Similarly, one can figure out the matrix $\Gamma_2(x)$, whose calculation is a bit messy. We can denote 重写

$$\Gamma_2(x) = \begin{pmatrix} \Gamma_2(x)_{xx} & \Gamma_2(x)_{x,S_1(x)} & \Gamma_2(x)_{x,S_2(x)} \\ \Gamma_2(x)_{S_1(x),x} & \Gamma_2(x)_{S_1(x),S_1(x)} & \Gamma_2(x)_{S_1(x),S_1(x)} \\ \Gamma_2(x)_{S_2(x),x} & \Gamma_2(x)_{S_2(x),S_1(x)} & \Gamma_2(x)_{S_2(x),S_2(x)} \end{pmatrix}$$

$\Gamma_2(x)$ is a symmetric matrix. For the moment, we only need three simple blocks $\Gamma_2(x)_{S_2(x),x}$, $\Gamma_2(x)_{S_2(x),S_1(x)}$, and $\Gamma_2(x)_{S_2(x),S_2(x)}$.

For convenience, we introduce the following notation:

$$P_{xy} = \begin{cases} \frac{1}{d_x}, & \text{if } x \sim y \\ 0, & \text{otherwise.} \end{cases}$$

P_{xy} is called the <u>transition rate</u> in discrete Markov chain theory.

Recall in this notation, $\Gamma(x)$ can be reformulated as

$$\Gamma(x) = \frac{1}{2} \begin{pmatrix} 1 & -P_{xy_1} & \cdots & -P_{xy_m} \\ -P_{xy_1} & P_{xy_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -P_{xy_m} & 0 & \cdots & P_{xy_m} \end{pmatrix}$$

On can check that

$$\left(\Gamma_2(x)\right)_{S_2(x),x} = \begin{pmatrix} \frac{1}{4}\sum_{y\in S_1(x)} P_{xy}P_{yz_1} \\ \vdots \\ \frac{1}{4}\sum_{y\in S_1(x)} P_{xy}P_{yz_n} \end{pmatrix}, \quad \left(\Gamma_2(x)\right)_{S_2(x),S_1(x)} = \begin{pmatrix} -\frac{1}{2}P_{xy_1}P_{y_1z_1} & \cdots & -\frac{1}{2}P_{xy_m}P_{y_mz_1} \\ \vdots & \ddots & \vdots \\ -\frac{1}{2}P_{xy_1}P_{y_1z_n} & \cdots & -\frac{1}{2}P_{xy_m}P_{y_mz_n} \end{pmatrix},$$

and

$$\left(\Gamma_2(x)\right)_{S_2(x),S_2(x)} = \begin{pmatrix} \frac{1}{4}\sum_{y\in S_1(x)} P_{xy}P_{yz_1} & & 0 \\ & \ddots & \\ 0 & & \frac{1}{4}\sum_{y\in S_1(x)} P_{xy}P_{yz_n} \end{pmatrix}$$

The point is that $(\Gamma_2(x))_{S_2(x), S_2(x)}$ is diagonal and invertible!

Let $f: V \to \mathbb{R}$ be nonzero s.t. $\Gamma_2(f)(x) = K\Gamma(f)(x)$. 重写

Then we have $\dfrac{\vec{f}^T(\Gamma_2(x) - K\Gamma(x))\vec{f}}{\vec{f}^T\vec{f}} = 0 \Rightarrow$ $\vec{f}$ is an eigenvector of $\Gamma_2(x) - K\Gamma(x)$ to the zero eigenvalue

That is,

$$\begin{pmatrix} \Gamma_2(x)_{B_1(x), B_1(x)} - K\Gamma(x) & \Gamma_2(x)_{B_1(x), S_2(x)} \\ & \\ \Gamma_2(x)_{S_2(x), B_1(x)} & \Gamma_2(x)_{S_2(x), S_2(x)} \end{pmatrix} \begin{pmatrix} f(x) \\ f(y_1) \\ \vdots \\ f(y_m) \\ f(z_1) \\ \vdots \\ f(z_n) \end{pmatrix} = 0$$

