Spectral Graph Theory

Social and Technological Networks

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Spectral methods

- Understanding a graph using eigen values and eigen vectors of the matrix
- We saw:
- Ranks of web pages: components of 1st eigen vector of suitable matrix
- Pagerank or HITS are algorithms designed to compute the eigen vector
- Random walks and local pageranks help in understanding community structure

Laplacian

- L = D – A [D is the diagonal matrix of degrees]

$$\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

- An eigen vector has one value for each node
- We are interested in properties of these values

Laplacian

- L = D – A [D is the diagonal matrix of degrees]

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- Symmetric. Real Eigen values.
- Row sum=0. Singular matrix. At least one eigen value =0.
- Positive semidefinite. Non-negative eigen values

Laplacian and random walks

- Suppose we are doing a random walk on a graph
- Let u(i) be the probability of the walk being at node i
  - E.g. initially it is at starting node s
  - After 10 steps, probability is higher near s, low at nodes farther away
  - Question: How does the probability change with time?
  - This probability diffuses with time. Like heat diffuses

Laplacian matrix

- Imagine a small and different quantity of heat at each node (say, in a metal mesh)
- we write a function u: u(i) = heat at i
- This heat will spread through the mesh/graph
- Question: how much heat will each node have after a small amount of time?

Heat diffusion

- Suppose nodes i and j are neighbors
  - Have temperature u(i) and u(j)
  - How much heat will flow from i to j?

Heat diffusion

- Suppose nodes i and j are neighbors
- In a short time, how much heat will flow from i to j?
- Proportional to the gradient: (u(i) - u(j))*Δt
  - Let us keep Δt fixed, and write just (u(i) - u(j))
- this is signed: negative means heat flows into i

Heat diffusion

- If i has neighbors j1, j2….
- Then heat flowing out of i is:

  = (u(i) - u(j1)) + (u(i) - u(j2)) + (u(i) - u(j3)) + …

  = degree(i)*u(i) - u(j1) - u(j2) - u(j3) - ….
- Hence L = D - A

$$\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

The heat equation

$$\frac{\partial u}{\partial t} = L(u)$$

- The net heat outflow of nodes in a time step
- The change in heat distribution in a small time step
  - The rate of change of heat distribution

The smooth heat equation

- The smooth Laplacian:

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}.$$

- The smooth heat equation:

$$\Delta f = \frac{\partial f}{\partial t}$$

Heat flow

- Will eventually converge to v[0] : the zeroth eigen vector, with eigen value $\lambda_0 = 0$

