Introduction to Data Science

Support Vector Machine

Arijit Mondal

Dept. of Computer Science & Engineering

Indian Institute of Technology Patna

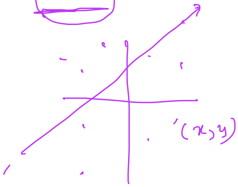
arijit@iitp.ac.in

Support Vector Machine

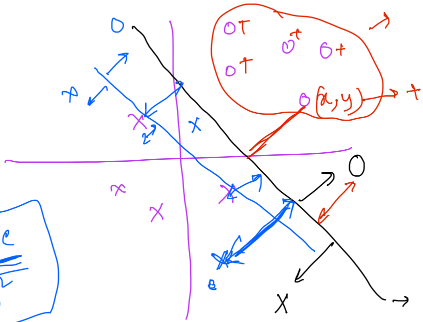
- An approach for classification
- Developed in 1990s
- Generalization of maximum margin classifier
  - Mostly limited to linear boundary
- Support vector classifier — broad range of classes
- SVM — Non-linear class boundary

Hyperplane

- In n dimensional space a hyperplane is a flat affine subspace of dimension $n-1$
- Mathematically it is defined as
  - For 2 dimensions — $w_0 + w_1x_1 + w_2x_2 = 0$
  - For n dimensions — $w_0 + w_1x_1 + \ldots + w_nx_n = 0$



$y = ax + b$



$$\frac{ax_1 + by_1 + c}{\sqrt{a^2+b^2}}$$

$(x_1, y_1) \to$ O, X

classifier

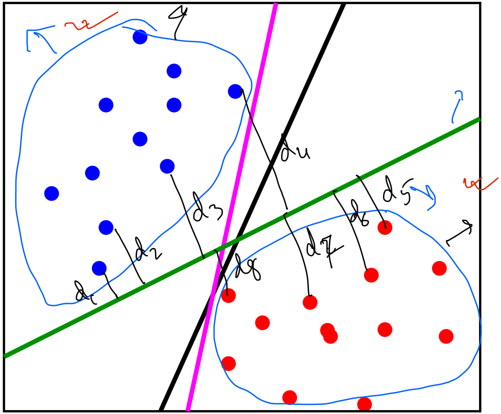
$ax + by + c = 0$

$+$, $-$

Classification using Hyperplane

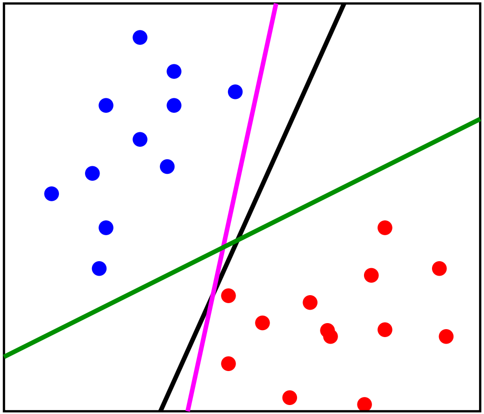
- Assume, *m* training observation in *n* dimensional space

$$\max \left\{ \boxed{\min_i \{ d_i \}} \right\}$$



Classification using Hyperplane

- Assume, *m* training observation in *n* dimensional space
- Separating hyperplane has the property
  - $w_0 + w_1x_1 + \ldots + w_nx_n > 0$ if $y_i = 1$
  - $w_0 + w_1x_1 + \ldots + w_nx_n < 0$ if $y_i = -1$



Classification using Hyperplane

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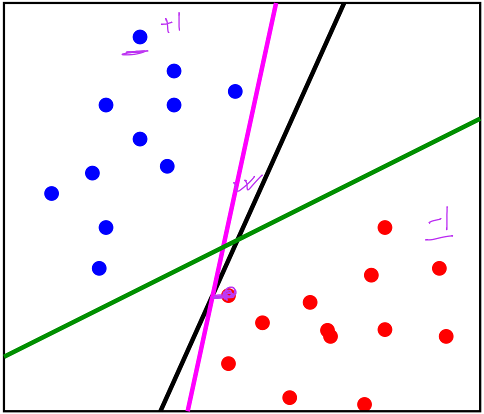
- Hence, $y_i(w_0 + w_1x_1 + \ldots + w_nx_n) > 0$
- Classification of test observation x^* is done based on the sign of

$$f(x^*) = w_0 + w_1x_1^* + \ldots + w_nx_n^*$$

>0, <0

- Magnitude of $f(x^*)$
  - Far from 0 — Confident about prediction
  - Close to 0 — Less certain



