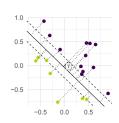
Introduction to Machine Learning

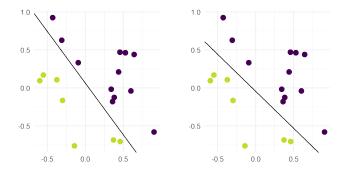
Linear Hard Margin SVM



Learning goals

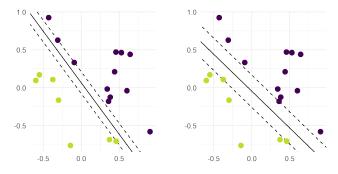
- Know that the hard-margin SVM maximizes the margin between data points and hyperplane
- Know that this is a quadratic program
- Know that support vectors are the data points closest to the separating hyperplane

LINEAR CLASSIFIERS



- We want study how to build a binary, linear classifier from solid geometrical principles.
- Which of these two classifiers is "better"?

LINEAR CLASSIFIERS



- We want study how to build a binary, linear classifier from solid geometrical principles.
- Which of these two classifiers is "better"?
- \rightarrow The decision boundary on the right has a larger **safety margin**.

SUPPORT VECTOR MACHINES: GEOMETRY

For labeled data
$$\mathcal{D} = ((\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)}))$$
, with $y^{(i)} \in \{-1, +1\}$:

• Assume linear separation by $f(\mathbf{x}) = \boldsymbol{\theta}^{\top} \mathbf{x} + \theta_0$, such that all +-observations are in the positive halfspace

$$\{\mathbf{x}^{(i)} \in \mathcal{X} : f(\mathbf{x}) > 0\}$$

and all —-observations are in the negative halfspace

$$\{\mathbf{x}\in\mathcal{X}:f(\mathbf{x})<0\}.$$

• For a linear separating hyperplane, we have

$$y^{(i)}\underbrace{\left(\boldsymbol{\theta}^{\top}\mathbf{x}^{(i)} + \theta_{0}\right)}_{=f\left(\mathbf{x}^{(i)}\right)} > 0 \quad \forall i \in \{1, 2, ..., n\}.$$

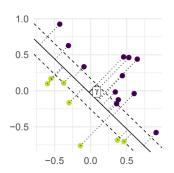
SUPPORT VECTOR MACHINES: GEOMETRY

0

$$d\left(f,\mathbf{x}^{(i)}\right) = \frac{y^{(i)}f\left(\mathbf{x}^{(i)}\right)}{\|\boldsymbol{\theta}\|} = y^{(i)}\frac{\boldsymbol{\theta}^{T}\mathbf{x}^{(i)} + \theta_{0}}{\|\boldsymbol{\theta}\|}$$

computes the (signed) distance to the separating hyperplane $f(\mathbf{x})$, positive for correct classifications, negative for incorrect.

• This expression becomes negative for misclassified points.

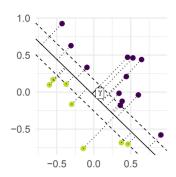


SUPPORT VECTOR MACHINES: GEOMETRY

• The distance of f to the whole dataset \mathcal{D} is the smallest distance

$$\gamma = \min_{i} \left\{ d\left(f, \mathbf{x}^{(i)}\right) \right\}.$$

• This represents the "safety margin", it is positive if *f* separates and we want to maximize it.



We formulate the desired property of a large "safety margin" as an optimization problem:

$$\begin{aligned} & \max_{\boldsymbol{\theta}, \theta_0} & \gamma \\ & \text{s.t.} & \quad \boldsymbol{d}\left(\boldsymbol{f}, \mathbf{x}^{(i)}\right) \geq \gamma & \forall \, i \in \{1, \dots, n\}. \end{aligned}$$

- The constraints mean: We require that any instance i should have a "safety" distance of at least γ from the decision boundary defined by $f = \boldsymbol{\theta}^T + \theta_0 \mathbf{x}$.
- Our objective is to maximize the "safety" distance.

