Machine Learning

Support Vector Machines

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Classification and Margin

Consider a classification problem with two classes:

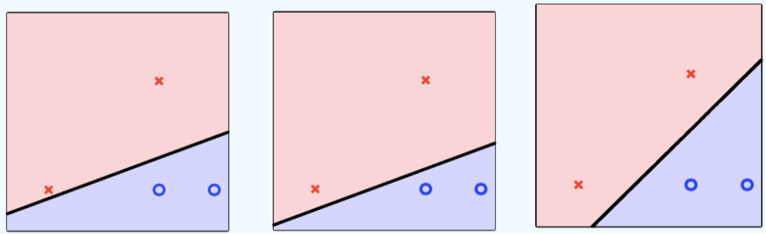
- instance set $\mathcal{X} = \mathbb{R}^d$
- label set $\mathcal{Y} = \{-1, 1\}$.

Training data: $S = ((\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m))$

Hypothesis set $\mathcal{H}$ = halfspaces

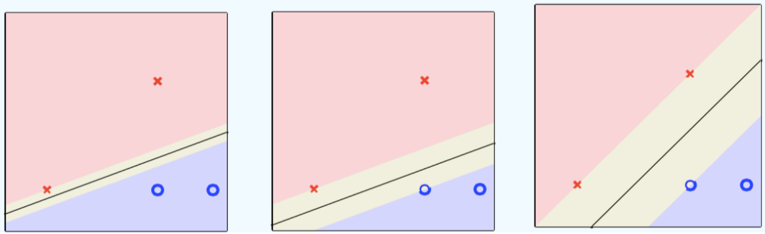
Assumption: data is linearly separable $\Rightarrow$ there exist a halfspace that perfectly classifies the training set

In general: multiple separating hyperplanes: $\Rightarrow$ which one is the best choice?



Classification and Margin

The last one seems the best choice, since it can tolerate more "noise".



Informally, for a given separating halfspace we define its *margin* as its minimum distance to an example in the training set S.

Intuition: best separating hyperplane is the one with largest margin.

How do we find it?

Linearly Separable Training Set

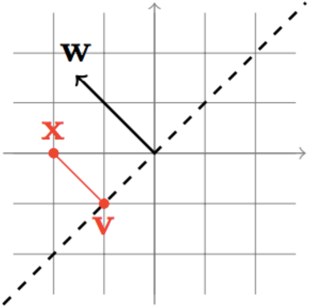
Training set $S = ((\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m))$ is *linearly separable* if there exists a halfspace $(\mathbf{w}, b)$ such that $y_i = \text{sign}(\langle \mathbf{w}, \mathbf{x}_i \rangle + b)$ for all $i = 1, \ldots, m$.

Equivalent to:

$$\forall i = 1, \ldots, m : y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) > 0$$

Informally: *margin* of a separating hyperplane is its minimum distance to an example in the training set S

Separating Hyperplane and Margin



Given hyperplane defined by $L = \{\mathbf{v} : \langle \mathbf{w}, \mathbf{v} \rangle + b = 0\}$, and given $\mathbf{x}$, the distance of $\mathbf{x}$ to L is

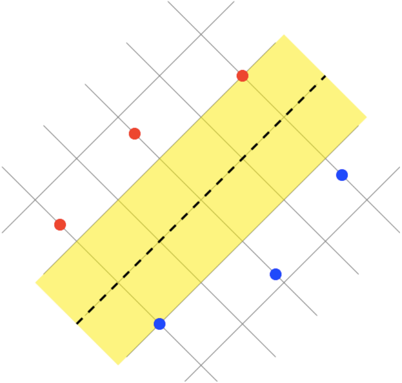
$$d(\mathbf{x}, L) = \min\{||\mathbf{x} - \mathbf{v}|| : \mathbf{v} \in L\}$$

Claim: if $||\mathbf{w}|| = 1$ then $d(\mathbf{x}, L) = |\langle \mathbf{w}, \mathbf{x} \rangle + b|$ (Proof: Claim 15.1 [UML])

Margin and Support Vectors

The *margin* of a separating hyperplane is the distance of the closest example in training set to it. If $||\mathbf{w}|| = 1$ the margin is:

$$\min_{i \in \{1,\ldots,m\}} |\langle \mathbf{w}, \mathbf{x}_i \rangle + b|$$



The closest examples are called *support vectors*

Support Vector Machine (SVM)

Hard-SVM: seek for the separating hyperplane with largest margin (only for linearly separable data)

Computational problem:

$$\arg \overbrace{\max_{(\mathbf{w},b):||\mathbf{w}||=1} \underbrace{\min_{i\in\{1,\dots,m\}} |\langle \mathbf{w}, \mathbf{x}_i\rangle + b|}_{\text{margin}}}^{\text{largest margin}}$$

subject to $\forall i : y_i(\langle \mathbf{w}, \mathbf{x}_i\rangle + b) > 0$

Equivalent formulation (due to separability assumption):

$$\arg \max_{(\mathbf{w},b):||\mathbf{w}||=1} \min_{i\in\{1,\dots,m\}} y_i(\langle \mathbf{w}, \mathbf{x}_i\rangle + b)$$

Hard-SVM: Quadratic Programming Formulation

- **input**: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)$
- **solve**:

$$(\mathbf{w}_0, b_0) = \arg\min_{(\mathbf{w},b)} ||\mathbf{w}||^2$$

subject to $\forall i : y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$

- **output**: $\hat{\mathbf{w}} = \frac{\mathbf{w}_0}{||\mathbf{w}_0||}, \hat{b} = \frac{b_0}{||\mathbf{w}_0||}$

Proposition

The output of algorithm above is a solution to the *Equivalent Formulation* in the previous slide.

