Support Vector Machines

ML Instruction Team, Fall 2022

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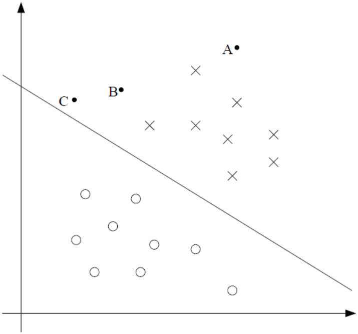
Intuition: Margins

- Separating Hyperplane



- 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.

Hyperplane

- **Hyperplane**: A hyperplane in *p* dimensions is a flat affine subspace of dimension *p-1*:

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p = 0$$

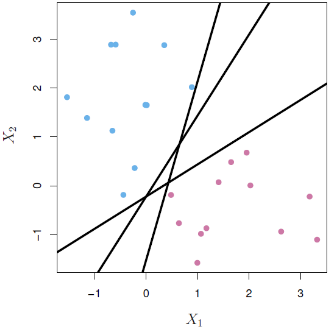
- The vector $\beta = (\beta_1, \beta_2, \ldots, \beta_p)$ is called the normal vector – it points in a direction orthogonal to the surface of the defined hyperplane.

- 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 ($f(X) > 0$ for one side and $f(X) < 0$ for the other side).

- So if we code $Y^{(i)} \in \{\pm 1\}$, then $\forall i$

$$Y^{(i)} f(X^{(i)}) > 0$$

Maximal Margin Classifier



- **Maximal(Optimal) Separating Hyperplane**: The separating hyperplane with the biggest margin between the classes.

$$
\begin{aligned}
\max_{\beta_0, \beta, M} \quad & M \\
\text{s.t.} \quad & \sum_{j=1}^{p} \beta_j^2 \\
& y^{(i)}(\beta^T x^{(i)} + \beta_0) \geq M \quad \forall i \in \{1, 2, \dots, N\}
\end{aligned}
\tag{1}
$$

Maximal Margin Classifier: Quadratic Program

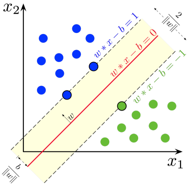
- Eq.(1) can be rephrased as a convex quadratic problem and be solved efficiently using QP solvers.

- (Euclidean) distance between two hyperplanes

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

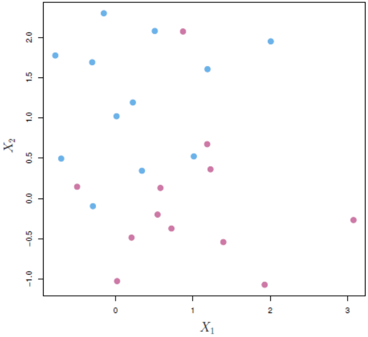
is **dist**($\mathcal{H}_1, \mathcal{H}_2$) $= 2/||\beta||_2$

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



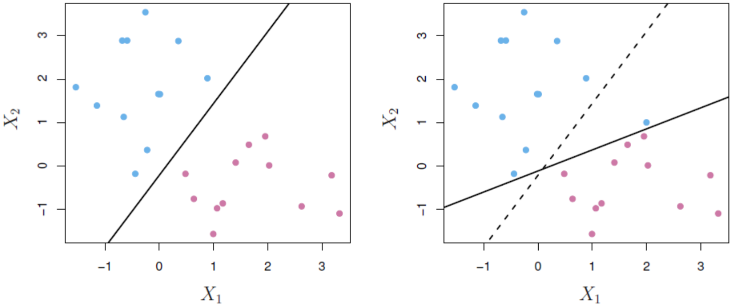
Non-linearly Separable Data

- In most cases however, the data are not linearly separable unless $N < p$.



Noisy Data

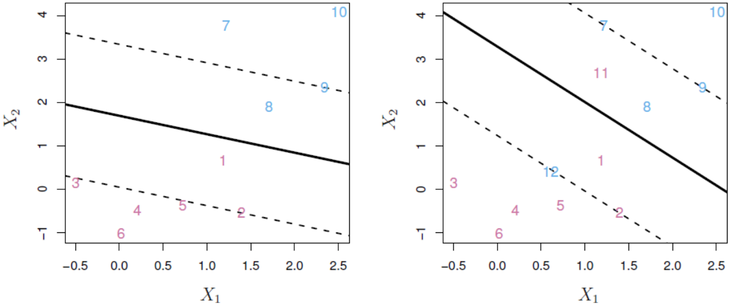
- Sometimes the data are linearly separable, but noisy. This can lead to a poor solution for the maximal margin classifier. Also, hard-margin classifier is sensitive to outliers.



