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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
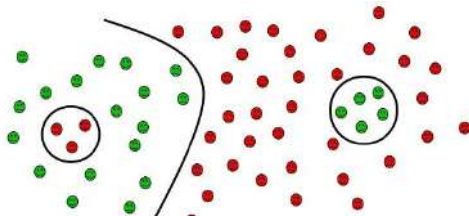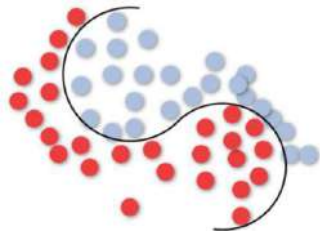
Linear separators

- 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?
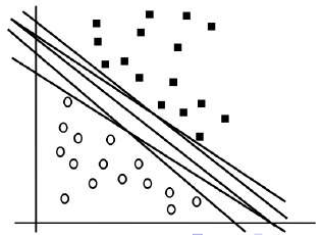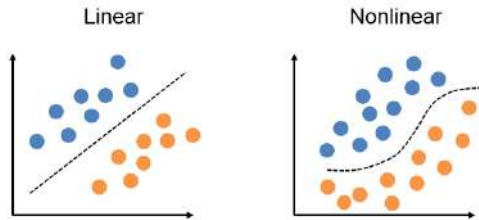
Linear separators

- Each input x has n attributes $\langle x_1, x_2, \ldots, x_n \rangle$

- Linear separator has the form
$$w_1 x_1 + w_2 x_2 + \cdots + w_n x_n + b$$

- Classification criterion
$$w_1 x_1 + \cdots + w_n x_n + b > 0, \quad \text{classify yes}, +1$$
$$w_1 x_1 + \cdots + w_n x_n + b < 0, \quad \text{classify no}, -1$$

- Dot product $\langle w \cdot x \rangle$
$$(w_1, \ldots, w_n) \cdot (x_1, \ldots, x_n) = w_1 x_1 + \cdots + w_n x_n$$

- Collapsed form
$$\langle w \cdot x \rangle + b > 0, \langle w \cdot x \rangle + b < 0 \qquad w_0$$

- Rename bias b as w_0, create fictitious $x_0 = 1$

- Equation becomes
$$\langle w \cdot x \rangle > 0, \langle w \cdot x \rangle < 0$$
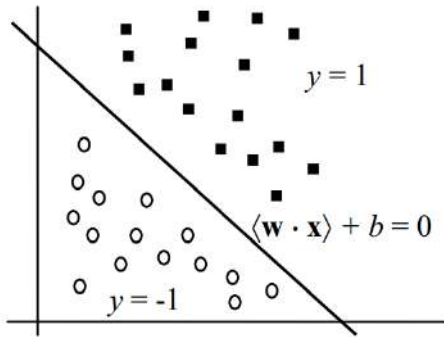
Perceptron algorithm

(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

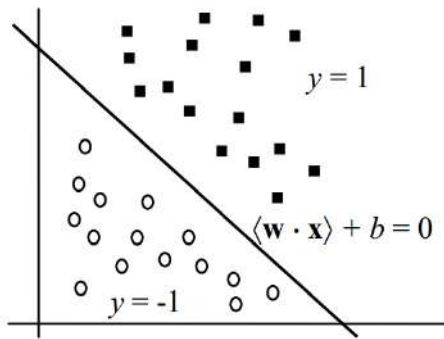*Initialize* $w = \langle 0, 0, \ldots, 0 \rangle$

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* $w + x_i$

$y = 1$

$\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$

$y = -1$

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
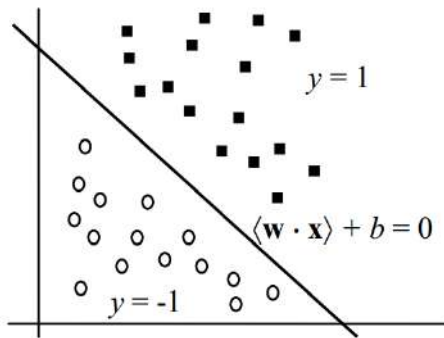
Theorem

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 $r = \max_i |x_i|$.

$$\left(w^* \cdot x_i\right)\left(\cdot y_i\right) \geq 1$$

$$w^* x_i \geq 1 \quad \text{if } y_i = +1$$
$$\leq -1 \quad \text{if } y_c = -1$$

Theorem

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- Assume w^* exists. Keep track of two quantities: $w^\top w^*$, $|w|^2$.

