Kernel methods and Graph kernels

Social and Technological Networks

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Kernels

- Kernels are a type of measures of similarity
- Important technique in Machine learning
- Used to increase power of many techniques

- Can be defined on graphs
- Used to compare, classify, cluster many small graphs
  - E.g. Molecules, neighborhoods of different people in social networks etc…

Graph kernels

- To compute similarity between two attributed graphs
  - Nodes can carry labels
  - E.g. Elements (C, N, H etc) in complex molecules
- Idea: It is not obvious how to compare two graphs
  - Instead compute walks, cycles etc on the graph, and compare those
- There are various types of kernels defined on graphs

Walk counting

- Count the number of walks of length k from i to j
- Idea: i and j should be considered close if
  - They are not far in the shortest path distance
  - And there are many walks of short length between them (so they are highly connected)
- So, there would be many walks of length $\leq k$

Walk counting

- Can be computed by taking k^th power of adjacency matrix A
- If $A^k(i,j) = c$, that means there are c walks of length k between i and j
  - Homework: Check this!
- Note: A^k is expensive, but manageable for small graphs
- Kernel: compare A^k for the two graphs

Common walk kernel

- Count how many walks are common between the two graphs

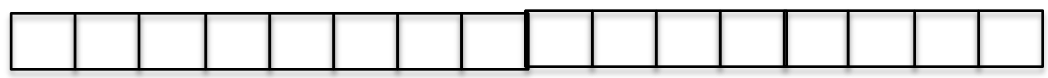
- That is, take all possible walks of length k on both graphs.
  - Count the number that are exactly the same
  - Two walks are same if they follow the same sequence of labels
    - (note that other than labels, there is no obvious correspondence between nodes)

Recap: dot product and cosine similarity

$$\text{similarity} = \cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\|\|\mathbf{B}\|} = \frac{\sum\limits_{i=1}^{n} A_i B_i}{\sqrt{\sum\limits_{i=1}^{n} A_i^2} \sqrt{\sum\limits_{i=1}^{n} B_i^2}}$$

Computation of A.B is the important element. Since |A||B| is just normalization. A.B can be seen as the unnormalized similarity.

Common walk kernel as a dot product or cosine similarity

- For graphs G_A and G_B
- Imagine vectors A and B representing all walks in graphs 
- Each position has a
  - Zero if that walk does not occur in the graph
  - One if the walk occurs in the graph
- Then A.B = number of common walks in the graph

Random walk kernel

- Perform multiple random walks of length k on both graphs
- Count the number of walks (label sequences) common to both graphs

- Check that this is analogous to a dot product

- Note that the vectors implied by the kernel do not need to be computed explicitly

Tottering

- Walks can move back and forth between adjacent vertices
  - Small structural similarities can produce a large score

- Usual technique: for a walk $v_1, v_2, \ldots$ prohibit return along an edge, ie prohibit $v_i = v_{i+2}$

Subtree kernel

- From each node, compute a neighborhood upto distance h

- From every pair of nodes in two graphs, compare the neighborhoods
  - And count the number of matches (nodes in common)

Shortest path kernel

- Compute all pairs shortest paths in two graphs
- Compute the number of common sequences

- Tottering problem does not appear

- Problem: there can be many (exponentially many) shortest paths between two nodes
  - Computational problems
  - Can bias the similairity

Shortest distance kernel

- Instead use shortest distance between nodes
- Always unique

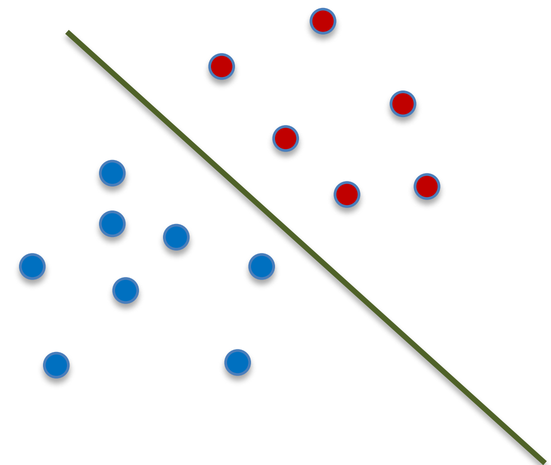
- Method:
  - Compute all shortest distances SD(G1) and SD(G2) in graphs G1 and G2
  - Define kernel (e.g. Gaussian kernel) over pairs of distances: $k(s_1, s_2)$, where $s_1 \in SD(G_1), s_2 \in SD(G_2)$
  - Define shortest path (SP)kernel between graphs as sum of kernel values over all pairs of distances between two graphs
    - $\mathrm{K}_{SP}(G_1, G_2) = \sum_{s_1} \sum_{s_2} k(s_1, s_2)$

