$$\Delta f(u) = \frac{1}{4} \sum_{i=1}^{4} (f(u_i) - f(u))$$

$$= \frac{1}{4} \cdot \left[\left(f(u_1) - f(u) \right) - \left(f(u) - f(u_2) \right) \right]$$

$$+ \frac{1}{4} \left[\left(f(u_3) - f(u) \right) - \left(f(u) - f(u_4) \right) \right].$$

Analogue to Laplacian on $\mathbb{R}^2$, $L = \frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial y^2}$.

<u>More serious treatment</u>:

Consider the set of functions on oriented edges E^{or}

$$i : E^{or} \to \mathbb{R}$$

s.t. $\quad i(u,v) = -i(v,u), \quad \forall \{u,v\} \in E.$

This is a linear space.

Define $\quad d : \mathbb{R}^{|V|} \to Q \quad$ s.t. $\forall f : V \to \mathbb{R}$

$$df(u,v) := f(u) - f(v)$$

Assign inner product structures.

$\forall f, g \in \mathbb{R}^{|V|}, \quad (f,g) := \sum_{v \in V} f(v) g(v) d_v \qquad (*)$

$\forall i, j \in Q, \quad (i,j)_Q := \sum_{\{u,v\} \in E} i(u,v) j(u,v)$

Let d^* be the adjoint operator of d s.t.

$$(df, i)_Q = (f, d^* i)$$

That is

$$\sum_{\{u,v\} \in E} (f(u) - f(v)) i(u,v) = \sum_{u \in V} f(u) d^* i(u) d_u$$

Observe that $\text{LHS} = \sum_{u \in V} f(u) \sum_{v : \{u,v\} \in E} i(u,v)$

That is, we have

$$\sum_{u \in V} f(u)\, d^* i(u)\, d_u = \sum_{u \in V} f(u) \sum_{v : \{u,v\} \in E} i(u,v), \quad \forall f$$

$$\Rightarrow d^* i(u) = \frac{1}{d_u} \sum_{v : \{u,v\} \in E} i(u,v)$$

Therefore, we have

$$\boxed{\Delta = -d^* d.} \qquad (**)$$

<u>Laplacian and its spectrum</u>

We continue the study of functions on a graph G, with the aim of understanding the structure of G. We hope to find a particular set of basis functions such that all functions can be decomposed in terms of basis functions. Of course, we hope these basis functions contain much of the characteristic properties of G. In that sense, we do not want to choose dirac functions $\{\delta_u : u \in V\}$. The set of eigenfunctions of L is a good choice.

~~We have the following immediate consequence of (**)~~.

① Assigning the inner product (*) to the set of all functions on $G = (V, E)$, we obtain a Hilbert space, denoted by $\ell^2(V)$. Then we have the following immediate consequence of (**) for the Laplacian operator $\Delta : \ell^2(V) \to \ell^2(V)$.

(i) Δ is selfadjoint. That is,

$$(f, \Delta g) = (f, -d^* d g) = -(df, dg)_Q$$
$$= -(d^* df, g) = (\Delta f, g), \quad \forall f, g \in \ell^2(V)$$

(ii) Δ is nonpositive, that is,

$$(\Delta f, f) = -(d^*df, f) = -(df, df)_Q$$

$$= -\sum_{\{u,v\}\in E} (f(u)-f(v))^2 \leq 0.$$

~~Definition~~: Therefore ~~Δ has real eigenvalues~~ the eigenvalues of Δ are real and nonpositive. We write them as $-\lambda_k$ so that the eigenvalue equation becomes

$$\Delta u_k + \lambda_k u_k = 0.$$

We list them as

$$0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N \quad \text{where } N = |V|.$$

(Notice that Δ can be represented as a $N \times N$ matrix. Therefore it has N eigenvalues counted by multiplicity).

By definition, $\Delta u = 0$ for a constant function u. Therefore $\lambda_1 = 0$.

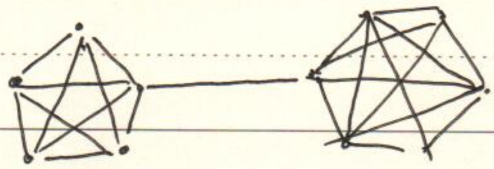
Lemma 1. Let $G = (V, E)$ be a connected finite simple graph. Then the 0 eigenvalue is simple. That is, the only harmonic fct on a connected graph is constant functions.

Proof: Let $f_1 : V \to \mathbb{R}$ be such that $\Delta f_1 = 0$.
Let $u \in V$ be a maximum of f_1, i.e. $f(v) \leq f(u)$, $\forall v \in V$.
Then $0 = \Delta f_1(u) = \frac{1}{d_u} \sum_{v:\{u,v\}\in E} (f_1(v) - f_1(u)) \leq 0$
"=" holds iff $f_1(v) = f_1(u)$ for any $v \sim u$.
Due to connectedness, we have $f_1 \equiv f_1(u)$ by induction. □

Lemma 2. Let $G = (V, E)$ be a finite simple graph. Then the multiplicity of zero eigenvalue equals the number of connected components.

