Pattern Classification

Lecture 06: Linear Discriminant Functions

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https://github.com/erkundanec/PatternClassification

Linear Machine: Support Vector Machine

Introduction

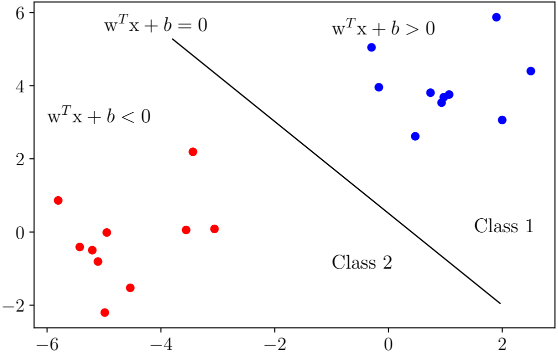
- Support vector machines (SVMs) are a linear machines initially developed for two class problems, which construct a hyperplane or set of hyperplanes in a high- or infinite-dimensional space.
- SVMs are a set of supervised learning methods used for
  - classification,
  - regression and
  - outliers detection.
- The advantages of support vector machines are:
  - Effective in high dimensional spaces.
  - Also, effective in cases where number of dimensions is greater than the number of samples.
  - Uses a subset of training points in the decision function (called support vectors), so it is also memory efficient.
  - Versatile: different SVM kernels can be specified for the decision function. Common kernels are provided, but it is also possible to specify custom kernels.

Introduction

- The disadvantages of support vector machines include:
  - If the number of features is much greater than the number of samples then choosing regularization to avoiding over-fitting is crucial.
  - SVMs do not directly provide probability estimates, these are calculated using an expensive five-fold cross-validation.
- In addition to performing linear classification, SVMs can efficiently perform a non-linear classification using what is called Kernel trick.
- Kernel trick implicitly maps their input into high-dimensional feature space.

Linear decision boundary

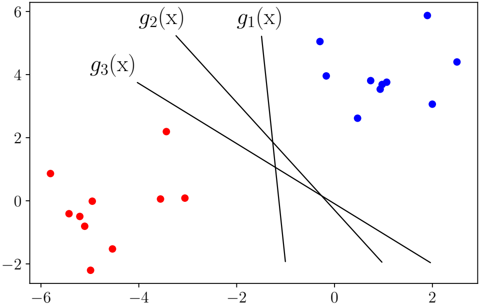
- Binary classification can be viewed as the task of separating classes in feature space using decision boundary:



$$f(x) = \text{sign}(w^T x + b)$$

What is a good Decision Boundary?

- Consider a two-class, linearly separable classification problem, many decision boundaries are possible.
- Are all decision boundaries equally good?
- Which of the linear separators is optimal?
- The perceptron algorithm can be used to find such a boundary.



Linear SVM: Objective

- Let us training data set, $\mathcal{D}$, a set of n points.

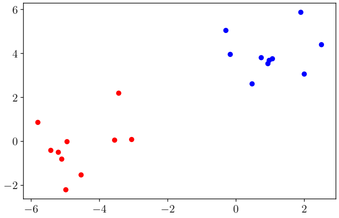
$$\mathcal{D} = \{(\mathrm{x}_i, y_i) \mid \mathrm{x}_i \in \Re^d, y_i \in \{-1, 1\}\}_{i=1}^{n}$$

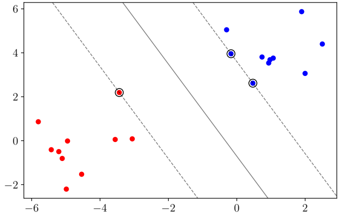
$\mathrm{x}_i \quad \rightarrow \quad d$-dimensional real vector

- Objective: find maximum-margin hyperplane

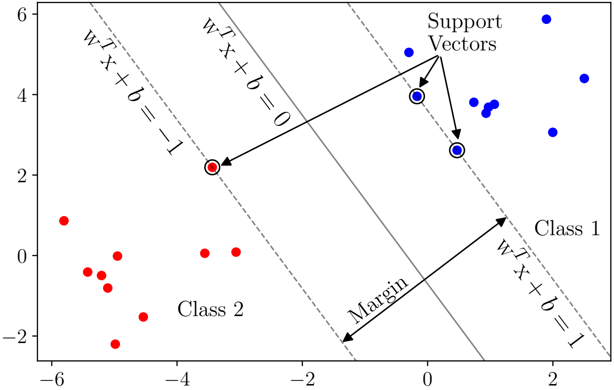
$$\mathrm{w}^T\mathrm{x} + b = 0$$

where w is the normal vector to the hyperplane and b is the bias/intercept.