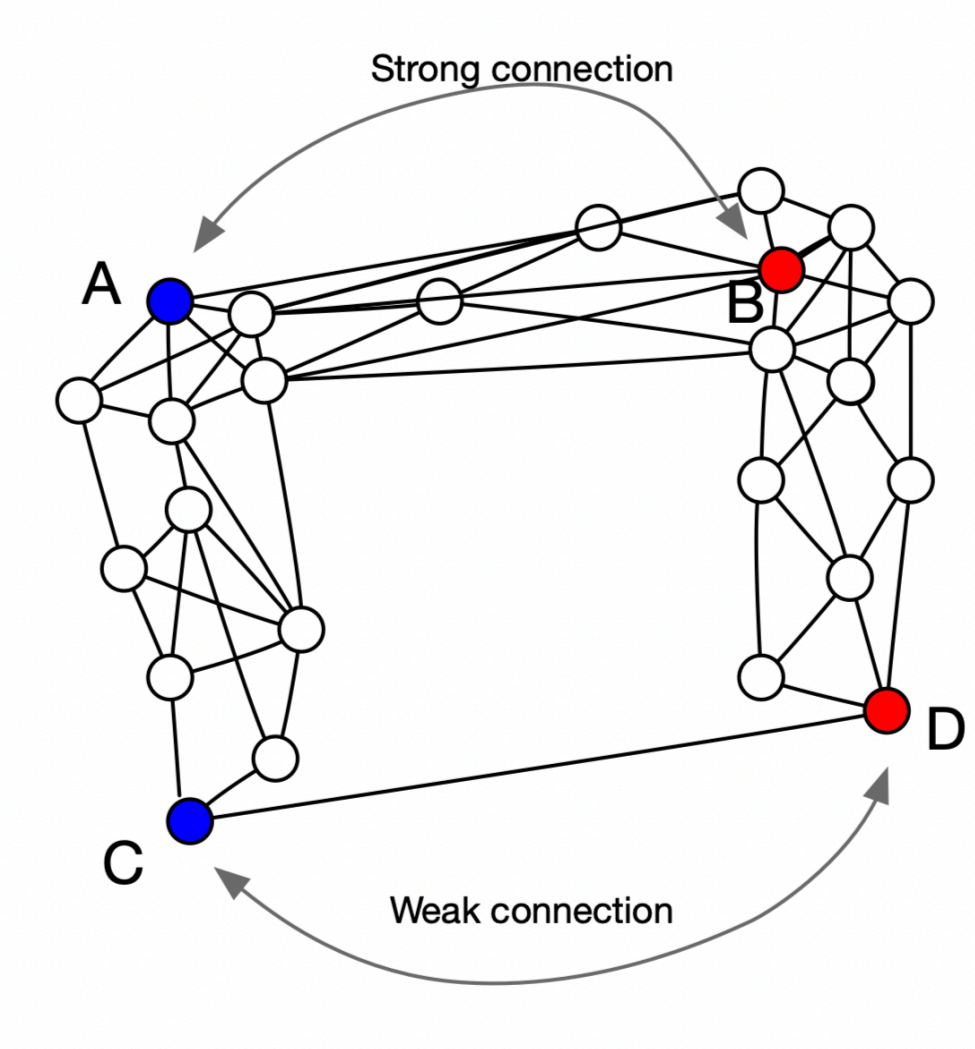
v[0] = const for the chain

Eigen vectors

- Other eigen vectors
- Encode various properties of the graph
  - Or, properties of diffusion in graph
- Have many applications

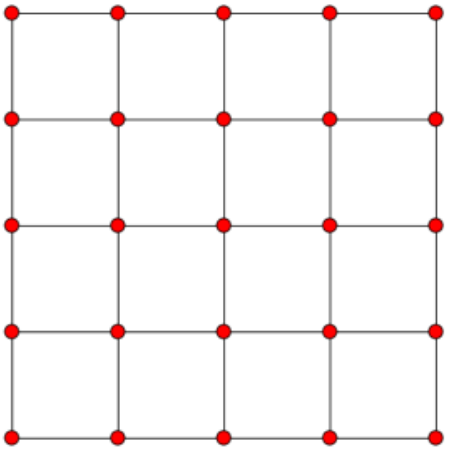
Diffusion as a distance feature

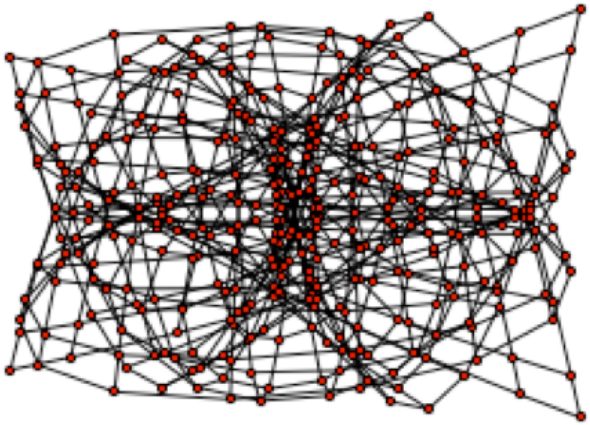
- CD is a weak connection
  - Fragile
  - Single short path
  - Diffusion from C to D is slow
- AB is a strong connection
  - Robust (to edge failure)
  - Many short paths
  - Diffusion from A to B is fast
- “Thick corridor” vs “Thin corridor”



Application 1: Drawing a graph (Embedding)

- Problem: Computer does not know what a graph is supposed to look like
- A graph is a jumble of edges
- Consider a grid graph:
- We want it drawn *nicely*



