Support Vector Machine

Bùi Tiến Lên

2024

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Contents

Notation

symbol	meaning
$a, b, c, N \dots$	scalar number
$\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{x}, \boldsymbol{y} \dots$	column vector
$\boldsymbol{X}, \boldsymbol{Y} \dots$	matrix
$\mathbb{R}$	set of real numbers
$\mathbb{Z}$	set of integer numbers
$\mathbb{N}$	set of natural numbers
$\mathbb{R}^D$	set of vectors
$\mathcal{X}, \mathcal{Y}, \dots$	set
$\mathcal{A}$	algorithm

operator	meaning
$\boldsymbol{w}^\intercal$	transpose
$\boldsymbol{X}\boldsymbol{Y}$	matrix multiplication
$\boldsymbol{X}^{-1}$	inverse
$\boldsymbol{x} \cdot \boldsymbol{y}$	dot

Linear Support Vector Machines

- The Separable Case
- The Non-Separable Case

Problem Statement

- Training set:

$$(\boldsymbol{x}_i, y_i)_{i=1\dots N} \in \mathbb{R}^D \times \{-1, 1\}$$

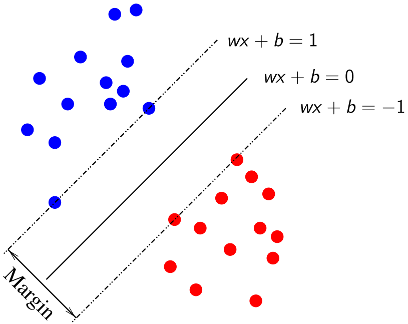
- We would like to find an hyperplane

$$\boldsymbol{w}^\intercal \boldsymbol{x} + b = 0, \quad (\boldsymbol{w} \in \mathbb{R}^D, b \in \mathbb{R})$$

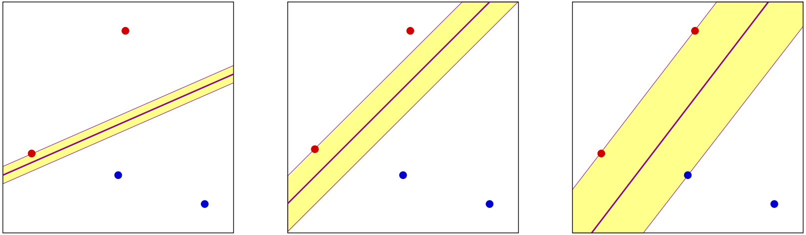
which **separates** the two classes.

Margin

- Let d_+ be the shortest distance from the hyperplane to the closest positive example.
- Let d_- be the shortest distance from the hyperplane to the closest negative example.
- Define the **margin** of the hyperplane to be $\min(d_+, d_-)$.



Better Linear Separation

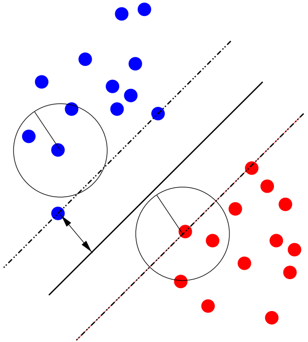


Two questions:

1. Why is bigger margin better?
2. Which $\boldsymbol{w}$, b maximizes the margin

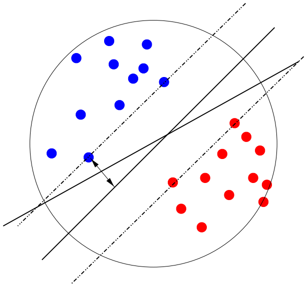
Why is it Good to Maximize the Margin?

- If training and test data come from the same distribution and all test data are within some Δ distance from the training points. If all points lie at a distance of at least Δ from the separator, and all points are in a bounded sphere, then a small perturbation of the definition of the separator will not hurt.



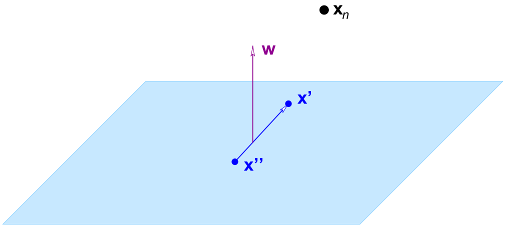
Why is it Good to Maximize the Margin? (cont.)

