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* Let W be the weight matrix and D be the diagonal matrix such that $D_{ii} = \sum_j w_{ij}$, let $P = D^{-1}W$ be random walk laplacian and let

$L_{sym} = D^{-0.5} W D^{-0.5}$ be normalized symmetric laplacian matrix.

Let $V = [v_1, \ldots, v_n]$ be eigenvectors of L_{sym}

=> Given $L_{sym} = V \Lambda V^T$, let $\Psi = D^{0.5} V$ and

$\Phi = D^{0.5} V$

prove the following

(i) The columns of Ψ and Φ form a biorthogonal system such that

$$\langle \psi_i, \phi_j \rangle = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

proof

=> For $\psi_i(s)$ solution we have the integral equation

$$\psi_i(s) = \lambda \int_a^b L_{sym}(s,t)\, \psi_i(t)\, dt$$

and similarly for $\phi_j(s)$ we have

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$$\phi_i(s) = \lambda \int_a^b L_{sym}(s,t)\, \phi_j(t)\, dt$$

=> Note that 2 systems ψ_i and ϕ_j form a biorthogonal system $\langle \psi_i, \phi_j \rangle$ if one-to-one correspondence can be established between them such that the integral of product of 2 corresponding functions is equal to unity otherwise is zero

=> Thus for a biorthogonal system $\langle \psi_i, \phi_j \rangle$ the function ψ_i, ϕ_j are linearly independent.

=> Now we suppose that there exist a linear relation such that

$$a_1\psi_1 + a_2\psi_2 + a_3\psi_3 + --- + a_n\psi_n = 0$$

=> We multiply the above by

$\phi_j \; (j = 1, 2, 3, ---, n)$ and integrating the function over the interval a to b we obtain

$$a_{ik} = \int \phi_i L_{sym} \phi_k \qquad \text{——— } (*)$$

=> Thus we have equation connecting $\{\psi_i\}$ and $\{\phi_i\}$ given as

$$P_i = \sum_{k=1}^{i} a_{ik} \psi_k \quad \text{and}$$

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$$\psi_i = \sum_{k=1}^{i} b_{ik} P_k \quad \text{--- (1)}$$

=> Multiplying eqn (1) by ϕ_j and integrating we get

$$\int \psi_i \phi_j = \sum_{k=1}^{i} b_{ik} \int P_k \phi_j$$

=> Substituting into (*) we have

$$\int \psi_i \phi_j = \sum_{k=1}^{i} b_{ik} a_{kj} \quad \text{--- (2)}$$

=> Now, since matrices (b_{ik}) and (a_{kj}) are inverses of each, ~~the~~ eqn (2) becomes

$$\int \psi_i \phi_j = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}$$

=> Since the 2 systems ψ_i and ϕ_j are an adjoint system of each other, we have the integral simplifying into

$$\langle \psi_i, \phi_j \rangle = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{"} \ i \neq j \end{cases}$$

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(ii) The vectors ψ_i are right eigenvectors of P while ϕ_i are left eigenvectors such that

$$P\psi_i = \lambda_i \psi_i \quad \text{and} \quad \phi_i^T P = \lambda_i \phi_i^T$$

Prouf

=) We consider the biorthogonal system $\langle \psi_i, \phi_j \rangle$ defined by the relation

$$\psi_i = \sum_{k=1}^{i} Z_k \quad \text{and} \quad \phi_j = Z_i - Z_{i+1}$$

=) Thus for a normalized symmetric Laplacian, we obtain a corresponding kernel matrix $K(s,t)$ defined by

$$K(s,t) = \sum_{i=1}^{\infty} \frac{\alpha_i(s)\,\alpha_i(t)}{1-\lambda_i}$$

whereby α_i is a sequence of constants such that $\frac{1}{\alpha_i}$ is a finite norm

=) Thus, above system simplifies into

$$\psi_i = \lambda_i Z_{2i-1} \quad \text{and} \quad \phi_j = \frac{Z_{2i-1} + \alpha_i Z_{2i}}{\lambda_i}$$

=) We note the biorthogonal system $\langle \psi_i, \phi_j \rangle$ has limited matrix $(a)_u$ and unlimited matrix $(b)_u$ and $(b)_v$