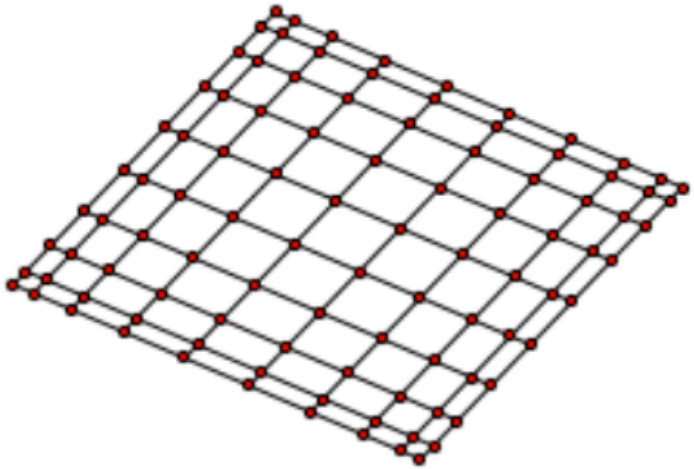


Graph embedding

- Find positions for vertices of a graph in low dimension (compared to n)
- Common objective: Preserve some properties of the graph e.g. approximate distances between vertices. Create a metric
  - Useful in visualization
  - Finding approximate distances
  - Clustering
- Using eigen vectors
  - One eigen vector gives x values of nodes
  - Other gives y-values of nodes … etc

Draw with v[1] and v[2]

- Suppose v[0], v[1], v[2]… are eigen vectors
  - Sorted by increasing eigen values
- Plot graph using X=v[1], Y=v[2]
- Produces the grid

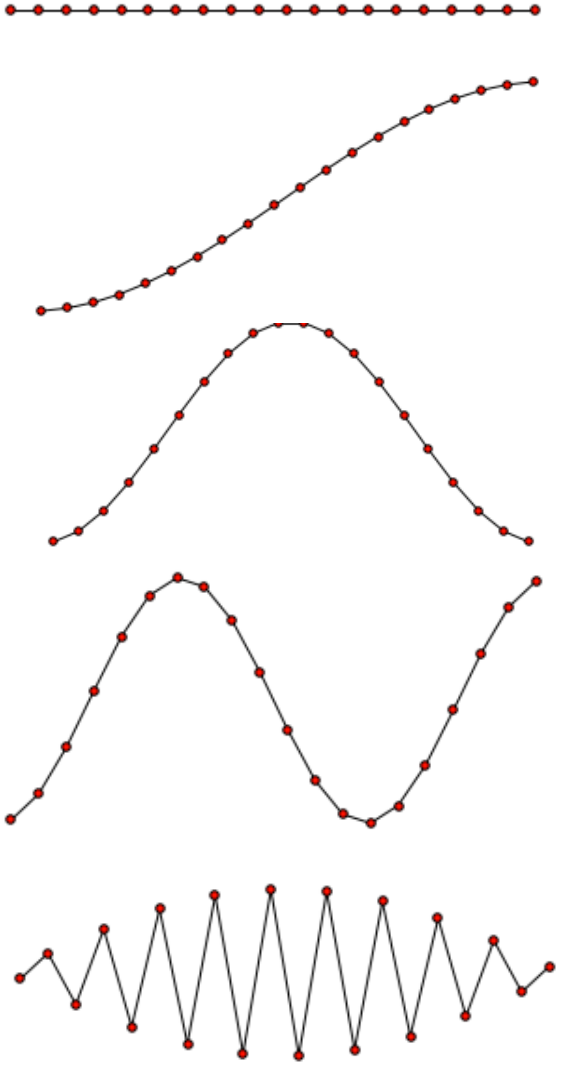


Intuitions: the 1-D case

- Suppose we take the jth eigen vector of a chain
- What would that look like?
- We are going to plot the chain along x-axis
- The y axis will have the value of the node in the jth eigen vector
- We want to see how these rise and fall