- The *support vector classifier* (SVC) maximizes a *soft* margin.

Support Vector Classifier(Soft Margin Classifier)

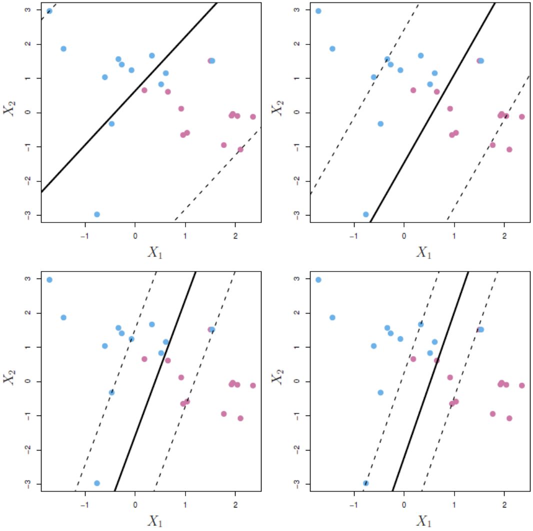
- Allowing some samples to violate the margin, with *slack variables*, in a controlled manner:



$$
\begin{aligned}
\min_{\beta,\beta_0,\xi} \quad & \frac{1}{2}||\beta||_2^2 + C\sum_{i=1}^{N}\xi_i \\
\text{s.t.} \quad & y^{(i)}(\beta^T x^{(i)} + \beta_0) \geq 1 - \xi_i \\
& \xi_i \geq 0 \quad \forall i \in \{1, 2, \ldots, N\}
\end{aligned} \tag{3}
$$

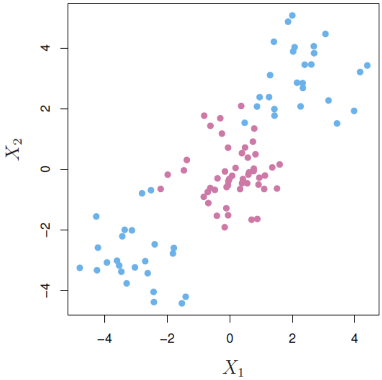
Effect of Regularization Parameter

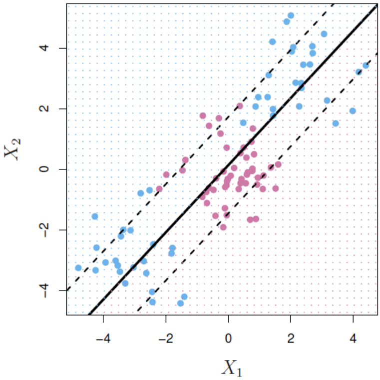
- C is a regularization parameter that controls the bias-variance trade-off of the support vector classifier.



The Need for Non-Linear Boundary

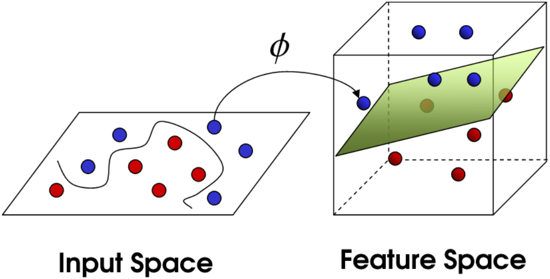
- Linear boundary can fail in many cases, regardless of the value of C.





Feature Expansion

- Enlarge the space of features by including transformations; e.g. $X_1^2, X_1^3, X_1X_2, X_1X_2^2, \ldots$. 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.



Dual Problem of SVC

- **Primal problem**:

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

- **Dual problem** (using the lagrangian):

$$\begin{aligned} \max_{\alpha_i} \quad & \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y^{(i)}y^{(j)}{x^{(i)}}^T x^{(j)} \\ \text{s.t.} \quad & \sum_{i=1}^{N}\alpha_i y^{(i)} = 0 \\ & 0 \leq \alpha_i \leq C \quad \forall i \in \{1, 2, \ldots, N\} \end{aligned} \tag{4}$$

KKT Conditions

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

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

- There can be 3 cases:

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

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:

$$f(x) = \beta_0 + \sum_{i=1}^{N} \alpha_i y^{(i)} x^T x^{(i)} = \beta_0 + \sum_{i=1}^{N} \alpha_i y^{(i)} \langle x, x^{(i)} \rangle \tag{5}$$

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

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i y^{(i)} \langle x, x^{(i)} \rangle \tag{6}$$

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

So, all we need is inner products!

