Support Vector Machines

ML Instruction Team, Fall 2022

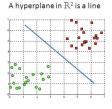
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Hyperplane

Hyperplane: A hyperplane in p dimensions is an affine subspace of dimension p-1:

$$\beta_0+\beta_1X_1+\beta_2X_2+\ldots+\beta_pX_p=0$$



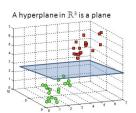


Figure: Hyperplanes, Source

- The vector $\boldsymbol{\beta} = (\beta_1, \beta_2, ..., \beta_p)$ is called the **normal vector** it points in a direction orthogonal to the surface of the defined hyperplane.
- If $f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p = \beta^T X + \beta_0$, then f(X) divides the p-dimensional feature space into two half-spaces.
- So if we code $Y^{(i)} \in \{\pm 1\}$, then $\forall i: \quad Y^{(i)}f(X^{(i)}) > 0$

Introduction Maximal Margin Classifier Support Vector Classifier Support Vector Machines

Intuition: Margins

Separating Hyperplane

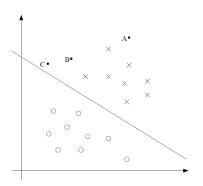


Figure: Separating Hyperplane, Source

- Our confidence about the prediction of classes of A, B and C relies on their distance from decision boundary.
- We try to find the optimal hyperplane that separates the classes in the feature space.

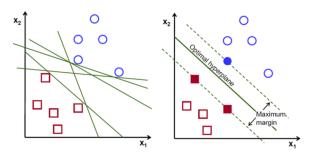


Figure: Maximal Separating Hyperplane, Source

Maximal (Optimal) Separating Hyperplane: The separating hyperplane with the largest between-class margin M.

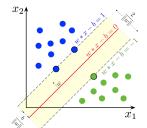
$$\max_{eta,eta_0,M} M$$
 s.t. $\sum_{j=1}^p eta_j^2 = 1$

 $distance: y^{(i)}(\beta^T x^{(i)} + \beta_0) \geq M \quad \forall i \in \{1, 2, ..., N\}$

- Eq.(1) can be rephrased as a **convex quadratic problem** and be solved efficiently using QP solvers.
- (Euclidean) distance between two hyperplanes

$$\mathcal{H}_1 = \{x|\beta^Tx + \beta_0 = 1\} \qquad \mathcal{H}_2 = \{x|\beta^Tx + \beta_0 = -1\}$$

is
$$\operatorname{dist}(\mathcal{H}_1, \mathcal{H}_2) = 2/||\beta||_2$$



$$\min_{\beta,\beta_0} \quad \frac{1}{2}||\beta||_2^2$$

$$\text{s.t.} \quad y^{(i)}(\beta^T x^{(i)} + \beta_0) \geq 1 \quad \forall i \in \{1,2,...,N\}$$

Figure: Optimal Hyperplane,

Source

Not-linearly Separable Data

In most cases however, the data are not linearly separable.

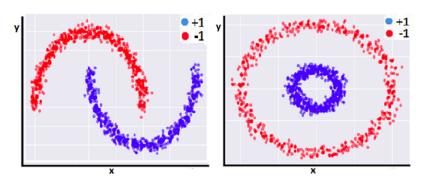


Figure: Not-linearly Separable Data, Source

Noisy Data

Sometimes the data are linearly separable, but noisy. This can lead to a poor solution for the maximal margin classifier. Also, hard-margin classifier is sensitive to outliers.

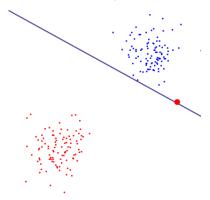


Figure: Noisy Data, Source

Support Vector Classifier (SVC) maximizes a soft margin.



