Commute Time:

$$CT(i,j) = H(i,j) + H(j,i)$$

- The *Commute time* $CT(i,j)$ on a graph is the expected time it takes a random walk to visit node j starting from node i and return.
- The *hitting time* $H(i,j)$ of a random walk on a graph is the expected time it takes to visit node j starting from node i.

The *commute time distance* can be expressed in terms of the *unnormalized* and *normalized* Laplacian.

- In terms of the eigen-system of the *unnormalized* Laplacian L:

$$CT(i,j) = \mathrm{vol}(V) \sum_{\alpha=2}^{|V|} \frac{1}{\lambda_\alpha} \left(v_{\alpha j} - v_{\alpha i} \right)^2 \tag{1}$$

- In terms of the eigen-system of the *normalized* Laplacian L_{sym}:

$$CT(i,j) = \mathrm{vol}(V) \sum_{\alpha=2}^{|V|} \frac{1}{\lambda_\alpha^{sym}} \left(\frac{v_{\alpha j}^{sym}}{\sqrt{D_{jj}}} - \frac{v_{\alpha i}^{sym}}{\sqrt{D_{ii}}} \right)^2 \tag{2}$$

Where $\mathrm{vol}(V) = \sum_i D_{ii}$ and $|V|$ denotes the cardinality of the set of nodes.

We can rewrite (1) and (2) in the following form:

- $$CT(i,j) = \sum_{\alpha=2}^{|V|} \left(\sqrt{\frac{\mathrm{vol}(V)}{\lambda_\alpha}} v_{\alpha j} - \sqrt{\frac{\mathrm{vol}(V)}{\lambda_\alpha}} v_{\alpha i} \right)^2$$

- $$CT(i,j) = \sum_{\alpha=2}^{|V|} \left(\sqrt{\frac{\mathrm{vol}(V)}{\lambda_\alpha^{sym} D_{jj}}} v_{\alpha j}^{sym} - \sqrt{\frac{\mathrm{vol}(V)}{\lambda_\alpha^{sym} D_{ii}}} v_{\alpha i}^{sym} \right)^2$$

The previous form express the CTD as Euclidean distances.

Commute time embedding:

Let Θ denote the new vector space that preserves the commute time distance of the nodes of the graph. The new coordinate matrix can be written:

- In terms of the *unnormalized* Laplacian L:

$$\Theta = \sqrt{vol(V)}\mathbf{\Lambda}^{-1/2}\mathbf{V}^T$$

- In terms of the *normalized* Laplacian L_{sym}:

$$\Theta_{sym} = \sqrt{vol(V)}\mathbf{\Lambda}_{L_{sym}}^{-1/2}\mathbf{V}_{L_{sym}}^T\mathbf{D}^{-1/2}$$

Let m denote the new dimension in the embedded space and n the dimension in the original space ($m < n$).

$\Rightarrow$ Θ and Θ_{sym} are $m \times n$ matrices, $\mathbf{\Lambda}$ and $\mathbf{\Lambda}_{sym}$ are $m \times m$ matrices and $\mathbf{V}$ and $\mathbf{V}_{sym}$ are $n \times m$ matrices.

Notice that the columns of Θ and Θ_{sym} are vectors of Cartesian co-ordinates.

Optimal embedding problem in terms of the unnormalized Laplacian (as defined in the paper)

The objective function:

$$\sum_{ij}(y_i - y_j)^2 W_{ij} \tag{3}$$

Which relates to the quadratic form of L:

$$\frac{1}{2}\sum_{ij}(y_i - y_j)^2 W_{ij} = \mathbf{y}'(D - W)\mathbf{y} = \mathbf{y}' L \mathbf{y}$$

The minimization problem can be reduced to finding a solution to:

$$\underset{y \in \mathbb{R}^n}{\arg\min} \quad \mathbf{y}' L \mathbf{y} \tag{4a}$$

$$\text{subject to} \quad \mathbf{y}' D \mathbf{y} = 1 \tag{4b}$$

$$\mathbf{y}' D \mathbb{1} = 0 \tag{4c}$$

The vector $\mathbf{y}$ that minimizes the objective function (4a) is given by the smallest eigenvalue solution of the generalized eigenvalue problem:

$$L\mathbf{y} = \lambda D\mathbf{y}$$

Recall:
λ is is an eigenvalue of L_{rw} with eigenvector y iff λ is an eigenvalue of L_{sym} with eigenvector $w = D^{1/2}y$.

