function of the angle ω , where ω is a parameterization of all weight vectors $w = (\cos(\omega), \sin(\omega))$ in \mathbb{R}^2 .

Optimal Projection

Lemma

The optimal projection $w^* = \underset{w \in \mathbb{R}^D}{\operatorname{arg max}} J(w)$ is given by

$$w^* = C_W^{-1}(m_+ - m_-).$$

Proof: We have

$$\nabla_{w}J(w)=2\frac{1}{\langle w,C_{W}w\rangle}C_{B}w-2\frac{\langle w,C_{B}w\rangle}{\langle w,C_{W}w\rangle^{2}}C_{W}w.$$

We solve for the extrema of J(w) and get

$$\frac{\langle w, C_W w \rangle}{\langle w, C_B w \rangle} C_B w = C_W w.$$

Now, $C_B w$ is always proportional to $m_+ - m_-$ and $\frac{\langle w, C_W w \rangle}{\langle w, C_B w \rangle}$ is just a scalar factor. Therefore

$$w^* \propto C_W^{-1}(m_+ - m_-).$$

LDA VI

• Final classifier:

$$f(x) = sign(\langle w, x \rangle + b).$$

Determine **the threshold** *b* by minimizing the training error.

Optimal Projection can also be derived using least squares.
 This yields the following optimization problem

$$(w',w_0') = \mathop{\arg\min}_{w \in \mathbb{R}^D, w_0 \in \mathbb{R}} \ \sum_{i=1}^n (Y_i - \langle w, X_i \rangle - w_0)^2.$$

One can prove (exercise)

$$w^* \sim w'$$
.

Dimensionality Reduction

In **Dimensionality Reduction** we would like to have

- a lower dimensional $m \ll D$ representation of the data,
- which preserves the "interesting" properties of the data
 ⇒ In classification: classifier should perform on the new
 m-dimensional space as well as on the original D-dimensional space.

Generalization to the multi-class case

The **between-class covariance** matrix C_B is defined as

$$C_B = \sum_{k=1}^K n_k (m_k - m)(m_k - m)^T.$$

and the total within-class covariance matrix C_W as

$$C_W = \sum_{k=1}^K \sum_{\{i \mid Y_i = k\}} (X_i - m_k)(X_i - m_k)^T,$$

The **Fisher criterion** J(w) stays the same

$$J(w) = \frac{\langle w, C_B w \rangle}{\langle w, C_W w \rangle}.$$

Generalization to the multi-class case

One needs generally a K-1-dimensional subspace in order to separate K classes !

Rayleigh-Ritz principle

Proposition (Rayleigh-Ritz principle)

Let $A \in \mathbb{R}^{d \times d}$ be a symmetric matrix, then

$$\lambda_{\max} = \max_{x \in \mathbb{R}^d} \frac{\langle x, Ax \rangle}{\langle x, x \rangle},$$

is the largest eigenvalue of A and the maximizing argument x_{max} is the corresponding eigenvector. Equivalently,

$$\lambda_{\mathsf{max}} = \max_{x \in \mathbb{R}^d, \ \|x\| = 1} \langle x, Ax \rangle.$$

Other eigenvalues and eigenvectors can be found as follows. Denote by u_1, \ldots, u_r the eigenvectors corresponding to the largest r eigenvalues, then the r+1 largest eigenvalue can be found as,

$$\lambda_{r+1} = \max_{x \in \mathbb{R}^d, \ \langle x, u_s \rangle = 0, \ s = 1, \dots, r} \frac{\langle x, Ax \rangle}{\langle x, x \rangle}.$$

LDA as Dimensionality Reduction

How can we get more projections from the Fisher criterion?

$$J(w) = \frac{\langle w, C_B w \rangle}{\langle w, C_W w \rangle}.$$

The Fisher criterion can be seen as the variational formulation of the **generalized eigenvalue problem**

$$C_{RW} = \lambda C_{WW}$$
.

Generalized Rayleigh-Ritz Principle!

m-dimensional projection is determined by the *m* eigenvectors corresponding to the *m* largest eigenvectors.