- One can use less bits to encode the separating hyperplane (**Minimum Description Length** principle)



Finding w with large margin

- Let $\mathbf{x}_n$ be the nearest data point to the plane $\mathbf{w}^\intercal \mathbf{x} + b = 0$. How far is it?



- The distance between $\mathbf{x}_n$ and the plane $\mathbf{w}^\intercal \mathbf{x} + b = 0$ where $|\mathbf{w}^\intercal \mathbf{x}_n + b| = 1$ (normalize $\mathbf{w}$ and b)

$$distance = \frac{1}{|\mathbf{w}|} \tag{1}$$

A Constrained Optimization Problem

- Representation of hypothesis set

$$\mathcal{H} : y = f(\boldsymbol{x}) = \text{sign}(\boldsymbol{w} \cdot \boldsymbol{x} + b) \tag{2}$$

- Evaluation

$$\begin{aligned} \arg\min_{\boldsymbol{w},b} \quad & \frac{1}{2}\|\boldsymbol{w}\|^2 && (3) \\ \text{subject to} \quad & y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) \geq 1, \quad i = 1, 2, \ldots, N && (4) \end{aligned}$$

The Dual Formulation

- Representation of hypothesis set

$$\mathcal{H} : y = f(\boldsymbol{x}) = \text{sign}\left(\sum_{i=1}^{N} \alpha_i y_i (\boldsymbol{x} \cdot \boldsymbol{x}_i) + b\right) \tag{5}$$

- Evaluation

$$\arg\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\boldsymbol{x}_i \cdot \boldsymbol{x}_j) - \sum_{i=1}^{N} \alpha_i \tag{6}$$

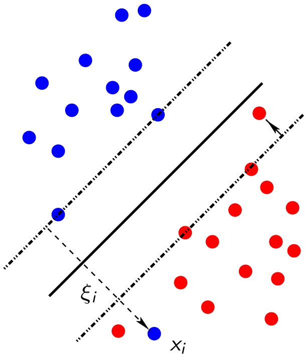
$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \tag{7}$$

$$\alpha_i \geq 0, \quad i = 1, 2, \ldots, N \tag{8}$$

- This can be solved using classical **quadratic programming optimization**

Bug

- This minimization problem does not have any solution if the two classes are not separable.



Fixing The Bug: "Soft" Margin

- Relax the constraints: use a **soft margin** instead of a **hard margin**.
- We would like to minimize:

$$\arg\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \quad \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{N}\xi_i \tag{9}$$

$$\text{subject to} \quad y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i + b) \geq 1 - \xi_i \tag{10}$$

$$\xi_i \geq 0, \quad i = 1, 2, \ldots, N \tag{11}$$

The Dual Formulation

- Representation of hypothesis set

$$\mathcal{H} : y = f(\boldsymbol{x}) = \text{sign}\left(\sum_{i=1}^{N} \alpha_i y_i (\boldsymbol{x} \cdot \boldsymbol{x}_i) + b\right) \tag{12}$$

- Evaluation

$$\arg\min_{\boldsymbol{\alpha}} \quad \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (\boldsymbol{x}_i \cdot \boldsymbol{x}_j) - \sum_{i=1}^{N} \alpha_i \tag{13}$$

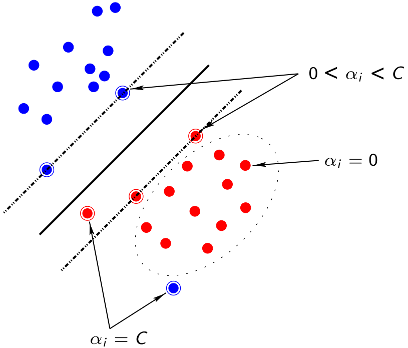
$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \tag{14}$$

$$0 \leq \alpha_i \leq C, \quad i = 1, 2, \ldots, N \tag{15}$$

Support Vector Terminology

- Training examples $\boldsymbol{x}_i$ with $\alpha_i > 0$ are **support vectors**.

