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Madhavan Mukund

https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning
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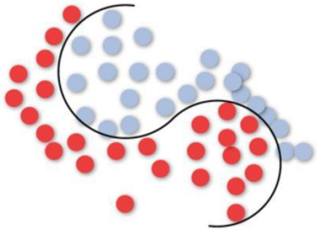
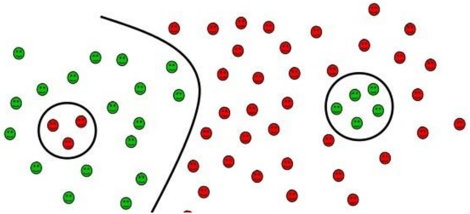
A geometric view of supervised learning

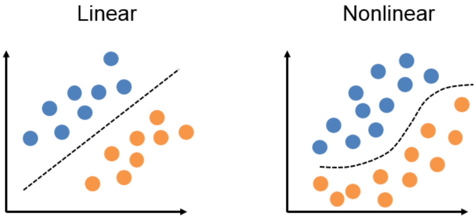
- Think of data as points in space
- Find a separating curve (surface)
- Separable case
  - Each class is a connected region
  - A single curve can separate them
- More complex scenario
  - Classes form multiple connected regions
  - Need multiple separators

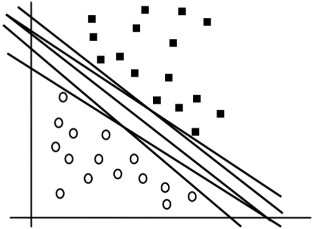




Linear separators

- 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?

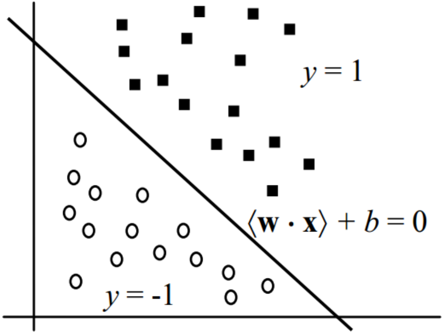




Linear separators

- Each input x has n attributes <x_1,x_2,…,x_n>
- Linear separator has the form
  $w_1x_1 + w_2x_2 + \cdots + w_nx_n + b$
- Classification criterion
  $w_1x_1 + \cdots + w_nx_n + b > 0, \quad \text{classify yes}, +1$
  $w_1x_1 + \cdots + w_nx_n + b < 0, \quad \text{classify no}, -1$
- Dot product $\langle w \cdot x \rangle$
  $(w_1, \ldots, w_n) \cdot (x_1, \ldots, x_n) = w_1x_1 + \cdots + w_nx_n$
- Collapsed form
  $\langle w \cdot x \rangle + b > 0, \langle w \cdot x \rangle + b < 0$
- Rename bias b as w_0, create fictitious $x_0 = 1$
- Equation becomes

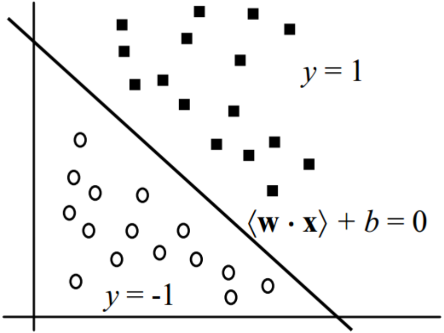
$$\langle w \cdot x \rangle > 0, \langle w \cdot x \rangle < 0$$



Perceptron algorithm

(Frank Rosenblatt, 1958)

- Each training input is (x_i, y_i) where $x_i = <x^i_1, x^i_2, \ldots, x^i_n>$ and $y_i = +1$ or -1
- Need to find $w = <w_0, w_1, \ldots, w_n>$. 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 $\langle w \cdot x_i \rangle < 0$, *or*
$y_i = -1$, and $\langle w \cdot x_i \rangle > 0$

