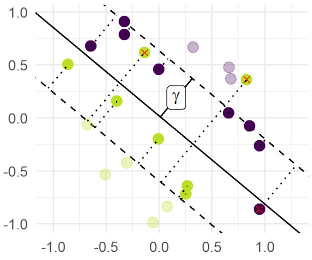
Introduction to Machine Learning

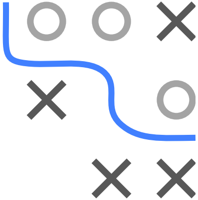
Linear Support Vector Machines
Soft-Margin SVM

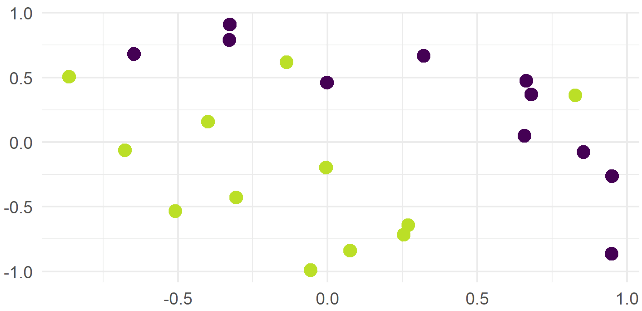


Learning goals

- 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





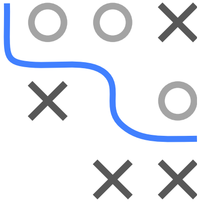
- Assume that dataset $\mathcal{D}$ is not linearly separable.
- Margin maximization becomes meaningless because the hard-margin SVM optimization problem has contradictory constraints and thus an empty **feasible region**.

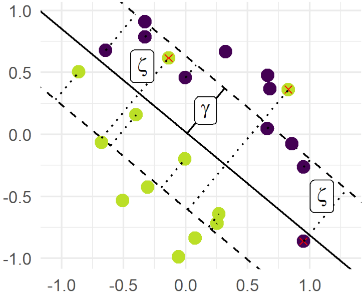
MARGIN VIOLATIONS

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

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

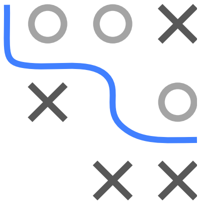
- Even for separable data, a decision boundary with a few violations and a large average margin may be preferable to one without any violations and a small average margin.



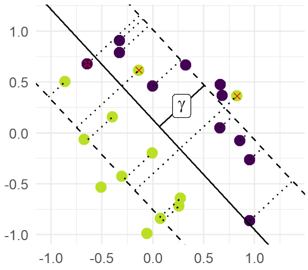


We assume $\gamma = 1$ to not further complicate presentation.

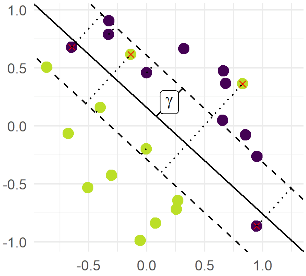
MARGIN VIOLATIONS



- 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.



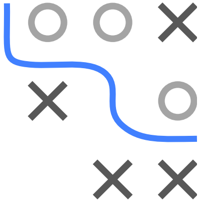
C = 0.5



C = 100

SOFT-MARGIN SVM

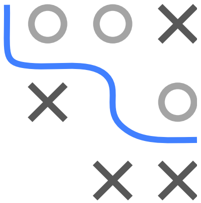
The linear **soft-margin** SVM is the convex quadratic program:



$$
\begin{aligned}
\min_{\boldsymbol{\theta},\boldsymbol{\theta}_0,\zeta^{(i)}} \quad & \frac{1}{2}\|\boldsymbol{\theta}\|^2 + C\sum_{i=1}^{n}\zeta^{(i)} \\
\text{s.t.} \quad & y^{(i)}\left(\left\langle\boldsymbol{\theta},\mathbf{x}^{(i)}\right\rangle + \boldsymbol{\theta}_0\right) \geq 1 - \zeta^{(i)} \quad \forall\, i \in \{1,\dots,n\}, \\
\text{and} \quad & \zeta^{(i)} \geq 0 \quad \forall\, i \in \{1,\dots,n\}.
\end{aligned}
$$

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:

$$\mathcal{L}(\boldsymbol{\theta}, \theta_0, \boldsymbol{\zeta}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = \frac{1}{2}\|\boldsymbol{\theta}\|_2^2 + C\sum_{i=1}^{n}\zeta^{(i)} - \sum_{i=1}^{n}\alpha_i\left(y^{(i)}\left(\left\langle\boldsymbol{\theta}, \mathbf{x}^{(i)}\right\rangle + \boldsymbol{\theta}_0\right) - 1 + \zeta^{(i)}\right)$$

$$- \sum_{i=1}^{n}\mu_i\zeta^{(i)} \quad \text{with Lagrange multipliers } \boldsymbol{\alpha} \text{ and } \boldsymbol{\mu}.$$

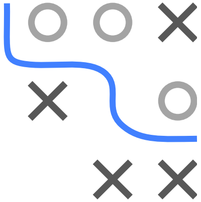
The KKT conditions for $i = 1, \dots, n$ are:

$$\begin{aligned}
\alpha_i &\geq 0, & \mu_i &\geq 0, \\
y^{(i)}\left(\left\langle\boldsymbol{\theta}, \mathbf{x}^{(i)}\right\rangle + \boldsymbol{\theta}_0\right) - 1 + \zeta^{(i)} &\geq 0, & \zeta^{(i)} &\geq 0, \\
\alpha_i\left(y^{(i)}\left(\left\langle\boldsymbol{\theta}, \mathbf{x}^{(i)}\right\rangle + \boldsymbol{\theta}_0\right) - 1 + \zeta^{(i)}\right) &= 0, & \zeta^{(i)}\mu_i &= 0.
\end{aligned}$$

With these, we derive (see our optimization course) that

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

SOFT-MARGIN SVM DUAL FORM



Can be derived exactly as for the hard margin case.

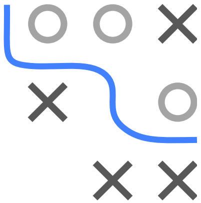
$$\begin{aligned} \max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} \left\langle \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \right\rangle \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \\ & \sum_{i=1}^{n}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

or, in matrix notation:

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

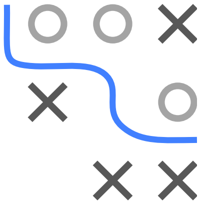
with $\boldsymbol{K} := \mathbf{X}\mathbf{X}^T$.

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.

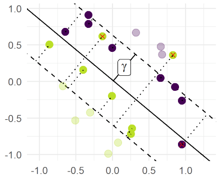
SUPPORT VECTORS



There are three types of training examples:

- Non-SVs have $\alpha_i = 0$ ($\Rightarrow \mu_i = C \Rightarrow \zeta^{(i)} = 0$) and can be removed from the problem without changing the solution. Their margin $yf(\mathbf{x}) \geq 1$. They are always classified correctly and are never inside of the margin.
- SVs with $0 < \alpha_i < C$ ($\Rightarrow \mu_i > 0 \Rightarrow \zeta^{(i)} = 0$) 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 $yf(\mathbf{x}) < 1$ (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.



UNIQUENESS OF THE SOLUTION

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