$$\begin{aligned} L_{sym}\ w &= \lambda w \\ (D^{1/2} - D^{-1/2}W)y &= \lambda D^{1/2}y \\ (I - D^{-1}W)y &= \lambda y \\ L_{rw}\ y &= \lambda y \\ (D^{-1}L)y &= \lambda y \\ Ly &= \lambda Dy \end{aligned} \tag{5}$$

Optimal embedding problem in terms of the unnormalized Laplacian

The unnormalized version of the optimal embedding problem is given by minimizing the following objective function:

$$\begin{aligned} \underset{y \in \mathbb{R}^n}{\arg\min} \quad & \mathbf{y}' L \mathbf{y} && \text{(6a)} \\ \text{subject to} \quad & \mathbf{y}'\mathbf{y} = 1 && \text{(6b)} \\ & \mathbf{y}'\mathbb{1} = 0 && \text{(6c)} \end{aligned}$$

Notice that this formulation is not the Laplacian eigenmap. The solution to (6a) is associated to the standard eigenvalue problem:

$$L\mathbf{y} = \lambda \mathbf{y}$$

Optimal embedding problem in terms of the normalized Laplacian

Let $\mathbf{u} = D^{1/2}\mathbf{y}$. We can rewrite the objective function (3):

$$\sum_{ij}(y_i - y_j)^2 W_{ij} = \sum_{ij}\left(\frac{u_i}{\sqrt{D_{ii}}} - \frac{u_j}{\sqrt{D_{jj}}}\right)^2 W_{ij}$$

Which relates to the quadratic form of L_{sym}:

$$\frac{1}{2}\sum_{ij}\left(\frac{u_i}{\sqrt{D_{ii}}} - \frac{u_j}{\sqrt{D_{jj}}}\right)^2 W_{ij} = \mathbf{u}' L_{sym}\mathbf{u}$$

$$\begin{aligned} &\arg\min_{u\in\mathbb{R}^n} \quad \mathbf{u}' L_{sym}\mathbf{u} && \text{(7a)} \\ &\text{subject to} \qquad \mathbf{u}'\mathbf{u} = 1 && \text{(7b)} \\ &\qquad\qquad\qquad \mathbf{u}'(D^{1/2}\mathbb{1}) = 0 && \text{(7c)} \end{aligned}$$

The vector $\mathbf{u}$ that minimizes the objective function in (7a) is given by the smallest eigenvalue solution of the standard eigenvalue problem:

$$L_{sym}\mathbf{u} = \lambda\mathbf{u}$$

Notice that

$$\underset{\mathbf{y},\ \ \mathbf{y}'D\mathbf{y}=1;\ \ D\mathbf{y}\perp\mathbb{1}}{\arg\min}\ \mathbf{y}'L\mathbf{y} = \underset{\mathbf{u},\ \ \mathbf{u}'\mathbf{u}=1;\ \ \mathbf{u}\perp D^{1/2}\mathbb{1}}{\arg\min}\ \mathbf{u}'L_{sym}\mathbf{u}$$

Commute time embedding for the Normalized Laplacian L_{sym}
The new Cartesian coordinate of the i:th data points:

$$\mathbf{x}_i = \sqrt{\mathrm{vol}(V)/\lambda_\alpha D_{ii}} \quad \cdot [v_{2i}, v_{3i}, ..., v_{mi}]$$

and:

$$x_{i\alpha} = v_{\alpha i} \frac{\sqrt{\mathrm{vol}(V)}}{\sqrt{\lambda_\alpha D_{ii}}}, \qquad \alpha > 1$$

$v_{\alpha i}$ refers to the i:th component of the α eigenvector of L_{sym}.
The first eigenvector of L_{sym}:

$$v_{1i} = \frac{\sqrt{D_{ii}}}{vol(V)} \qquad \lambda_1 = 0$$

Statistical properties of the data point $x_{i\alpha}$

From the constraints (7b), (7c):

$$\begin{cases} \sum_i v_{\alpha i}\sqrt{D_{ii}} = 0, & \text{for} \quad \alpha > 1 \\ \sum_i v_{\alpha i}^2 = 1, & \text{for all} \quad \alpha \end{cases}$$