Logistic Regression

Logistic Regression:

Original Formulation: Maximum likelihood estimation using the following model for the conditional probability

$$P(Y=1|X=x, w) = \frac{1}{1+e^{-\langle w,\phi(x)\rangle}}.$$

Definition

Given a training sample $T_n = (X_i, Y_i)_{i=1}^n$ with $X_i \in \mathcal{X}$ and $Y_i \in \{-1, 1\}$ and the function space $\mathcal{F} = \{\sum_{i=1}^D w_i \phi_i(x) \mid w \in \mathbb{R}^D\}$ we define **logistic regression** as the mapping $\mathcal{A} : T_n \to \mathcal{F}$ with,

$$T_n \mapsto f_n = \operatorname*{arg\,min}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \log \Big(1 + \exp(-Y_i \langle w, \phi(X_i) \rangle) \Big).$$
 (1)

Empirical risk minimization using the logistic loss!

Logistic Regression II

- no analytical solution,
- solution using a Newton-type gradient descent method. Gradient and the Hessian of the empirical risk:

$$R_{\mathrm{emp}}(w) = \frac{1}{n} \sum_{i=1}^{n} \log \Big(1 + \exp(-Y_i \langle w, \phi(X_i) \rangle) \Big),$$

as

$$\frac{\partial R_{\text{emp}}}{\partial w_{s}}(w) = -\frac{1}{n} \sum_{i=1}^{n} y_{i} \, \phi_{s}(X_{i}) \frac{\exp(-Y_{i} \, \langle w, \phi(X_{i}) \rangle)}{1 + \exp(-Y_{i} \, \langle w, \phi(X_{i}) \rangle)},$$

$$\frac{\partial^{2} R_{\text{emp}}}{\partial w_{r} \partial w_{s}}(w) = \frac{1}{n} \sum_{i=1}^{n} \phi_{s}(X_{i}) \phi_{r}(X_{i}) \frac{\exp(-Y_{i} \, \langle w, \phi(X_{i}) \rangle)}{\left(1 + \exp(-Y_{i} \, \langle w, \phi(X_{i}) \rangle)\right)^{2}}.$$

Logistic Regression III

Newton-Raphson algorithm: with stepsize fixed to 1,

$$w_{\mathrm{new}} = w_{\mathrm{old}} - \left(\frac{\partial^2 R_{\mathrm{emp}}}{\partial w_r \partial w_s}(w)\right)^{-1} \nabla_w R_{\mathrm{emp}}(w),$$

With the diagonal matrices W and D with diagonal entries

$$W_{ii} = \frac{\exp(-Y_i \langle w, \phi(X_i) \rangle)}{(1 + \exp(-Y_i \langle w, \phi(X_i) \rangle)^2}, \qquad D_{ii} = \frac{\exp(-Y_i \langle w, \phi(X_i) \rangle)}{1 + \exp(-Y_i \langle w, \phi(X_i) \rangle)},$$

we can write the gradient and Hessian $H(R_{\mathrm{emp}})$ of R_{emp} as

$$\nabla_w R_{\text{emp}}(w) = -\frac{1}{n} \Phi^T DY, \qquad H(R_{\text{emp}})\big|_w = \frac{1}{n} \Phi^T W \Phi.$$

Logistic Regression IV

Thus we can write the **Newton-Raphson update** as

$$w_{\text{new}} = w_{\text{old}} + \left(\Phi^T W \Phi\right)^{-1} \Phi^T D Y$$

= $\left(\Phi^T W \Phi\right)^{-1} \Phi^T W \left(\Phi w_{\text{old}} + W^{-1} D Y\right) = \left(\Phi^T W \Phi\right)^{-1} \Phi^T W Z$,

with $Z = \Phi w_{\text{old}} + W^{-1}DY$.

Logistic Regression IV

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$$w_{\text{new}} = w_{\text{old}} + \left(\Phi^T W \Phi\right)^{-1} \Phi^T D Y$$

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with $Z = \Phi w_{\text{old}} + W^{-1}DY$.

Weighted least squares problem:

$$\sum_{i=1}^{n} \gamma_{i} (Y_{i} - \langle w, \Phi(X_{i}) \rangle)^{2} = \langle Y - \Phi w, W(Y - \Phi w) \rangle,$$

where $W = \operatorname{diag}(\gamma)$ and solution $w^* = (\Phi^T W \Phi)^{-1} \Phi^T WY$. Each update is the solution of a weighted least squares with output Z

iteratively reweighted least squares

Logistic Regression V

Problem: Empirical risk minimization is prone to overfitting.

Solution: Add regularizer!