Linear SVM: pictorial representation

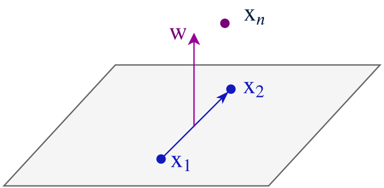


Preliminary concepts

- Let x_n be the nearest data point to the plane $\mathrm{w}^T\mathrm{x} + b = 0$.
- How far is it?
- Normalize w and b such that:

$$|\mathrm{w}^T\mathrm{x}_n + b| = 1$$

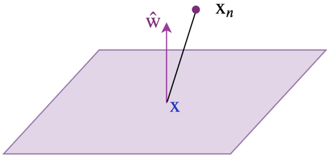
  - Now, we need to compute the distance between x_n and the plane $\mathrm{w}^T\mathrm{x} + b = 0$, where $|\mathrm{w}^T\mathrm{x}_n + b| = 1$.
  - The vector w is $\perp$ to the plane in the $\mathcal{X}$ space:
  - Take x_1 and x_2 on the plane



$$\mathrm{w}^T\mathrm{x}_1 + b = 0 \text{ and } \mathrm{w}^T\mathrm{x}_2 + b = 0 \qquad \Rightarrow \quad \mathrm{w}^T(\mathrm{x}_1 - \mathrm{x}_2) = 0$$

Preliminary concepts

The distance between x_n and the plane:



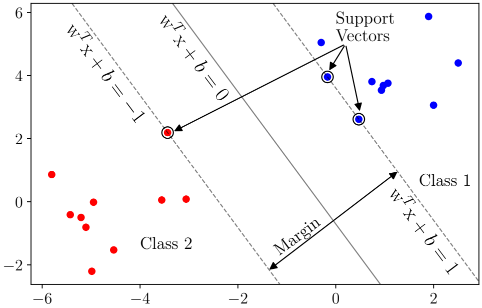
- Take any point x on the plane
- Projection of $\mathrm{x}_n - \mathrm{x}$ on $\hat{\mathrm{w}}$

$$\hat{\mathrm{w}} = \frac{\mathrm{w}}{||\mathrm{w}||}$$

$$\Rightarrow \quad \text{distance} = |\hat{\mathrm{w}}^T(\mathrm{x}_n - \mathrm{x})|$$

$$\text{distance} = \frac{1}{||\mathrm{w}||}|\mathrm{w}^T\mathrm{x}_n - \mathrm{w}^T\mathrm{x}| = \frac{1}{||\mathrm{w}||}|\mathrm{w}^T\mathrm{x}_n + b - \mathrm{w}^T\mathrm{x} - b| = \frac{1}{||\mathrm{w}||}$$

Problem formulation



- Two hyperplanes

$$\mathrm{w}^T\mathrm{x} + b = 1$$
$$\mathrm{w}^T\mathrm{x} + b = -1$$

- So the distance between the hyperplane is

$$\frac{b+1}{||\mathrm{w}||} - \frac{b-1}{||\mathrm{w}||} = \frac{2}{||\mathrm{w}||}$$

(need to be maximize)

- Therefore, $||\mathrm{w}||$ need to be minimize.

