Machine Learning

Support Vector Machines

Try to find the "best" linear model
that maximizes the margin

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Linearly Separable Training Set

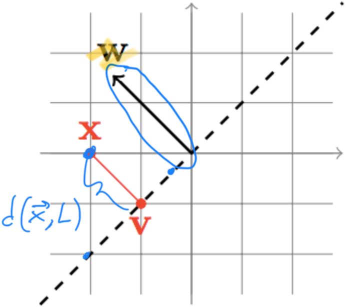
Training set $S = ((\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m))$ is *linearly separable* if there exists a halfspace $(\mathbf{w}, b)$ such that $y_i = \text{sign}(\langle \mathbf{w}, \mathbf{x}_i \rangle + b)$ for all $i = 1, \ldots, m$.

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

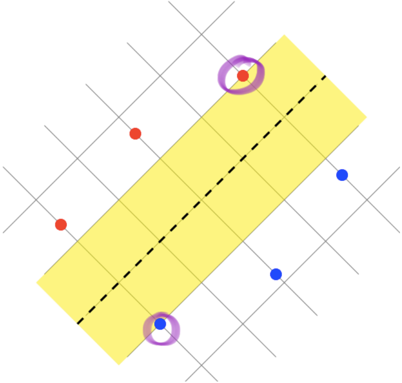
$$d(\mathbf{x}, L) = \min\{||\mathbf{x} - \mathbf{v}|| : \mathbf{v} \in L\}$$

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)

margin for the separating hyperplane $\vec{w}, b$

(*) **Computational problem**:

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

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

Equivalent formulation (due to separability assumption):

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

Solving it, is $\underbrace{\text{equivalent}}_{\text{we get the same solution}}$ to solve (*)

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.

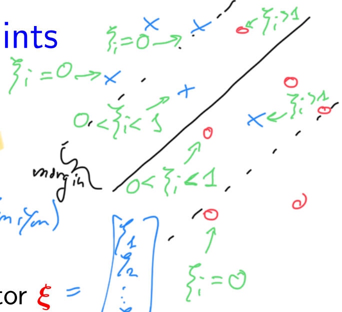
What if data is not linearly separable? $\Rightarrow$ soft-SVM

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:

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



for $(\vec{x}_1, y_1)$ for $(\vec{x}_m, y_m)$

Soft-SVM constraints:

- *slack variables*: $\xi_1, \ldots, \xi_m \geq 0 \Rightarrow$ vector $\boldsymbol{\xi}$ $= \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_m \end{bmatrix}$
- 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**:

regularization

training error?

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

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

- **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

Soft-SVM: Solution

We need to solve:

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

where

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

How?

- standard solvers for optimization problems
- **Stochastic Gradient Descent**

SGD for Solving Soft-SVM

We want to solve

$$\min_{\mathbf{w}} \left(\frac{\lambda}{2} ||\mathbf{w}||^2 + \frac{1}{m} \sum_{i=1}^{m} \max\{0, 1 - y \langle \mathbf{w}, \mathbf{x}_i \rangle \} \right)$$

Note: it's standard to add a $\frac{1}{2}$ in the regularization term to simplify some computations.

SGD algorithm:

$\boldsymbol{\theta}^{(1)} \leftarrow \mathbf{0}$;

for $t \leftarrow 1$ *to* T **do**

  $\eta^{(t)} \leftarrow \frac{1}{\lambda t}$; $\mathbf{w}^{(t)} \leftarrow \eta^{(t)} \boldsymbol{\theta}^{(t)}$;

  choose i uniformly at random from $\{1, \ldots, m\}$;

  if $y_i \langle \boldsymbol{w}^{(t)}, \boldsymbol{x}_i \rangle < 1$ **then** $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} + y_i \mathbf{x}_i$;

  else $\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)}$;

return $\bar{\mathbf{w}} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{w}^{(t)}$;