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Data Mining and Machine Learning
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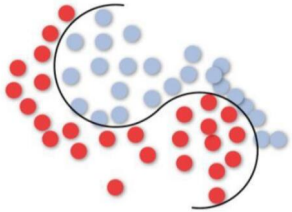
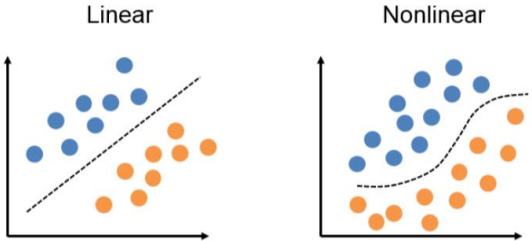
A geometric view of supervised learning

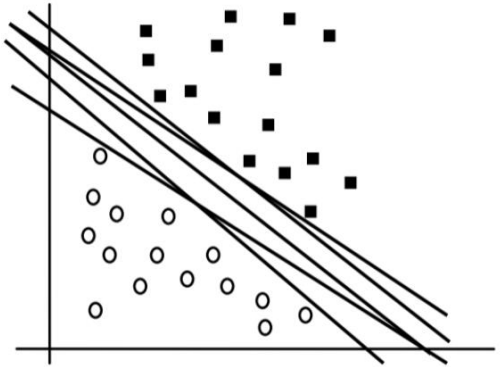
- Think of data as points in space
- Find a separating curve (surface)
- Separable case
  - Each class is a connected region
  - A single curve can separate them
- Simplest case — linearly separable data
- Dual of linear regression
  - Find a line that passes close to a set of points
  - Find a line that separates the two sets of points





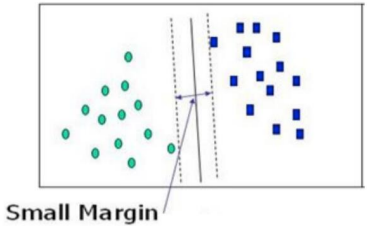
Linear separators

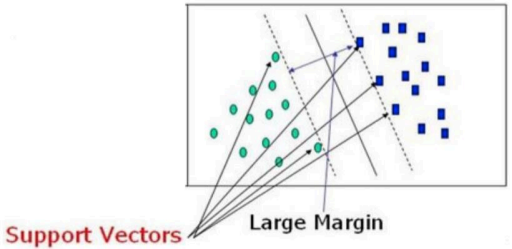
- Perceptron algorithm is a simple procedure to find a linear separator, if one exists
- Many lines are possible
  - Does the Perceptron algorithm find the best one?
  - What is a good notion of "cost" to optimize?



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

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

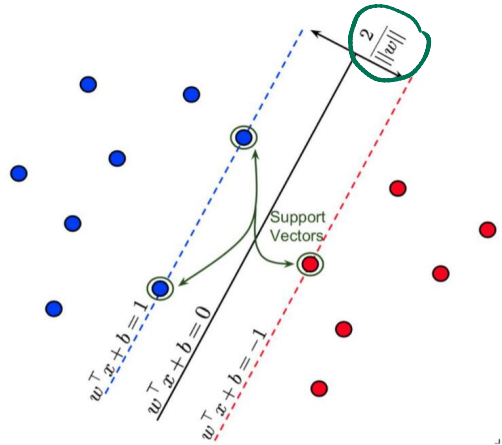
Subject to

$w_1 x_1^i + w_2 x_2^i + \cdots w_n x_n^i + b > 1$, if $y_i = 1$

$w_1 x_1^i + w_2 x_2^i + \cdots w_n x_n^i + b < -1$, 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