Support Vector Classifier (Soft Margin Classifier)

Allowing some samples to violate the margin, with slack variables (ξ), in a controlled manner:

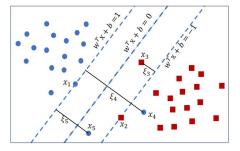


Figure: Soft Margin Classifier, Source

$$\begin{split} \min_{\beta,\beta_0,\xi} \quad & \frac{1}{2}||\beta||_2^2 + C\sum_{i=1}^N \xi_i \\ \text{s.t.} \quad & y^{(i)}(\beta^T x^{(i)} + \beta_0) \geq 1 - \xi_i \\ & \xi_i \geq 0 \quad \forall i \in \{1,2,\dots,N\} \end{split}$$

Effect of Regularization Parameter

C is a regularization parameter that controls the width of the margin in the support vector classifier.

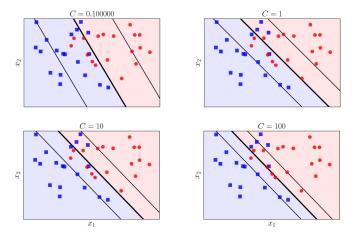


Figure: Regularization Effect, Source



Dual Problem of SVC

Primal problem:

$$\begin{split} \min_{\beta,\beta_0,\xi} & & \frac{1}{2}||\beta||_2^2 + C\sum_{i=1}^N \xi_i \\ \text{s.t.} & & y^{(i)}(\beta^T x^{(i)} + \beta_0) \geq 1 - \xi_i \\ & & \xi_i \geq 0 \quad \forall i \in \{1,2,...,N\} \end{split}$$

Dual problem (using the lagrangian):

$$\begin{aligned} & \max_{\alpha_i} & & \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y^{(i)} y^{(j)} x^{(i)^T} x^{(j)} \\ & \text{s.t.} & & \sum_{i=1}^N \alpha_i y^{(i)} = 0 \\ & & & 0 \leq \alpha_i \leq C \quad \forall i \in \{1,2,...,N\} \end{aligned}$$



KKT Conditions

From Karush-Kuhn-Tucker (KKT) conditions and complementary slackness we have:

$$\begin{split} \alpha_i (1 - \xi_i - y^{(i)} (\beta^T x^{(i)} + \beta_0)) &= 0 \\ (C - \alpha_i) \xi_i &= 0 \end{split}$$

There can be 3 cases:

$$\begin{cases} \alpha_i = 0 \rightarrow \pmb{\xi_i} = 0 \Rightarrow 1 - y^{(i)}(\beta^T x^{(i)} + \beta_0) < 0 \colon & \text{Non-Support} \\ 0 < \alpha_i < C \rightarrow \pmb{\xi_i} = 0 \Rightarrow 1 - y^{(i)}(\beta^T x^{(i)} + \beta_0) = 0 \colon & \text{Support} \\ \alpha_i = C \rightarrow \pmb{\xi_i} > 0 \Rightarrow 1 - \xi_i - y^{(i)}(\beta^T x^{(i)} + \beta_0) = 0 \colon & \text{Support} \end{cases}$$

Classification Function

- $f(x) = \beta^T x + \beta_0$
- Also, when minimizing the conjugate function of primal problem, we get:

$$\beta = \sum_{i=1}^N \alpha_i y^{(i)} x^{(i)}$$

This results in the following classification function for SVC:

$$f(x) = \beta_0 + \sum_{i=1}^N \alpha_i y^{(i)} x^T x^{(i)} = \beta_0 + \sum_{i=1}^N \alpha_i y^{(i)} \langle x, x^{(i)} \rangle$$

It turns out that most of the $\hat{\alpha}_i$ can be zero:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i y^{(i)} \langle x, x^{(i)} \rangle$$

where S is the support set of indices i such that $\hat{\alpha}_i > 0$.

So, all we need is **inner products**!



The Need for Non-Linear Boundary

Linear boundary can fail in many cases, regardless of the value of C.

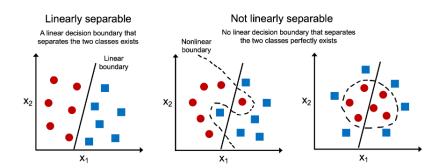


Figure: The Need for Non-linear Boundary, Source

Feature Expansion

- Enlarge the space of features by including transformations; e.g. $X_1^2, X_1^3, X_1X_2, X_1X_2^2, \dots$ Hence increasing the dimension of the original p-dimensional input space.
- Then we can fit a support vector classifier in the enlarged space.
- This results in **non-linear decision boundaries** in the original feature space.

