Brain information flow

-Technical note

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Diffusion maps exploits the charactersistic of random walk Markov chain. The basic observation is that if we take a random walk on the data, walking to a nearby data-point is more likely than walking to another that is far away.

Given a dataset **X**, Define the probality of walking x to y in one step as:

$$k(x,y) = exp(-\frac{||x-y||^2}{\epsilon})$$

- $k(x,y) = k(y,x)$
- $k(x,y) \geq 0$
- captures the local geometry

markov chain
$d(x) = \int_{\mathbf{X}} k(x,y) d\mu(y)$
and define:

$$p(x,y) = \frac{k(x,y)}{d(x)}$$

not symmetric but positivity-preserving property
$\int_{\mathbf{X}} p(x,y) d\mu(y) = 1$

Diffusion pmrocess

Define the diffusion matirx L : $L_{i,j} = k(x_i, x_j)$, a version of graph laplacian matrix.
New kernel:

$$L_{i,j}^{\alpha} = k^(\alpha)(x_i, x_j) = \frac{L_{i,j}}{\left(d(x_i)d(x_j)\right)^{\alpha}}$$

or equivalently, $L(\alpha) = D^{-\alpha} L D^{-\alpha}$. After graph Laplacian normalization, we get transition matrix M.

$$p(x_j, t | x_i) = M_{i,j}^{t}$$

The eigendecomposition of the matrix M^t yields

$$M_{i,j}^{t} = \sum_{l} \lambda_l^t \psi_l(x_i) \phi_l(x_j)$$

Diffusion distance

The diffusion distance at time t:

$$D_t(x_i, x_j)^2 = \sum_y \frac{(p(y, t|x_i) - p(y, t|x_j)^2)}{\Phi_0(y)}$$

where $\phi_0(y)$ is stationary distribution of the markov chain, given by the first left eigenvector of M:

$$\phi_0(y) = \frac{d(y)}{\sum_{z \in \mathbf{X}} d(z)}$$

low dimension embedding
the eigenvectors can be used as a new set of coordinates, then the original data can be embedded into

$$\Psi_t(x) = \left(\lambda_1^t \psi_1(x), \lambda_2^t \psi_2(x), \ldots, \lambda_k^t \psi_k(x)\right)$$

The above diffusion distance is equal to Euclidean distance in the diffusion coordinates

$$\begin{aligned} D_t\left(x_i, x_j\right)^2 &= \left\|\Psi_t\left(x_i\right) - \Psi_t\left(x_j\right)\right\|^2 \\ &= \sum_l \lambda_l^{2t}\left(\psi_l\left(x_i\right) - \psi_l\left(x_j\right)\right)^2 \end{aligned}$$