How do we get a solution? Quadratic optimization problem: objective is convex quadratic function, constraints are linear inequalities $\Rightarrow$ Quadratic Programming solvers!

Equivalent Formulation and Support Vectors

Equivalent formulation (homogeneous halfspaces): assume first component of $\mathbf{x} \in \mathcal{X}$ is 1, then

$$\mathbf{w}_0 = \min_{\mathbf{w}} ||\mathbf{w}||^2 \text{ subject to } \forall i : y_i \langle \mathbf{w}, \mathbf{x}_i \rangle \geq 1$$

"Support Vectors" $=$ vectors at minimum distance from $\mathbf{w}_0$

The support vectors are the only ones that matter for defining $\mathbf{w}_0$!

Proposition

Let $\mathbf{w}_0$ be as above. Let $I = \{i : |\langle \mathbf{w}_0, \mathbf{x}_i \rangle| = 1\}$. Then there exist coefficients $\alpha_1, \ldots, \alpha_m$ such that

$$\mathbf{w}_0 = \sum_{i \in I} \alpha_i \mathbf{x}_i$$

"Support vectors" $= \{\mathbf{x}_i : i \in I\}$

Note: Solving Hard-SVM is equivalent to find α_i for $i = 1, \ldots, m$, and $\alpha_i \neq 0$ only for support vectors

Soft-SVM

Hard-SVM works if data is linearly separable.

What if data is not linearly separable? $\Rightarrow$ soft-SVM

Idea: modify constraints of Hard-SVM to allow for some violation, but take into account violations into objective function

Soft-SVM Constraints

Hard-SVM constraints:

$$y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$$

Soft-SVM constraints:

- *slack variables*: $\xi_1, \ldots, \xi_m \geq 0 \Rightarrow$ vector $\boldsymbol{\xi}$
- for each $i = 1, \ldots, m$: $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i$
- ξ_i: how much constraint $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$ is violated

Soft-SVM minimizes combinations of

- norm of $\mathbf{w}$
- average of ξ_i

Tradeoff among two terms is controlled by a parameter $\lambda \in \mathbb{R}, \lambda > 0$

Soft-SVM: Optimization Problem

- **input**: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)$, parameter $\lambda > 0$
- **solve**:

looks like a regularization problem

$$\min_{\mathbf{w}, b, \xi} \left(\lambda ||\mathbf{w}||^2 + \frac{1}{m} \sum_{i=1}^{m} \xi_i \right)$$

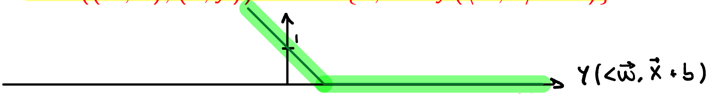
"training error"

subject to $\forall i : y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$

- **output**: $\mathbf{w}, b$

Equivalent formulation: consider the *hinge loss*

$$\ell^{\text{hinge}}((\mathbf{w}, b), (\mathbf{x}, y)) = \max\{0, 1 - y(\langle \mathbf{w}, \mathbf{x} \rangle + b)\}$$



Given $(\mathbf{w}, b)$ and a training S, the empirical risk $L_S^{\text{hinge}}((\mathbf{w}, b))$ is

$$L_S^{\text{hinge}}((\mathbf{w}, b)) = \frac{1}{m} \sum_{i=1}^{m} \ell^{\text{hinge}}((\mathbf{w}, b), (\mathbf{x}_i, y_i))$$

Soft-SVM as RLM

Soft-SVM: solve

$$\min_{\mathbf{w},b,\xi} \left(\lambda ||\mathbf{w}||^2 + \frac{1}{m} \sum_{i=1}^{m} \xi_i \right)$$

subject to $\forall i : y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$

Equivalent formulation with hinge loss:

$$\min_{\mathbf{w},b} \left(\lambda ||\mathbf{w}||^2 + L_S^{\text{hinge}}(\mathbf{w}, b) \right)$$

that is

$$\min_{\mathbf{w},b} \left(\lambda ||\mathbf{w}||^2 + \frac{1}{m} \sum_{i=1}^{m} \ell^{\text{hinge}}((\mathbf{w}, b), (\mathbf{x}_i, y_i)) \right)$$

Note:

- $\lambda ||\mathbf{w}||^2$: ℓ_2 regularization
- $L_S^{\text{hinge}}(\mathbf{w}, b)$: empirical risk for hinge loss

Exercise 4

Assuming we have the following dataset ($x_i \in \mathbb{R}^2$) and by solving the SVM for classification we get the corresponding optimal dual variables:

i	x_i^T	y_i	α_i^*
1	[0.2 -1.4]	-1	0
2	[-2.1 1.7]	1	0
3	[0.9 1]	1	0.5
4	[-1 -3.1]	-1	0
5	[-0.2 -1]	-1	0.25
6	[-0.2 1.3]	1	0
7	[2.0 -1]	-1	0.25
8	[0.5 2.1]	1	0

Answer to the following:

(A) What are the support vectors?

(B) Draw a schematic picture reporting the data points (approximately) and the optimal separating hyperplane, and mark the support vectors. Would it be possible, by moving only two data points, to obtain the SAME separating hyperplane with only 2 support vectors? If so, draw the modified configuration (approximately).