Support vector machines

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Ecole des Ponts - ParisTech

SOCN course 2014

Outline

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1. Constrained optimization, Lagrangian duality and KKT

2. Support vector machines

Constrained optimization, Lagrangian duality and KKT

Review: Constrained optimization

Optimization problem in canonical form

$$\begin{aligned} \min_{\mathbf{x}\in\mathcal{X}} \quad & f(\mathbf{x}) \\ \text{s.t.} \quad & h_i(\mathbf{x}) = 0, \quad i \in [\![1, n]\!] \\ & g_j(\mathbf{x}) \leq 0, \quad j \in [\![1, m]\!] \end{aligned}$$

with

- $\mathcal{X} \subset \mathbb{R}^p$.
- f, g_j functions,
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The problem is convex if f, g_j and $\mathcal{X}$ are convex (w.l.o.g $\mathring{\mathcal{X}} \neq \varnothing$).

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Lagrangian

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\mathbf{x}) + \sum_{i=1}^{n} \lambda_i \, h_i(\mathbf{x}) + \sum_{j=1}^{m} \mu_j \, g_j(\mathbf{x})$$

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Primal vs Dual problem

$$p^* = \min_{\mathbf{x} \in \mathcal{X}} \quad \max_{\boldsymbol{\lambda} \in \mathbb{R}^n, \boldsymbol{\mu} \in \mathbb{R}^m_+} \quad \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) \qquad \text{(P)}$$

$$d^* = \max_{\boldsymbol{\lambda} \in \mathbb{R}^n, \boldsymbol{\mu} \in \mathbb{R}^m_+} \quad \min_{\mathbf{x} \in \mathcal{X}} \quad \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) \qquad \text{(D)}$$

Maxmin inequalities

$$\max_y \min_x f(x,y) \leq \min_x \max_y f(x,y)$$

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Strong duality

In some cases, we have strong duality:

- $d^* = p^*$
- Solutions to (P) and (D) are the same

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Slater's conditions requires that there exists a feasible point which is strictly feasible for all non-affine constraints.

Karush-Kuhn-Tucker conditions

Theorem

For a convex problem defined by differentiable functions f, h_i, g_j, x is an optimal solution if and only if there exists $(\boldsymbol{\lambda}, \boldsymbol{\mu})$ such that the KKT conditions are satisfied.

KKT conditions

$$\nabla f(\mathbf{x}) + \sum_{i=1}^{n} \lambda_i \nabla h_i(\mathbf{x}) + \sum_{j=1}^{m} \mu_j \nabla g_j(\mathbf{x}) = 0 \quad \text{(Lagrangian stationarity)}$$

$$h(\mathbf{x}) = 0, \quad g(\mathbf{x}) \leq 0 \quad \text{(primal feasibility)}$$

$$\mu_j \geq 0 \quad \text{(dual feasibility)}$$

$$\forall j \in [\![1, m]\!], \quad \mu_j \, g_j(\mathbf{x}) = 0 \quad \text{(complementary slackness)}$$

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This leads to

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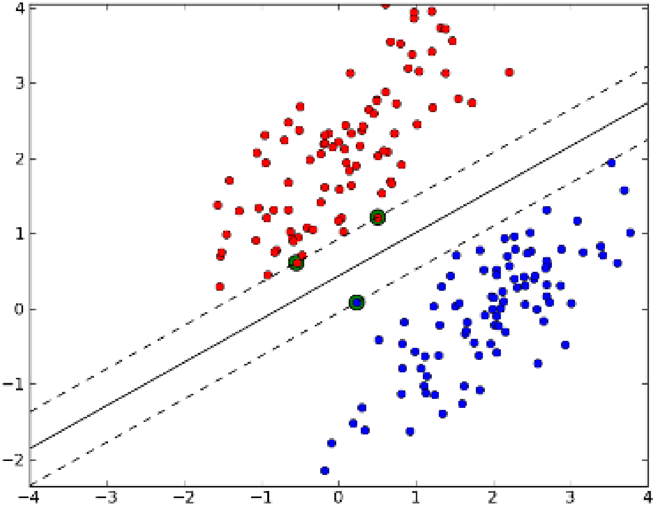
- quadratic program (not a so useful property nowadays)
- unfeasible if the data is not separable

Hard-margin SVM



Soft margin SVM

- Authorize some points to be on the wrong side of the margin
- Penalize by a cost proportional to the distance to the margin
- Introduce some slack variables ξ_i measuring the violation for each datapoint.