Problem formulation

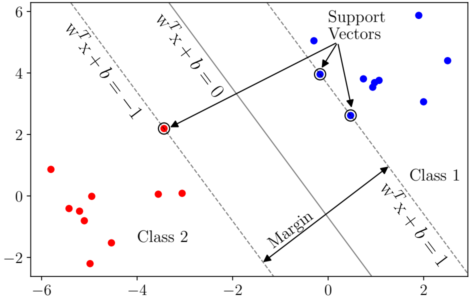
- We need to minimize $||\mathrm{w}||$ to maximize the margin.
- We also have to restrict data points from falling into the margin, so add the following constraints:
  - $\mathrm{w}^T \mathrm{x}_i + b \geq 1$ for x_i of the 1st class.
  - $\mathrm{w}^T \mathrm{x}_i + b \leq -1$ for x_i of the 2nd class.
- This can be written as

$$y_i(\mathrm{w}^T \mathrm{x}_i + b) \geq 1 \quad \text{for} \quad i = 1, 2, \ldots, n$$

- Combining the above two

$$\underset{\mathrm{w}, b}{\text{Minimize}} \quad ||\mathrm{w}||$$

subject to $y_i(\mathrm{w}^T \mathrm{x}_i + b) \geq 1 \quad \text{for} \quad i = 1, 2, \ldots, n$



Problem formulation

- Problem is difficult to solve because it depends on $||\mathrm{w}||$, the norm of w, which involves a square root.
- Substitute $||\mathrm{w}||$ with $\frac{1}{2}||\mathrm{w}||^2$ (just for mathematical convenience)
- Then problem is formulated as

$$\underset{\mathrm{w},b}{\text{Minimize}} \quad \frac{1}{2}||\mathrm{w}||^2$$
$$\text{subject to} \quad y_i(\mathrm{w}^T\mathrm{x}_i + b) \geq 1 \quad \text{for} \quad i = 1, 2, \ldots, n$$

- The above problem is constraint optimization problem.

Problem solution: Lagrange formulation

- There is no direct solution of the formulated constraint optimization problem.
- To obtain the dual, take positive Lagrange multiplier α_i multiplied by each constraint and subtract from the objective function.

$$\text{Minimize} \quad \mathcal{L}(\mathrm{w}, b, \alpha) = \frac{1}{2}\mathrm{w}^T\mathrm{w} - \sum_{i=1}^{n} \alpha_i(y_i(\mathrm{w}^T\mathrm{x}_i + b) - 1)$$

w.r.t. w and b and maximize w.r.t. each $\alpha_i \geq 0$

- We can find the constraint as

$$\nabla_{\mathrm{w}}\mathcal{L} = \mathrm{w} - \sum_{i=1}^{n} \alpha_i y_i \mathrm{x}_i = 0$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^{n} \alpha_i y_i = 0$$

Problem solution: Lagrange formulation

- We obtained

$$\mathrm{w} = \sum_{i=1}^{n} \alpha_i y_i \mathrm{x}_i \qquad \text{and} \qquad \sum_{i=1}^{n} \alpha_i y_i = 0$$

- Substitute in Lagrangian optimization problem,

$$\mathcal{L}(\mathrm{w}, b, \alpha) = \frac{1}{2}\mathrm{w}^T\mathrm{w} - \sum_{i=1}^{n} \alpha_i (y_i(\mathrm{w}^T\mathrm{x}_i + b) - 1)$$

we get

$$\mathcal{L}(\alpha) = \sum_{n=1}^{n} \alpha_n - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathrm{x}_i^T \mathrm{x}_j$$

Maximize w.r.t. to α subject to $\alpha_i \geq 0$ for $i = 1, \ldots, n$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$

The solution - quadratic programming

$$\min_{\alpha} \quad \frac{1}{2}\alpha^T \begin{bmatrix} y_1y_1x_1^Tx_1 & y_1y_2x_1^Tx_2 & \cdots & y_1y_nx_1^Tx_n \\ y_2y_1x_2^Tx_1 & y_2y_2x_2^Tx_2 & \cdots & y_2y_nx_2^Tx_n \\ \vdots & \vdots & \ddots & \vdots \\ y_ny_1x_n^Tx_1 & y_ny_2x_n^Tx_2 & \cdots & y_ny_nx_n^Tx_n \end{bmatrix} \alpha + \left(-1^T\right)\alpha$$