Proof. By the proof of Lemma 1, $\Delta f = 0 \Rightarrow f$ is constant on each connected component. All such functions forms a k-dim. linear space where $k = \#$ connected components. That is the dim of the eigenspace of 0 is k. $\square$

From the above property, we see that when the graph G is "close" to be disconnected, then λ_2 should be very small.



[Jost, Mathematical Methods in Biology and Neurobiology, Universitext, Springer, 2014, Chap. 2]

Courant's minimax principle

We iteratively define the following Hilbert spaces:

$H_1 := \ell^2(V)$, $\mu_1 = 0$, f_1 is the constant fct with $(f_1, f_1) = 1$.

$H_2 := \{ f \in \ell^2(V) ;\ (f, f_1) = 0 \}$

Define:

$$\mu_2 := \inf_{f \in H_2 \setminus \{0\}} \frac{(df, df)_Q}{(f, f)}$$

Rayleigh Quotient

~~Then~~ Observe that

$$\frac{(df, df)_Q}{(f,f)} = \frac{\sum_{\{u,v\} \in E} (f(u) - f(v))^2}{\sum_{u \in V} f(u)^2 d_u}$$

remains unchanged when a function u is multiplied by a nonzero constant. So

$$\mu_2 := \inf_{\substack{f \in H_2 \setminus \{0\} \\ (f,f) = 1}} (df, df)_Q$$

Since $\{f \in H_2 \setminus \{0\}, (f,f)=1\}$ is compact. we can always find a function f_2 realize μ_2, that is

$$\mu_2 = \frac{(df_2, df_2)_Q}{(f_2, f_2)}.$$

Now, we have H_2, μ_2, f_2.

We can continue to define H_3, μ_3, f_3, and iteratively any H_k, μ_k, f_k s.t.

$$H_k := \{ f \in \ell^2(V) : (f, f_1) = \cdots = (f, f_{k-1}) = 0 \}$$

$$\mu_k := \inf_{f \in H_k \setminus \{0\}} \frac{(df, df)_Q}{(f, f)}$$

and f_k is the one with $(f_k, f_k)=1$ and

$$\mu_k = \frac{(df_k, df_k)_Q}{(f_k, f_k)}.$$

Hence, in the end, we arrive at an orthonormal basis

$$f_1, f_2, \cdots, f_N, \text{ with } N = |V|.$$

By definition, we have $\mu_k \geq \mu_{k-1}$. $\forall\, k = 2, \cdots, N$.

<u>Lemma 3</u>. Let $\mu_1, \cdots, \mu_N$ be defined as above. Then

$$\mu_k = \lambda_k, \quad k = 1, \cdots, N.$$

~~That is~~ Indeed, $\Delta f_k = -\lambda_k f_k$, $k = 1, \cdots, N$.

<u>Proof</u>: By definition

$$\mu_k = \frac{(df_k, df_k)}{(f, f)} = \inf_{f \in H_k \setminus \{0\}} \frac{(df, df)}{(f, f)}$$

For any $\varphi \in H_k$, we have $f_k + t\varphi \in H_k$, and

$$\frac{(d(f_k+t\varphi),\ d(f_k+t\varphi))}{(f_k+t\varphi,\ f_k+t\varphi)} \geq \mu_k$$

where "=" is achieved when $t=0$.

Therefore

$$0 = \frac{d}{dt}\Big|_{t=0} \frac{(d(f_k+t\varphi),\ d(f_k+t\varphi))}{(f_k+t\varphi,\ f_k+t\varphi)} = \frac{2(df_k, d\varphi)(f_k,f_k) - 2(df_k, df_k)(f_k,\varphi)}{(f_k, f_k)^2}$$

$$= \frac{2(df_k, d\varphi)(f_k,f_k) - 2\mu_k(f_k,f_k)(f_k,\varphi)}{(f_k,f_k)^2}$$

$$= 2(df_k, d\varphi) - 2\mu_k(f_k,\varphi)$$

$$= 2(d^*d f_k - \mu_k f_k, \varphi) = -2(\Delta f_k + \mu_k f_k, \varphi)$$

$$\Rightarrow \quad (\Delta f_k + \mu_k f_k, \varphi) = 0, \quad \forall \varphi \in H_k \qquad (*)$$

Observe that, $(*)$ actually holds true for any $\varphi \in \ell^2(V)$.