Update w *to* $w + x_i$

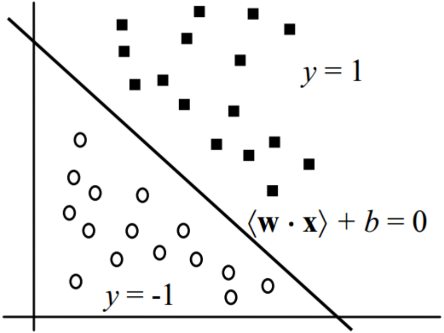
Perceptron algorithm

- 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

- 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

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

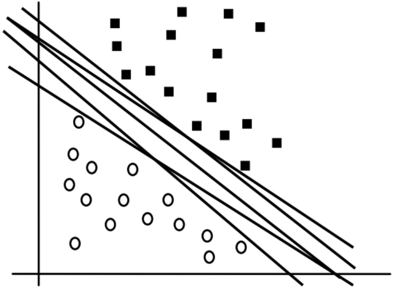
  - Note that we update only when $x_i^\top y_i w < 0$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates
- 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 $\sum_i n_i x_i$

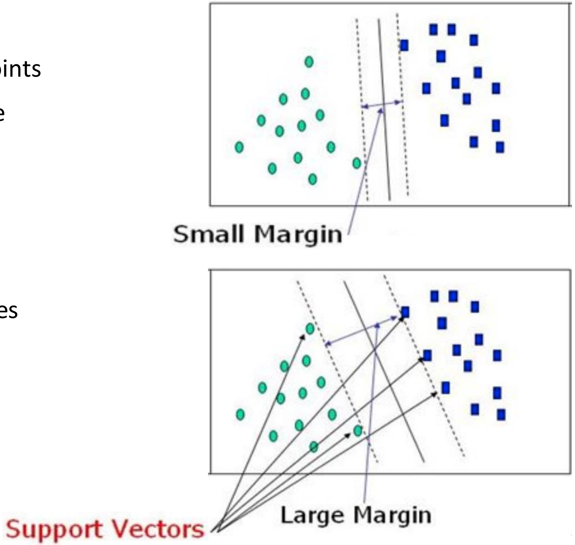
Linear separators

- 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

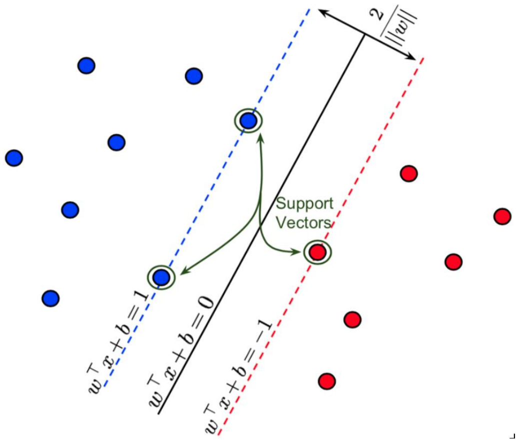
$$\begin{aligned} w_1x_1 + \cdots + w_nx_n + b > 0, &\quad \text{classify yes}, +1 \\ w_1x_1 + \cdots + w_nx_n + b < 0, &\quad \text{classify no}, -1 \end{aligned}$$

- Scale margin so that separation is 1 on either side

$$\begin{aligned} w_1x_1 + \cdots + w_nx_n + b > 1, &\quad \text{classify yes}, +1 \\ w_1x_1 + \cdots + w_nx_n + b < -1, &\quad \text{classify no}, -1 \end{aligned}$$

- Using Pythagoras's theorem, perpendicular distance to nearest support vector is $\dfrac{1}{||w||}$,