- Rewrite as dual
- Maximize

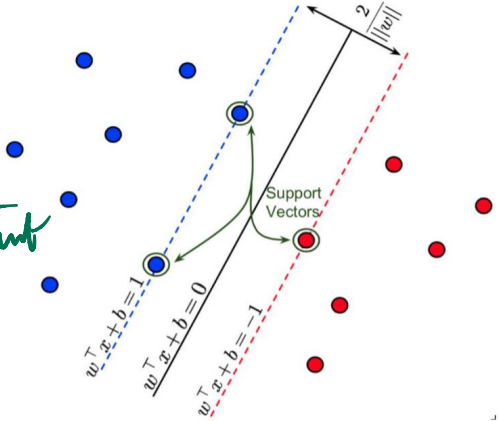
$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \; x_i \cdot x_j$$

Subject to

$\alpha_i \geq 0, i \in 1, 2, \ldots N$

One per constraint

- Lagrange multipliers α_1, α_2, $\ldots$, α_N, one multiplier per training input

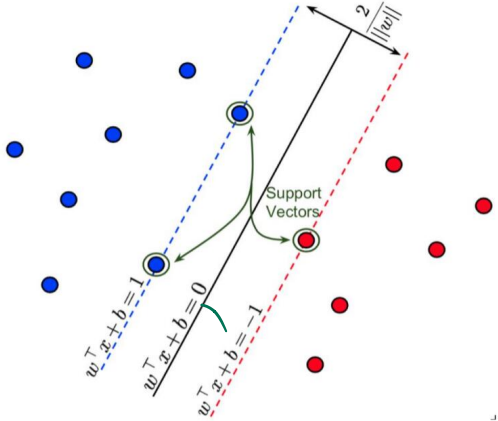


Support Vector Machine (SVM)

Final classifier is of the form

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

- 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



Soft margin optimization

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

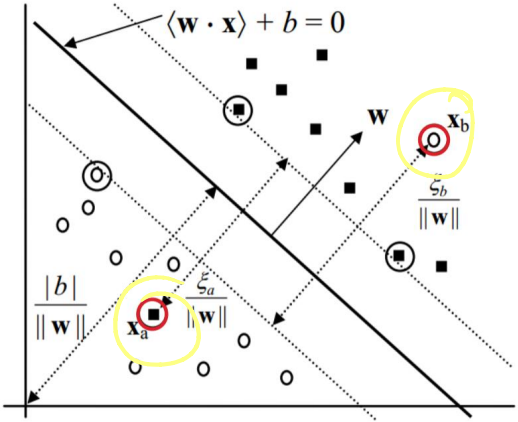
Subject to

$\xi_i \geq 0$

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

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

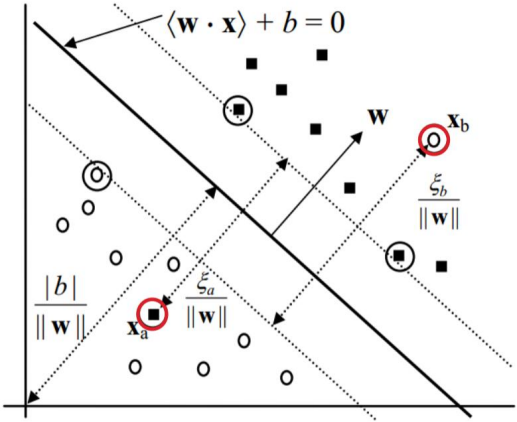
- Constraints include requirement that error terms are non-negative
- Again the objective function is quadratic



Soft margin optimization

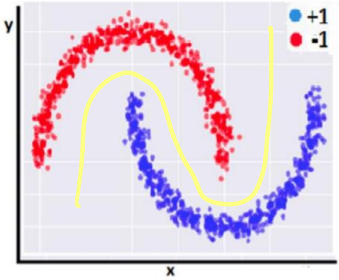
- Can again be solved using the dual
- Form of the solution turns out to be the same as the hard margin case
  - Expression in terms of Lagrange multipliers α_i
  - Only terms corresponding to support vectors are actively used

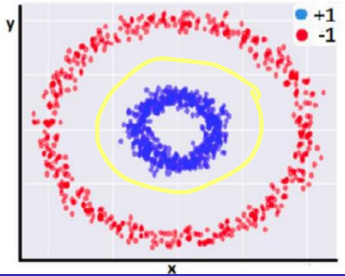
$$\text{sign}\left[\sum_{i \in sv} y_i \alpha_i (x_i \cdot z) + b\right]$$



The non-linear case

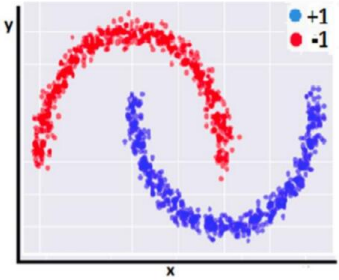
- How do we deal with datasets where the separator is a complex shape?