Kernels and SVMs

- 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.

- Kernel matrix: $K_{i,j} = K(x^{(i)}, x^{(j)})$
  A valid kernel function is the one that results in a symmetric positive semi-definite kernel matrix for any set of samples. (Necessary and sufficient: Mercer theorem)

- 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

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i y^{(i)} K(x, x^{(i)}) \tag{7}$$

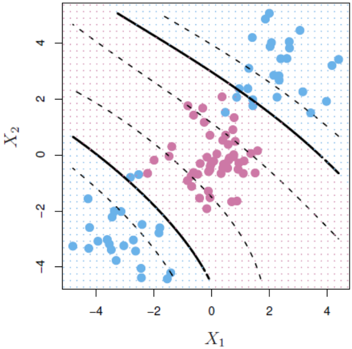
Polynomial Kernels

$$K(x, y) = (1 + \langle x, y \rangle)^d \tag{8}$$

- e.g. Feature transformation from 2D kernels:

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

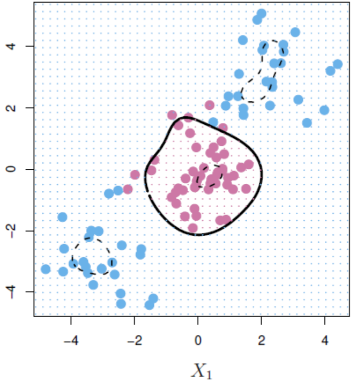
- e.g. Polynomial kernel of degree 3:



Radial Basis Kernels

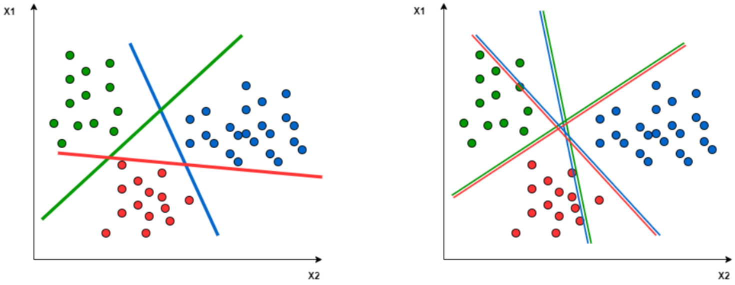
$$K(x, y) = \mathsf{exp}(-\gamma \|x - y\|_2^2) \quad (9)$$

- γ is the hyperparameter to be chosen to control the bias-variance trade-off.
- e.g. Radial basis functions (RBF) kernel:



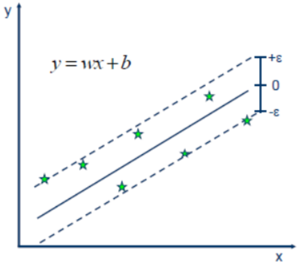
Multi-class SVM

- **One-vs-All**: Fit all K different 2-class SVM classifiers $\hat{f}_k(x), \forall k \in \{1, 2, \ldots, K\}$; 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.



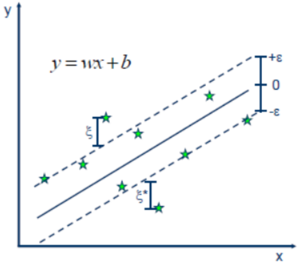
(a) One-vs-All (b) One-vs-One

Support Vector Regression



$$\min_{\beta, \beta_0} \quad \frac{1}{2}||\beta||_2^2$$
$$\texttt{s.t.} \quad |y^{(i)} - (\beta^T x^{(i)} + \beta_0)|_2 \leq \epsilon \quad \forall i \in \{1, 2, \ldots, N\} \tag{10}$$

Soft Support Vector Regression



$$
\begin{aligned}
\min_{\beta, \beta_0} \quad & \frac{1}{2}||\beta||_2^2 + C\sum_{i=1}^{N}\xi_i \\
\text{s.t.} \quad & |y^{(i)} - (\beta^T x^{(i)} + \beta_0)|_2 \leq \epsilon + \xi_i \\
& \xi_i \geq 0 \quad \forall i \in \{1, 2, \ldots, N\}
\end{aligned} \tag{11}
$$

Final Notes

Thank You!

Any Question?