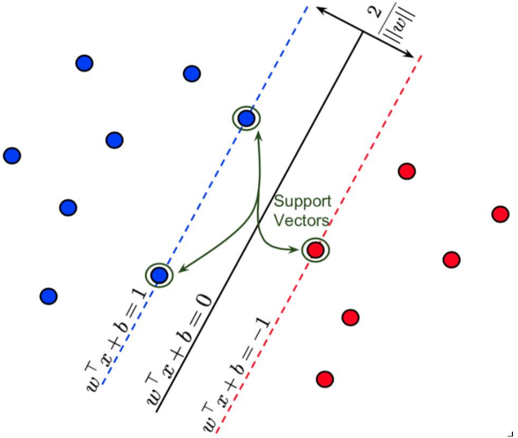
where $||w|| = \sqrt{w_1^2 + w_2^2 + \cdots + w_n^2}$



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

$$\begin{array}{ll} w_1 x_1^i + \cdots + w_n x_n^i + b > 1, & \text{if } y_i = 1 \\ w_1 x_1^i + \cdots + w_n^i x_n + b < -1, & \text{if } y_i = -1 \end{array}$$



Optimization problem

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

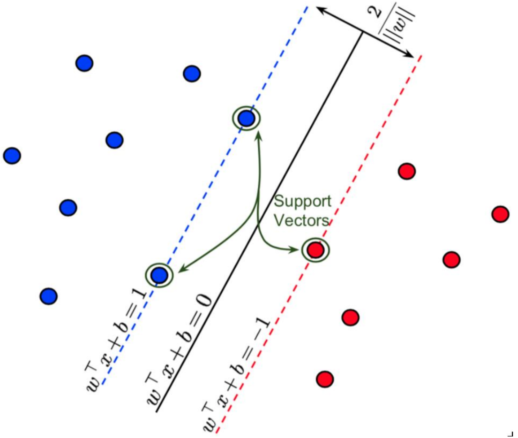
Subject to

$$\begin{aligned} w_1 x_1^i + \cdots + w_n x_n^i + b > 1, &\quad \text{if } y_i = 1 \\ w_1 x_1^i + \cdots + w_n^i x_n + b < -1, &\quad \text{if } y_i = -1 \end{aligned}$$

- 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

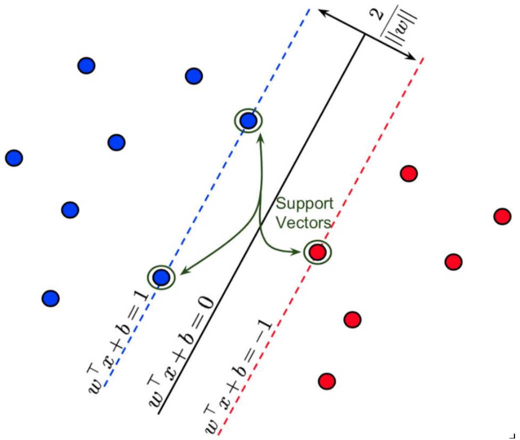


Solution to optimization problem

- 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

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

- *sv* is set of support vectors

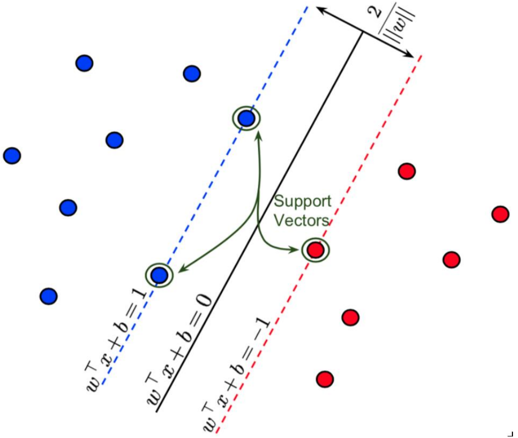


Support Vector Machine (SVM)

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

Support Vector Machine (SVM)