Perceptron Algorithm — Proof

> ## Theorem
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> 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.
$$(w + x_i y_i)^\top w^* = w^\top w^* + x_i^\top y_i w^* \geq w^\top w^* + 1$$

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 $r = \max_i |x_i|$.

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

- 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

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- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$

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- $m \quad \leq \quad |w||w^*|$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates

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-
$$
\begin{aligned}
m &\leq |w||w^*| \\
m/|w^*| &\leq |w|
\end{aligned}
$$

- Assume Perceptron Algorithm makes m updates

- Then, $w^\top w^* \geq m$, $|w|^2 \leq mr^2$

- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \\ m/|w^*| &\leq r\sqrt{m} \end{aligned}$$

Perceptron Algorithm — Proof (cont'd)

- Assume Perceptron Algorithm makes m updates

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\sqrt{m} &\leq r|w^*|
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Perceptron Algorithm — Proof (cont'd)

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m &\leq r^2|w^*|^2
\end{aligned}
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- $$\begin{aligned} m &\leq |w||w^*| \\ m/|w^*| &\leq |w| \\ m/|w^*| &\leq r\sqrt{m} \\ \sqrt{m} &\leq r|w^*| \\ m &\leq r^2|w^*|^2 \end{aligned}$$

Suppose I want to classify a new x'

$$W \cdot x' > 0 \text{ or } < 0 ?$$

$$\left(\Sigma n_i x_i \right) \cdot x'$$

$n_1 x_1 \cdot x'$
$+ n_2 x_2 \cdot x'$
$+ \cdots + n_k x_k \cdot x'$

- Note (for later) that final w is of the form $\sum_i n_i x_i$
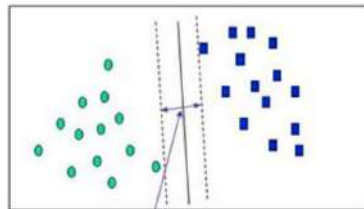
Linear separators

- 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?
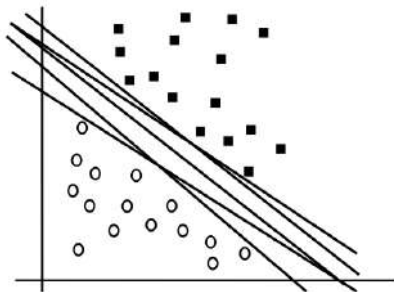
Margin

- 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

Small Margin
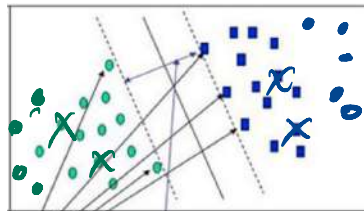
Support Vectors

Large Margin

Finding a maximum margin classifier

- Recall our original linear classifier

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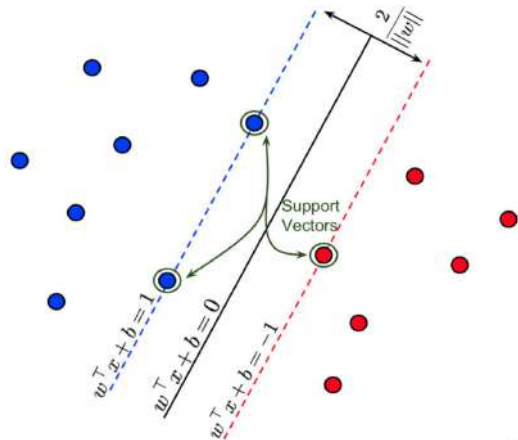$$w_1x_1 + \cdots + w_nx_n + b < 0, \quad \text{classify no}, -1$$

- Scale margin so that separation is 1 on either side

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

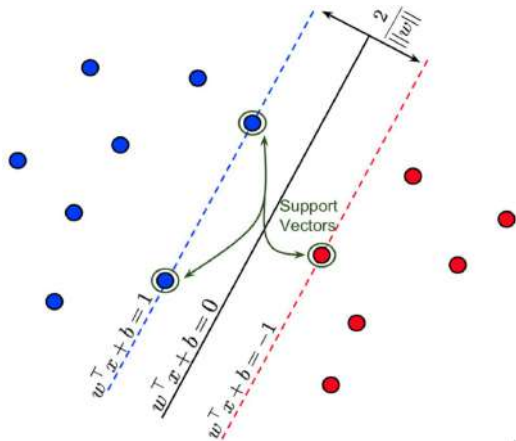- Using Pythagoras's theorem, perpendicular distance to nearest support vector is $\dfrac{1}{||w||}$,