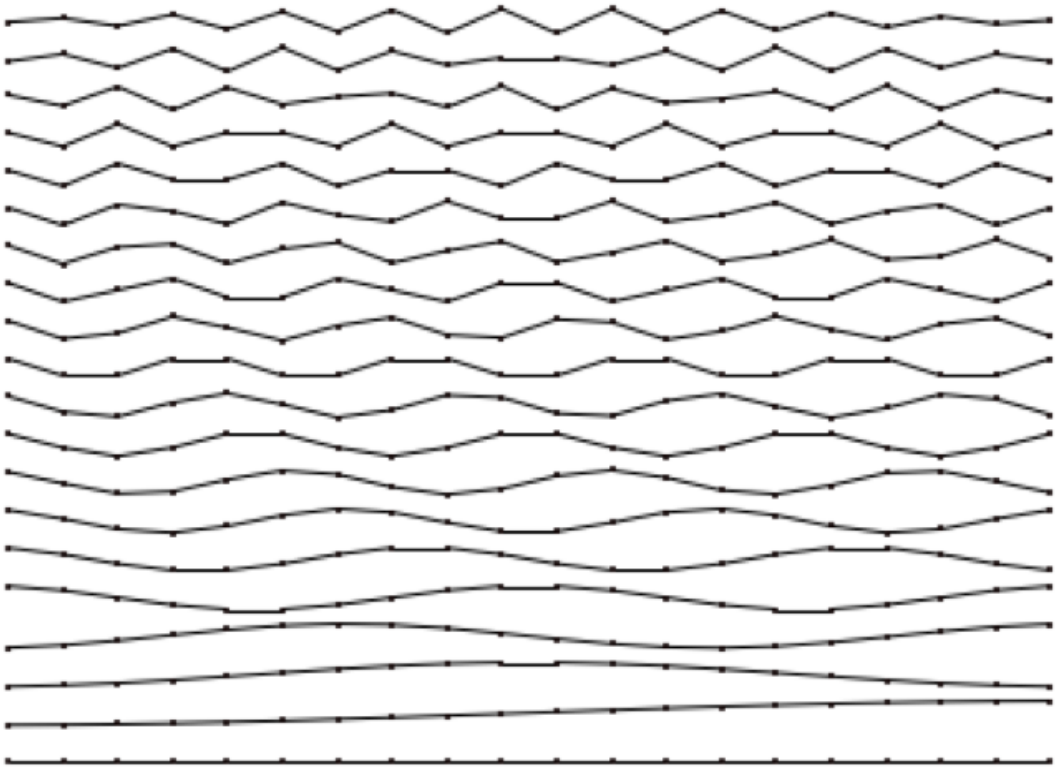
Observations (20 node chain)