- 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



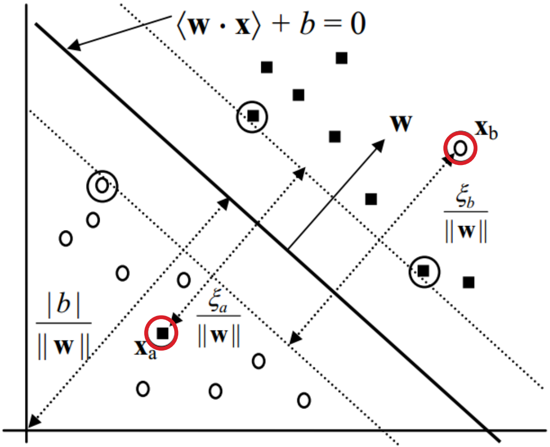
The non-linear case

- 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

$$
\begin{array}{ll}
\langle w \cdot x \rangle + b > 1, & \text{if } y_i = 1 \\
\langle w \cdot x \rangle + b < -1, & \text{if } y_i = -1
\end{array}
$$

we have

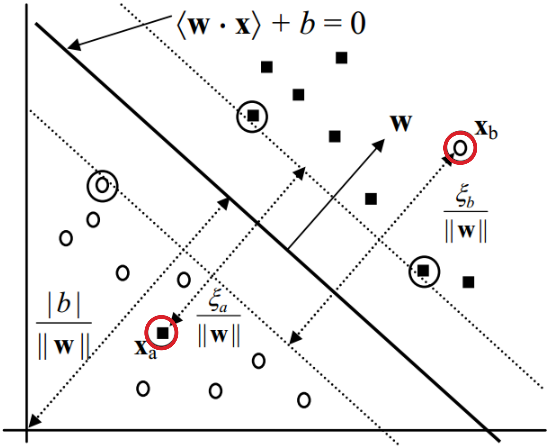
$$
\begin{array}{ll}
\langle w \cdot x \rangle + b > 1 - \xi_i, & \text{if } y_i = 1 \\
\langle w \cdot x \rangle + b < -1 + \xi_i, & \text{if } y_i = -1
\end{array}
$$



Soft margin classifier

$$\begin{aligned} \langle w \cdot x \rangle + b &> 1 - \xi_i, & \text{if } y_i &= 1 \\ \langle w \cdot x \rangle + b &< -1 + \xi_i, & \text{if } y_i &= -1 \end{aligned}$$

- Error term always non-negative, $\xi_i \geq 0$
- 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



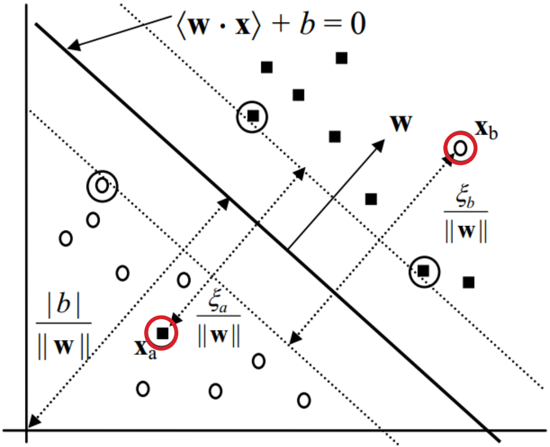
Soft margin optimization

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

Subject to

$$\begin{aligned} &\xi_i \geq 0 \\ &\langle w \cdot x \rangle + b > 1 - \xi_i, \quad \text{if } y_i = 1 \\ &\langle w \cdot x \rangle + b < -1 + \xi_i, \quad \text{if } y_i = -1 \end{aligned}$$