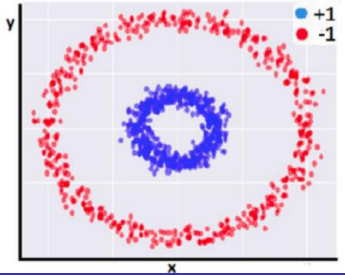




The non-linear case

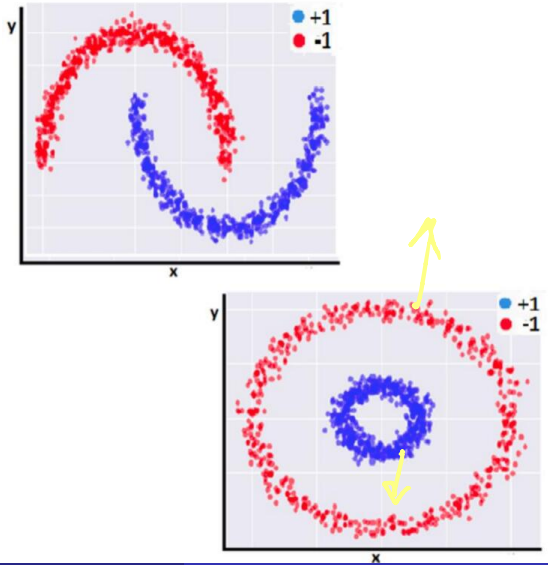
- How do we deal with datasets where the separator is a complex shape?
- Geometrically transform the data
  - Typically, add dimensions





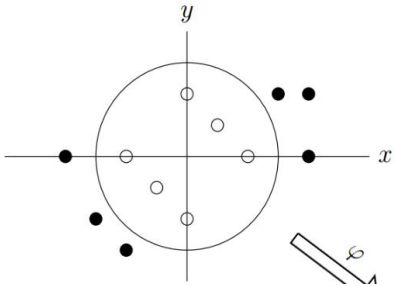
The non-linear case

- 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 $x^2 + y^2 = 1$



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- Consider two sets of points separated by a circle of radius 1
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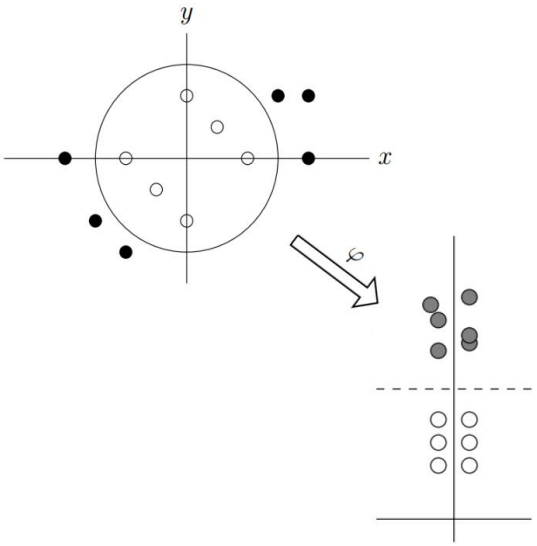