- j = 0
- j=1
- j=2
- j =3
- j = 19



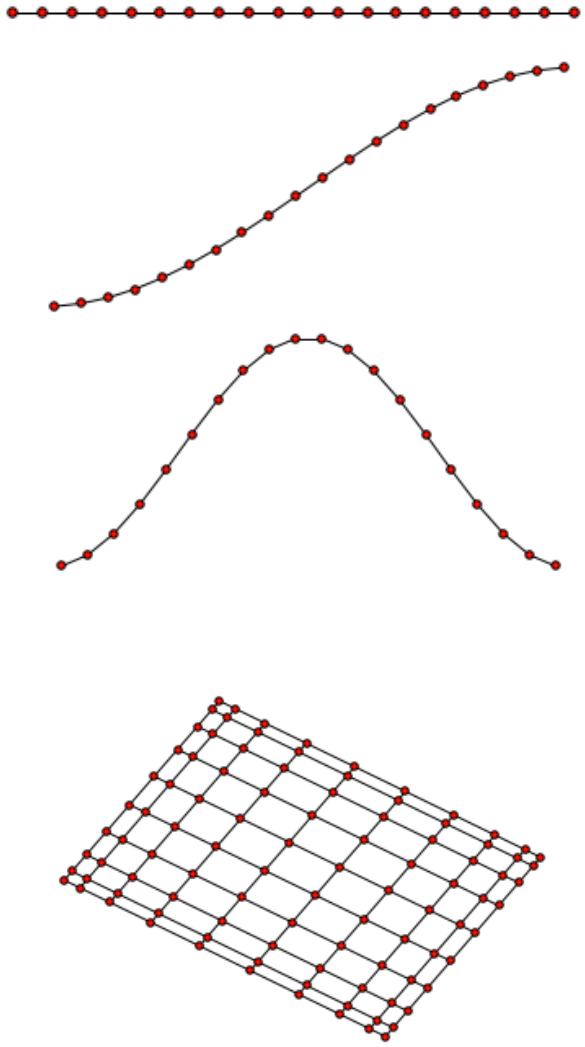
For All j

- Low ones at bottom
- High ones at top
- Code on web page

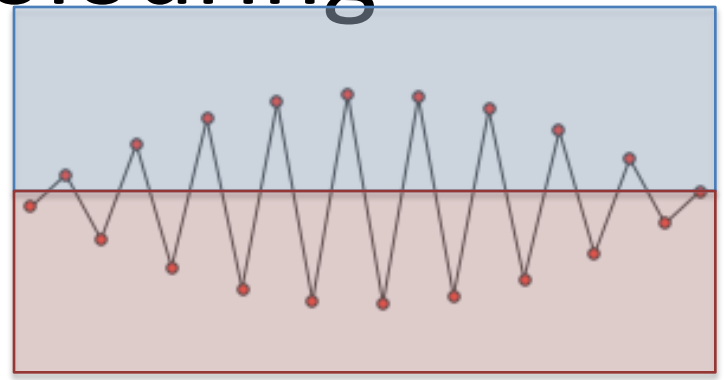


Observations

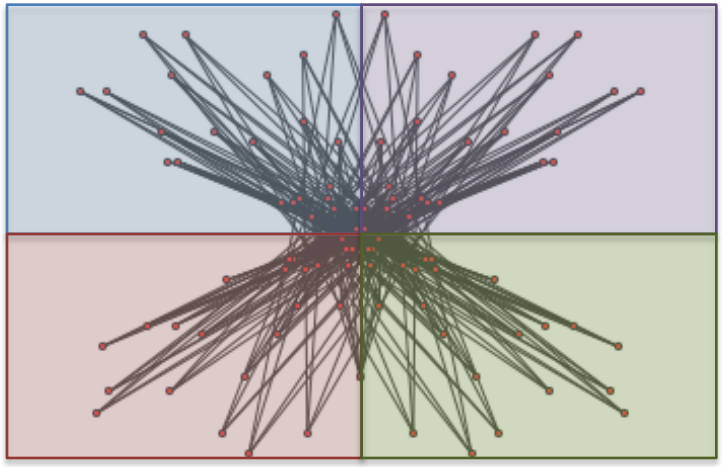
- In Dim 1 grid:
  - v[1] is monotone
  - v[2] is not monotone
- In dim 2 grid:
  - both v[1] and v[2] are monotone in suitable directions
- For low values of j:
  - Nearby nodes have similar values
    - Useful for embedding
- Similar to PCA



Application 2: Colouring



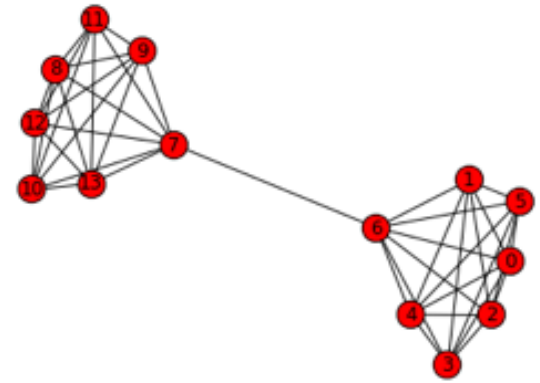
- Colouring: Assign colours to vertices, such that neighboring vertices do not have same colour
  - E.g. Assignment of radio channels to wireless nodes. Good colouring reduces interference

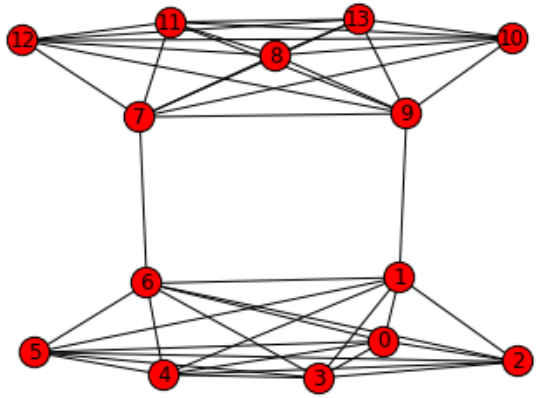


- Idea: High eigen vectors give *dissimilar* values to nearby nodes
- Use for colouring!