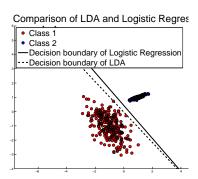
Definition

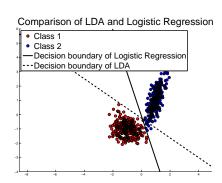
Given a training sample $T_n = (X_i, Y_i)_{i=1}^n$ with $X_i \in \mathcal{X}$ and $Y_i \in \{-1, 1\}$ and the function space $\mathcal{F} = \{\sum_{i=1}^D w_i \phi_i(x) \mid w \in \mathbb{R}^D\}$ we define L_2 -regularized logistic regression as the mapping $\mathcal{A} : T_n \to \mathcal{F}$ with,

$$T_n \mapsto f_n = \operatorname*{arg\,min}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \log \left(1 + \exp(-Y_i \langle w, \phi(X_i) \rangle) \right) + \lambda \|w\|_2^2,$$

where λ is the regularization parameter.

Comparison LDA vs Logistic Regression

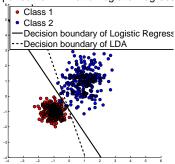




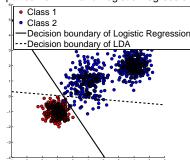
Left: A linearly separable problem, Right: A non-separable problem.

Comparison LDA vs Logistic Regression II

Comparison of LDA and Logistic Regress



Comparison of LDA and Logistic Regression



Left: Original data, **Right:** Adding the second Gaussian blob should not change the decision boundary. However, LDA changes its decision completely.

Support Vector Machines

The linear **support vector machine** can be motivated from different perspectives.

Geometric Perspective: Maximum margin hyperplane

Unique hyperplane which correctly classifies the data and has maximal distance/margin from the training data.

- hard margin case: linearly separable data.
- soft margin case: all kind of data allowed.

Support Vector Machines II

• Linear classifier is determined by the weight vector w and the offset b.

$$f(x) = sign(\langle w, x \rangle + b).$$

- **decision boundary** $\langle w, x \rangle + b = 0$ is the most interesting quantity.
- classifier and the decision boundary are not unique. For $\gamma > 0$, $\tilde{w} = \gamma w$ and $\tilde{b} = \gamma b$ gives same classifier. \Rightarrow fix using canonical hyperplane.

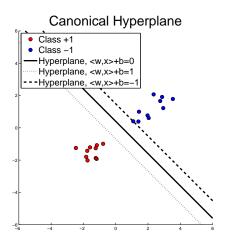
Definition

The pair $(w, b) \in \mathbb{R}^d \times \mathbb{R}$ is said to be in **canonical** form with respect to $X_1, \ldots, X_n \in \mathbb{R}^d$, if it scaled such that

$$\min_{i=1,\ldots,n} |\langle w, X_i \rangle + b| = 1,$$

which implies that the point closest to the hyperplane $h=\{x|\langle w,x\rangle+b=0\}$ has distance $\rho=\frac{1}{\|w\|}$. We call ρ the **geometrical margin** of the hyperplane.

Support Vector Machines III



The canonical hyperplane for a set of training points $(X_i)_{i=1}^n$.

Support Vector Machines IV

Maximum margin hyperplane: a hyperplane which correctly classifies the data and has maximum distance/margin to the data.

Definition

A maximum margin hyperplane (w, b) for a linearly separable set of training data $(X_i, Y_i)_{i=1}^n$ is defined as

$$\max_{w \in \mathbb{R}^d, \ b \in \mathbb{R}} \min\{\|x - X_i\| \mid \langle w, x \rangle + b = 0, \ x \in \mathbb{R}^d, \ i = 1, \dots, n\},\$$

where we optimize over all (w, b) such that $Y_i(\langle w, X_i \rangle + b) > 0$.

Support Vector Machines V

Equivalent formulation:

$$\max_{w \in \mathbb{R}^d, \ b \in \mathbb{R}} \frac{1}{\|w\|}$$
 subject to: $Y_i(\langle w, X_i \rangle + b) \ge 1, \quad \forall i = 1, \dots, n$

Second equivalent formulation:

$$\begin{aligned} & \min_{w \in \mathbb{R}^d, \ b \in \mathbb{R}} \frac{1}{2} \|w\|^2 \\ & \text{subject to:} \ Y_i(\langle w, X_i \rangle + b) \geq 1, \quad \forall i = 1, \dots, n \end{aligned}$$

convex optimization problem: quadratic program

Support Vector Machines VI

Lagrange function: Let $w \in \mathbb{R}^d$ and $\alpha \in \mathbb{R}^n$

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 + \sum_{i=1}^{n} \alpha_i \Big[1 - Y_i(\langle w, X_i \rangle + b) \Big],$$

where $\alpha_i \geq 0$, $\forall i = 1, ..., n$, are the Lagrange multipliers.