It follows that:

$$\sum_i v_{\alpha i}\sqrt{D_{ii}} = 0 \Rightarrow \sum_i x_{i\alpha}\left(\frac{D_{ii}}{\mathrm{vol}(V)}\right) = 0 = E[x_{i\alpha}] = \mu_\alpha \qquad (8)$$

$$\sum_i v_{\alpha i}^2 = 1 \Rightarrow E[X_{i\alpha}^2] - E[X_{i\alpha}]^2 = \sum_{i=1}^{n} x_{i\alpha}^2\left(\frac{D_{ii}}{\mathrm{vol}(V)}\right) = \frac{1}{\lambda_\alpha} \qquad (9)$$

Covariance Matrix

$$\Lambda_{\alpha\alpha'} = \sum_i x_{i\alpha} x_{i\alpha'} \left(\frac{D_{ii}}{\mathrm{vol}(V)} \right) = \sum_{i=1}^{n} \frac{v_{i\alpha} v_{i\alpha'}}{\sqrt{\lambda_\alpha \lambda_{\alpha'}}} = \frac{1}{\lambda_\alpha} \gamma_{\alpha\alpha'} \qquad (10)$$

$$\sum_i v_{\alpha i} v_{\alpha' i} = \gamma_{\alpha\alpha'} \quad \text{(orthonormal)}$$

$$\begin{cases} \gamma_{\alpha\alpha'} = 0, & \alpha \neq \alpha' \\ \gamma_{\alpha\alpha'} = 1, & \alpha = \alpha' \end{cases}$$

- Points are weighted by their degree.

Some questions to think about

- What is the meaning of the eigenvalues λ_α?
- What does it mean that the covariance matrix is diagonalized?
- How can we relate to Principal Component Analysis?

- The inverse of the eigenvalues correspond to the variance of the data points when we project to one of the axis.
- The variance is the inverse of the eigenvalues only if we are using Cartesian coordinates.
- From (10) it is clear that Λ is diagonalized given the orthogonality of the eigenvectors.
- The new Cartesian coordinates are uncorrelated and linearly independent (but not independent).
- The eigenvector space coincides with the Principal Components in the projected space.

Commute time embedding for the unnormalized Laplacian L

$$\mathbf{x}_i = \sqrt{\mathrm{vol}(V)/\lambda_\alpha} \;\; [v_{2i}, v_{3i}, \ldots, v_{mi}]$$

Meaning that for the α dimension

$$x_{i\alpha} = v_{i\alpha} \frac{\sqrt{\mathrm{vol}(V)}}{\sqrt{\lambda_\alpha}}, \qquad \alpha > 1$$

The first eigenvector of L:

$$v_{1i} = \frac{1}{\sqrt{|V|}}, \qquad \lambda_1 = 0$$

Statistical properties of the data point $x_{i\alpha}$

From the constraints (6b), (6c):

$$\begin{cases} \sum_i v_{i\alpha} = 0, & \text{for} \quad \alpha > 1 \\ \sum_i v_{i\alpha}^2 = 1, & \text{for all} \quad \alpha \end{cases}$$

it follows that:

$$\sum_i v_{i\alpha} = 0 \Rightarrow \sum_i x_{i\alpha} \left(\frac{1}{|V|} \right) = 0 = E[X_\alpha] = \mu_\alpha$$

$$\sum_i v_{i\alpha}^2 = 1 \Rightarrow E[X_\alpha^2] - E[X_\alpha]^2 = \sum_{i=1}^{n} x_{i\alpha}^2 \left(\frac{1}{|V|} \right) = \frac{1}{\lambda_\alpha} \frac{\mathrm{Vol(V)}}{|V|} \tag{11}$$

Covariance Matrix

$$\Lambda_{\alpha\alpha'} = \sum_i x_{i\alpha} x_{i\alpha'} \left(\frac{1}{|V|} \right) = \sum_{i=1}^{n} \frac{v_{i\alpha} v_{i\alpha'}}{\sqrt{\lambda_\alpha \lambda_{\alpha'}}} \frac{\mathrm{Vol(V)}}{|V|} = \frac{1}{\lambda_\alpha} \frac{\mathrm{Vol(V)}}{|V|} \gamma_{\alpha\alpha'}$$

- Each data point contributes equally, regardless of the degree distribution.
- The spread of the points non trivially depend on the number of nodes and volume.
- L_{sym} is much simpler.