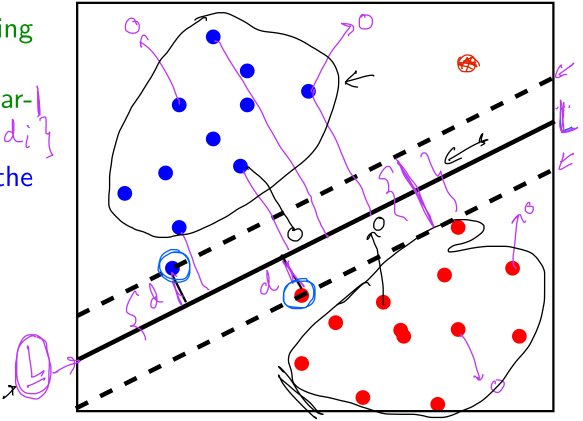
Maximal margin classifier

- Also known as optimal separating hyperplane
- Separating hyperplane farthest from training observation
  - Compute perpendicular distance from training point to the hyperplane
  - Smallest of these distances represents the margin

    min $\{d_i\}$
- Target is to find the hyperplane for which the margin is the largest

$$\max_{L} \left\{ \min_{i} \{d_i\} \right\}$$

$$M = \min \{d_i\}$$



Construction of maximal margin classifier

- Input — m points in n dimension space ie. $\mathrm{x}_1, \mathrm{x}_2, \ldots, \mathrm{x}_m$
- Input — labels $y_1, y_2, \ldots, y_m$ for each point x_i where $y_i \in \{-1, 1\}$
- Need to solve the following optimization problem

$$\max_{w_0, w_1, \ldots, w_n, M} M$$

subject to

$$y_i(w_0 + w_1 x_{i1} + w_{i2} + \ldots + w_{in} x_{in}) \geq M \quad \forall i = 1, \ldots, m$$