Application 3: Cuts/segmentation/clustering

- Find the smallest ‘cut’
- A small set of edges whose removal disconnects the graph
- Clustering, community detection…
- Idea: Use spectral embedding followed by standard clustering





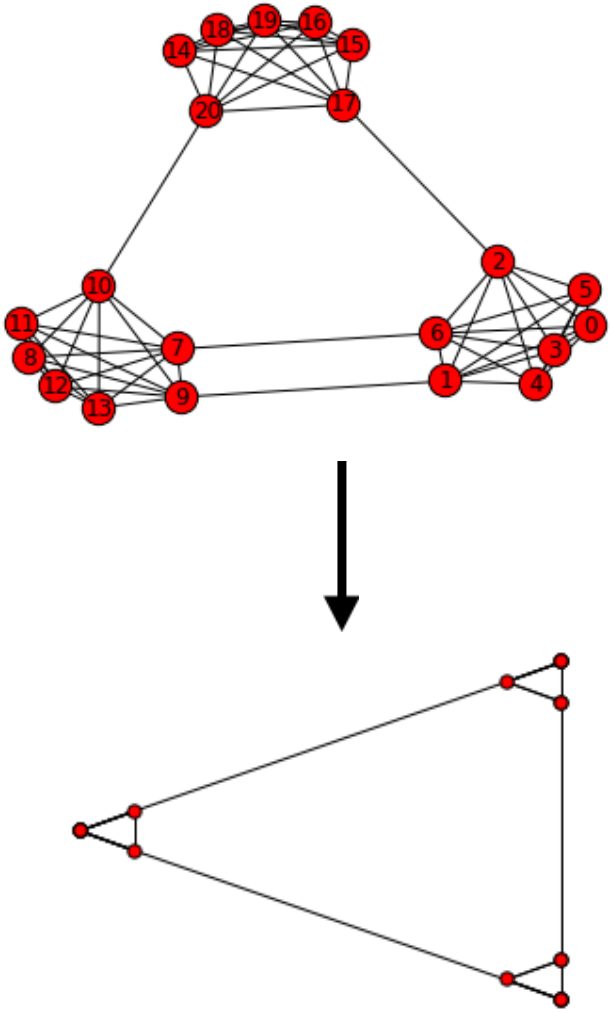
Clustering/community detection

- v[1] tends to stretch the narrow connections: discriminates different communities
- V[1] is sufficient to detect 2 communities
- Can be applied repeatedly for hierarchical clustering

Clustering: community detection

- More communities
- Spectral embedding needs higher dimensions

- Warning: it does not always work so cleanly
- In this case, the data is very symmetric clustered



Spectral clustering

- Objective: Cluster a given set of items

1. Define similarity graph between items
   - E.g. By creating edge between nearby items
   - Edge implies similar items, no edge implies dissimar items
   - Other graph construction methods are possible
2. Compute laplacian and spectra
3. Embed using first k eigen vectors
4. Perform k-means or similar k-clustering

How many dimensions to use?