Dual Lagrange function:

$$q(\alpha) = \inf_{w \in \mathbb{R}^d, \ b \in \mathbb{R}} L(w, b, \alpha).$$

- since L is convex we can compute the dual using the stationary point,
- Slater condition fulfilled if data is linearly separable ⇒ strong duality, we can solve primal problem via the dual problem.

Support Vector Machines VII

Derivatives:

$$\nabla_{w}L(w,b,\alpha)=w-\sum_{i=1}^{n}\alpha_{i}Y_{i}X_{i}, \qquad \frac{\partial L(w,b,\alpha)}{\partial b}=-\sum_{i=1}^{n}\alpha_{i}Y_{i}.$$

Conditions for global minimum:

$$w = \sum_{i=1}^{n} \alpha_i Y_i X_i, \qquad \sum_{i=1}^{n} \alpha_i Y_i = 0.$$

Plugging these expressions into $L(w, b, \alpha)$ we get the dual Lagrangian

$$q(\alpha) = -\frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j Y_i Y_j \langle X_i, X_j \rangle + \sum_{i=1}^{n} \alpha_i,$$

where $\alpha_i > 0$, $\forall i = 1, ..., n$.

Support Vector Machines VIII

Dual problem:

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j Y_i Y_j \langle X_i, X_j \rangle,$$
 subject to: $\alpha_i \geq 0, \quad i = 1, \dots, n,$
$$\sum_{i=1}^n Y_i \alpha_i = 0.$$

- The dual problem is solved in practice using the SMO (Sequential minimal optimization) method.
- complexity is in the worst case cubic in *n* but often much faster.

Support Vector Machines IX

Karush-Kuhn-Tucker (KKT) conditions: The most important one is the complementary slackness condition:

$$lpha_i > 0 \quad {
m if} \quad \left[1 - Y_i (\langle w, X_i \rangle + b) \right] = 0$$
 and $lpha_i = 0 \quad {
m if} \quad \left[1 - Y_i (\langle w, X_i \rangle + b) \right] < 0.$

or more compactly

$$\alpha_i \Big[1 - Y_i (\langle w, X_i \rangle + b) \Big] = 0.$$

The offset b can thus be determined by averaging the value $b = Y_i - \langle w, X_i \rangle$ over all points with $\alpha_i > 0$:

$$b = \frac{1}{\sum_{i=1}^n \mathbb{1}_{\alpha_i > 0}} \sum_{i=1}^n \mathbb{1}_{\alpha_i > 0} (Y_i - \sum_{i=1}^n \alpha_i Y_i \langle X_i, X_j \rangle).$$

Support Vectors

Final weight vector:

$$w = \sum_{i=1}^{n} \alpha_i Y_i X_i.$$

Only the points closest to the decision boundary contribute to solution

$$\alpha_i > 0 \quad \Leftrightarrow \quad \left[1 - Y_i(\langle w, X_i \rangle + b)\right] = 0,$$

These points are called **support vectors**. The area between the two supporting hyperplanes $\{x \mid \langle w, x \rangle + b = 1\}$ and $\{x \mid \langle w, x \rangle + b = -1\}$ is called the **margin**.

- **1** The weight vector of the support vector machine is typically **sparse** in terms of α .
- Modifications of the training points matter only if they move into the margin.

Convex hull formulation

Equivalent reformulation of the dual problem:

$$\min_{\alpha \in \mathbb{R}^n} \left\| \sum_{i=1, Y_i=1}^n \alpha_i X_i - \sum_{j=1, Y_j=-1}^n \alpha_j X_j \right\|^2,$$
subject to: $\alpha_i \ge 0, \quad i = 1, \dots, n,$

$$\sum_{i=1, Y_i=1}^n \alpha_i = \sum_{j=1, Y_i=-1}^n \alpha_j = 1.$$

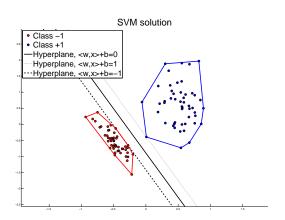
 \Longrightarrow distance between the convex hulls of positive and negative class.