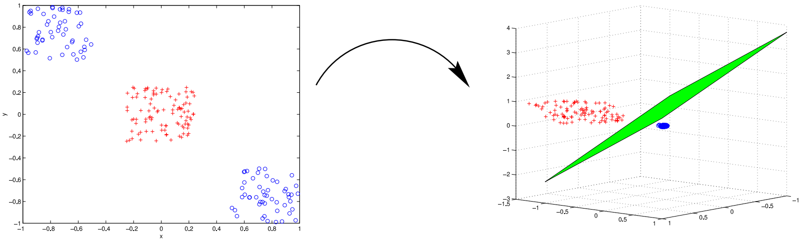
$$\begin{aligned} \alpha_i = 0 &\Rightarrow y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) > 1 \\ \alpha_i = C &\Rightarrow y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) < 1 \\ 0 < \alpha_i < C &\Rightarrow y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) = 1 \end{aligned} \tag{16}$$



Kernels Support Vector Machines

Non-Linear SVMs

- Project the data into a **higher dimensional space** (**feature space**): it should be easier to separate the two classes.
- Given a function $\phi : \mathbb{R}^D \rightarrow \mathcal{F}$, work with $\phi(\boldsymbol{x}_i)$ instead of working with $\boldsymbol{x}_i$.



The Kernel Function

Concept 1

A **kernel** is a function $k(\boldsymbol{x}, \boldsymbol{z})$ which represents a dot product in a "hidden" feature space of ϕ.

$$k(\boldsymbol{x}, \boldsymbol{z}) = \phi(\boldsymbol{x}) \cdot \phi(\boldsymbol{z}) \tag{17}$$

- **Note that**: we have only dot products $\phi(\boldsymbol{x}_i) \cdot \phi(\boldsymbol{x}_j)$ to compute; however, this could be very expensive in a high dimensional space.
- **Kernel trick**:

$$\text{instead of } \phi(\boldsymbol{x}) = \phi\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{pmatrix}, \text{ use } k(\boldsymbol{x}, \boldsymbol{z}) = (\boldsymbol{x} \cdot \boldsymbol{z})^2$$

Common Kernels

- Polynomial:

$$k(\boldsymbol{x}, \boldsymbol{z}) = (u\boldsymbol{x} \cdot \boldsymbol{z} + v)^p \ (u \in \mathbb{R}, v \in \mathbb{R}, p \in \mathbb{N}) \tag{18}$$

- Gaussian:

$$k(\boldsymbol{x}, \boldsymbol{z}) = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{z}\|^2}{\sigma^2}\right), \sigma \in \mathbb{R}^+ \tag{19}$$

Techniques for Construction of Kernels

In all the following, $k_1, k_2, ..., k_j$ are assumed to be valid kernel functions

1. **Scalar multiplication**: The validity of a kernel is conserved after multiplication by a positive scalar, i.e., for any $\alpha > 0$, the function

$$k(\boldsymbol{x}, \boldsymbol{z}) = \alpha k_1(\boldsymbol{x}, \boldsymbol{z}) \tag{20}$$

2. **Adding a positive constant**: For any positive constant $\alpha > 0$, the function

$$k(\boldsymbol{x}, \boldsymbol{z}) = \alpha + k_1(\boldsymbol{x}, \boldsymbol{z}) \tag{21}$$

Techniques for Construction of Kernels (cont.)

3. **Linear combination**: A linear combination of kernel functions involving only positive weights, i.e.,

$$k(\boldsymbol{x}, \boldsymbol{z}) = \sum_{j=1}^{m} \alpha_j k_j(\boldsymbol{x}, \boldsymbol{z}), \qquad \text{with } \alpha_j > 0 \tag{22}$$

   is a valid kernel function.

4. **Product**: The product of two kernel functions, i.e.,

$$k(\boldsymbol{x}, \boldsymbol{z}) = k_1(\boldsymbol{x}, \boldsymbol{z}) k_2(\boldsymbol{x}, \boldsymbol{z}) \tag{23}$$

   is a valid kernel function.