subject to $\mathrm{y}^T\alpha = 0$ and $0 \leqslant \alpha \leqslant \infty$

QP hand us α

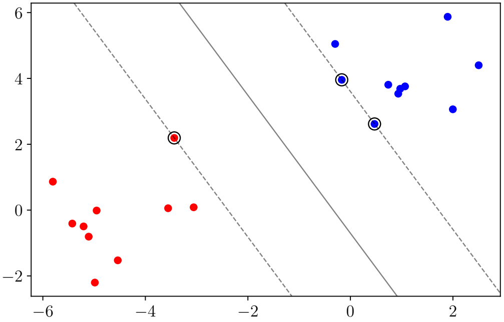
- Solution: $\alpha = \alpha_1, \dots, \alpha_n$

$$\Rightarrow \mathrm{w} = \sum_{i=1}^{n} \alpha_i y_i \mathrm{x}_i$$

- KKT condition: For $i = 1, \dots, n$

$$\alpha_i(y_i(\mathrm{w}^T \mathrm{x}_i + b) - 1) = 0$$

- For non-zero value of α ($\alpha_n > 0$), x_n are support vectors.



Support vectors

- Closest x_i's to the plane achieve the margin

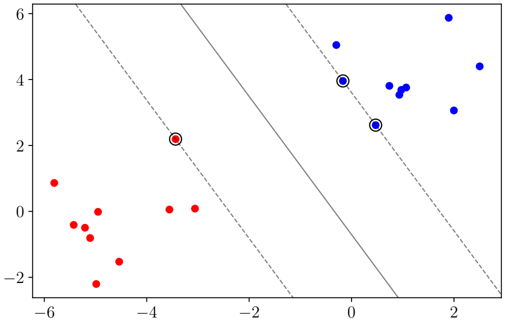
$$\Rightarrow y_i(\mathrm{w}^T \mathrm{x_i} + b) = 1$$

- We have the weight vector

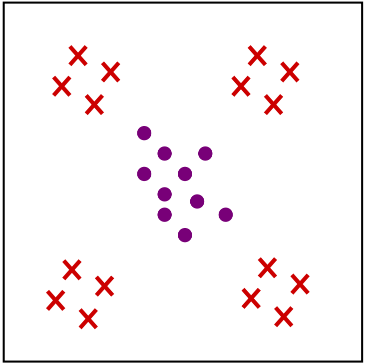
$$\mathrm{w} = \sum_{x_i \text{ is SV}} \alpha_i y_i \mathrm{x}_i$$

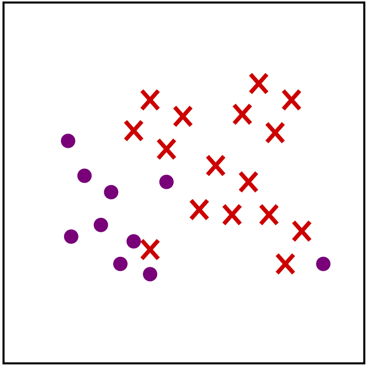
- Solve for b: using any Support vector (SV):

$$y_i(\mathrm{w}^T \mathrm{x}_i + b) = 1$$



Non-separable features



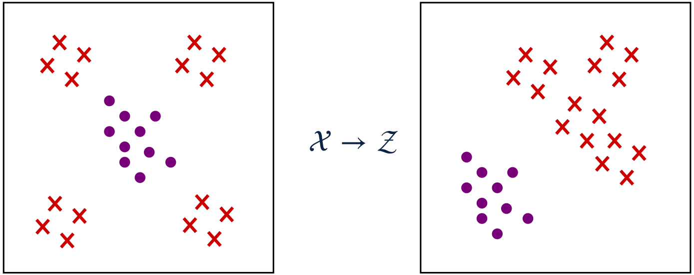


Kernel trick: z instead of x

- Dual problem:

$$\boxed{\mathcal{L}(\alpha) = \sum_{n=1}^{n} \alpha_n - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathrm{z}_i^T \mathrm{z}_j}$$

Maximize w.r.t. to α subject to $\alpha_i \geq 0$ for $i = 1, \ldots, n$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$