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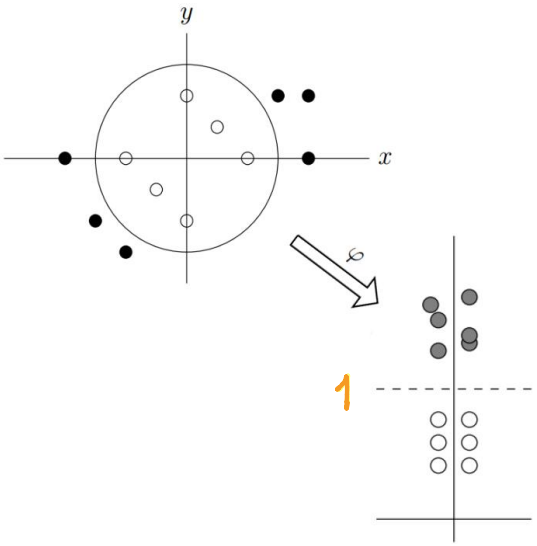
  $\varphi : (x, y) \mapsto (x, y, x^2 + y^2)$



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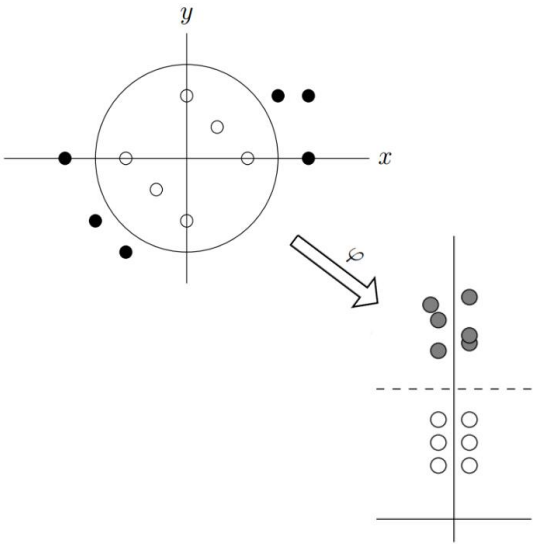
  $$\varphi : (x, y) \mapsto (x, y, x^2 + y^2)$$
- Points inside circle lie below $z = 1$
- Point outside circle lifted above $z = 1$

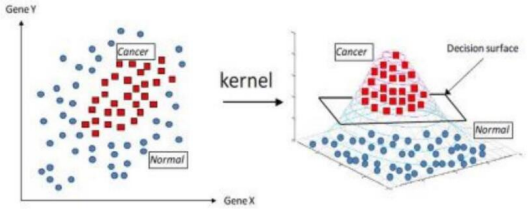


SVM after transformation

- SVM in original space

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

$x \longmapsto \varphi(x)$



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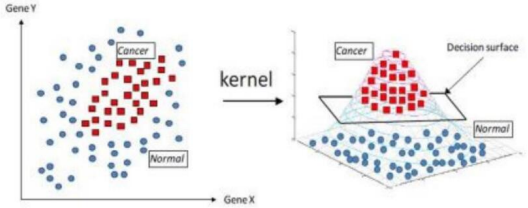
$$\text{sign}\left[\sum_{i \in sv} y_i \alpha_i (\varphi(x_i) \cdot \varphi(z)) + b\right]$$



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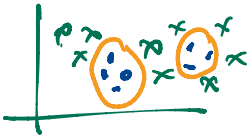
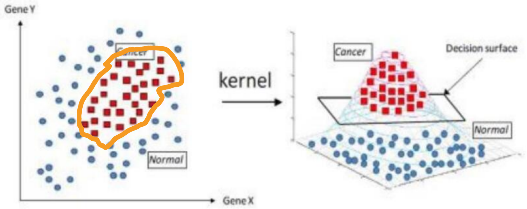
- Training: maximize

$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y_i y_j \alpha_i \alpha_j \; \varphi(x_i) \cdot \varphi(x_j)$$





What is φ?