Techniques for Construction of Kernels (cont.)

5. **Polynomial functions of a kernel output**: Given a polynomial $f : \mathbb{R} \to \mathbb{R}$ with positive coefficients, the function

$$k(\boldsymbol{x}, \boldsymbol{z}) = f(k_1(\boldsymbol{x}, \boldsymbol{z})) \tag{24}$$

is a valid kernel function.

6. **Exponential function of a kernel output**: The function

$$k(\boldsymbol{x}, \boldsymbol{z}) = \exp(k_1(\boldsymbol{x}, \boldsymbol{z})) \tag{25}$$

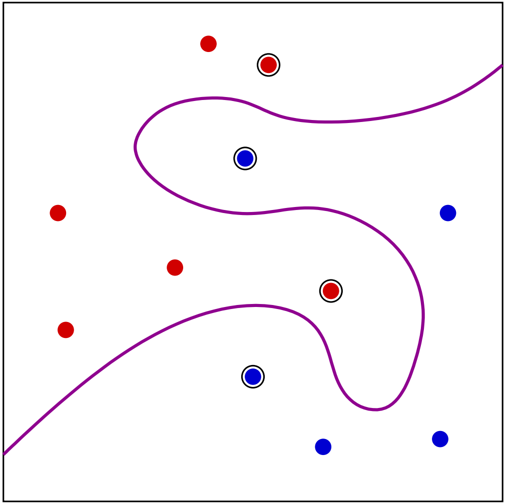
is a valid kernel function.

7. **Product of matrix** and **vectors**:

$$k(\boldsymbol{x}, \boldsymbol{z}) = \boldsymbol{x}^{\mathsf{T}} A \boldsymbol{z} \tag{26}$$

where A is a symmetric positive semidefinite matrix.

Decision Boundary and Support Vectors



SVMs in Practice

- In order to tune the **capacity**, the kernel is the most important parameter to choose.
  - Polynomial kernel: increasing the degree will increase the **capacity**.
  - Gaussian kernel: increasing σ will decrease the capacity.
- Tune C, the trade-off between the **margin** and the **errors**.
  - For non-noisy data sets, C usually has not much influence.
  - Carefully choose C for noisy data sets: small values usually give better results.

Multi-class SVM

Multiclass SVM formulations

- There are a few ways of formulating the SVM over multiple classes:
  - One-vs-all
  - One-vs-one
  - Hierarchical
  - **Multiclass**

Score function

Concept 2

The **score function** f that maps the raw features to class scores.

$$\boldsymbol{z} = f(\boldsymbol{x}; W) = W\boldsymbol{x} \tag{27}$$

input image

$$\underbrace{\begin{bmatrix} 1.1 & 0.2 & -0.5 & 0.1 & 2.0 \\ 3.2 & 1.5 & 1.3 & 2.1 & 0.0 \\ -1.2 & 0 & 0.25 & 0.2 & -0.3 \end{bmatrix}}_{W} \times \underbrace{\begin{bmatrix} 1 \\ 56 \\ 231 \\ 24 \\ 2 \end{bmatrix}}_{\boldsymbol{x}} = \begin{bmatrix} -96.8 \\ 437.9 \\ 61.95 \end{bmatrix} \begin{array}{l} \text{cat score} \\ \text{dog score} \\ \text{ship score} \end{array}$$

Multiclass SVM loss

- Given the input vector $\boldsymbol{x}_i$ and the label y_i that specifies the index of the correct class. The multiclass SVM loss (**hinge loss**) for the vector $\boldsymbol{x}_i$ is then formalized as follows