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

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

Optimization problem

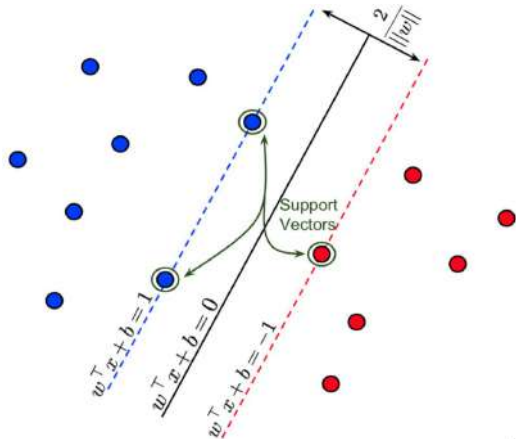Minimize $\dfrac{||w||}{2}$

Subject to

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

- 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
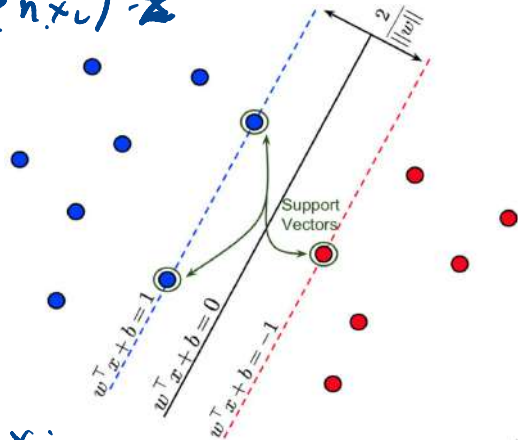
Solution to optimization problem

$w \cdot z$

- 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

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

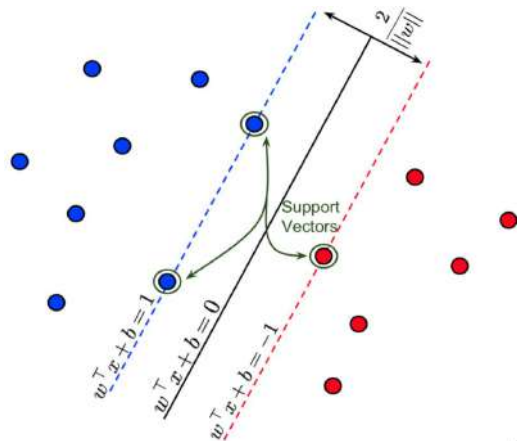- sv is set of support vectors

$\left(\sum n_i x_i\right) \cdot z$

$w = \sum y_i \alpha_i x_i$

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
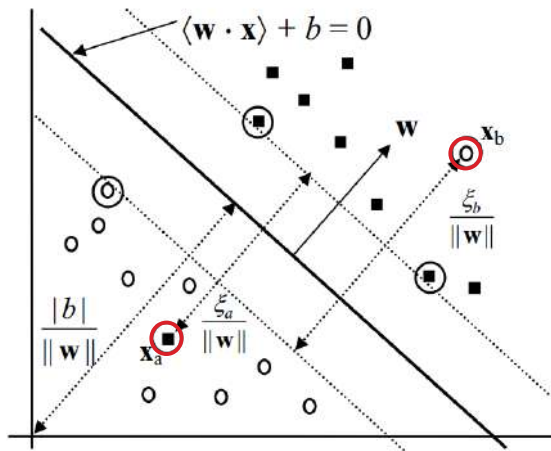 - Will be used later, in the non-linear case

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

$$\langle w \cdot x \rangle + b > 1, \qquad \text{if } y_i = 1$$
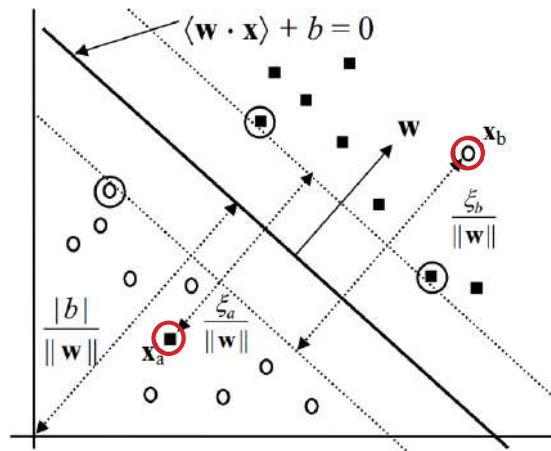$$\langle w \cdot x \rangle + b < -1, \qquad \text{if } y_i = -1$$