$\Rightarrow$ Therefore resulting mb

$$\psi_i = \frac{\lambda_i Z_{2i}}{\alpha_i} \quad \text{and} \quad \phi_j = \frac{Z_{2i-1} + \alpha_i Z_{2i}}{\lambda_i}$$

$$= \phi_j = \frac{\phi_j^T}{\lambda_j}$$

$\Rightarrow$ Note that Z_{2i} is a complete system of normalized biorthogonal function, simplifying further mb

$$\int \rho \psi_i = \frac{\lambda_i}{\alpha_i}$$

$\Rightarrow$ Multiplying the above relation with ψ_i and taking kernel matrix intergral from a to b we have

$$P\psi_i = \int_a^b \frac{\lambda_i \psi_i}{\alpha_i} \quad \text{with } \frac{1}{\alpha_i} = \alpha_i \quad \forall i = 1, 2, 3, --$$

$$\Rightarrow P\psi_i = \int_a^b \lambda_i \psi_i$$

$$= \underline{\underline{P\psi_i = \lambda_i \psi_i}}$$

$\Rightarrow$ Similarly for a complete $\{\phi_j\}$ of normalized biorthogonal function, we obtain a P function such that

$$\phi_j = \frac{P}{\sqrt{\int p^2}} \quad \text{for } \phi_{j+1}^T = \phi_j$$

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$\Rightarrow$ But from $\phi_j = \frac{\phi_j^T}{\lambda}$, we substitute into above equation to obtain

$$\frac{\phi_j^T}{\lambda} P = \phi_j = \phi_{j+1}^T$$

$$\Rightarrow \frac{\phi_j^T}{\lambda} P = \phi_{j+1}^T$$

for $i = j+1 \quad \forall i = 1, 2, 3, ---$

$\Rightarrow$ Therefore

$$\frac{\phi_i^T P}{\lambda_i} = \phi_i^T$$

$$\Rightarrow \phi_i^T P = \lambda_i \phi_i^T$$

i) We have diffusion distance between 2 points x_i, x_j and time t

$$\Delta_t (x_i, x_j) = \sum_k \frac{((P^t)_{ik} - (P^t)_{jk})^2}{D_{kk}}$$

We need to show that

$$\Delta_0 (x_i, x_j) = \frac{1}{D_{ii}} + \frac{1}{D_{jj}}$$

<u>Proof</u>

$\Rightarrow$ First we note that P_{ij}^t in componentwise is equivalent to

$$P^t_{ij} = \sum_{k=1}^{n} \phi_k(i)\,\psi_k(j)$$

=> Thus, we have that

$$\sum_k \left((P^t)_{ik} - (P^t)_{jk}\right)^2 = \sum_{L=1}^{n} \frac{\left[\sum_{k=1}^{n} \phi_k(i)\psi_k(L) - \phi_k(j)\psi_k(L)\right]^2}{D_{kk}}$$

$$= \sum_{L=1}^{n} \sum_{k,k'}^{n} \frac{(\phi_k(i) - \phi_k(j))\,\psi_k(L)\,(\phi_{k'}(i) - \phi_{k'}(j))\,\psi_{k'}(L)}{D_{kk}}$$

$$= \sum_{k,k'}^{n} (\phi_k(i) - \phi_k(j))(\phi_{k'}(i) - \phi_{k'}(j))\,\delta_{kk'}$$

$$\Rightarrow \sum_{k=1}^{n} (\phi_k(i) - \phi_k(j))^2 = \sum_{k=1}^{n} \phi_k(i)\phi_k(j) = (\phi\phi^T)_{ij} = \frac{1}{D_{ij}}$$

=> Thus, at time $t=0$, and $k=1$, we have that

$$\sum_{k=1}^{\omega} (\phi_k(i) - \phi_k(j))^2 = \frac{1}{D_{ii}} + \frac{1}{D_{jj}} + 0 \Rightarrow$$

$$\Rightarrow D_0(x_i, x_j) = \frac{1}{D_{ii}} + \frac{1}{D_{jj}}$$

(iv) prove that

$$\left| D_t(x_i, x_j) - \sum_{k=1}^{k} \left(\bar{\psi}_{k}(i) - \bar{\psi}_{k}(j)\right)^2 \right| \le \lambda_{k+1}^{2t} \left(\frac{1}{D_{ii}} + \frac{1}{D_{jj}} \right)$$

given that

$$D_t(x_i, x_j) = \sum_{k=1}^{n} \lambda_k^{2t} \left(\psi_k(i) - \psi_k(j)\right)^2 = \sum_{k} \bar{\psi}_k(i) - \bar{\psi}_k(j)^2$$

with

$$x_i \longrightarrow [\bar{\psi}_1(i), \ldots, \bar{\psi}_k(j)]$$

proof

$\Rightarrow$ First we write a corresponding componentwise equivalent of P_{ij}^t as