Don't care

SVM after transformation

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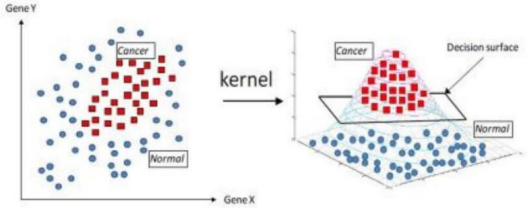
- All we need to know is how to compute dot products in transformed space

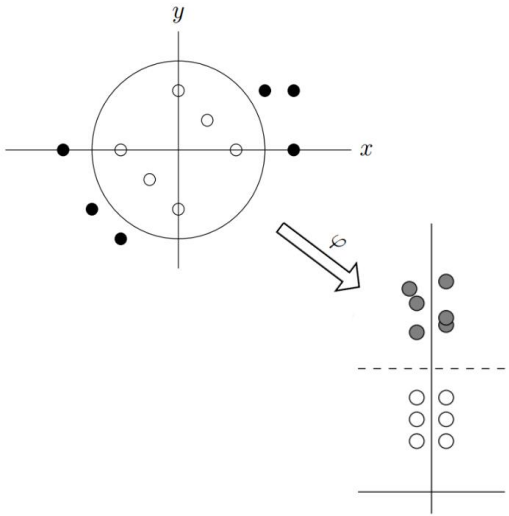


Dot products

- Consider the transformation

$\varphi : (x_1, x_2) \mapsto (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2)$

2D ⟶ 6D



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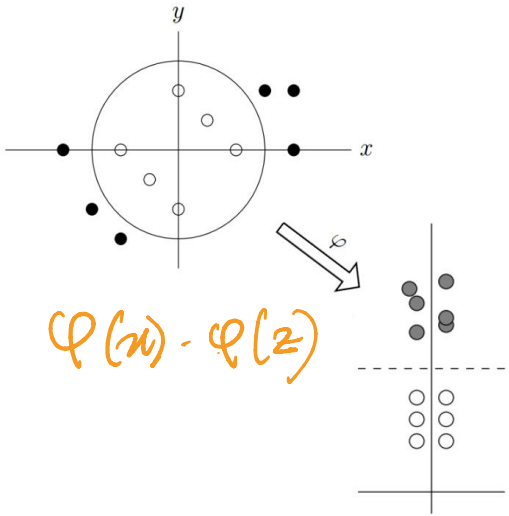
- Dot product in transformed space

$$\begin{aligned} \varphi(x) \cdot \varphi(z) &= 1 + 2x_1z_1 + 2x_2z_2 + x_1^2z_1^2 \\ &\quad +2x_1x_2z_1z_2 + x_2^2z_2^2 \\ &= (1 + x_1z_1 + x_2z_2)^2 \end{aligned}$$



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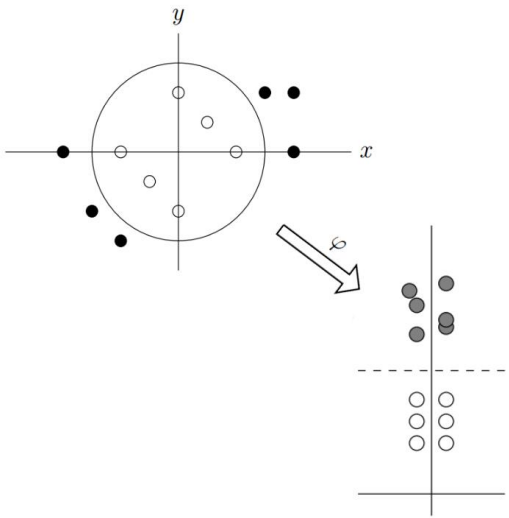
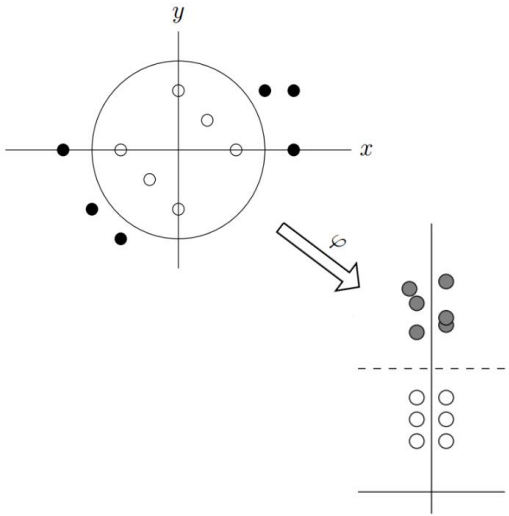
- Transformed dot product can be expressed in terms of original inputs

