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Data Mining and Machine Learning
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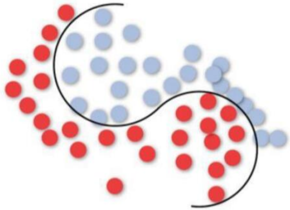
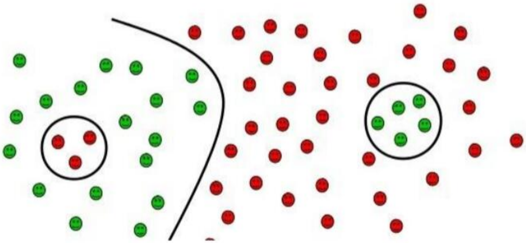
A geometric view of supervised learning

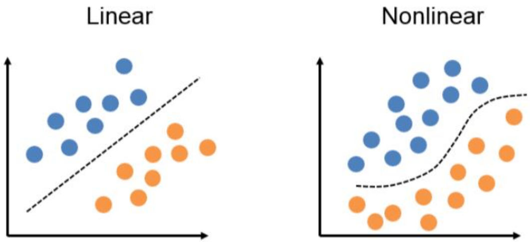
- Think of data as points in space
- Find a separating curve (surface)
- Separable case
  - Each class is a connected region
  - A single curve can separate them
- More complex scenario
  - Classes form multiple connected regions
  - Need multiple separators

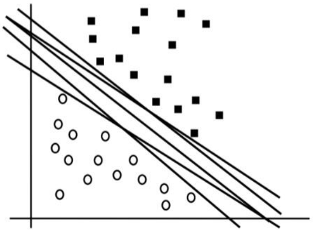




Linear separators

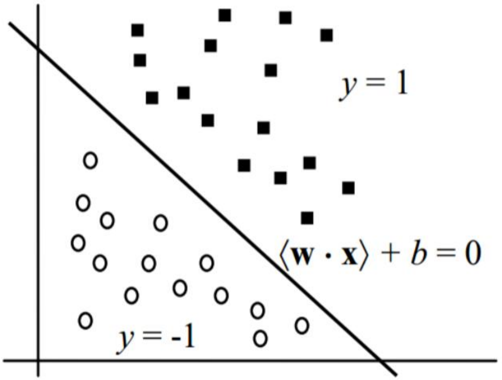
- Simplest case — linearly separable data
- Dual of linear regression
  - Find a line that passes close to a set of points
  - Find a line that separates the two sets of points
- Many lines are possible
  - How do we find the best one?
  - What is a good notion of “cost” to optimize?





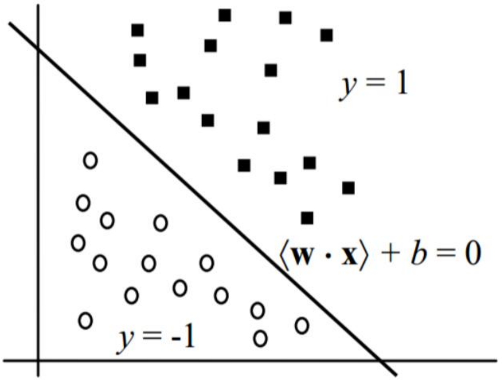
Linear separators

- Each input x has n attributes $\langle x_1, x_2, \ldots, x_n \rangle$
- Linear separator has the form $w_1x_1 + w_2x_2 + \cdots w_nx_n + b$
- Classification criterion
  - $w_1x_1 + w_2x_2 + \cdots w_nx_n + b > 0$, classify yes, $+1$
  - $w_1x_1 + w_2x_2 + \cdots w_nx_n + b < 0$, classify no, -1



Linear separators

- Dot product $w \cdot x$
  $\langle w_1, w_2, \ldots, w_n \rangle \cdot \langle x_1, x_2, \ldots, x_n \rangle = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$
- Collapsed form
  $w \cdot x + b > 0$, $w \cdot x + b < 0$
- Rename bias b as w_0, create fictitious $x_0 = 1$
- Classification criteria become
  $w \cdot x > 0$, $w \cdot x < 0$



Perceptron algorithm

(Frank Rosenblatt, 1958)

- Each training input is (x_i, y_i), where $x_i = \langle x_{i_1}, x_{i_2}, \ldots, x_{i_n} \rangle$ and $y_i = +1$ or -1
- Need to find $w = \langle w_0, w_1, \ldots, w_n \rangle$
  - Recall $x_{i_0} = 1$, always