$$P_{ij}^t = \sum_{k=1}^{n} \lambda_k^t \, \phi_k(i) \, \psi_k(j)$$

Thus, we have

$$\sum_k \frac{\left((P^t)_{ik} - (P^t)_{jk}\right)^2}{D_{kk}} \quad \text{becoming}$$

$$\Rightarrow \sum_{l=1}^{n} \frac{\left[\sum_{k=1}^{n} \lambda_k^t \phi_k(i) \psi_k(l) - \lambda_k^t \phi_k(j) \psi_k(l) \right]^2}{D_{kk}}$$

$$\Rightarrow \sum_{l=1}^{n} \sum_{k,k'}^{n} \frac{\lambda_k^t \left(\phi_k(l) - \phi_k(j)\right) \psi_k(l) \, \lambda_{k'}^t \left(\phi_{k'}(i) - \phi_{k'}(j)\right) \psi_{k'}(l)}{D_{kk}}$$

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$$\Rightarrow \sum_{k,k'}^{n} \lambda_k^t \lambda_{k'}^t \left(\phi_k(i) - \phi_k(j)\right)\left(\phi_{k'}(i) - \phi_{k'}(j)\right) \sum_{i=1}^{n} \frac{\psi_k(l)\psi_{k'}(l)}{D_{kk}}$$

$$\Rightarrow \sum_{k=1}^{n} \lambda_{k+1}^{2t} \left(\phi_k(i) - \phi_k(j)\right)^2 = D_t^2(x_i, x_j)$$

$\Rightarrow$ Note that in practice we truncate diffusion map ϕ_t^δ that will make use of less coordinate system

$\Rightarrow$ This implies that ϕ_t^δ will use only eigenvectors for which its eigenvalues satisfy

$$|\lambda_k|^t > \delta$$

$\Rightarrow$ Thus, we have

$$\sum_{k=1}^{n} \phi_k(i) - \phi_k(j)^2 \leq \frac{2}{D_{min}} (1 - \delta_{ij}) \quad \forall i,j = 1,2,3,\dots,n$$

$\Rightarrow$ This simplifies into

$$\left[D_t^\delta(x_i, x_j)\right]^2 = D_t^2(x_i, x_j) - \sum_{k;\, |\lambda_k|^t < \delta} \lambda_{k+1}^{2t} \left(\phi_k(i) - \phi_k(j)\right)^2$$

$$\geq D_t^2(x_i, x_j) - \delta^2 \sum_{k=1}^{\infty} \left(\phi_k(i) - \phi_k(j)\right)^2$$

$$= D_t^2(x_i, x_j) \geq \frac{2\delta^2}{D_{min}} (1 - \delta_{ij}) \quad \text{where}$$

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$$\left[D_t^{\delta}(x_i, x_j)\right]^2 \leq D_t^2(x_i, x_j)$$

whereby

$$D_t^{\delta}(x_i, x_j) = \sum_{k=1}^{k}\left(\bar{\psi}_k(i) - \bar{\psi}_k(j)\right)^2$$

and

$$D_t^2(x_i, x_j) = \sum_{k=1}^{n} \lambda_{k+1}^{2t}\left(\phi_k(i) - \phi_k(j)\right)^2$$

From (iii) we know that

$$\sum_{k=1}^{n}\left(\phi_k(i) - \phi_k(j)\right)^2 = \frac{1}{D_{ii}} + \frac{1}{D_{jj}}$$

=> Thus, substituting into $D_t^2(x_i, x_j)$, we obtain

$$\Rightarrow D_t^2(x_i, x_j) = \sum_{k=1}^{n} \lambda_{k+1}^{2t}\left(\frac{1}{D_{ii}} + \frac{1}{D_{jj}}\right) \quad \text{———} \; (*)$$

=> Therefore for small δ, the truncated diffusion distance $D_t(x_i, x_j)$ in general is given by

$$\left|D_t(x_i, x_j) - D_t^{\delta}(x_i, x_j)\right| \leq D_t^2(x_i, x_j)$$

$$\Rightarrow \left|D_t(x_i, x_j) - \sum_{k=1}^{k}\left(\bar{\psi}_k(i) - \bar{\psi}_k(j)\right)^2\right| \leq \sum_{k=1}^{n} \lambda_{k+1}^{2t}\left(\phi_k(i) - \phi_k(j)\right)^2$$

=> Substituting (*) we have.

$$\left|D_t(x_i, x_j) - \sum_{k=1}^{k}\left(\bar{\psi}_k(i) - \bar{\psi}_k(j)\right)^2\right| \leq \lambda_{k+1}^{2t}\left(\frac{1}{D_{ii}} + \frac{1}{D_{jj}}\right) \quad \boxtimes$$

THANK YOU!!!