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$$\min_{\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad \forall i, \begin{cases} y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \\ \xi_i \geq 0 \end{cases}$$

Lagrangian of the SVM

$$\mathcal{L}(w, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\nu})$$

$$= \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\big(1 - \xi_i - y_i(\mathbf{w}^\top \mathbf{x}_i + b)\big) - \sum_{i=1}^{n}\nu_i\xi_i$$

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$$\begin{aligned} &= \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i + \sum_{i=1}^{n}\alpha_i\left(1 - \xi_i - y_i(\mathbf{w}^\top\mathbf{x}_i + b)\right) - \sum_{i=1}^{n}\nu_i\xi_i \\ &= \frac{1}{2}\|\mathbf{w}\|^2 - \mathbf{w}^\top\left(\sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i\right) + \sum_{i=1}^{n}\xi_i\left(C - \alpha_i - \nu_i\right) - \sum_{i=1}^{n}\alpha_i y_i b + \sum_{i=1}^{n}\alpha_i \end{aligned}$$

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$$= \frac{1}{2}\|\mathbf{w}\|^2 - \mathbf{w}^\top\Big(\sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i\Big) + \sum_{i=1}^{n}\xi_i\,(C - \alpha_i - \nu_i) - \sum_{i=1}^{n}\alpha_i y_i b + \sum_{i=1}^{n}\alpha_i$$

Stationarity of the Lagrangian

$$\nabla_{\mathbf{w}}\mathcal{L} = \mathbf{w} - \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i, \quad \frac{\partial \mathcal{L}}{\partial \xi_i} = C - \alpha_i - \nu_i \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial b} = \sum_{i=1}^{n}\alpha_i y_i.$$

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So that $\nabla\mathcal{L} = 0$ leads to

$$\mathbf{w} = \sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i, \quad 0 \le \alpha_i \le C \quad \text{and} \quad \sum_{i=1}^{n}\alpha_i y_i = 0.$$

Dual of the SVM

$$\max_{\boldsymbol{\alpha}} \; -\frac{1}{2}\Big\|\sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i\Big\|^2 + \sum_{i=1}^{n}\alpha_i$$

$$\text{s.t.} \quad \sum_{i=1}^{n}\alpha_i y_i = 0, \qquad \forall i,\; 0 \le \alpha_i \le C.$$

$$\max_{\boldsymbol{\alpha}} \; -\frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{D_y K D_y}\boldsymbol{\alpha} + \boldsymbol{\alpha}^\top \mathbf{1}$$

$$\text{s.t.} \quad \boldsymbol{\alpha}^\top \mathbf{y} = 0, \qquad 0 \le \boldsymbol{\alpha} \le C.$$

with

- $\mathbf{y}^\top = (y_1, \ldots, y_n)$ the vector of labels
- $\mathbf{D_y} = \mathrm{Diag}(\mathbf{y})$ a diagonal matrix with the label
- $\mathbf{K}$ the Gram matrix with $\mathbf{K}_{ij} = \mathbf{x}_i^\top \mathbf{x}_j$

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$$\max_{\boldsymbol{\alpha}} -\frac{1}{2}\sum_{1\leq i,j\leq n} \alpha_i\alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j + \sum_{i=1}^{n} \alpha_i$$

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The set S of support vectors is therefore composed of some points on the margin and all incorrectly placed points.

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- The optimal solution is $\mathbf{w}^* = \sum_{i \in S} \alpha_i^* y_i \mathbf{x}_i$, i.e. a weighted combination of the support vectors
- The solution does not depend on the well-classified points

$\rightarrow$ Leads to working set strategies.

$\rightarrow$ Computational gain

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Representer property for the SVM

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f^*(\mathbf{x}) &= \mathbf{w}^{*\top}\mathbf{x} + b \\
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$\rightarrow$ Can we use another dot product than the one associated to the usual Euclidean distance in $\mathbb{R}^p$?

Hinge loss interpretation of the SVM

$$\min_{\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad \forall i, \begin{cases} y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i \\ \xi_i \geq 0 \end{cases}$$

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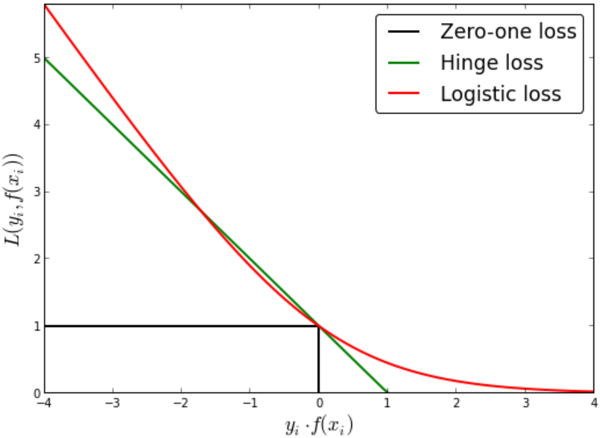
Our problem is now of the form

$$\min_{\mathbf{w}} \sum_{i=1}^{n} \ell(f(\mathbf{x}_i), y_i) + \frac{1}{2C}\|\mathbf{w}\|^2 \qquad \text{with} \quad f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b.$$

Hinge loss vs other losses



The hinge loss is the "least convex" loss which upper bounds the 0-1 loss and equals 0 for large scores.

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→ Penalizes more strongly misclassified points

→ Less robust to outliers

→ Tends to be less sparse

→ Score in $[0, 1]$ for n large, interpretable as a probability.

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- Naive choice: $C_+ = C/n_+$ and $C_- = C/n_-$

  ⚠ Is suboptimal in theory and in practice !!

  $\rightarrow$ Better to search for the optimal hyperparameter pair (C_+, C_-).