Kernel Trick: What do we need from the $\mathcal{Z}$ space?

$$\boxed{\mathcal{L}(\alpha) = \sum_{n=1}^{n} \alpha_n - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j \mathrm{z}_i^T \mathrm{z}_j}$$

Constraints: $\alpha \geq 0$ for $i = 1, \ldots, n$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$

$$\boxed{g(\mathrm{x}) = \text{sign}(\mathrm{w}^T \mathrm{z} + b)} \qquad \text{need} \quad \mathrm{z}_i^T \mathrm{z}$$

where

$$\mathrm{w} = \sum_{\mathrm{z}_i \text{ is SV}} \alpha_i y_i z_i$$

and b:

$$y_j(\mathrm{w}^T \mathrm{z}_j + b) = 1 \qquad \text{need } \mathrm{z}_i^T \mathrm{z}_j$$

Kernel Trick: generalized inner product

- Given two points x and $\mathrm{x}' \in \mathcal{X}$, we need $\mathrm{z}^T\mathrm{z}'$.
- Let $\mathrm{z}^T\mathrm{z}' = K(\mathrm{x}, \mathrm{x}')$ (the kernel: inner product of x and x')
- Example: $\mathrm{x} = (x_1, x_2)^T \rightarrow$ 2nd-order Φ

$$\mathrm{z} = \Phi(\mathrm{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

$$K(\mathrm{x}, \mathrm{x}') = \mathrm{z}^T\mathrm{z}' = 1 + x_1 x_1' + x_2 x_2' + x_1^2 {x'}_1^2 + x_2^2 {x'}_2^2 + x_1 {x'}_1 x_2 {x'}_2$$

Kernel Trick

- Can we compute $K(\mathrm{x}, \mathrm{x}')$ without transforming x and x'?
- Consider:

$$K(\mathrm{x}, \mathrm{x}') = (1 + \mathrm{x}^T \mathrm{x}')^2 = (1 + x_1 {x'}_1 + x_2 {x'}_2)^2$$
$$= 1 + x_1^2 {x'_1}^2 + x_2^2 {x'_2}^2 + 2x_1 {x'}_1 + 2x_2 {x'}_2 + 2x_1 {x'}_1 x_2 {x'}_2$$

- This is the inner production of

$$(1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2)$$

$$(1, {x'_1}^2, {x'_2}^2, \sqrt{2}{x'}_1, \sqrt{2}{x'}_2, \sqrt{2}{x'}_1 {x'}_2)$$

Non-linear Kernels

- Following are some basic non-linear kernels:
  - Linear:

$$K(\mathrm{x}_i, \mathrm{x}_j) = \mathrm{x}_i^T \mathrm{x}_j$$

  - Polynomial:

$$K(\mathrm{x}_i, \mathrm{x}_j) = (\gamma \mathrm{x}_i^T \mathrm{x}_j + r)^d, \gamma > 0$$

  - Radial basis function:

$$K(\mathrm{x}_i, \mathrm{x}_j) = \exp\left(-\gamma \|\mathrm{x}_i - \mathrm{x}_j\|^2\right), \gamma > 0$$

  - Sigmoid:

$$K(\mathrm{x}_i, \mathrm{x}_j) = \tanh\left(\gamma \mathrm{x}_i^T \mathrm{x}_j + r\right), \gamma > 0$$

where, γ, r, and d are kernel parameters.

Kernel formulation of SVM

- Remember quadratic programming?
- The only difference in quadratic coefficients as:

$$\min_{\alpha} \quad \frac{1}{2}\alpha^T \begin{bmatrix} y_1y_1z_1^Tz_1 & y_1y_2z_1^Tz_2 & \cdots & y_1y_nz_1^Tz_n \\ y_2y_1z_2^Tz_1 & y_2y_2z_2^Tz_2 & \cdots & y_2y_nz_2^Tz_n \\ \vdots & \vdots & \ddots & \vdots \\ y_ny_1z_n^Tz_1 & y_ny_2z_n^Tz_2 & \cdots & y_ny_nz_n^Tz_n \end{bmatrix} \alpha + \left(-1^T\right)\alpha$$