We reformulate the problem:

$$\label{eq:starting_problem} \begin{split} \max_{\boldsymbol{\theta}, \boldsymbol{\theta}_0} \quad & \gamma \\ \text{s.t.} \quad & \frac{y^{(i)} \left(\left< \boldsymbol{\theta}, \mathbf{x}^{(i)} \right> + \boldsymbol{\theta}_0 \right)}{\|\boldsymbol{\theta}\|} \geq \gamma \quad \forall \, i \in \{1, \dots, n\}. \end{split}$$

ullet The inequality is rearranged by multiplying both sides with $\|oldsymbol{ heta}\|$:

$$\begin{aligned} & \max_{\boldsymbol{\theta}, \boldsymbol{\theta}_0} \quad \gamma \\ & \text{s.t.} \quad \boldsymbol{y}^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \boldsymbol{\theta}_0 \right) \geq \|\boldsymbol{\theta}\| \gamma \quad \forall \, i \in \{1, \dots, n\}. \end{aligned}$$

 Note that the same hyperplane does not have a unique representation:

$$\{\mathbf{x} \in \mathcal{X} \mid \boldsymbol{\theta}^{\top} \mathbf{x} = \mathbf{0}\} = \{\mathbf{x} \in \mathcal{X} \mid \boldsymbol{c} \cdot \boldsymbol{\theta}^{\top} \mathbf{x} = \mathbf{0}\}$$

for arbitrary $c \neq 0$.

• To ensure uniqueness of the solution, we make a reference choice – we only consider hyperplanes with $\|\theta\| = 1/\gamma$:

$$\begin{array}{ll} \max\limits_{\boldsymbol{\theta}, \theta_0} & \gamma \\ \text{s.t.} & \mathbf{y}^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \theta_0 \right) \geq 1 \quad \forall \, i \in \{1, \dots, n\}. \end{array}$$

• Substituting $\gamma = 1/\|\boldsymbol{\theta}\|$ in the objective yields:

$$\begin{array}{ll} \max _{\boldsymbol{\theta}, \theta_0} & \frac{1}{\|\boldsymbol{\theta}\|} \\ \text{s.t.} & y^{(i)}\left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \theta_0\right) \geq 1 \quad \forall \, i \in \{1, \dots, n\}. \end{array}$$

• Maximizing $1/\|\theta\|$ is the same as minimizing $\|\theta\|$, which is the same as minimizing $\frac{1}{2}\|\theta\|^2$:

$$\min_{\boldsymbol{\theta}, \theta_0} \quad \frac{1}{2} \|\boldsymbol{\theta}\|^2
\text{s.t.} \quad y^{(i)} \left(\left\langle \boldsymbol{\theta}, \mathbf{x}^{(i)} \right\rangle + \theta_0 \right) \ge 1 \quad \forall i \in \{1, \dots, n\}.$$

QUADRATIC PROGRAM

We derived the following optimization problem:

$$\begin{split} \min_{\boldsymbol{\theta}, \theta_0} & \quad \frac{1}{2} \|\boldsymbol{\theta}\|^2 \\ \text{s.t.} & \quad \boldsymbol{y}^{(i)} \left(\left\langle \boldsymbol{\theta}, \boldsymbol{x}^{(i)} \right\rangle + \theta_0 \right) \geq 1 \quad \forall \, i \in \{1, \dots, n\}. \end{split}$$

This turns out to be a **convex optimization problem** – particularly, a **quadratic program**: The objective function is quadratic, and the constraints are linear inequalities.

This is called the **primal** problem. We will later show that we can also derive a dual problem from it.

We will call this the linear hard-margin SVM.

SUPPORT VECTORS

- There exist instances $(\mathbf{x}^{(i)}, y^{(i)})$ with minimal margin $y^{(i)}f(\mathbf{x}^{(i)}) = 1$, fulfilling the inequality constraints with equality.
- They are called **support vectors (SVs)**. They are located exactly at a distance of $\gamma = 1/\|\theta\|$ from the separating hyperplane.
- It is already geometrically obvious that the solution does not depend on the non-SVs! We could delete them from the data and would arrive at the same solution.