  we have

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

Soft margin classifier

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

- 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

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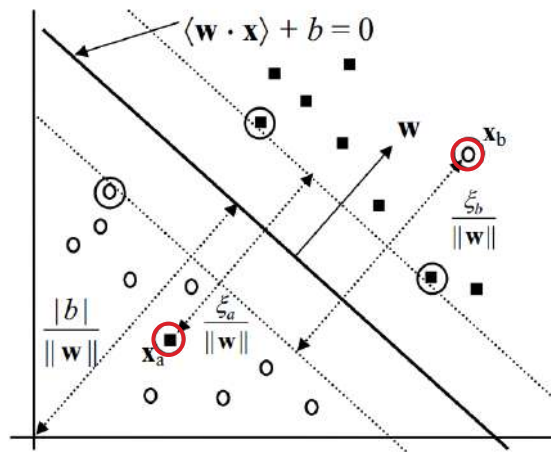## Soft margin optimization

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

Subject to

$\xi_i \geq 0$

$\langle w \cdot x \rangle + b > 1 - \xi_i, \quad \text{if } y_i = 1$

$\langle w \cdot x \rangle + b < -1 + \xi_i, \quad \text{if } y_i = -1$

- 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

$$\text{sign}\left[\sum_{i \in sv} y_i \alpha_i \langle x_i \cdot z \rangle + b\right]$$
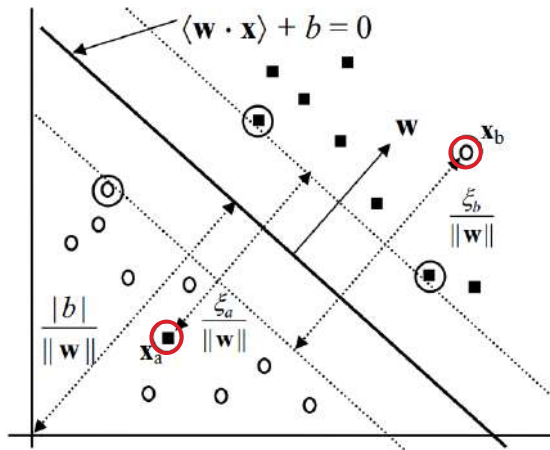
- How do we deal with datasets where the separator is a complex shape?

- Geometrically transform the data
  - Typically, add dimensions

- For instance, if we can "lift" one class, we can find a planar separator between levels
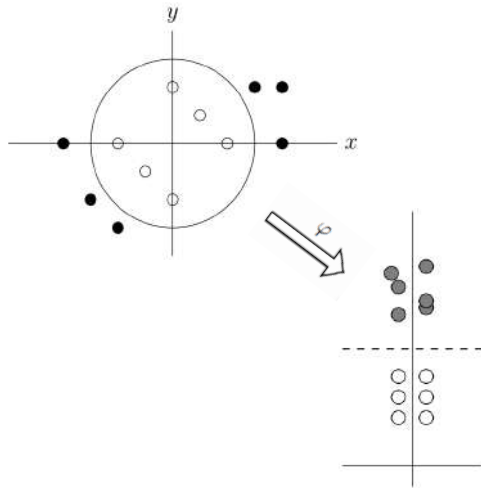

input space   mapped space
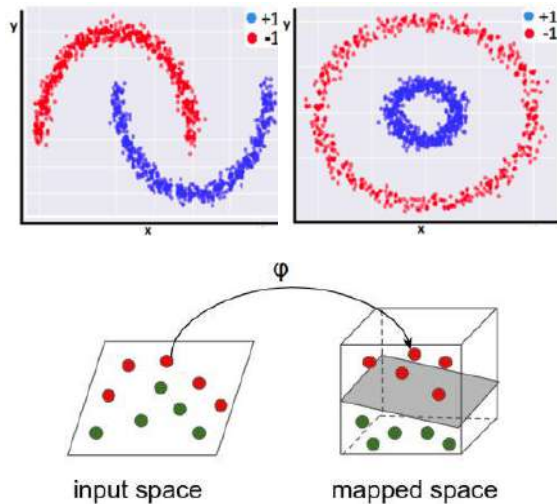
Geometric tranformation

- 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

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

- After transformation

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

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