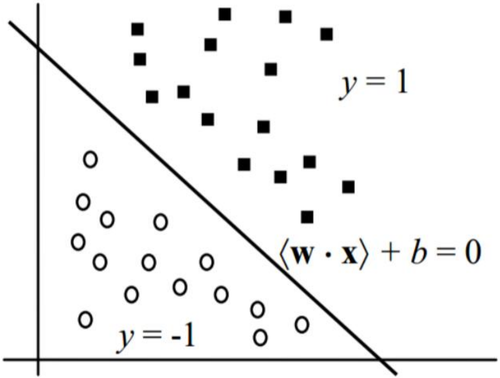
Initialize $w = \langle 0, 0, \ldots, 0 \rangle$

While there exists x_i, y_i *such that*

$y_i = +1$ *and* $w \cdot x_i < 0$, *or*

$y_i = -1$ *and* $w \cdot x_i > 0$

Update w *to* $w + x_i y_i$

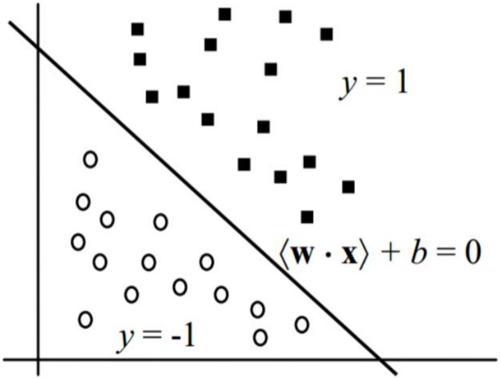


Perceptron algorithm ...

- Keep updating w as long as some training data item is misclassified
- Update is an offset by misclassified input
- Need not stabilize, potentially an infinite loop

Theorem

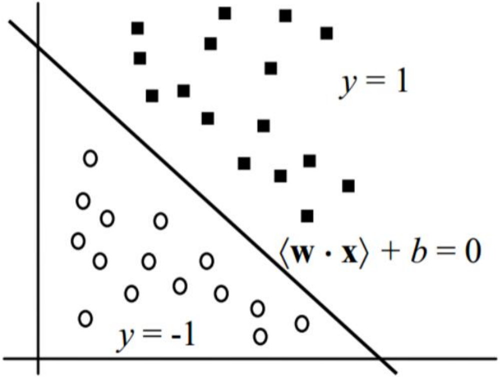
If the points are linearly separable, the Perceptron algorithms always terminates with a valid separator



Theorem

If the points are linearly separable, the Perceptron algorithms always terminates with a valid separator

- Termination time depends on two factors
  - Width of the band separating the positive and negative points
    - Narrow band takes longer to converge
  - Magnitude of the x values
    - Larger spread of points takes longer to converge



Perceptron Algorithm — Proof

Theorem

If there is w^* satisfying $(w^* \cdot x_i)y_i \geq 1$ for all i, then the Perceptron Algorithm finds a solution w with $(w \cdot x_i)y_i > 0$ for all i in at most $r^2|w^*|^2$ updates, where $r = \max_i |x_i|$.

- Assume w^* exists. Keep track of two quantities: $w^\top w^*$, $|w|^2$.
- Each update increases $w^\top w^*$ by at least 1.

$$(w + x_i y_i)^\top w^* = w^\top w^* + x_i^\top y_i w^* \geq w^\top w^* + 1$$

- Each update increases $|w|^2$ by at most r^2

$$(w + x_i y_i)^\top (w + x_i y_i) = |w|^2 + 2x_i^\top y_i w + |x_i y_i|^2 \leq |w|^2 + |x_i|^2 \leq |w|^2 + r^2$$

  - Note that we update only when $x_i^\top y_i w < 0$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$
- $m \;\leq\; |w||w^*|$, because $a \cdot b = |a||b| \cos\theta$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$
- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \end{aligned}$$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$
- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \\ m/|w^*| &\leq r\sqrt{m}, \text{ because } |w|^2 \leq mr^2 \end{aligned}$$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$
- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \\ m/|w^*| &\leq r\sqrt{m} \\ \sqrt{m} &\leq r|w^*| \end{aligned}$$

Perceptron Algorithm — Proof (cont'd)

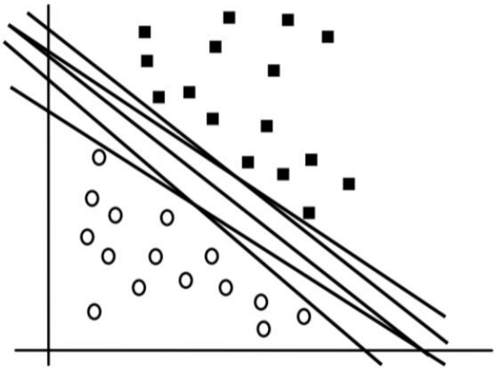
- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$
- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \\ m/|w^*| &\leq r\sqrt{m} \\ \sqrt{m} &\leq r|w^*| \\ m &\leq r^2|w^*|^2 \end{aligned}$$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$
- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \\ m/|w^*| &\leq r\sqrt{m} \\ \sqrt{m} &\leq r|w^*| \\ m &\leq r^2|w^*|^2 \end{aligned}$$
- Note (for later) that final w is of the form $\sum_i n_i x_i$