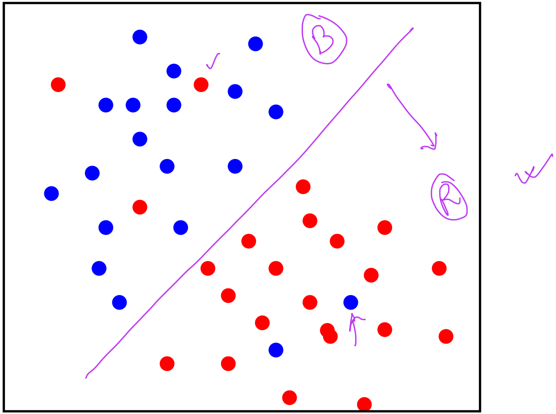
$$\sum_{i=1}^{n} w_i^2 = 1$$

$$\frac{a x_1 + b x_1 + c}{\sqrt{a^2 + b^2}}$$

$$\sqrt{a^2+b^2} = 1$$

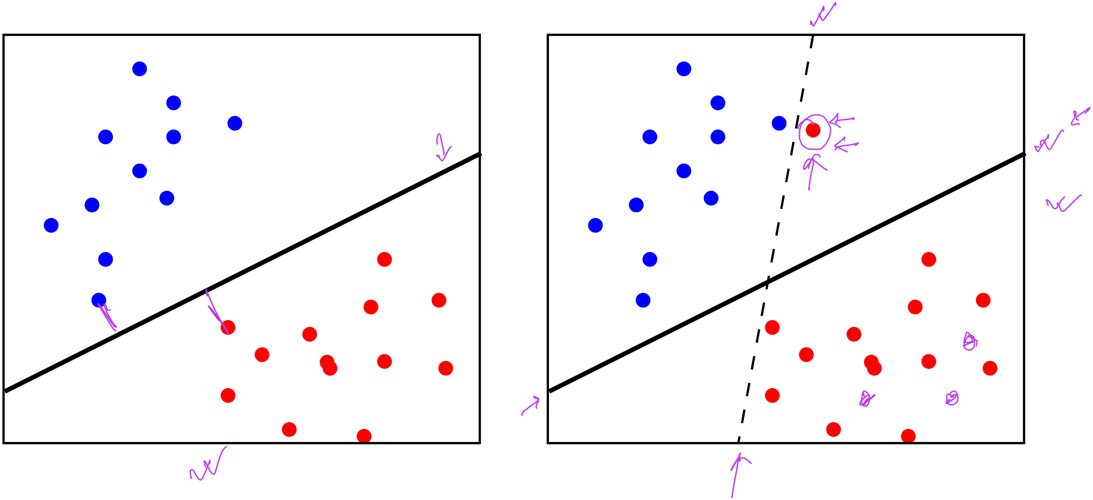
Issues

- Maximal margin classifier fails to provide classification in case of overlap



Issues

- Single observation point can change the hyperplane drastically

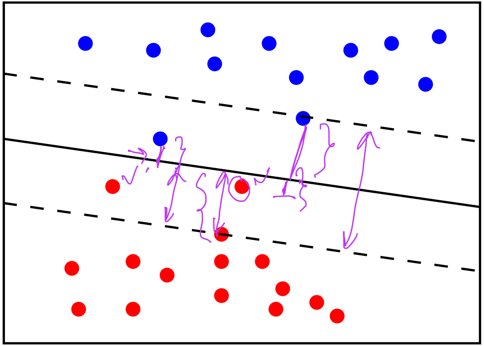


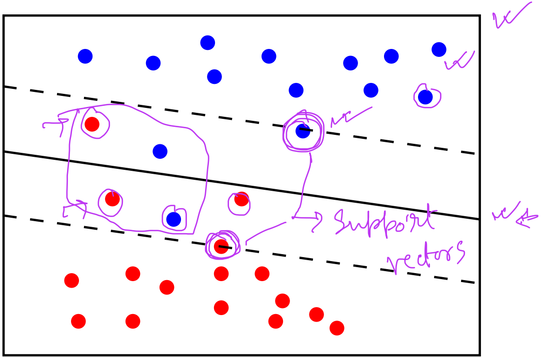
Support Vector Classifier

- Provides greater robustness to individual observations
- Better classification of most of the training observations
- Worthwhile to misclassify a few training observations
- Also known as soft margin classifier

Support Vector Classifier

- Points can lie within the margin or wrong side of hyperplane





Optimization with misclassification

- Input — $x_1, x_2, \ldots, x_m$ and $y_1, y_2, \ldots, y_m$
- Need to solve the following optimization problem

$$\max_{w_0, w_1, \ldots, w_n, M} \quad M$$

subject to

$$y_i(w_0 + w_1 x_{i1} + \ldots + w_{in} x_{in}) \geq M(1 - \epsilon_i) \quad \forall i = 1, \ldots, m$$

$$\sum_{i=1}^{n} w_i^2 = 1, \quad \boxed{\sum_{i=1}^{m} \epsilon_i \underset{\le}{=} C}$$

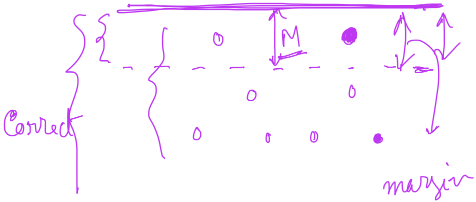
$\epsilon_i = 0$

$0 < \epsilon_i < 1$

$\epsilon_i > 1$

wrong

- C is non-negative tuning parameter, ϵ_i - slack variable
- Classification of test observation remains the same



Observations

- $\epsilon_i = 0$ — ith observation is on the correct side of margin
- $\epsilon_i > 0$ — ith observation is on the wrong side of margin
- $\epsilon_i > 1$ — ith observation is on the wrong side of hyperplane
- C — budget for the amount that the margin can be violated by m observations
  - $C = 0$ — No violation, ie. maximal margin classifier
  - $C > 0$ — No more than C observation can be on the wrong side of hyperplane
  - C is small — Narrow margin, highly fit to data, low bias and high variance
  - C is large — Fitting data is less hard, more bias and may have less variance