Kernel based ML

- Kernels are powerful methods in machine learning
- We will briefly review general kernels and their use

The main ML question

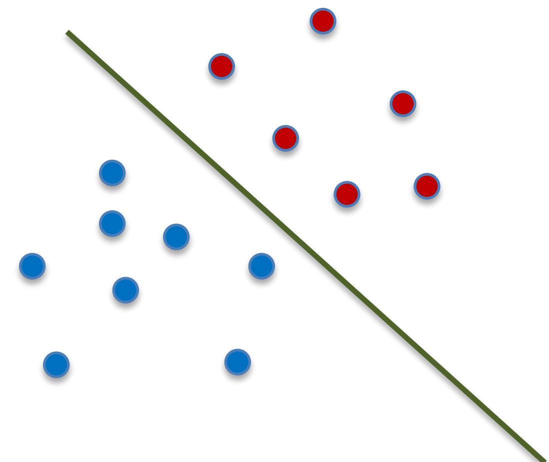
- For classes that can be separated by a line
  - ML is easy
  - E.g. Linear SVM, Single Neuron

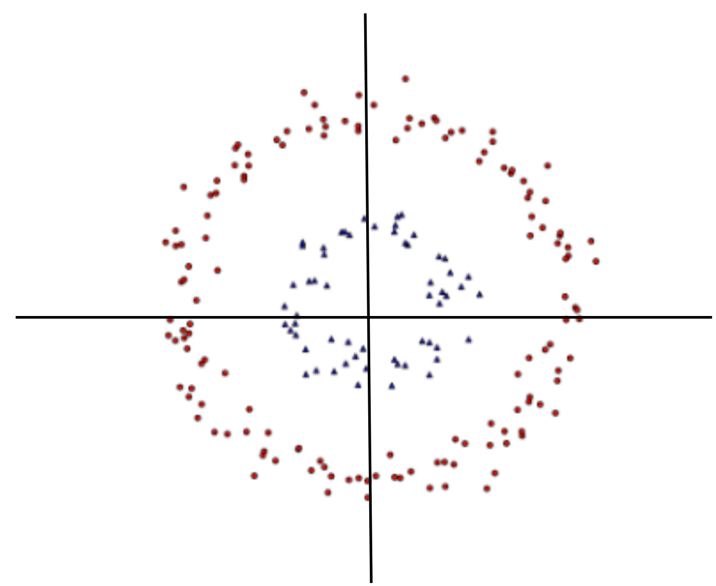


- But what if the separation is more complex?

The main ML question

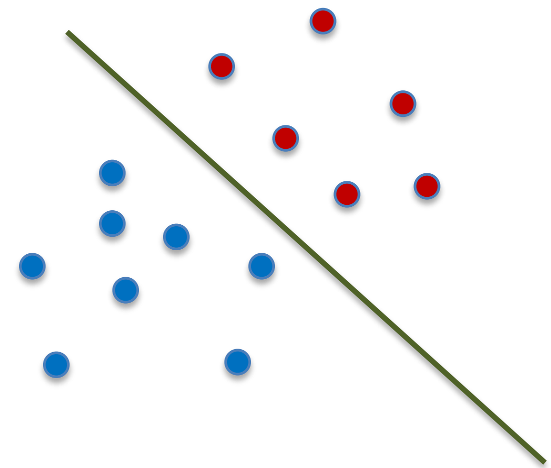
- For classes that can be separated by a line
  - ML is easy
  - E.g. Linear SVM, Single Neuron
- What if the structure is more complex?
  - Cannot separated linearly