  $\varphi(x) \cdot \varphi(z) = K(x, z) = (1 + x_1z_1 + x_2z_2)^2$



Kernels

- K is a kernel for transformation φ if $K(x, z) = \varphi(x) \cdot \varphi(z)$

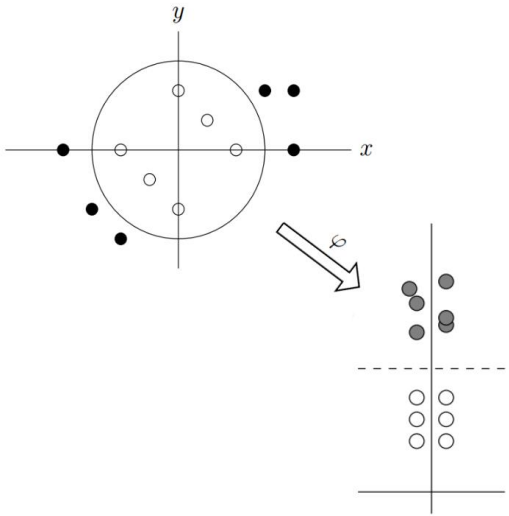


Kernels

- K is a kernel for transformation φ if $K(x, z) = \varphi(x) \cdot \varphi(z)$
- If we have a kernel, we don't need to explicitly compute transformed points
- All dot products can be computed implicitly using the kernel on original data points

$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \, \varphi(x_i) \cdot \varphi(x_j)$$

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



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$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} y_i y_j \alpha_i \alpha_j \; K(x_i, x_j)$$

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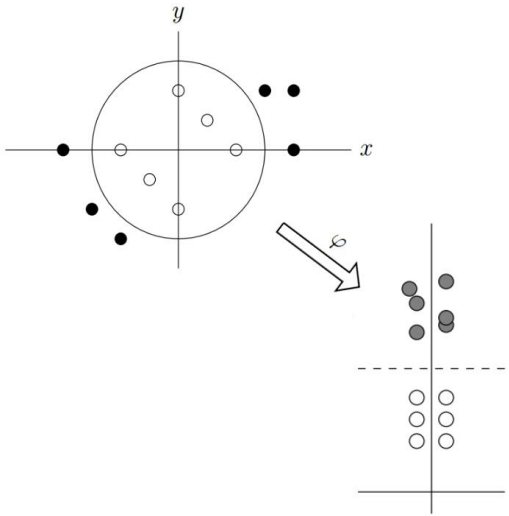
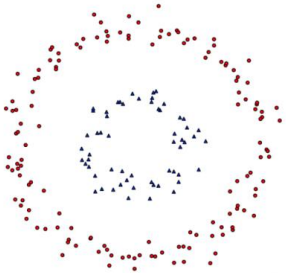
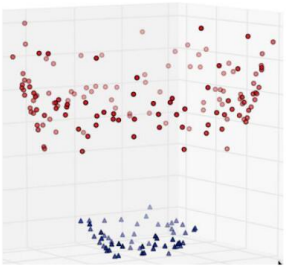


Kernels

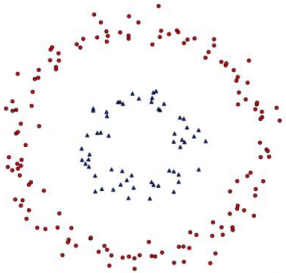
- If we know K is a kernel for some transformation φ, we can blindly use K without even knowing what φ looks like!

