Introduction to Machine Learning

Linear Support Vector Machines Soft-Margin SVM



Learning goals

- Understand that the hard-margin SVM problem is only solvable for linearly separable data
- Know that the soft-margin SVM problem therefore allows margin violations
- The degree to which margin violations are tolerated is controlled by a hyperparameter



NON-SEPARABLE DATA





- $\bullet\,$ Assume that dataset ${\cal D}$ is not linearly separable.
- Margin maximization becomes meaningless because the hard-margin SVM optimization problem has contradictory constraints and thus an empty **feasible region**.

MARGIN VIOLATIONS

- We still want a large margin for most of the examples.
- We allow violations of the margin constraints via slack vars $\zeta^{(i)} \ge 0$

$$y^{(i)}\left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \boldsymbol{\theta}_0\right) \geq 1 - \zeta^{(i)}$$

• Even for separable data, a decision boundary with a few violations and a large average margin may be preferable to one without any violations and a small average margin.





We assume $\gamma = 1$ to not further complicate presentation.

MARGIN VIOLATIONS

- Now we have two distinct and contradictory goals:
 - Maximize the margin.
 - 2 Minimize margin violations.
- Let's minimize a weighted sum of them: $\frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n \zeta^{(i)}$
- Constant C > 0 controls the relative importance of the two parts.





SOFT-MARGIN SVM

The linear **soft-margin** SVM is the convex quadratic program:

$$\begin{array}{ll} \min_{\boldsymbol{\theta},\boldsymbol{\theta}_{0},\boldsymbol{\zeta}^{(i)}} & \frac{1}{2} \|\boldsymbol{\theta}\|^{2} + C \sum_{i=1}^{n} \boldsymbol{\zeta}^{(i)} \\ \text{s.t.} & \boldsymbol{y}^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \boldsymbol{\theta}_{0} \right) \geq 1 - \boldsymbol{\zeta}^{(i)} \quad \forall i \in \{1, \dots, n\}, \\ \text{and} & \boldsymbol{\zeta}^{(i)} \geq 0 \quad \forall i \in \{1, \dots, n\}. \end{array}$$

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This is called "soft-margin" SVM because the "hard" margin constraint is replaced with a "softened" constraint that can be violated by an amount $\zeta^{(i)}$.

LAGRANGE FUNCTION AND KKT

The Lagrange function of the soft-margin SVM is given by:

$$\mathcal{L}(\boldsymbol{\theta}, \theta_0, \boldsymbol{\zeta}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2} \|\boldsymbol{\theta}\|_2^2 + C \sum_{i=1}^n \zeta^{(i)} - \sum_{i=1}^n \alpha_i \left(y^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \theta_0 \right) - 1 + \zeta^{(i)} \right) - \sum_{i=1}^n \mu_i \zeta^{(i)} \quad \text{with Lagrange multipliers } \boldsymbol{\alpha} \text{ and } \boldsymbol{\mu}.$$

The KKT conditions for i = 1, ..., n are:

$$\begin{aligned} \alpha_i &\geq \mathbf{0}, \qquad \mu_i \geq \mathbf{0}, \\ \mathbf{y}^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \boldsymbol{\theta}_{\mathbf{0}} \right) - \mathbf{1} + \zeta^{(i)} \geq \mathbf{0}, \qquad \zeta^{(i)} \geq \mathbf{0}, \\ \alpha_i \left(\mathbf{y}^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \boldsymbol{\theta}_{\mathbf{0}} \right) - \mathbf{1} + \zeta^{(i)} \right) &= \mathbf{0}, \qquad \zeta^{(i)} \mu_i = \mathbf{0}. \end{aligned}$$

With these, we derive (see our optimization course) that $\boldsymbol{\theta} = \sum_{i=1}^{n} \alpha_i \boldsymbol{y}^{(i)} \mathbf{x}^{(i)}, \quad \mathbf{0} = \sum_{i=1}^{n} \alpha_i \boldsymbol{y}^{(i)}, \quad \alpha_i = \boldsymbol{C} - \mu_i \quad \forall i = 1, \dots, n.$

SOFT-MARGIN SVM DUAL FORM

Can be derived exactly as for the hard margin case.

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_j \alpha_j y^{(i)} y^{(j)} \left\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right\rangle$$
s.t. $0 \le \alpha_i \le C$,
 $\sum_{i=1}^n \alpha_i y^{(i)} = 0$,

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or, in matrix notation:

$$\begin{split} \max_{\boldsymbol{\alpha} \in \mathbb{R}^n} & \mathbf{1}^T \boldsymbol{\alpha} - \frac{1}{2} \boldsymbol{\alpha}^T \operatorname{diag}(\mathbf{y}) \boldsymbol{K} \operatorname{diag}(\mathbf{y}) \boldsymbol{\alpha} \\ \text{s.t.} & \boldsymbol{\alpha}^T \mathbf{y} = \mathbf{0}, \\ & \mathbf{0} \leq \boldsymbol{\alpha} \leq \boldsymbol{C}, \end{split}$$

with $\boldsymbol{K} := \boldsymbol{X} \boldsymbol{X}^{T}$.

COST PARAMETER C

- The parameter *C* controls the trade-off between the two conflicting objectives of maximizing the size of the margin and minimizing the frequency and size of margin violations.
- It is known under different names, such as "trade-off parameter", "regularization parameter", and "complexity control parameter".
- For sufficiently large *C* margin violations become extremely costly, and the optimal solution does not violate any margins if the data is separable. The hard-margin SVM is obtained as a special case.

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SUPPORT VECTORS

There are three types of training examples:

- Non-SVs have α_i = 0 (⇒ μ_i = C ⇒ ζ⁽ⁱ⁾ = 0) and can be removed from the problem without changing the solution. Their margin yf(x) ≥ 1. They are always classified correctly and are never inside of the margin.
- SVs with 0 < α_i < C (⇒ μ_i > 0 ⇒ ζ⁽ⁱ⁾ = 0) are located exactly on the margin and have yf(x) = 1.
- SVs with α_i = C have an associated slack ζ⁽ⁱ⁾ ≥ 0. They can be on the margin or can be margin violators with yf(x) < 1 (they can even be misclassified if ζ⁽ⁱ⁾ ≥ 1).

As for hard-margin case: on the margin we can have SVs and non-SVs.





UNIQUENESS OF THE SOLUTION

The primal and the dual form of the SVM are convex problems, so each local minimum is a global minimum.

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