subject to $\mathrm{y}^T\alpha = 0$ and $0 \leqslant \alpha \leqslant \infty$

The final hypothesis

- Express $g(\mathrm{x}) = \mathrm{sign}(\mathrm{w}^{\mathrm{T}}\mathrm{z} + \mathrm{b})$ in terms of $K(\_,\_)$

$$w = \sum_{z_n in SV} \alpha_n y_n z_n \Rightarrow g(x) = sign\left(\sum_{\alpha_n > 0} \alpha_n y_n K(x_n, x) + b\right)$$

Express $\quad g(\mathbf{x}) = \mathrm{sign}\left(\mathbf{w}^{\intercal}\mathbf{z} + b\right) \quad$ in terms of $K(-,-)$

$$\mathbf{w} = \sum_{\mathbf{z}_n \text{ is SV}} \alpha_n y_n \mathbf{z}_n \quad \Longrightarrow \quad g(\mathbf{x}) = \mathrm{sign}\left(\sum_{\alpha_n > 0} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b\right)$$

$$\text{where} \quad b = y_m - \sum_{\alpha_n > 0} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}_m)$$

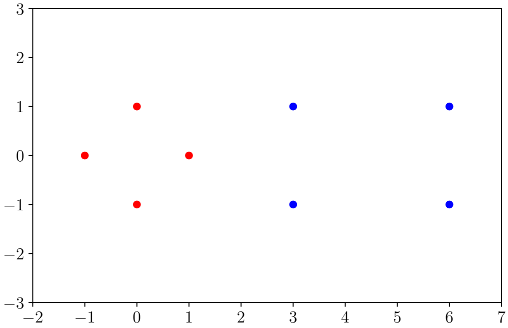
Example: Linear (trivial problem)

- Suppose we are given the following positively labeled data points in $\Re^2$:

$$\left\{ \begin{pmatrix} 3 \\ 1 \end{pmatrix}, \begin{pmatrix} 3 \\ -1 \end{pmatrix}, \begin{pmatrix} 6 \\ 1 \end{pmatrix}, \begin{pmatrix} 6 \\ -1 \end{pmatrix} \right\}$$

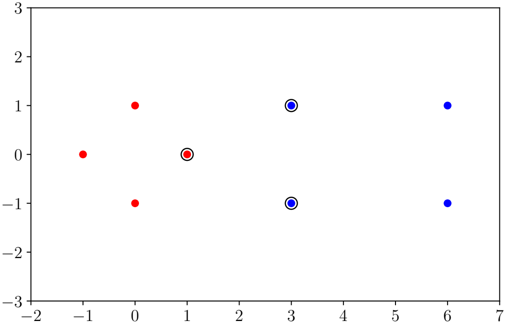
- and the following negatively labeled data points in $\Re^2$

$$\left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix} \right\}$$



Solution

- Since the data is linear separable, we can use a linear SVM.
- By inspection, it should be obvious that there are three support vectors.



Soft Margin Classification

- In basic SVM, the optimization problem is formulated for margin maximization when the feature vectors are linearly separable.
- However, a greater margin can be achieved by allowing classifier for some misclassification error during training itself.
- After allowing the misclassification of some features, the inequality constraint in basic SVM is replaced with $y_i(\mathrm{w}^T\mathrm{x}_i + b) \geq 1 - \xi_i$, where $\xi_i \geq 0$ are slack variables.

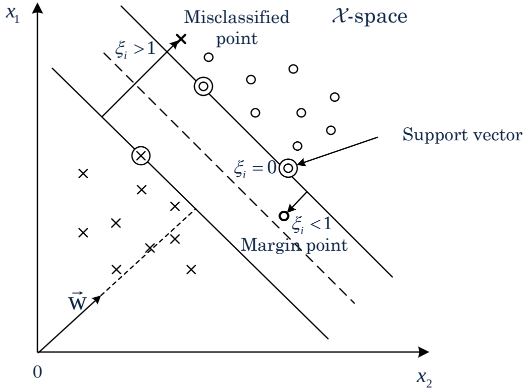


Figure: $\mathcal{X}$-space with support vector, penalized misclassification, and margin error

