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

 $\overline{\mathbf{C}}$

- Assume that dataset 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 $\zeta^{(i)}\geq 0$

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

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

SOFT-MARGIN SVM

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

$$
\min_{\theta, \theta_0, \zeta^{(i)}} \quad \frac{1}{2} \|\theta\|^2 + C \sum_{i=1}^n \zeta^{(i)}
$$
\ns.t.
$$
y^{(i)} \left(\left\langle \theta, \mathbf{x}^{(i)} \right\rangle + \theta_0 \right) \ge 1 - \zeta^{(i)} \quad \forall i \in \{1, ..., n\},
$$
\nand
$$
\zeta^{(i)} \ge 0 \quad \forall i \in \{1, ..., n\}.
$$

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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 ζ (*i*) .

LAGRANGE FUNCTION AND KKT

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

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

$$
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$$

The KKT conditions for $i = 1, \ldots, n$ are:

$$
\alpha_i \geq 0, \qquad \mu_i \geq 0,
$$

$$
y^{(i)}\left(\left\langle \theta, \mathbf{x}^{(i)} \right\rangle + \theta_0\right) - 1 + \zeta^{(i)} \geq 0, \qquad \zeta^{(i)} \geq 0,
$$

$$
\alpha_i\left(y^{(i)}\left(\left\langle \theta, \mathbf{x}^{(i)} \right\rangle + \theta_0\right) - 1 + \zeta^{(i)}\right) = 0, \qquad \zeta^{(i)}\mu_i = 0.
$$

With these, we derive (see our optimization course) that P*n* P*n* (*i*)

$$
\boldsymbol{\theta} = \sum_{i=1} \alpha_i \mathbf{y}^{(i)} \mathbf{x}^{(i)}, \quad 0 = \sum_{i=1} \alpha_i \mathbf{y}^{(i)}, \quad \alpha_i = C - \mu_i \quad \forall i = 1, \ldots, n.
$$

SOFT-MARGIN SVM DUAL FORM

Can be derived exactly as for the hard margin case.

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

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:

$$
\max_{\alpha \in \mathbb{R}^n} \quad \mathbf{1}^T \alpha - \frac{1}{2} \alpha^T \operatorname{diag}(\mathbf{y}) \mathbf{K} \operatorname{diag}(\mathbf{y}) \alpha
$$
\ns.t. $\alpha^T \mathbf{y} = 0$,
\n $0 \le \alpha \le C$,

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

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.

SUPPORT VECTORS

There are three types of training examples:

- Non-SVs have $\alpha_i = \mathsf{0} \ (\Rightarrow \mu_i = \mathsf{C} \Rightarrow \zeta^{(i)} = \mathsf{0})$ 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 $<\alpha_{i}<{\cal C} \,(\Rightarrow\mu_{i}>0\Rightarrow\zeta^{(i)}=0)$ are located exactly on the margin and have $yf(\mathbf{x}) = 1$.
- SVs with $\alpha_i = C$ have an associated slack $\zeta^{(i)} \geq 0$. They can be on the margin or can be margin violators with $yf(x) < 1$ (they can even be misclassified if $\zeta^{(i)} \geq 1$).

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

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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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