Look at the last n linear equations, we have

$$\Gamma_2(x)_{S_2(x), B_1(x)} \begin{pmatrix} f(x) \\ f(y_1) \\ \vdots \\ f(y_m) \end{pmatrix} + \Gamma_2(x)_{S_2(x), S_2(x)} \begin{pmatrix} f(z_1) \\ \vdots \\ f(z_n) \end{pmatrix} = 0. \qquad (\ast\ast\ast)$$

Since $\Gamma_2(x)_{S_2(x), S_2(x)}$ is invertible, the values $\begin{pmatrix} f(z_1) \\ \vdots \\ f(z_n) \end{pmatrix}$ is uniquely determined by ~~that~~ the values $\begin{pmatrix} f(x) \\ f(y_1) \\ \vdots \\ f(y_m) \end{pmatrix}$. Moreover, this "determination" is irrelated to the number K!

<u>Lemma III.6.5</u>: Let $f: V \to \mathbb{R}$ be a nonzero function s.t.

$$\Gamma_2(f)(x) = K\Gamma(f)(x), \quad \text{for some } x \in V$$

Then $\vec{f}|_{S_2(x)}$ is uniquely determined by $\vec{f}|_{B_1(x)}$. More precisely, we have

$$\frac{f(x) + f(z)}{2} = \frac{\sum_{y \in S_1(x)} P_{xy} P_{yz} f(y)}{\sum_{y \in S_1(x)} P_{xy} P_{yz}}. \qquad (\star)$$

Proof. One only need to write out explicitly from $(\ast\ast\ast)$ that for any $z \in S_2(x)$, that

$$\left(\frac{1}{4}\sum_{y \in S_1(x)} P_{xy} P_{yz}\right) \cdot f(x) - \frac{1}{2}\sum_{y \in S_1(x)} f(y) P_{xy} P_{yz} + \left(\frac{1}{4}\sum_{y \in S_1(x)} P_{xy} P_{yz}\right) f(z) = 0. \quad \square$$

We next show certain eigenvalue sharpness also lead to similar consequence on distance function as in the case 重写 of diameter sharpness.

<u>Lemma III 6.6</u>. Let G satisfies $CD(K,\infty)$, $K>0$. Let K be an eigenvalue of Δ with eigenfunction φ, i.e. $\Delta\varphi + K\varphi = 0$.

Then (i) $\Gamma_2(\varphi)(x) = K\Gamma(\varphi)(x)$, $\forall x \in V$

(ii) $\Gamma(\varphi) \equiv \text{const}$.

<u>Proof</u>: Recall that

$$\langle \Gamma(f,g), \mathbb{1} \rangle = -\langle \Delta f, g \rangle \quad \forall f,g: V \to \mathbb{R}.$$

Then we have

$$K^2 \langle \varphi, \varphi \rangle = \langle K\varphi, K\varphi \rangle = \langle \Delta\varphi, \Delta\varphi \rangle = -\langle \Gamma(\varphi, \Delta\varphi), \mathbb{1} \rangle$$

$$= \langle \tfrac{1}{2}\Delta\Gamma(\varphi) - \Gamma(\varphi,\Delta\varphi), \mathbb{1} \rangle$$

$$= \langle \Gamma_2(\varphi,\varphi), \mathbb{1} \rangle \underset{CD(K,\infty)}{\geq} \langle K\Gamma(\varphi), \mathbb{1} \rangle = -K \langle \varphi, \Delta\varphi \rangle$$

$$= K^2 \langle \varphi, \varphi \rangle.$$

This forces $\langle \Gamma_2(\varphi) - K\Gamma(\varphi), \mathbb{1} \rangle = 0$. Since $\Gamma_2(\varphi)(x) - K\Gamma(\varphi)(x) \geq 0$ at any $x \in V$, we derive

