A 邻接矩阵. D, 度矩阵.

$L = D - A$. 拉普拉斯矩阵

$L_{sym} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$ 归一化拉普拉斯矩阵

谱图理论

1. L 和 L_{sym} 半正定

设 $G(i,j) = \begin{pmatrix} \ddots & & & \\ & 1 & -1 & \\ & -1 & 1 & \\ & & & \ddots \end{pmatrix}$ 第 (i,i), (j,j) 为 1，(i,j) (j,i) 为 -1

$$L = D - A = \sum^{n(i)} G(i,j)$$

$G(i,j)$ 的 (i,j) 和 (j,i) 与 $-A$ 相同，

其 (i,i) 与 (j,j) 的合为 D

$$\therefore \frac{\vec{x}^T L \vec{x}}{\vec{x}^T \vec{x}} = \frac{\vec{x}^T \sum^{n} G(i,j) \vec{x}}{\vec{x}^T \vec{x}}$$

$$= \vec{x}^T \begin{pmatrix} \vdots \\ x_i - x_j \\ x_j - x_i \\ \cdots \end{pmatrix} = x_i(x_i - x_j) - x_j(x_j - x_i)$$

$$= (x_i - x_j)^2 \geq 0$$

$\therefore$ 半正定

2. $L_{sym} \in [0,2]$

令 $G^{(2)}(i,j) = \begin{pmatrix} \ddots & & & \\ & 1 & 1 & \\ & 1 & 1 & \\ & & & \ddots \end{pmatrix}$

$$D+A = \sum^{n} G(i,j)$$

$$\frac{\vec{x}^T(D+A)\vec{x}}{\vec{x}^T\vec{x}} = \frac{\vec{x}^T(\sum G^{(2)}(i,j))\vec{x}}{\vec{x}^T\vec{x}}$$

$$\vec{x}^T(\sum G(i,j))\vec{x} = \vec{x}^T \begin{pmatrix} \vdots \\ x_i + x_j \\ x_j + x_i \\ \vdots \end{pmatrix} = (x_i + x_j)^2 \geq 0$$

$$(D+A)_{sym} = D^{-\frac{1}{2}}(D+A)D^{-\frac{1}{2}} = I + D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$$

$$= \sum\left(\frac{x_i}{\sqrt{d_i}} + \frac{x_j}{\sqrt{d_j}}\right)^2 \geq 0$$

$$\vec{x}^T(D+A)_{sym}\vec{x} = \sum\left(\frac{x_i}{\sqrt{d_i}} + \frac{x_j}{\sqrt{d_j}}\right)^2 \geq 0$$

$$\vec{x}^T(I + D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\vec{x} = \vec{x}^T\vec{x} + \vec{x}^T D^{-\frac{1}{2}}AD^{-\frac{1}{2}}\vec{x} \geq 0$$

$$2\vec{x}^T\vec{x} \geq \vec{x}^T\vec{x} - \vec{x}^T D^{-\frac{1}{2}}AD^{-\frac{1}{2}}\vec{x}$$

$$2\vec{x}^T\vec{x} \geq \vec{x}^T(I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\vec{x}$$

$$I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}} = L_{sym}$$

$$\therefore \frac{2\vec{x}^T\vec{x}}{\vec{x}^T\vec{x}} \geq \frac{\vec{x}^T(I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}})\vec{x}}{\vec{x}^T\vec{x}} \qquad \therefore 2 \geq L_{sym} \geq 0$$

$\therefore L_{sym} \in [0,2]$

图的卷积

$g_\theta * X = U g_\theta U^T X$ 其复杂度太高

所以改成 $g_\theta * X \approx \sum_{k=0}^{K} \theta_k T_k(\tilde{L}) X$

再近似成 $g_\theta * X \approx \theta(I + D^{-\frac{1}{2}} A D^{-\frac{1}{2}}) X$

$F(A) = L / L_{sym}$

$F(A) = U \Lambda U^T = L_{sym} - I$

$g_\theta * X = U g_\theta(\Lambda) U^T X = U(\sum T_k(\Lambda)) U^T X$

$= \sum_{k=0}^{K} \theta_k U T_k(\Lambda) U^T X = \sum_{k=0}^{K} \theta_k T_k(U \Lambda U^T) X$

$= \sum_{k=0}^{K} \theta_k T_k(L_{sym} - I) X$

$g_\theta(\Lambda) = \theta_0 \Lambda^0 + \theta_1 \Lambda^1 \cdots + \theta_n \Lambda^n$

$U g_\theta(\Lambda) U^T = g_\theta(U \Lambda U^T) = g_\theta(F(A))$

$(U \Lambda U^T)^k = U \Lambda U^T U \Lambda U^T \cdots U \Lambda U^T = U \Lambda^k U^T$

切比雪夫多项式 $T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$　　$T_0 = 1$

$T_n(\cos\theta) = \cos n\theta$　$[-1,1]$　　$T_1 = x$

$K = 2$

$$L_{sym} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

八、$g_\theta * x = \sum_{k=0}^{K} \theta_k T_k(-D^{-\frac{1}{2}} A D^{-\frac{1}{2}})x$

$$\approx \theta_0 T_0(L_{sym} - I)x + \theta_1 T_1(L_{sym} - I)x$$

$$= \theta_0 T_0 x - \theta_1 D^{-\frac{1}{2}} A D^{-\frac{1}{2}} x$$

令 $\theta_0 = -\theta_1$

$$= \theta_0 (I + D^{-\frac{1}{2}} A D^{-\frac{1}{2}})x$$

$\Downarrow$ 归一化

$$\hat{D}^{-\frac{1}{2}} \hat{A} \hat{D}^{-\frac{1}{2}} x$$

$\hat{D}, \hat{A}$ 为加上自环

八、快速卷积公式

$$H^{(l+1)} = f(H^{l}, A) = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}H^{(l)}W^{(l)})$$

广义到C个输入，即信号X和F个滤波器中，特征映射式子为

$$Z = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}X\Theta$$