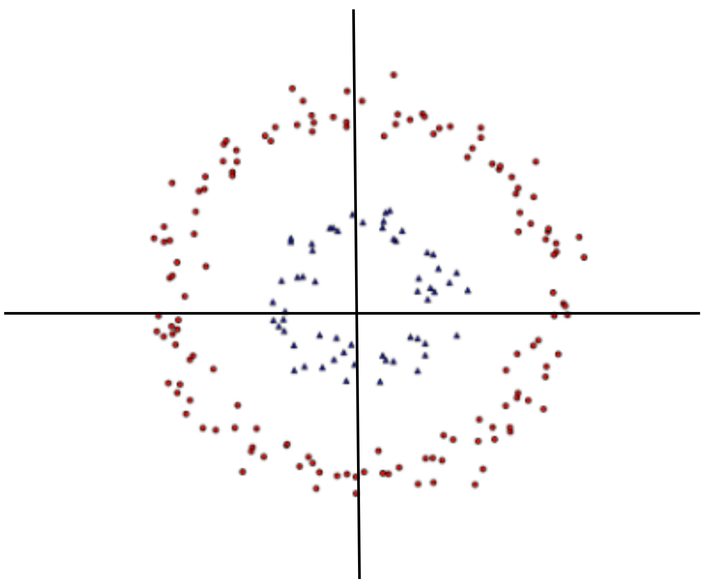




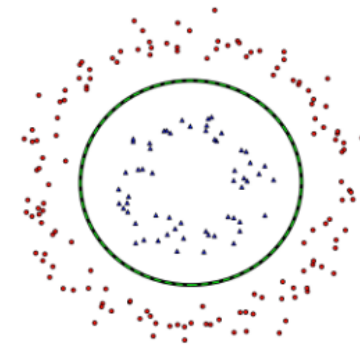
Non linear separators

- Method 1:
  - Search within a class of non linear separators
  - E.g. Search over all possible circles, parabola etc.
  - higher degree polynomials allow more curved lines

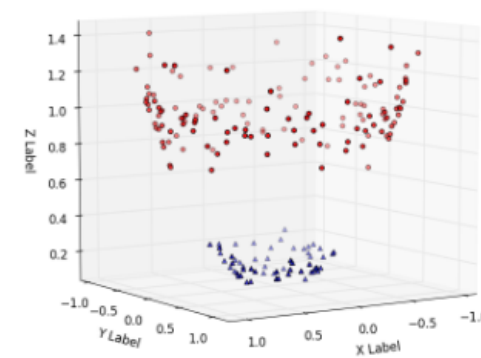




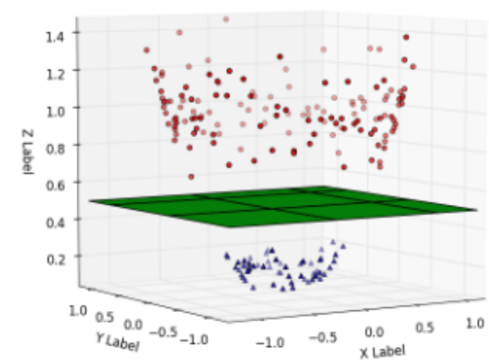
Method 2: Lifting to higher dimensions



- Suppose we lift every (x,y) point to
- $(x, y) \rightarrow (x, y, \mathrm{x}^2 + \mathrm{y}^2)$:

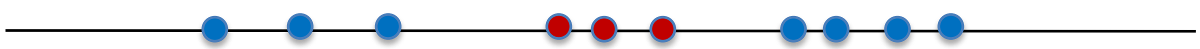


- Now there is a linear separator!



Exercise

- Suppose we have the following data:



- How would you lift and classify?

- Assuming there is a mechanism to find linear separators (in any dimension) if they exist

Kernels

- A similarity measure $K: X \times X \rightarrow \mathbb{R}$ is a kernel if:

- There is an embedding ψ (usually to higher dimension),
  - Such that: $\mathrm{K}(\boldsymbol{u}, \boldsymbol{v}) = \langle \psi(\boldsymbol{u}), \psi(\boldsymbol{v}) \rangle$
  - Where $\langle , \rangle$ represents inner product
    - Dot product is a type of inner product

Benefit of Kernels

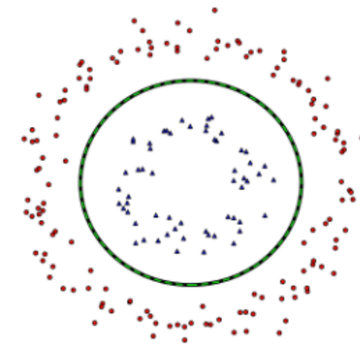
- High dimensions have power to represent complex structures
  - We have seen in reference to complicated networks
- Lifting data to high dimensions can be used to separate complex structures that cannot be distinguished in low domensions
  - But lifting to higher dimensions can be expensive (storage, computation)
  - Particularly when the data itself is already high dimensional