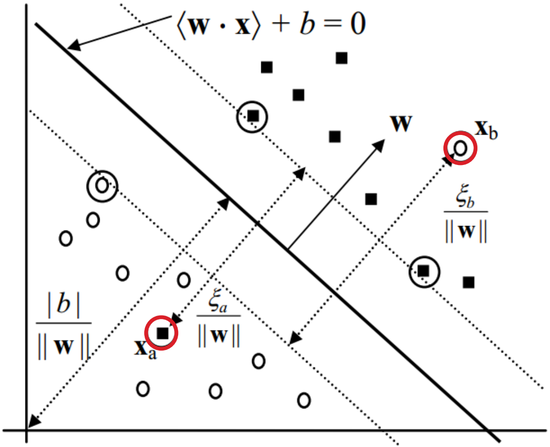
- Constraints include requirement that error terms are non-negative
- Again the objective function is quadratic



Soft margin optimization

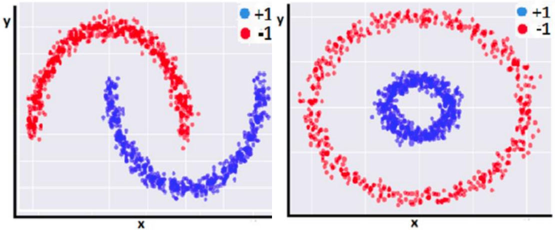
- Can again be solved using convex optimization theory
- Form of the solution turns out to be the same as the hard margin case
  - Expression in terms of Lagrange multipliers α_i
  - Only terms corresponding to support vectors are actively used

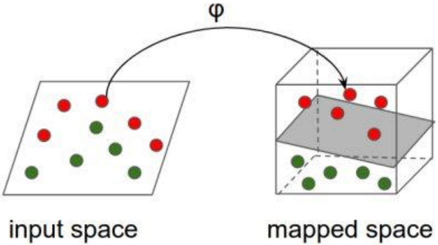
$$\operatorname{sign}\left[\sum_{i \in sv} y_i \alpha_i \langle x_i \cdot z \rangle + b\right]$$



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



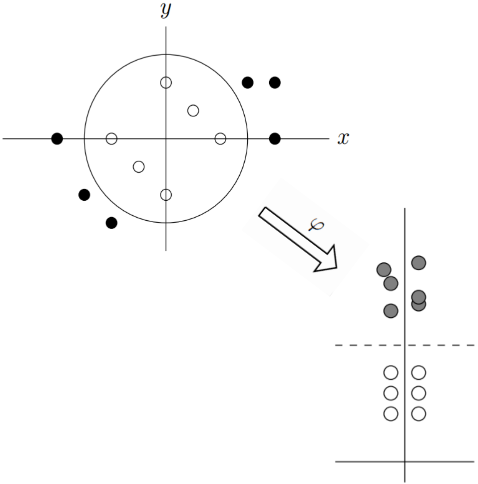


Geometric tranformation

- Consider two sets of points separated by a circle of radius 1
- Equation of circle is $x^2 + y^2 = 1$
- Points inside the circle $x^2 + y^2 < 1$
- Points outside circle $x^2 + y^2 > 1$
- Transformation

$$\varphi : (x, y) \mapsto (x, y, x^2 + y^2)$$

- Points inside circle lie below z = 1
- Point outside circle lifted above z = 1



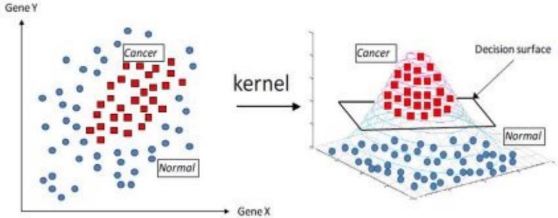
SVM after transformation

- SVM in original space

$$\operatorname{sign}\left[\sum_{i\in sv} y_i\alpha_i\langle x_i \cdot z\rangle + b\right]$$

- After transformation

$$\operatorname{sign}\left[\sum_{i\in sv'} y_i\alpha_i\langle \varphi(x_i) \cdot \varphi(z)\rangle + b\right]$$



- All we need to know is how to compute dot products in transformed space