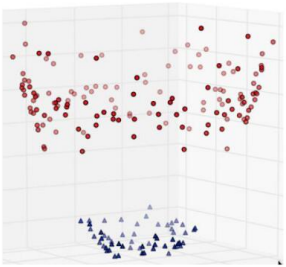




Kernels

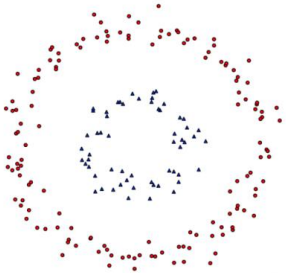
- If we know K is a kernel for some transformation φ, we can blindly use K without even knowing what φ looks like!
- When is a function a valid kernel?

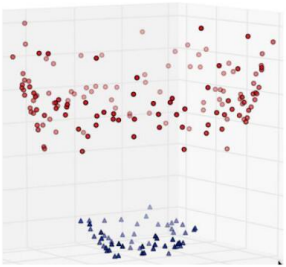




Kernels

- If we know K is a kernel for some transformation φ, we can blindly use K without even knowing what φ looks like!
- When is a function a valid kernel?
- Has been studied in mathematics — Mercer's Theorem
  - Criteria are non-constructive





Kernels

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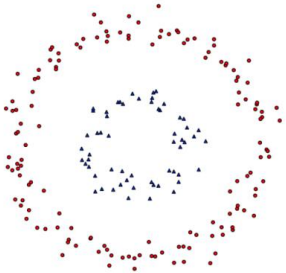
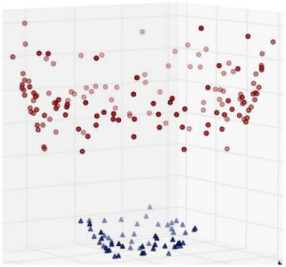
- When is a function a valid kernel?
- Has been studied in mathematics — Mercer's Theorem
  - Criteria are non-constructive
- Can define sufficient conditions from linear algebra



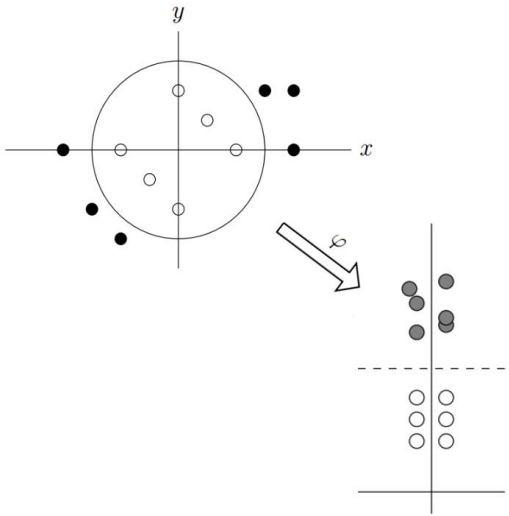


Kernels

- Kernel over training data $x_1, x_2, \ldots, x_N$ can be represented as a gram matrix

$$K = \begin{array}{c} \\ x_1 \\ x_2 \\ \vdots \\ x_N \end{array} \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & \cdots & x_N \end{array} \\ \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \end{array}$$

- Entries are values $K(x_i, x_j)$

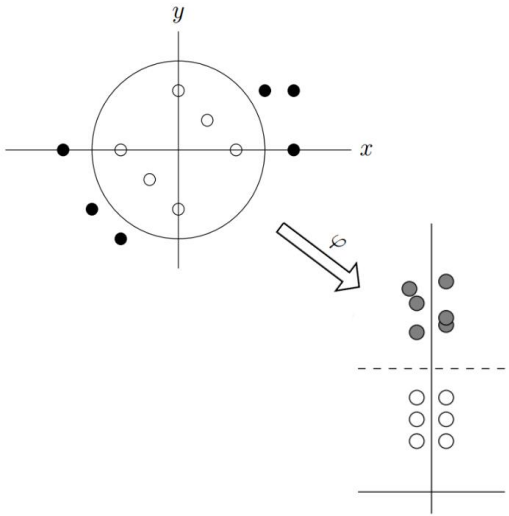


Kernels

- Kernel over training data $x_1, x_2, \ldots, x_N$ can be represented as a gram matrix