- Common heuristic:
- The biggest gap among successive eigen values

$$\max_k \left|\lambda_k - \lambda_{k-1}\right|$$

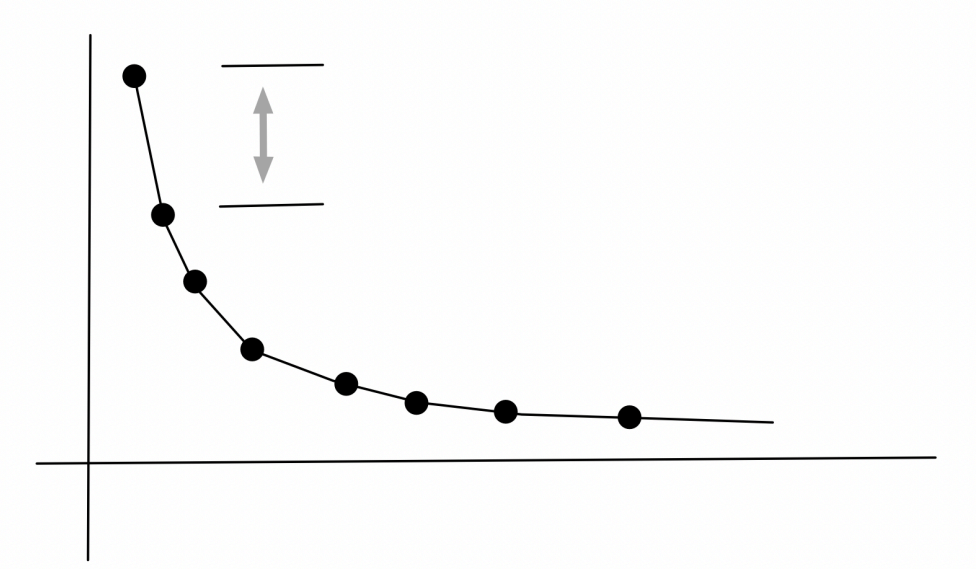


Image segmentation

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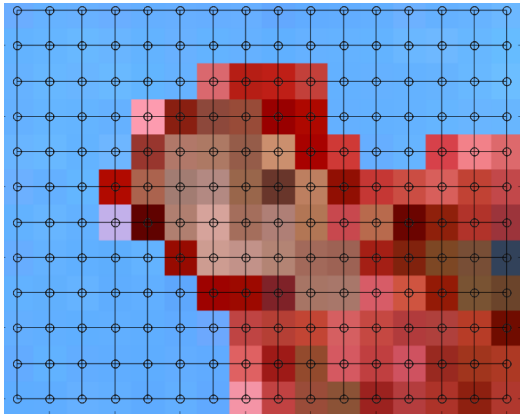
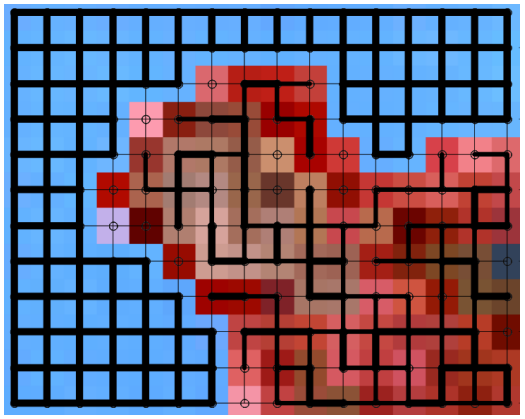


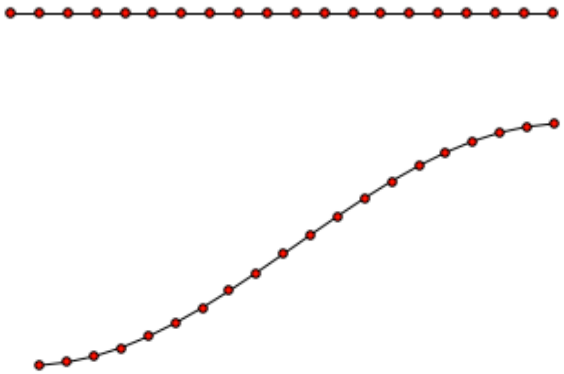
$v[1]$

$weight(i,j) \approx e^{-(px_i - px_j)^2}$



Eigen vectors of Laplacian

- Change implied by L on any input vector can be represented by sum of action of its eigen vectors (we saw this for HITS MM^T)
- v[0] is the slowest component of the change
  - With multiplier $\lambda_0=0$
  - The steady state component
- v[1] is slowest non-zero component
  - with multiplier λ_1



Spectral gap

- $\lambda_1 - \lambda_0$

- Determines the overall speed of change
  - And therefore speed of convergence
- If the slowest component v[1] changes fast
  - Then overall the values must be changing fast
  - Fast diffusion
- If the slowest component is slow
  - Convergence will be slow
- Examples:
  - Expanders and random graphs have large spectral gaps
  - Grids and dumbbells have small gaps ~ 1/n

Application 4: isomorphism testing

- Eigen values being different implies graphs are different
- Though not necessarily the other way

Spectral methods

- Wide applicability inside and outside networks
- Related to many fundamental concepts
  - PCA
  - SVD
- Random walks, diffusion, heat equation…
- Results are good many times, but not always
- Relatively hard to prove and understand properties
- Inefficient: eig. computation costly on large matrix
- (Somewhat) efficient methods exist for more restricted problems
  - e.g. when we want only a few smallest/largest eigen vectors