This is because, for any f_i, $i = 0, 1, \ldots, k-1$, we have

$$(\mu_k f_k, f_i) = 0$$

and $(\Delta f_k, f_i) = -(df_k, df_i) = (f_k, \Delta f_i)$

$$= -\mu_i (f_k, f_i) = 0.$$

Therefore, we have

$$(\Delta f_k + \mu_k f_k, \varphi) = 0, \quad \forall \varphi \in \ell^2(V).$$

$$\Rightarrow \quad \Delta f_k + \mu_k f_k = 0.$$

Hence $\mu_k = \lambda_k$, and f_k is the corresponding eigenfunctions $\square$

<u>Remark</u>. We have constructed an orthonormal basis of $\ell^2(V)$ consisting of eigenfunctions of Δ. Then for any function

$f \in \ell^2(V)$, we can decompose it as

$$f = \sum_k (f, f_k) f_k .$$

Hence $\quad (f, f) = \sum_k (f, f_k)^2 \quad$ since $(f_k, f_\ell) = \delta_{k\ell}$.

Moreover $\quad (df, df)_Q = (d^* df, f)_Q = -(\Delta f, f)_Q$

$$= -\left(\sum_k (f, f_k) \Delta f_k, f\right)$$

$$= \sum_k (f, f_k)^2 \lambda_k$$

Theorem. (Courant's minimax principle) Let G be a ~~connected~~ finite simple graph. Let P^k be the collection of all k dimensional linear subspaces of $\ell^2(V)$. Then we have

$$\lambda_k = \max_{L \in P^{k-1}} \min \left\{ \frac{(df, df)}{(f, f)} : f \neq 0, (f, h) = 0, \forall h \in L \right\} \quad (1)$$

and dually

$$\lambda_k = \min_{L \in P^k} \max \left\{ \frac{(df, df)}{(f, f)} : f \in L \setminus \{0\} \right\} \quad (2)$$

Remark. In (1), the minimum is taken under "$k-1$ constraints", and we maximize w.r.t. the constraints. In (2), we consider the maximum for k degree of freedom, and we minimize w.r.t. those degree of freedom.

Proof. Since $\quad \dfrac{(df, df)_Q}{(f, f)} = \dfrac{\sum_{i=1}^N (f, f_i)^2 \lambda_i}{\sum_{i=1}^N (f, f_i)^2}$,

we have $\quad \lambda_k = \min \left\{ \dfrac{(df, df)_Q}{(f, f)} : f \neq 0, (f, f_j) = 0, j = 1 \cdots k-1 \right\}$

and $\quad \lambda_k = \max \left\{ \dfrac{(df, df)_Q}{(f, f)} : f \neq 0, f \in \operatorname{span}\{f_1, \cdots, f_k\} \right\}$

the min is realized by f_k, and the max is also realized by f_k.

For any $L \in P^k$, we solve

$$\begin{cases} (g, f_j) = 0, & j = 1, \cdots, k-1 \\ g \in L \end{cases}$$

By dimension consideration, we always have a nonzero solution.

Moreover $\frac{(dg, dg)_Q}{(g,g)} = \frac{\sum_{j \geq k} \lambda_j (g, f_j)^2}{\sum_{j \geq k} (g, f_j)^2} \geq \lambda_k$

Therefore $$\max_{f \in L \setminus \{0\}} \frac{(df, df)}{(f,f)} \geq \lambda_k$$

Of course, for $L_0 = \text{span}\{f_1, \cdots, f_k\}$, we have

$$\max_{f \in L_0 \setminus \{0\}} \frac{(df, df)}{(f,f)} = \lambda_k$$

That is, $\lambda_k = \min_{L \in P^k} \max_{f \in L \setminus \{0\}} \frac{(df, df)}{(f,f)}$.

In a dual manner, for any $L_0 \in P^{k-1}$, we solve

$$\begin{cases} h \perp L_0 \\ h \in \text{span}\{f_1, \cdots, f_k\} \end{cases}$$

We are looking for a h in a k-dim subspace that is vertical to a $(k-1)$-dim space. We can always find such a nonzero h.

Moreover $\frac{(dh, dh)_Q}{(h,h)} = \frac{\sum_{1 \leq j \leq k} \lambda_j (h, f_j)^2}{\sum_{1 \leq j \leq k} (h, f_j)^2} \leq \lambda_k$

Therefore

$$\therefore \min_{f \in L^{\perp} \setminus \{0\}} \frac{(df, df)_Q}{(f, f)} \leq \lambda_k$$

And hence $\displaystyle \lambda_k = \max_{L \in P^{k-1}} \min_{f \in L^{\perp} \setminus \{0\}} \frac{(df, df)_Q}{(f, f)}$. $\square$

Laplacian Eigenvalues.

$$0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N \leq 2$$

By the new variational formula, we can ~~do~~ easily understand $\lambda_1 = 0$, and multiplicity of 0 = # connected components.