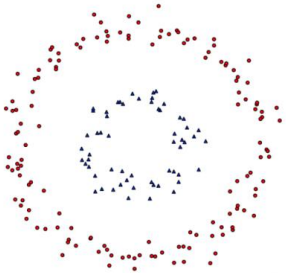
$$K = \begin{array}{c} \\ x_1 \\ x_2 \\ \vdots \\ x_N \end{array} \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & \cdots & x_N \end{array} \\ \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \end{array}$$

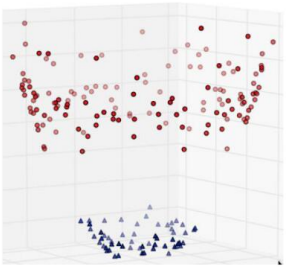
- Entries are values $K(x_i, x_j)$
- Gram matrix should be positive semi-definite for all $x_1, x_2, \ldots, x_N$



Known kernels

- Fortunately, there are many known kernels



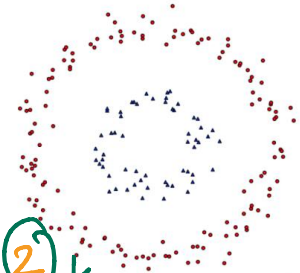


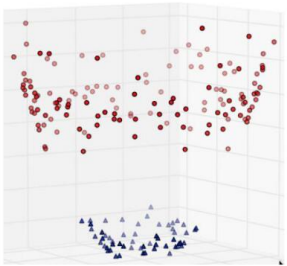
Known kernels

- Fortunately, there are many known kernels
- Polynomial kernels

$$K(x, z) = (1 + x \cdot z)^k$$

$(1 + (x \cdot z))^2 k$





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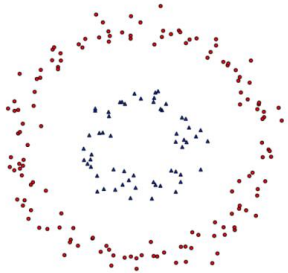
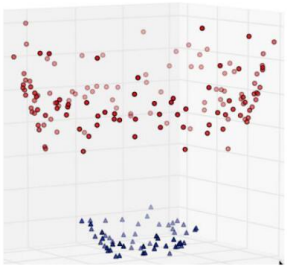
$$K(x, z) = (1 + x \cdot z)^k$$

- Any $K(x, z)$ representing a similarity measure



$d(x, z)$

Similarity $\frac{1}{d(x, z)}$



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$$K(x, z) = (1 + x \cdot z)^k$$

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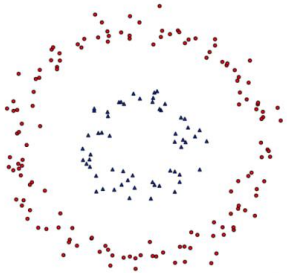
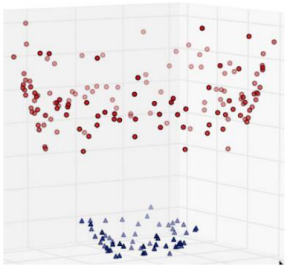
- Gaussian radial basis function — similarity based on inverse exponential distance

$$K(x, z) = e^{-c|x-z|^2}$$

distance





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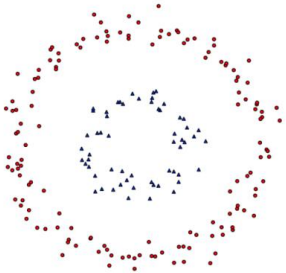

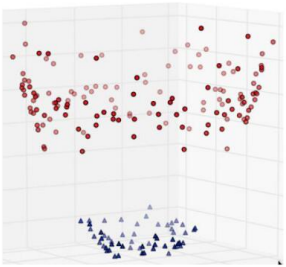

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