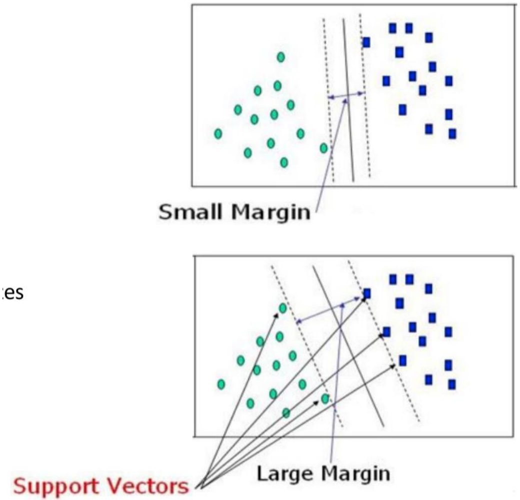
Linear separators

- Simplest case — linearly separable data
- Perceptron algorithm is a simple procedure to find a linear separator, if one exists
- Many lines are possible
  - Does the Perceptron algorithm find the best one?
  - What is a good notion of "cost" to optimize?



Margin

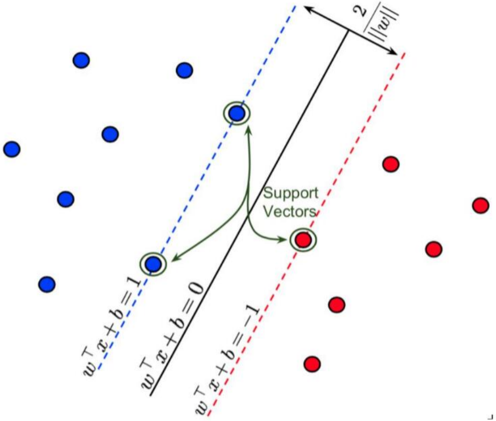
- Each separator defines a margin
  - Empty corridor separating the points
  - Separator is the centre line of the margin
- Wider margin makes for a more robust classifier
  - More gap between the classes
- Optimum classifier is one that maximizes the width of its margin
- Margin is defined by the training data points on the boundary
  - Support vectors



Finding a maximum margin classifier

- Recall our original linear classifier
  $w_1x_1 + w_2x_2 + \cdots w_nx_n + b > 0$, classify yes, $+1$
  $w_1x_1 + w_2x_2 + \cdots w_nx_n + b < 0$, classify no, -1

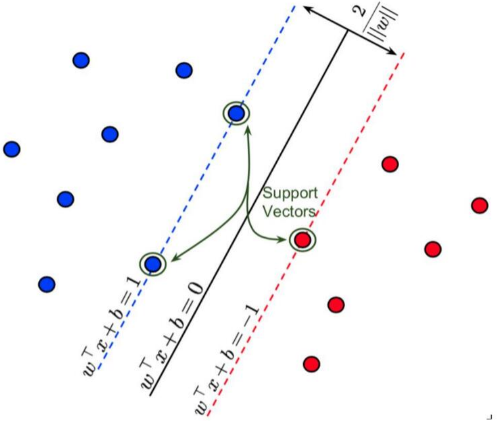
- Scale margin so that separation is 1 on either side
  $w_1x_1 + w_2x_2 + \cdots w_nx_n + b > 1$, classify yes, $+1$
  $w_1x_1 + w_2x_2 + \cdots w_nx_n + b < -1$, classify no, -1



Finding a maximum margin classifier

- Scale margin so that separation is 1 on either side
  $w_1x_1 + w_2x_2 + \cdots w_nx_n + b > 1$, classify yes, $+1$
  $w_1x_1 + w_2x_2 + \cdots w_nx_n + b < -1$, classify no, -1

- Using Pythagoras's theorem, perpendicular distance to nearest support vector is $\frac{1}{|w|}$, where
  $|w| = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}$

