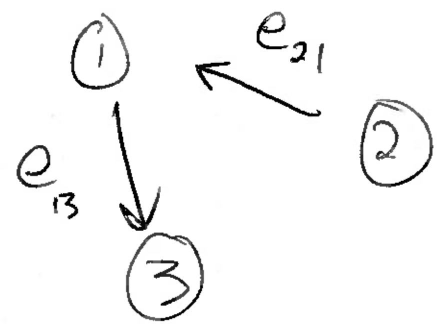
Today

- Intro to graphs, graph calculus
- The graph laplacian
- Graph Exterior Calculus
- Applications

Define $G(N,E)$ as graph w/ nodes and directed edges

$e_{ij} \in E$ points $j \to i$

$n_i \in N$ is node



We refer to N, E as chains ($N \to$ 0-chains, $E \to$ 1-chains)

def k-chain oriented set of $k+1$ vertices

~~We define~~ $$C^0 \xleftarrow{\partial_0} C^1$$

∂_k is a boundary operator $\partial_k : C^{k+1} \to C^k$

ex $$\partial_0 e_{ij} = n_j - n_i$$

We can assign real numbers to chains to develop graph functions (think of the grid functions in FDM as a function on 0-chains).

<u>Def</u> $f_{*}^{k} \in C_k = \mathbb{R}^{\dim(C^k)}$

co-chain (note <u>sub</u> script)

(often in math, co- means a real number associated w/ an object)

<u>Note</u> $f_{ij} \in C_1$, $f_{ij} = -f_{ji}$

<u>Def</u> co-boundary is a mapping

$$d_k : C_k \to C_{k+1}$$

<u>ex</u> Let $\phi \in C_0 \to \phi = \{\phi_1, \dots \phi_{\dim(C_0)}\}$

$d_0 \phi_{ij} = \phi_j - \phi_i$ is called the <u>graph gradient</u>

<u>Why?</u> In traditional calc, $\int_{e_{ij}} \nabla u \cdot dl = u_j - u_i$ by FTC

Final ingredient

Def Co-differential is the adjoint of coboundary

Note $\delta_K : \mathbb{R}^{\dim(C_K)} \to \mathbb{R}^{\dim(C_{K+1})}$

$$\Rightarrow \delta_K \in \mathbb{R}^{\dim(C_{K+1}) \times \dim(C_K)}$$

$v \in C_K,\ u \in C_{K+1}$

$$\langle v, \underbrace{\delta_K^* u}_{\text{codifferential}} \rangle = \langle \delta_K v, u \rangle$$

or more explicitly

$$\begin{aligned}
\langle \delta_K v, u \rangle &= \sum_{i,j,K} \delta_{ij,K}\, v_K\, u_{ij} \\
&= \sum_K v_K \underbrace{\left(\sum_{ij} \delta_{ij,K}\, u_{ij} \right)}_{\delta^* u} \\
&= \sum_K v_K\, \delta^* u_K \\
&= \langle v, \delta^* u \rangle
\end{aligned}$$

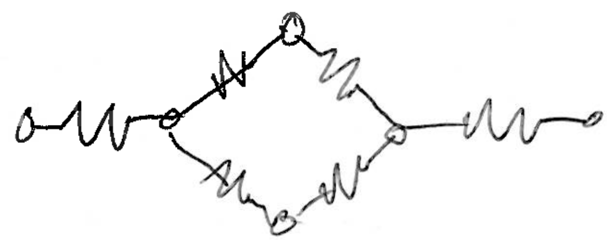
Alternatively, we can also define δ^* w.r.t. a weighted inner product

$$\langle v, \delta^* u \rangle_{W_k} = \langle \delta v, u \rangle_{W_{k+1}}$$

$$\Rightarrow \boxed{\delta^* u = W_k^{-1} \delta^T W_{k+1} u}$$

May seem a little abstract – some examples of common problems cast in this framework:

– Circuit analysis



Ohm's Law

$$I_{ij} = R_{ij}^{-1}(V_j - V_i)$$

Kirchoffs Law

$$\sum_{j \sim i} I_{ij} = 0$$

Can be recast

$$I = R^{-1}\delta_0 V$$

$$\delta_0^* I = 0$$

$$\Rightarrow \boxed{\delta_0^* R^{-1} \delta_0 V = 0}$$

– Graph Attention / Message passing networks

For a gat layer

$$m_{ij}^n = F(x_i^n, x_j^n \mid \theta_m)$$

$$x^{n+1} = x^n + \sigma\Big(\sum_{j \sim i} \alpha_{ij}(x_i^n, x_j^n)\; m_{ij}^n\Big)$$

can be rewritten

$$x^{n+1} = x^{n} + G(\delta_0^* m)$$

where the attention is inducing the codifferential

$$\rightarrow \delta^* m = \delta_0^T \underset{W_{K+1}}{\alpha} m$$

Notes

- GATs are notoriously hard to train deep. - over squashing / over smoothing
- w/ some physics ideas we'll show how to keep them big