$$\Gamma_2(\varphi)(x) = K\Gamma(\varphi)(x), \quad \forall x \in V.$$

Moreover, $K\Gamma(\varphi) = \Gamma_2(\varphi) = \frac{1}{2}\Delta\Gamma(\varphi) - \Gamma(\varphi, \Delta\varphi)$

$$= \tfrac{1}{2}\Delta\Gamma(\varphi) + K\Gamma(\varphi,\varphi)$$

$\Rightarrow \Delta\Gamma(\varphi) = 0$. $\Rightarrow \Gamma(\varphi) \equiv \text{const}$. since 0 is a simple eigenvalue of Δ on a finite graph. □

Combining Lemma III.6.6 and Lemma III 6.5 leads to the

<u>Lemma III 6.7</u>. Let G satisfy $CD(K,\infty)$, $K>0$, Let φ_1, φ_2 be eigenfcts to K, and $\varphi_1|_{B_1(x)} = \varphi_2|_{B_1(x)}$.

Then $\varphi_1 = \varphi_2$

<u>Proof</u>: By induction over spheres $S_k(x)$. □

A natural question is that: given $f: B_1(x) \to \mathbb{R}$ s.t. $\Delta f + Kf = 0$ at x, can we always extend it to be an eigenfunction of K?

<u>Lemma III.6.8</u>. (Extension). Let G satisfy $CD(K,\infty)$, $K>0$. Let $x\in V$ be a vertex. Suppose $\lambda_{d_x+1} = K$. Then for any $f: V\to\mathbb{R}$ with $\Delta f(x) + Kf(x) = 0$. at $x \in V$, there exists an eigenfunction φ to K s.t. $\varphi|_{B_1(x)} = f|_{B_1(x)}$.

<u>Proof</u>: Higher multiplicity means high dimension of eigenspace. Which ensure all local fcts (of finite dim) are restrictions of eigenfunctions.

Denote by $\Phi := \{\varphi : \Delta\varphi + K\varphi = 0\}$ eigenspace to K.

and $\Phi_{|B_1(x)} := \{\varphi|_{B_1(x)} : \Delta\varphi + K\varphi = 0\}$.

They are both linear spaces. Consider the linear map

$$\eta : \Phi \longrightarrow \Phi_{|B_1(x)}$$
$$\varphi \longmapsto \varphi|_{B_1(x)}.$$

So Lemma III.6.7 simply says η is injective, & $\dim(\Phi_{|B_1(x)}) \geq \dim\Phi$

The assumption $\lambda_{d_x} = K$ ensures $\dim\Phi \geq d_x$. Therefore,

$\dim\left(\Phi_{|B_1(x)}\right) \geq d_x$ $\langle 1 \rangle$

Notice that $\varphi_{|B_1(x)} \in \mathbb{R}^{|B_1(x)|} = \mathbb{R}^{d_x+1}$.

However $\Delta\varphi + K\varphi = 0$, $K>0$ tells φ is not const.

Hence, we have $\dim\left(\Phi_{|B_1(x)}\right) \leq d_x+1-1 = d_x$ $\langle 2 \rangle$

Combining $\langle 1 \rangle$ and $\langle 2 \rangle$ yields $\dim\left(\Phi_{|B_1(x)}\right) = d_x$.

$\therefore$ This forces $\dim \Phi = \dim\left(\Phi_{|B_1(x)}\right)$.

That is, η is an injective linear map between two linear spaces of the same dimension. $\Rightarrow$ η is surjective. $\square$

Rmk: Due to the injectivity of η, we have the multiplicity $K>0$ as an eigenvalue $\leq \min_{x\in V} d_x$

Lemma III.6.9: Let G satisfy $CD(K,\infty)$, $K>0$, and $x_0 \in V$ be a vertex. Suppose $\lambda_{d_{x_0}+1} = K$.

Then $\varphi(x) := d(x_0,x) - \frac{1}{K}$ is an eigenfunction to K.