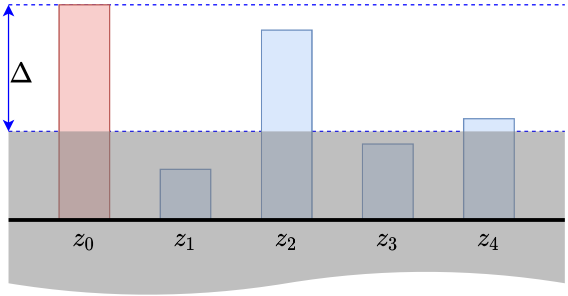
$$L_i = \sum_{j \neq y_i} \max(0, z_j - z_{y_i} + \Delta) \tag{28}$$

where $\boldsymbol{z} = f(\boldsymbol{x}_i; W) = W\boldsymbol{x}_i$

Example

- Suppose that we have five classes $\{0, 1, 2, 3, 4\}$ that receive the scores $\boldsymbol{z} = [17, 4, 15, 6, 8]$ and the true class $y_i = 0$
- Also assume that $\Delta = 10$

$$L_i = \max(0, 4 - 17 + 10) + \max(0, 15 - 17 + 10) + \max(0, 6 - 17 + 10) + \max(0, 8 - 17 + 10) = 9$$



Regularization loss

- The most common regularization penalty is the L_2 norm that discourages large weights through an elementwise quadratic penalty over all parameters:

$$R(W) = \sum_k \sum_l W_{k,l}^2 \tag{29}$$

- The data loss (which is the average loss L_i over all examples) and the regularization loss. That is, the full multiclass SVM loss becomes:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \mathcal{L}_{\text{reg}} = \underbrace{\frac{1}{N}\sum_i L_i}_{\text{data loss}} + \underbrace{\lambda R(W)}_{\text{regularization loss}} \tag{30}$$

- **Learning goal**: Find W that minimize

$$\arg\min_W \mathcal{L} \tag{31}$$

Practical considerations

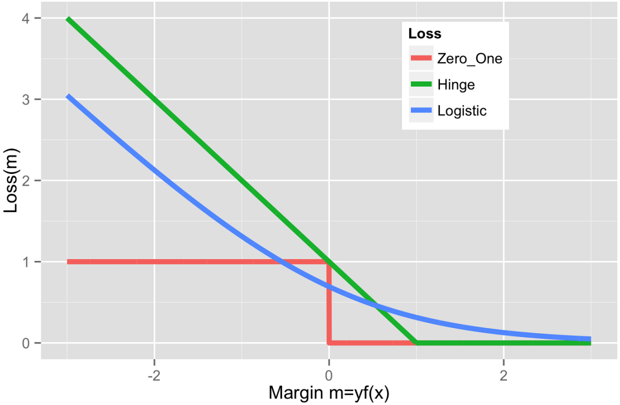
- **Setting Delta**: It can safely be set to $\Delta = 1.0$ in all cases
- **Relation to Binary Support Vector Machine**: The loss for the i-th example $(\boldsymbol{x}_i, y_i)$ can be written as

$$L_i = C \max(0, 1 - y_i \boldsymbol{w}^\top \boldsymbol{x}_i) + R(\boldsymbol{w}) \tag{32}$$

where C is a hyperparameter, and $y_i \in \{-1, 1\}$

Binary classification losses

- Perceptron (zero-one)
- SVM (hinge)
- Logistic



SGD for hinge loss

- Consider linear hypothesis space:

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = \boldsymbol{w}^\intercal \boldsymbol{x} \tag{33}$$

- Hinge loss of $(\boldsymbol{x}, y)$

$$\mathcal{L}(x) = \max(0, 1 - y\boldsymbol{w}^\intercal \boldsymbol{x}) \tag{34}$$

- Gradient of hinge loss $(\boldsymbol{x}, y)$:

$$\nabla_{\boldsymbol{w}}\mathcal{L}(\boldsymbol{x}) = \begin{cases} -y\boldsymbol{x} & \text{if } yh_{\boldsymbol{w}}(\boldsymbol{x}) < 1 \\ 0 & \text{if } yh_{\boldsymbol{w}}(\boldsymbol{x}) > 1 \\ \text{undefined} & \text{if } yh_{\boldsymbol{w}}(\boldsymbol{x}) = 1 \end{cases} \tag{35}$$

- A point with margin $m = yh_{\boldsymbol{w}}(\boldsymbol{x}) = 1$ is correctly classified $\rightarrow$ we can skip SGD update for these points.

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