Definition

Given a set T of points $(X_i)_{i=1}^n$ in \mathbb{R}^d . The **convex hull** of T is defined as the set

$$\bigg\{\sum_{i=1}^n \alpha_i X_i \mid \sum_{i=1}^n \alpha_i = 1, \quad \alpha_i \geq 0, \quad i = 1, \dots, n\bigg\}.$$

Example: linearly separable case



A linearly separable problem. The hard margin solution of the SVM is shown together with the convex hulls of the positive and negative class. The points on the margin, that is $\langle w, x \rangle + b = \pm 1$, are called **support** vectors.

Transition to soft-margin

Problems of the hard margin case:

- not all data is linearly separable,
- the hard margin case is often too strict since it is sensitive to outliers.

Relaxation of the constraints:

$$Y_i(\langle w, X_i \rangle + b) \geq 1 - \xi_i$$

where $\xi_i > 0$ are the slack variables.

Primal problem of the soft-margin case:

$$\min_{w \in \mathbb{R}^d, \ b \in \mathbb{R}, \ \xi \in \mathbb{R}^n} \frac{1}{2} \|w\|^2 + \frac{C}{n} \sum_{i=1}^n \xi_i$$
subject to: $Y_i(\langle w, X_i \rangle + b) \ge 1 - \xi_i, \quad \forall i = 1, \dots, n,$

$$\xi_i \ge 0, \quad \forall i = 1, \dots, n$$

Soft Margin as RERM

At the optimum: with $\xi_i \geq 0$,

$$\xi_i = \max \Big(0, 1 - Y_i(\langle w, X_i \rangle + b)\Big).$$

With $f(X_i) = \langle w, X_i \rangle + b$ we note that $\max (0, 1 - y_i f(X_i))$ is nothing else than the **hinge loss**.

Soft Margin SVM is RERM with Hinge loss and L_2 -regularization:

$$\min_{w \in \mathbb{R}^d, \ b \in \mathbb{R}} C \frac{1}{n} \sum_{i=1}^n \max \left(0, 1 - y_i (\langle w, x_i \rangle + b) \right) + \left\| w \right\|^2,$$

Error parameter C is inverse to the regularization parameter $\lambda = \frac{1}{C}$

Lagrangian of Soft Margin

Lagrangian of the soft margin problem:

$$L(w, b, \xi, \alpha, \beta) = \frac{1}{2} \|w\|^2 + \frac{C}{n} \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \alpha_i \left[1 - \xi_i - Y_i(\langle w, X_i \rangle + b) \right] - \sum_{i=1}^{n} \beta_i \xi_i$$

where $\alpha_i \geq 0$, $i = 1, \ldots, n$ and $\beta_i \geq 0$, $i = 1, \ldots, n$.

Conditions for stationary point:

$$w = \sum_{i=1}^{n} \alpha_i Y_i X_i, \qquad \sum_{i=1}^{n} \alpha_i Y_i = 0, \qquad \beta = \frac{C}{n} 1 - \alpha.$$

The last equation can be used to get rid of β . Due to the positivity of β we get the new constraint for α

$$0 \leq \alpha_i \leq \frac{C}{n}, \quad i = 1, \dots, n.$$

Lagrangian of Soft Margin

Dual Lagrangian of the soft margin problem:

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j Y_i Y_j \left\langle X_i, X_j \right\rangle,$$

subject to:
$$0 \le \alpha_i \le \frac{C}{n}$$
, $i = 1, ..., n$, $\sum_{i=1}^n Y_i \alpha_i = 0$.

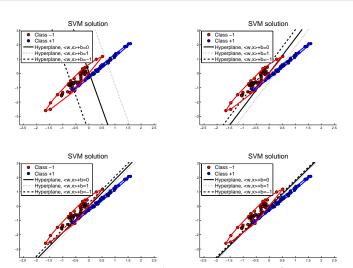
Complementary slackness conditions (part of KKT conditions):

$$\alpha_i \Big[1 - \xi_i - Y_i (\langle w, X_i \rangle + b) \Big] = 0, \quad \text{and} \quad \beta_j \xi_j = 0, \quad i, j = 1, \dots, n.$$

Three classes of points:

- $\alpha_i = 0$: outside the margin and all correctly classified.
- $0 < \alpha_i < \frac{C}{n}$: lie exactly on the margin are all correctly classified.
- $\alpha_i = \frac{C}{n}$: inside the margin, can be misclassified.

Comparison of different C



Top row: error parameter $C=10^1$ (left) and $C=10^2$ (right), Bottom row: error parameter $C=10^3$ (left) and $C=10^4$ (right).