In particular, we have $\Gamma_2(f_0) = K\Gamma(f_0)$ where $f_0(\cdot) := d(x_0,\cdot)$.

Proof: Let $\psi: V \to \mathbb{R}$ be the function such that

$$\psi(y) := d(x_0,y) + C, \quad \forall y \in V.$$

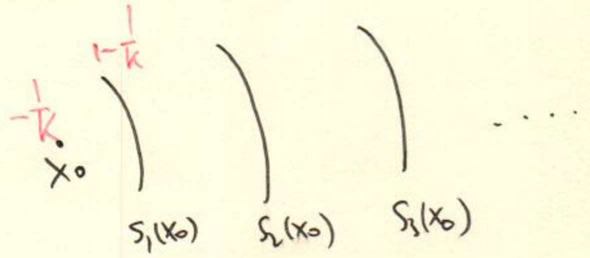
Then
$$\Delta\psi(x_0) = \frac{1}{d_{x_0}} \sum_{y: y\sim x_0} \left(\psi(y) - \psi(x_0)\right) = \frac{1}{d_{x_0}} \sum_{y:y\sim x_0} \left(1+C-C\right)$$
$$= 1$$

Therefore $\Delta\psi(x_0) + K\psi(x_0) = 1 + K\cdot C = 0$ if $C = \frac{-1}{K}$.

By Lemma III.6.8, $\exists$ an eigenfunct φ to K such that

$$\varphi|_{B_1(x_0)} = \psi|_{B_1(x_0)}. \quad \left(\text{Recall } \psi(x_0) = -\frac{1}{K},\ \psi(y) = 1-\frac{1}{K},\ \forall y \in S_1(x_0)\right)$$

By ($\star$) pp. 235, we know φ is uniquely determined by ~~satisfies~~ ($\star$) and $\psi|_{B_1(x_0)}$ at every $x \in V$.



In our case, $f(y) = 1-\frac{1}{K}$ $\forall y \in S_1(x_0)$

$$\forall z \in S_2(x_0): \quad \frac{\varphi(x_0)+\varphi(z)}{2} = \frac{\sum_{y\in S_1(x_0)} p_{x_0y}\, p_{yz}\, f(y)}{\sum_{y\in S_1(x_0)} p_{x_0y}\, p_{yz}}.$$

$$\Rightarrow \varphi(z) = 2\left(1-\frac{1}{K}\right) - \varphi(x_0) = 2 - \frac{2}{K} + \frac{1}{K} = 2 - \frac{1}{K}, \ \forall z \in S_2(x_0)$$

So one can easily show inductively, that φ is constant on each sphere $S_k(x_0)$, and $\varphi|_{S_k(x_0)} = k - \frac{1}{K}$.

That is, $\varphi(\cdot) = d(x_0,\cdot) - \frac{1}{K}$. $\square$

Let us summarize our results about diameter sharpness and eigenvalue sharpness from Lemma III 6.4 and Lemma III 6.9.

Theorem III.6.10 (Sharpness) Let G satisfy $CD(K,\infty)$, $K>0$

(i) If $\operatorname{diam}(G) = \frac{2}{K}$, then for any $x_0 \in V$ s.t. $\exists\, y_0 \in V$ satisfying $d(x_0,y_0) = \operatorname{diam}(G)$, we have

$$\Gamma_2(f_0) = K\Gamma(f_0), \quad f_0(\cdot) := d(x_0,\cdot).$$

(ii) If K is an eigenvalue of multiplicity r, then for any $x_0 \in V$ s.t. $d_{x_0} \le r$, we have

$$\Gamma_2(f_0) = K\Gamma(f_0), \quad f_0(\cdot) := d(x_0,\cdot).$$

Moreover, the fct $\varphi = f_0 - \frac{1}{K}$ satisfies $\Delta\varphi + K\varphi = 0$. $(\maltese)$.

Indeed, we have $(\maltese)$ is equivalent to $\Gamma_2(f_0) = K\Gamma(f_0)$.