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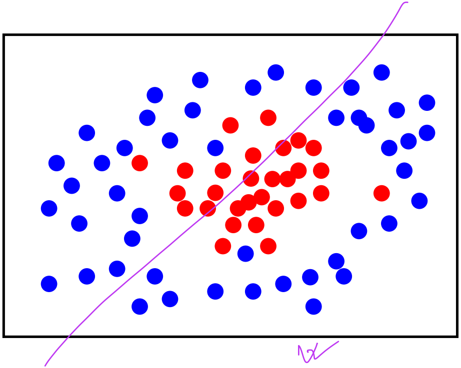
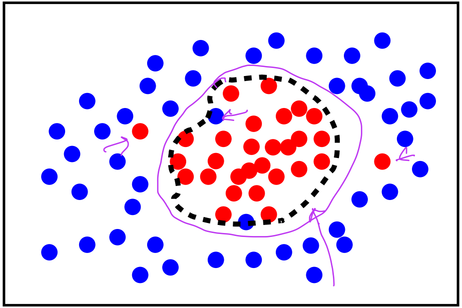
Classification with non-linear boundaries





x_1^2, $x_1^2 x_2$

Classification with non-linear boundaries

- Performance of linear regression can suffer for non-linear data
- Feature space can be enlarged using function of predictors
  - For example, instead of fitting with $x_1, x_2, \ldots, x_n$ features we could use $x_1, x_1^2, x_2, x_2^2 \ldots, x_n, x_n^2$ as features
- Optimization problem becomes

$$\max_{w_0, w_{11}, w_{12} \ldots, w_{n1}, w_{n2}, \epsilon_i, M} M$$

subject to

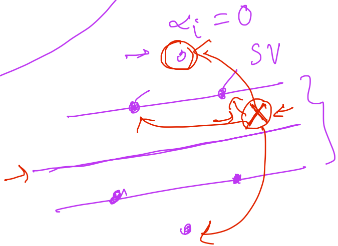
$$y_i \left(w_0 + \sum_{j=1}^{n} w_{j1} x_{ij} + \sum_{j=1}^{n} w_{j2} x_{ij}^2 \right) \geq M(1 - \epsilon_i) \quad \forall i = 1, \ldots, m$$

$$\sum_{i=1}^{n} \sum_{j=1}^{2} w_{ij}^2 = 1, \quad \sum_{i=1}^{m} \epsilon_i \leq C, \quad \epsilon_i \geq 0$$

Support Vector Machine

- Extension of support vector classifier that results from enlarging feature space
- It involves inner product of the observations $f(x) = w_0 + \sum_{i=1}^{m} \alpha_i \langle x, x_i \rangle$ where α_i - one per training example
  - To estimate α_i and w_0, we need $m(m-1)/2$ inner products, $\langle x_i, x_{i'} \rangle$
- It turns out that $\alpha_i \neq 0$ for support vectors

$$f(x) = w_0 + \sum_{i \in S} \alpha_i \langle x, x_i \rangle$$ where S - set of support vectors



Support Vector Machine

- Inner product is replaced with kernel, K or $K(\mathrm{x}_i, \mathrm{x}_{i'})$
- Kernel quantifies similarity between observations $K(\mathrm{x}_i, \mathrm{x}_{i'}) = \sum_{j=1}^{n} x_{ij} x_{i'j}$
  - Above one is Linear kernel ie. Pearson correlation
- Polynomial kernel $K(\mathrm{x}_i, \mathrm{x}_{i'}) = \left(1 + \sum_{j=1}^{n} x_{ij} x_{i'j}\right)^d$ where d is positive integer > 1
- Support vector classifier with non-linear kernel is known as support vector machine and the function will look

$$\boxed{f(x) = w_0 + \sum_{i \in S} \alpha_i K(\mathrm{x}, \mathrm{x}_i)}$$

- Radial kernel: $K(\mathrm{x}_i, \mathrm{x}_{i'}) = \exp\left(-\gamma \sum_{i=1}^{n} (x_{ij} - x_{i'j})^2\right)$ where $\gamma > 0$