Prob 3 Recommender systems

Given n ratings of movies, can you suggest other movies someone will like

0-cochain → score
1-cochain → movie preference

Similar graph analytics for social networks epidemiology

Stability Analysis

Let $W = \mathrm{diag}(w_1, \ldots, w_{N_{edges}}) > 0$

Define the weighted graph Laplacian

$$L_W[u]_i = \sum_{j \sim i} w_{ij} (u_j - u_i)$$

e.g. $w_{ij} = R_{ij}^{-1}$

Consider the problem

$$L_W[u]_i = f_i$$

We can mimick the Galerkin procedure, using the l_2- inner product in

$$\langle f, g \rangle = \sum_i f_i g_i$$

instead of integration

$\forall\, v \in C_0$

$$\langle v, L_W[u]_i \rangle = \langle v, f \rangle$$

LHS $\quad \displaystyle\sum_{i,j} v_i w_{ij} (u_j - u_i)$

$$= \frac{1}{2} \sum_{i,j} v_i w_{ij} (u_j - u_i) + v_i w_{ij} (u_j - u_i)$$

$$= \frac{1}{2} \sum_{i,j}' v_i w_{ij} (u_j - u_i) + v_j w_{ji} (u_i - u_j)$$

$$= -\frac{1}{2} \sum_{i,j}' (v_j - v_i) w_{ij} (u_j - u_i)$$

$$= -\frac{1}{2} (\delta v)^T W \delta u$$

$$:= a(u,v)$$

Like before, we have identified a variational problem

$$a(u,v) = \langle f, v \rangle$$

w/ energy norm

$$\|u\|_E = a(u,u) = \langle u, u \rangle_{\delta^T W \delta}$$

We can therefore see that we have all of our FEM machinery.

To invoke Lax-Milgram, we need to prove coercivity of energy norm

$$\|u\|_E^2 > \alpha \langle u, u \rangle$$

Rayleigh-Quotients + eigenanalysis

Let $M = M^T$ w/ orthogonal eigenpairs (λ_i, v_i)

i.e $v_i^T v_j = \delta_{ij}$

So $M v_i = \lambda_i v_i$ for i^{th} eigenpair

$v_i^T M v_i = \lambda_i v^T v_i = \lambda_i$

Fact

Symm Matrices have real non-neg eigvalues

<u>Def</u> The <u>Rayleigh-quotient</u>

$$R(M, x) = \frac{x^T M x}{x^T x}$$

Expanding x in eigen basis

$$\vec{x} = \sum_i \hat{y}_i \vec{v}_i$$

$$\hat{y}_i = \langle v_i, x \rangle$$

i.e the basis expansion coeffs projecting x onto v's

Then

$$R(M, x) = \frac{\sum_i \lambda_i y_i^2}{\sum_j y_j^2}$$

We can see that max/min of R gives max/min eigenvalues

$$\lambda_{min} \leq \lambda_{min} \frac{\sum y_j^2}{\sum y_j^2} \leq \frac{\sum_i \lambda_i y_i^2}{\sum_j y_j^2} \leq \lambda_{max} \frac{\sum_j y_j^2}{\sum_j y_j^2} \leq \lambda_{max}$$

Let d_v denote the degree of vertex v

Spectral Graph Theory
Fan Chung

Denote $T = \mathrm{diag}(d_v)_{v=1}^{N_{edges}}$

Def degree scaled Laplacian

$$\mathcal{L}_{ij} = \begin{cases} 1 & i=j, \ d_v \neq 0 \\ -\frac{1}{\sqrt{d_i d_j}} & j \sim i \end{cases}$$

$$\mathcal{L} = T^{-1/2} L \, T^{-1/2}$$

$\boxed{\text{Eigen values of } L \text{ match those of } \mathcal{L} \text{ scaled by degree!}}$

Consider the Rayleigh quotient

$$\frac{\langle g, \mathcal{L} g \rangle}{\langle g, g \rangle} = \frac{\langle g, T^{-1/2} L \, T^{-1/2} g \rangle}{\langle g, g \rangle}$$

Let $f = T^{-1/2} g$

$$= \frac{\langle f, Lf \rangle}{\langle T^{1/2} f, T^{1/2} f \rangle} = \frac{\sum_{j \sim i} (f_i - f_j)^2}{\sum_K f_K^2 d_K}$$