Theorem III.6.11 Let $G=(V,E)$ satisfy $CD(K,\infty)$, $K>0$. ~~Let $x_0 \in V$ and $f_0 := d(x_0,\cdot)$.~~ Let $f_0 : V \to \mathbb{R}$ be any fct.

TFAE:

(i) $\Gamma_2(f_0) = K\Gamma(f_0)$

(ii) $f_0 = \varphi + C$ for a const C and an eigenfunction φ to K of Δ. (i.e. $\Delta\varphi + K\varphi = 0$).

Proof: (ii) $\Rightarrow$ (i). $\Gamma_2(f_0) = \Gamma_2(\varphi)$, $\Gamma(f_0) = \Gamma(\varphi)$.

Hence, it remains to show

$$\Gamma_2(\varphi) = K\Gamma(\varphi) \quad \text{for any } \varphi \text{ s.t. } \Delta\varphi + K\varphi = 0.$$

This is done in Lemma III 6.6)

(i) $\Rightarrow$ (ii). We first observe

$$-K\langle f_0, \Delta f_0\rangle = K\langle \Gamma(f_0), \mathbb{1}\rangle \overset{(i)}{=} \langle \Gamma_2(f_0), \mathbb{1}\rangle$$

$$= \langle \tfrac{1}{2}\Delta\Gamma(f_0) - \Gamma(f_0, \Delta f_0), \mathbb{1}\rangle = -\langle \Gamma(f_0,\Delta f_0), \mathbb{1}\rangle \qquad \text{◎}$$

$$= \langle \Delta f_0, \Delta f_0\rangle.$$

Let $\{\varphi_i\}$ be an orthonormal basis of eigenfunctions of Δ, s.t. $\Delta\varphi_i + \lambda_i\varphi_i = 0$, $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_N$

Then we have $f_0 = \sum_{i=1}^{N} \langle f_0, \varphi_i\rangle \varphi_i$

$$\text{LHS of ◎} = -K\langle f_0, \Delta f_0\rangle = -K\Big\langle \sum_i \langle f_0,\varphi_i\rangle\varphi_i, -\sum_j \langle f_0,\varphi_j\rangle \lambda_j \varphi_j\Big\rangle$$

$$= K\sum_i \lambda_i \langle f_0 \varphi_i\rangle^2$$

$$\text{RHS of ◎} = \Big\langle \sum_i \lambda_i \langle f_0,\varphi_i\rangle\varphi_i, \sum_j \lambda_j \langle f_0,\varphi_j\rangle\varphi_j\Big\rangle$$

$$= \sum_i \lambda_i^2 \langle f_0, \varphi_i\rangle^2$$

This leads to $\sum_i \lambda_i(\lambda_i - K)\langle f_0,\varphi_i\rangle^2 = 0.$

Recall that $\lambda_2 \geq K$ by Lichnerowicz estimate.

Therefore each summand $\lambda_i(\lambda_i - K)\langle f_0, \varphi_i\rangle^2$, $i \geq 2$ is nonnegative. (The first summand $\lambda_1(\lambda_1-K)\langle f_0, \varphi_1\rangle^2 = 0$)

This forces $\lambda_i(\lambda_i - K)\langle f_0, \varphi_i\rangle^2 = 0$, $\forall i = 2, \cdots, N$.

$\Rightarrow \langle f_0, \varphi_i\rangle = 0$, whenever $i = 2, \cdots, N$ and $\lambda_i \neq K$.

Therefore $f_0 = \varphi + C$ with $\Delta\varphi + K\varphi = 0$ and constant C. □

Rmk. Indeed, one can show (i) $\Leftrightarrow$ (ii) $\Leftrightarrow$ (iii) $\Leftrightarrow$ (iii') ; where

(iii) : $\Gamma(P_t f_0) = e^{-2Kt} P_t \Gamma(f_0)$ at $x_0 \in V$

(iii') : $\Gamma(P_t f_0) = e^{-2Kt} P_t \Gamma(f_0)$ at any $x \in V$.

