MATH 5340 Fall '23

Lecture 16

Part 3: Graphs, Laplacians, and Markov chains

A graph is a pair:

G – a set of points called nodes (or vertices)

$$G = \{x_1, \dots, x_N\}$$

W – a weight matrix

$$W_{ij} \geq 0 \quad i,j = 1, \dots, N$$

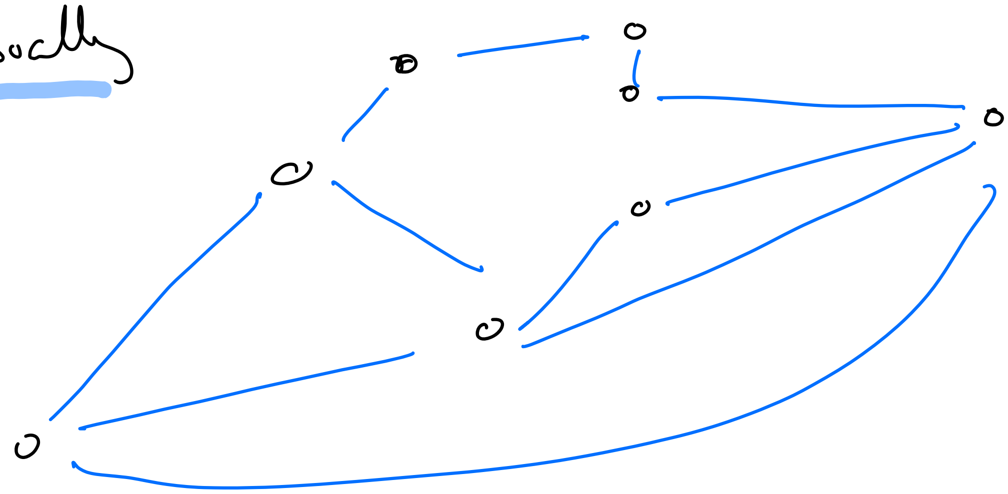
The matrix W is assumed symmetric (otherwise, one is talking about directed graphs)

Edges: Any pair (x_i, x_j) with $W_{ij} > 0$ will be called an **edge**.

If W_{ij} only takes the values $\{0,1\}$ what we have is commonly called a simple graph and in this case W is called the edge matrix.

In what follows we will assume $W_{ii}=0$ for all i's (one says there are no self-loops)

Visually



In our interpretation, W_{ij} measures the "affinity" between x_i and x_j, and the larger W_{ij}, the "closer" or stronger the bond between x_i and x_j.

Example: We are given points

$x_1, \dots, x_N$ (N is possibly very large, in practice $N = 10^6$)

and we fix a parameter $\rho > 0$. Then we define

$$W_{ij} = \begin{cases} 1 & \text{if } |x_i - x_j| < \rho \\ 0 & \text{otherwise.} \end{cases}$$

Definitions: Given x_i, the set of **neighbors** of x_i are those x_j's s.t. $W_{ij} > 0$, i.e. s.t. (x_i, x_j) is an edge.

A path in G is a sequence of nodes such that any two consecutive nodes in the sequence are neighbors. (visually, you are moving along the edges):

i.e. $x_{i_1}, x_{i_2}, \dots, x_{i_m}$: $W_{i_k i_{k+1}} > 0 \ \forall k$.

Given two nodes in G, we say they are connected in G if there is a path that starts in one and ends in the other. A graph G is called connected if any two nodes are connected.

Functions in G

We will denote by $C(G)$ the set of all functions $f : G \longrightarrow \mathbb{R}$, note that this is a real vector space isomorphic to $\mathbb{R}^N$, where an isomorphism is given by:

$$i : C(G) \longrightarrow \mathbb{R}^N$$

$$f \xrightarrow{i} (f(x_1), f(x_2), \dots, f(x_N))$$

In particular one can define inner products in $C(G)$, one could use the weights W to do so, but for now will only work with the usual inner product.

$$(f,g) = \sum_{i=1}^{N} f(x_i)\,g(x_i)$$

Note one could talk about the "canonical" or "nodal" basis for $C(G)$, namely

$$e_i \in C(G), \quad i = 1, \ldots, N$$

where

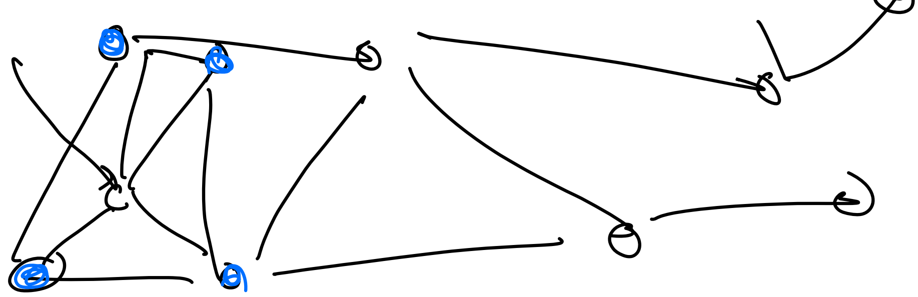
$$e_i(x_j) = \delta_{ij} \qquad \forall\ i,j.$$

The Laplacian on G

This is a linear transformation from $C(G)$ to itself, denoted by L and defined as follows:

$$(Lf)(x_i) = \sum_{j=1}^{N} \big(f(x_j) - f(x_i)\big) W_{ij}$$

x_i



How does L relate to the inner product?

$$(Lf, g) = \sum_{i=1}^{N} (Lf)(x_i) g(x_i)$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} (f(x_j) - f(x_i)) W_{ij} g(x_i)$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} f(x_j) g(x_i) W_{ij}$$

$$- \sum_{i=1}^{N} \sum_{j=1}^{N} f(x_i) g(x_i) W_{ij}$$

Observe:

$$\sum_{i=1}^{N} \sum_{j=1}^{N} f(x_i) g(x_i) W_{ij} = \sum_{j=1}^{N} \sum_{i=1}^{N} f(x_j) g(x_j) W_{ji}$$

Since $W_{ij} = W_{ji}$ $\forall\, i, j$, we have

$$\sum_{i=1}^{N} \sum_{j=1}^{N} f(x_i) g(x_i) W_{ij} = \sum_{i=1}^{N} \sum_{j=1}^{N} f(x_j) g(x_j) W_{ij}$$

Putting this back in (Lf, g),

$$(Lf, g) = \sum_{i=1}^{N} \sum_{j=1}^{N} f(x_j)\, g(x_i)\, W_{ij}$$

$$- \sum_{i=1}^{N} \sum_{j=1}^{N} f(x_j)\, g(x_j)\, W_{ij}$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} f(x_j)\big(g(x_i) - g(x_j)\big) W_{ij}$$

$$= (f, Lg)$$

This means that L is a symmetric linear transformation.