The new optimization problem: C-SVM

- Slack variables ξ_i can be added to allow misclassification of difficult or noisy examples, resulting margin called soft.
- Slack variables account for the misclassification and margin errors.
- The primal optimization problem with penalized misclassification and margin error becomes.

$$
\begin{aligned}
\underset{\mathrm{w},b}{\text{minimize}} \quad & \frac{1}{2}\|\mathrm{w}\|^2 + C\sum_{i=1}^{n}\xi_i \\
\text{subject to :} \quad & y_i(\mathrm{w}^{\mathrm{T}}\mathrm{x}_i + b) \geq 1 - \xi_i, \text{ and} \\
& \xi_i \geq 0, \ i = 1, 2, \ldots, n,
\end{aligned} \tag{1}
$$

- where C is a regularization parameter which sets the trade-off between margin maximization and minimizing the amount of slack (misclassifications and margin error).

Lagrange formulation

Using Lagrange multipliers, the dual problem is expressed in terms of Lagrangian coefficients as

Lagrange formulation

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\,\mathbf{w}^{\intercal}\mathbf{w} + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N}\alpha_n(y_n\,(\mathbf{w}^{\intercal}\mathbf{x}_n + b) - 1 + \xi_n) - \sum_{n=1}^{N}\beta_n\,\xi_n$$

Minimize w.r.t. $\mathbf{w}$, b, and $\boldsymbol{\xi}$ and maximize w.r.t. each $\alpha_n \geq 0$ and $\beta_n \geq 0$

$$\nabla_{\mathbf{w}}\mathcal{L} = \mathbf{w} - \sum_{n=1}^{N}\alpha_n y_n \mathbf{x}_n = \mathbf{0}$$

$$\frac{\partial\mathcal{L}}{\partial b} = -\sum_{n=1}^{N}\alpha_n y_n = 0$$

$$\frac{\partial\mathcal{L}}{\partial \xi_n} = C - \alpha_n - \beta_n = 0$$

and the solution is ...

$$\text{Maximize} \quad \mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \, \alpha_n \alpha_m \, \mathbf{x}_n^{\intercal} \mathbf{x}_m \quad \text{w.r.t. to } \boldsymbol{\alpha}$$

$$\text{subject to } \; 0 \le \alpha_n \le C \; \text{ for } \; n = 1, \cdots, N \quad \text{and} \quad \sum_{n=1}^{N} \alpha_n y_n = 0$$

$$\Longrightarrow \quad \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$$

$$\text{minimizes} \quad \frac{1}{2} \mathbf{w}^{\intercal} \mathbf{w} + C \sum_{n=1}^{N} \xi_n$$

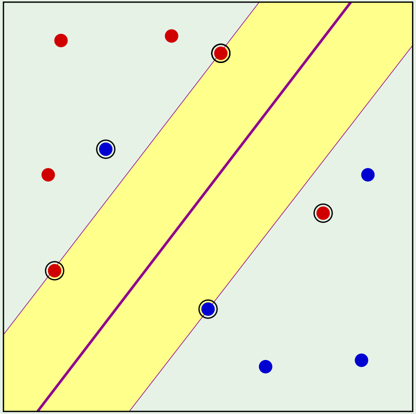
Types of support vectors

margin support vectors $(0 < \alpha_n < C)$

$$y_n\left(\mathbf{w}^\intercal\mathbf{x}_n + b\right) = 1 \qquad (\xi_n = 0)$$

non-margin support vectors $(\alpha_n = C)$

$$y_n\left(\mathbf{w}^\intercal\mathbf{x}_n + b\right) < 1 \qquad (\xi_n > 0)$$



Two technical observations

1. Hard margin: What if data is not linearly separable?

$$\text{``primal} \longrightarrow \text{dual''} \quad \text{breaks down}$$

2. $\mathcal{Z}$: What if there is w_0?

$$\text{All goes to } b \text{ and } w_0 \to 0$$

References

Thank you!