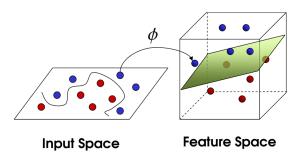


Figure: The Need for Non-inear Boundary, Source

Consider the feature mapping $T: x \to \phi(x)$, we define the corresponding kernel to be

$$K(x, x') = \langle \phi(x), \phi(x') \rangle.$$

Now we can simply replace all inner products by K(x, x'), and our algorithm would now be learning using the features ϕ .

- $K_{i,j} = K(x^{(i)}, x^{(j)})$ Kernel matrix: A valid kernel function is the one that results in a symmetric positive semi-definite kernel matrix for any set of samples. (Mercer theorem: necessary and sufficient condition)
- Calculating kernel matrix may be very inexpensive, even though $\phi(x)$ itself may be very expensive to calculate (perhaps because it is an extremely high dimensional vector).
- The classification function solution has the form

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i y^{(i)} K(x, x^{(i)})$$



Polynomial Kernels

$$K(x,y) = (1 + \langle x, y \rangle)^d$$

e.g. Feature transformation from 2D kernels:

$$K(x,y)=(1+\langle x,y\rangle)^2\Rightarrow\phi(x)=(1,\sqrt{2}x_1,\sqrt{2}x_2,x_1^2,x_2^2)$$

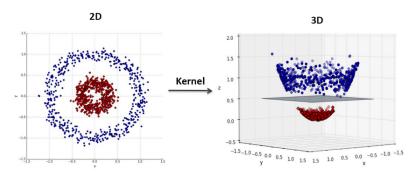


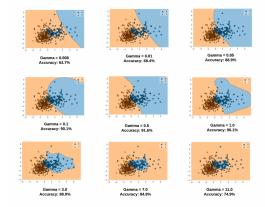
Figure: 2nd Order Polynomial Kernel, Source



Radial Basis Kernels

$$K(x,y) = \exp(-\gamma \|x-y\|_2^2)$$

- Measure of similarity!
- γ is the hyperparameter to be chosen to control the bias-variance trade-off.



Multi-class SVM

- One-vs-All : Fit all K different 2-class SVM classifiers $\hat{f}_k(x), \forall k \in \{1, 2, ..., K\};$ each class versus the rest. Classify x^* to the class for which $\hat{f}_k(x)$ is the largest.
- One-vs-One: Fit all $\binom{K}{2}$ pairwise classifiers $\hat{f}_{kl}(x)$. Classify x^* to the class that wins the most pairwise competitions.

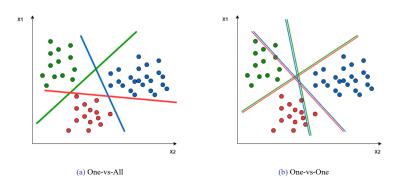


Figure: Multi-class SVM, Source



Support Vector Regression

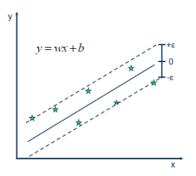


Figure: Support Vector Regression, Source

$$\begin{split} & \min_{\beta,\beta_0} & \frac{1}{2} ||\beta||_2^2 \\ \text{s.t.} & |y^{(i)} - (\beta^T x^{(i)} + \beta_0)|_2 \leq \epsilon \quad \forall i \in \{1,2,...,N\} \end{split}$$



Soft Support Vector Regression

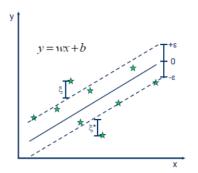


Figure: Soft Support Vector Regression, Source

$$\begin{split} \min_{\beta,\beta_0} \quad & \frac{1}{2}||\beta||_2^2 + C\sum_{i=1}^N \xi_i \\ \text{s.t.} \quad & |y^{(i)} - (\beta^T x^{(i)} + \beta_0)|_2 \leq \epsilon + \xi_i \\ & \xi_i \geq 0 \quad \forall i \in \{1,2,...,N\} \end{split}$$

Final Notes

Thank You!

Any Question?