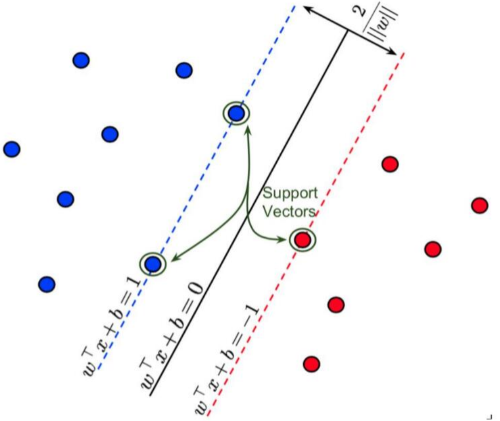


Optimization problem

- Want to maximize the overall margin $\dfrac{2}{|w|}$
- Equivalently, minimize $\dfrac{|w|}{2}$
- Also, w should classify each (x_i, y_i) correctly

  $w_1x_1^i + w_2x_2^i + \cdots w_nx_n^i + b > 1$,
  if $y_i = 1$

  $w_1x_1^i + w_2x_2^i + \cdots w_nx_n^i + b < -1$,
  if $y_i = -1$



Optimization problem

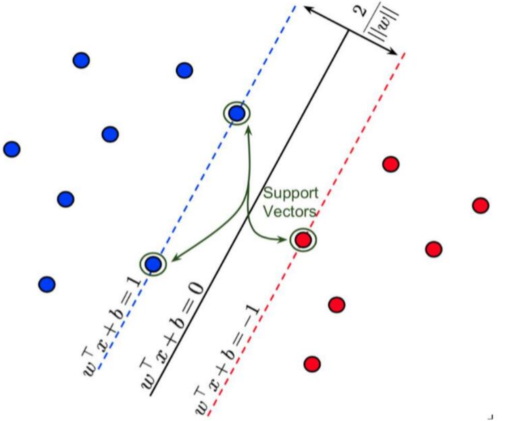
Minimize $\dfrac{|w|}{2}$

Subject to

$w_1x_1^i + w_2x_2^i + \cdots w_nx_n^i + b > 1$, if $y_i = 1$

$w_1x_1^i + w_2x_2^i + \cdots w_nx_n^i + b < -1$, if $y_i = -1$

- The constraints are linear
- The objective function is not linear
  $|w| = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}$
- This is a quadratic optimization problem, not linear programming

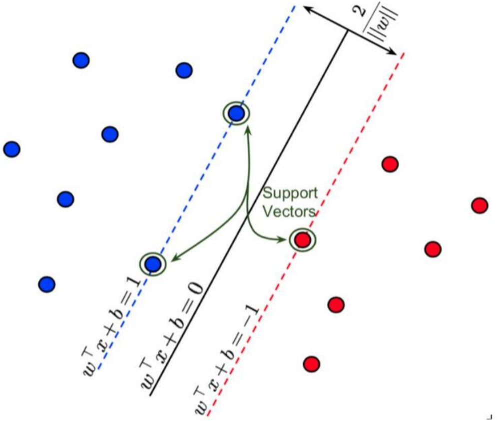


Solution to optimization problem

- Convex optimization theory
- Can be solved using computational techniques
- Solution expressed in terms of Lagrange multipliers $\alpha_1, \alpha_2, \ldots, \alpha_N$, one multiplier per training input
- α_i is non-zero iff x_i is a support vector
- Final classifier for new input z

$$\text{sign}\left[\sum_{i \in sv} y_i \alpha_i (x_i \cdot z) + b\right]$$

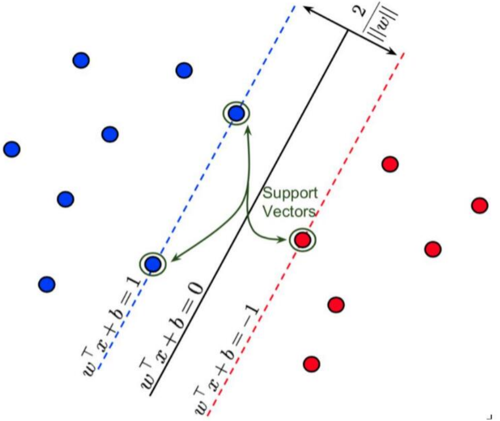
- sv is set of support vectors



Support Vector Machine (SVM)

$$\text{sign}\left[\sum_{i \in sv} y_i \alpha_i (x_i \cdot z) + b\right]$$

- Solution depends only on support vectors
  - If we add more training data away from support vectors, separator does not change
- Solution uses dot product of support vectors with new point
  - Will be used later, in the non-linear case