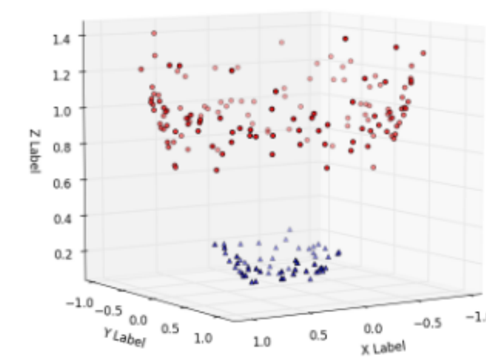
- Kernels define a similarity that is easy to compute
  - Equivalent to a high dimensional lift
  - Without having to compute the high-d representation

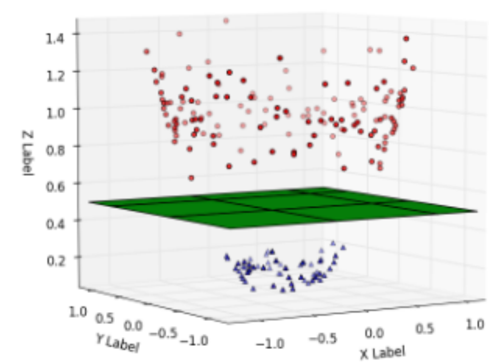
- Called the “Kernel trick”

Example kernel

- For the examples we saw earlier, the following kernel helps:
- $K(u, v) = (u \cdot v)^2$







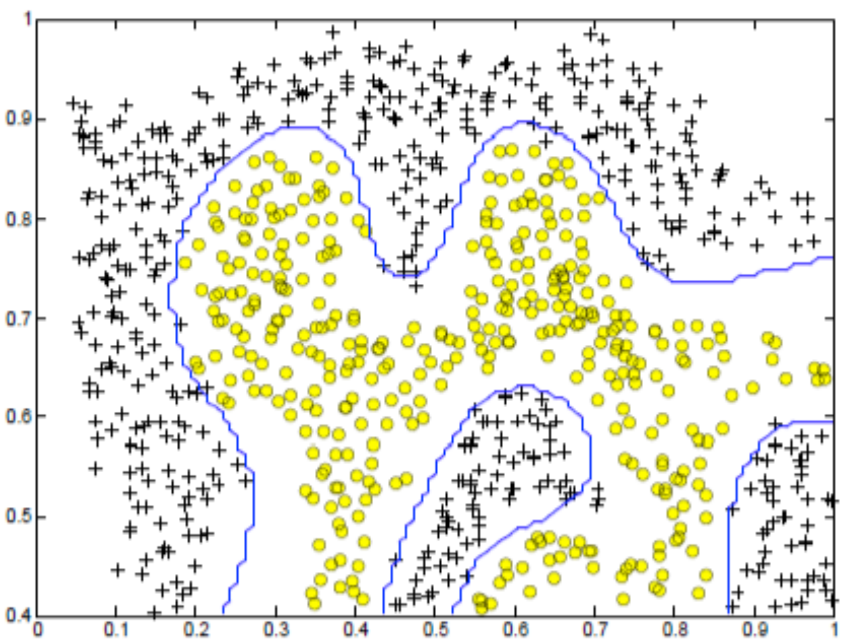
Example kernel

- For the examples we saw earlier, the following kernel helps:
- $K(u, v) = (u \cdot v)^2$
  - The implied lifting map is:
    $\psi(u) = \left(u_x^2, \sqrt{2}\, u_x u_y, u_y^2\right)$
  - Try it out!

More examples

- General Polynomial Kernel
- $K(u, v) = (1 + (u \cdot v))^k$

- Gaussian Kernel
- $K(u, v) = e^{-\frac{|u-v|^2}{2\sigma^2}}$
  - Sometimes called Radial Basis Function (RBF) kernel
  - Extremely useful in practice when you do not have specific knowledge of data



Heat Kernel or diffusion kernel

- Suppose heat diffuses for time t
- The rate at which heat moves from u to v is given by the Laplacian:

$$\frac{\partial}{\partial t} k_t(u, v) = \Delta k_t(u, v)$$

- The solution to this differential equation is the Gaussian!

$$k_t(u, v) = \frac{1}{(4\pi t)^{D/2}} e^{-|u-v|^2/4t}$$