Infact

$$\lambda_1 = \inf_{f \neq 0} \frac{(df, df)_Q}{(f, f)} = \inf_{f \neq 0} \frac{\sum_{\{u,v\} \in E} (f(u) - f(v))^2}{\sum_{u \in V} f(u)^2 d_u}$$

The strategy ~~to~~ for obtaining ~~the~~ an eigenfunction for λ_1 is to do the same as one's neighbors. This can be always achieved no matter what graphs we have.

By way of contrast, according to Courant's minimax principle, the largest eigenvalue is given by

$$\lambda_N = \max_{f \neq 0} \frac{(df, df)_Q}{(f, f)} = \max_{f \neq 0} \frac{\sum_{\{u,v\} \in E} (f(u) - f(v))^2}{\sum_{u \in V} f(u)^2 d_u}$$

The stategy for obtaining an eigenfunction for λ_N is to do the opposite what one's neighbors are doing. Thus, the corresponding eigenfunction exhibit oscillations with the highest possible frequency. However, in contrast to the case of λ_1, here we may have obstacles: for example, in C_3, $\triangle$, the strategy of doing the opposite to your neighbors does not work!!

~~Theorem~~ Lemma: Let G be a finite simple graph with $|V|=N$. We have
$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N \leq 2.$$
with $\lambda_N = 2$ iff G has a nontrivial connected component bipartite.

In fact, the multiplicity of eigenvalue 2 equals the number of bipartite connected components of G.

Remark: A bipartite graph $G=(V,E)$ is a graph s.t.
$$V = V_1 \sqcup V_2$$
and all edges connect vertices from different V_i's.

A graph is bipartite iff it contains no odd cycle.

Proof: This follows from the fact that
$$(f(u)-f(v))^2 \leq 2f(u)^2 + 2f(v)^2$$
where "=" iff $f(u) = -f(v)$.

In fact,
$$\lambda_N = \max_{f\neq 0} \frac{\sum_{\{u,v\}\in E} (f(u)-f(v))^2}{\sum_{u\in V} f(u)^2 d_u}$$
$$\leq \max_{f\neq 0} \frac{2\sum_{\{u,v\}\in E} (f(u)^2+f(v)^2)}{\sum_{u\in V} f(u)^2 d_u}$$
$$= 2 \max_{f\neq 0} \frac{\sum_{u\in V} f(u)^2 d_u}{\sum_{u\in V} f(u)^2 d_u} = 2$$

"=" iff $f(u) = -f(v)$ for any edge $\{u,v\}$ in E.

Under the constraints that $f(u) = -f(v)$ $\forall \{u,v\}\in E$, ~~we know~~ we can find nonzero such f on each connected component iff ~~G~~ this component contains no odd cycle.

That is, "=" iff G has a bipartite connected component. $\square$

Indeed, we have the following spectral characterization:

Theorem. Let G be a finite simple connected graph. Then G is bipartite iff for each λ_i, the value $2-\lambda_i$ is also an eigenvalue of G.

Pf. "$\Leftarrow$" easy: since G always has $\lambda_1 = 0$. Hence $2-0=2$ is an eigenvalue. $\Rightarrow$ G bipartite.

"$\Rightarrow$" Denote $\Delta f_i + \lambda_i f_i = 0$. Suppose the bipartition is $V = V_1 \sqcup V_2$.

Then define
$$\tilde{f}_i(u) = \begin{cases} f_i(u), & \text{if } u \in V_1 \\ -f_i(u), & \text{if } u \in V_2 \end{cases}$$

~~$\Delta f_i + \lambda_i f_i = 0 \Rightarrow$~~

One can check directly that
$$\Delta \tilde{f}_i + (2-\lambda_i)\tilde{f}_i = 0.$$
$\square$

G connected

"=" iff bipartite.
$$0 = \lambda_1 < \lambda_2 \le \lambda_3 \le \cdots \le \lambda_{N-1} \le \lambda_N \le 2$$

Example. Complete graphs with $|V| = N$. A graph is called complete if any two vertices are connected by an edge. Then it has constant vertex degree $d = N-1$.

Let f be a fct which is vertical to constant fcts, i.e.
$$\sum_{u\in V} f(u)\, d_u = 0 \Rightarrow \sum_{u \in V} f(u) = 0.$$

We compute for $u \in V$
$$\Delta f(u) = \frac{1}{d_u} \sum_{v:\{u,v\}\in E} f(v) - f(u)$$
$$= \frac{1}{N-1} \sum_{v\in V, v\neq u} f(v) - f(u)$$
$$= \frac{1}{N-1}(-f(u)) - f(u) = -\frac{N}{N-1} f(u).$$