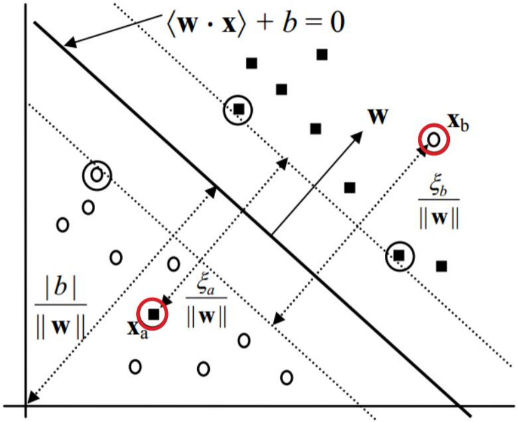
The non-linear case

- Some points may lie on the wrong side of the classifier
- How do we account for these?
- Add an error term to the classifier requirement
- Instead of

  $w \cdot x + b > 1$, if $y_i = 1$
  $w \cdot x + b < -1$, if $y_i = -1$

  we have

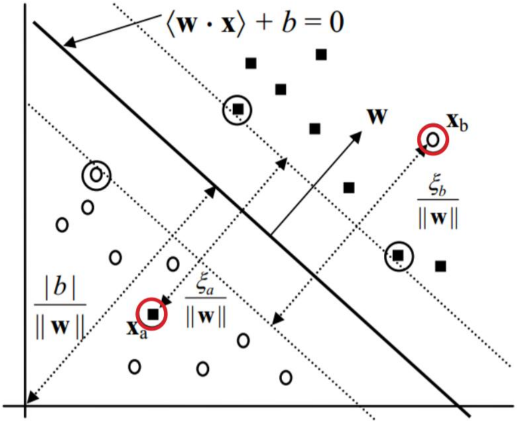
  $w \cdot x + b > 1 - \xi_i$, if $y_i = 1$
  $w \cdot x + b < -1 + \xi_i$, if $y_i = -1$



Soft margin classifier

$w \cdot x + b > 1 - \xi_i$, if $y_i = 1$
$w \cdot x + b < -1 + \xi_i$, if $y_i = -1$

- Error term always non-negative,
- If the point is correctly classified, error term is 0
- Soft margin — some points can drift across the boundary
- Need to account for the errors in the objective function
  - Minimize the need for non-zero error terms



Soft margin optimization

Minimize $\frac{|w|}{2} + \sum_{i=1}^{N} \xi_i^2$

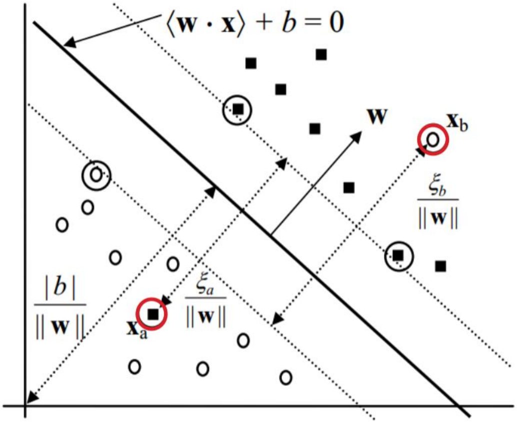
Subject to

$\xi_i \geq 0$

$w \cdot x_i + b > 1 - \xi_i$, if $y_i = 1$

$w \cdot x_i + b < -1 + \xi_i$, if $y_i = -1$

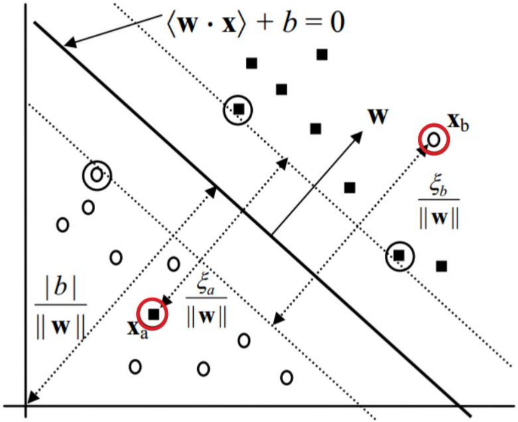
- Constraints include requirement that error terms are non-negative
- Again the objective function is quadratic



Soft margin optimization

- Can again be solved using convex optimization theory
- Form of the solution turns out to be the same as the hard margin case
  - Expression in terms of Lagrange multipliers α_i
  - Only terms corresponding to support vectors are actively used

$$\text{sign}\left[\sum_{i \in sv} y_i \alpha_i (x_i \cdot z) + b\right]$$



The non-linear case

- How do we deal with datasets where the separator is a complex shape?
- Geometrically transform the data
  - Typically, add dimensions
- For instance, if we can "lift" one class, we can find a planar separator between levels