We leave it as an exercise. □.

What is special for distance function?

For given $x_0 \in V$, we define $\qquad \frac{a_{zy}}{d_z} = \frac{1}{d_z}$ $z \sim y$

$$\forall z \in V, \quad d_-^{x_0}(z) := \sum_{d(y,x_0) < d(z,x_0)} p_{zy}$$

$$\forall z \in V \quad d_+^{x_0}(z) := \sum_{d(y,x_0) > d(z,x_0)} p_{zy}$$

Let us introduce the N-dim hypercube shell structure:

Def. (N-dim Hypercube shell structure HSS (N, x_0))

We say a graph $G = (V, E)$ has the Hypercube shell structure HSS (N, x_0) with dimension $N \in (0, \infty)$ w.r.t. $x_0 \in V$, if

(1) G is bipartite

(2) $d_-^{x_0}(x) = \frac{d(x_0, x)}{N}$, $\forall x \in V$.

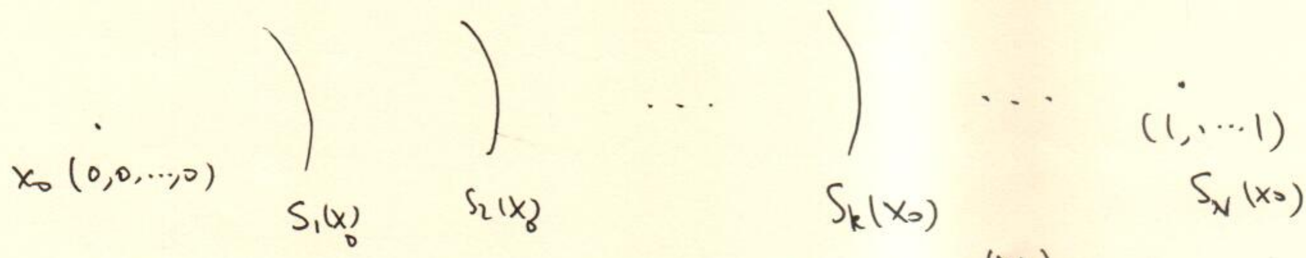
Why the name "hypercube"?

H^N is the graph with vertex set

$$V = \{(x_1, \dots, x_N) : x_i \in \{0,1\}\}$$

$$(x_1, \dots, x_N) \sim (y_1, \dots, y_N) \text{ iff } \sum_{i=1}^{N} |x_i - y_i| = 1.$$

For an N-hypercube, take $x_0 = (0, \dots, 0)$ for example,



$$|S_k(x_0)| = \binom{N}{k}$$

vertex degree $= N = \mathrm{diam}(H^N)$

What can we read from HSS (N, x_0)?

① G is bipartite $\Rightarrow$ $1 = d_-^{x_0}(x) + d_+^{x_0}(x)$.

By (1), we have $d_+^{x_0}(x) = \dfrac{N - d(x_0, x)}{N}$

② For $x \in S_1(x_0)$, (2) tells

$$\frac{1}{d_x} = d_-^{x_0}(x) = \frac{1}{N}, \text{ that is, } d_x = N, \ \forall x \in S_1(x_0).$$

③ We can determine the volume of each "shell" $S_k(x_0)$.

$$\left.\begin{array}{l} k=0, \quad \mathrm{vol}(\{x_0\}) = d_{x_0} \\ k=1, \quad \mathrm{vol}(S_1(x_0)) = d_{x_0} \cdot N \end{array}\right\} \Rightarrow \frac{\mathrm{vol}(S_1(x_0))}{\mathrm{vol}(S_0(x_0))} = N.$$

In general, we claim

$$\frac{\mathrm{vol}(S_{k+1}(x_0))}{\mathrm{vol}(S_k(x_0))} = \frac{N-k}{k+1}.$$