As a Rayleigh quotient, we can note

- λ_i are all positive.
- $\min(\lambda) = \lambda_0 = 0$ w/ vec $v = \vec{1}$
- For a non-simply connected graph w/ K-connected components $\lambda_0, \dots \lambda_{K-1} = 0$

For a simply connected graph, the constant we need for Lax-Milgram is

$$\alpha = \lambda_1 = \min_{f \perp \vec{1}} \frac{\sum_{j \sim i} (f_i - f_j)^2}{\sum_k f_k^2 d_k}$$

Notes – λ_1 is called Fiedler eigenvector & used in spectral graph theory, graph cut algorithms, diffusion problems, spectral clustering

– this α only holds for $f \perp v_0$, so when we solve the variational problem we need to choose grid functions orthogonal to the constant vector

Estimates for λ_1

Option 1 – For a fixed graph, can always solve eigenvalue problem

– Arnoldi iteration gives a scalable estimate for large graphs.

Option 2 The following proof is to estimate how scaling depends on # nodes + edges

Some definitions:

<u>Volume</u> $\mathrm{vol}(G) = \sum_i d_i$

<u>distance</u> $d(v_i, v_j)$ = shortest path connecting v_i, v_j

<u>diameter</u> $D = \max_{i,j \in V} d(v_i, v_j)$

<u>Thm</u> For simply connected graph G w/ diameter D

$$\lambda_1 \geq \frac{1}{D\,\mathrm{vol}(G)}$$

<u>Pf</u>

- For smallest eigvec $f_0 = \vec{1}$
- By orthogonality of eigenvectors $\langle f_0, f_1 \rangle = 0$

$$\Rightarrow \sum_i f_1(v_i) = 0$$

- Choose v_0 as a vertex satisfying

$$|f(v_0)| = \max_v |f(v)|$$

- Since $\sum_i f(v_i) = 0$, we can find a vertex u_0 such that $f(u_0)\,f(v_0) < 0$
- Pick path P joining u_0, v_0

$$\lambda_1 = \frac{\sum_{j \sim i} (f_j - f_i)^2}{\sum_K f_K^2 d_K} \geq \frac{\sum_{j,K \in P} (f_j - f_i)^2}{\mathrm{vol}\, G \;\; f^2(v_0)}$$

$$> \frac{\frac{1}{D} (f(v_0) - f(u_0))^2}{\mathrm{vol}(G) \;\; f^2(v_0)} > \frac{1}{D\, \mathrm{vol}\, G}$$

Graph div / grad / curl

So far we only introduced graph grad and div

For higher order chains, extend the coboundary

$$C^k = [v_1, \dots v_k]_{v_i \in V}$$

anti symmetric wrt vertex swap

$$\partial^k_{k-1}[v_1, \dots v_k]$$

$$= \sum_{i=1}^{k} (-1)^{i-1} [n_1, \dots \hat{n}_i, \dots n_k]$$

$\hat{}$ means leave this vertex out

<u>ex</u> Given edge $[v_1, v_2] = -[v_2, v_1]$

$$\partial_0 [v_1, v_2] = (-1)^0 v_2 + (-1)^1 v_1 = v_2 - v_1$$

<u>Thm</u> $\partial_{k-1} \circ \partial_k = 0$

$$\partial_{k-1} \partial_k = \sum_{i=1}^{k} (-1)^{i-1} \partial_{k-1} [n_1, \dots \hat{n}_i, \dots n_k]$$

$$= \sum_{i,j} (-1)^{i-1} (-1)^{j-1} [n_1, \dots \hat{n}_i, \dots \hat{n}_j \dots n_k]$$

anti symmetric

$$= \sum_{i,j} \alpha_{ij}$$

$= -\alpha_{ji}$

$$= 0$$

A similar algebraic definition of coboundary can be obtained

$$\langle f, \partial_{K+1} c \rangle = \langle d_K f, c \rangle$$

Ex $\quad \delta_0 \phi_{ij} = \phi_j - \phi_i \qquad$ grad

$\quad \delta_1 \phi_{ijK} = \phi_{ij} + \phi_{jK} + \phi_{Ki} \qquad$ curl

Similarly $\quad \delta_K \delta_{K-1} = 0$

Ex $\quad \delta_1 \delta_0 \phi = \delta_0 \phi_{ij} + \delta_0 \phi_{jK} + \delta_0 \phi_{Ki}$

$$= \phi_j - \phi_i + \phi_K - \phi_j + \phi_i - \phi_K$$

$$= 0$$

We will use these properties to define flows on graphs