Diffusion on Networks

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Physics of Diffusion

Diffusion is a spontaneus penetration of molecules of one type among molecules of the other type, from regions of higher concentration to the regions of lower concentration. Diffusion happens due to random motion of molecules

- Let $\Phi(r, t)$ -concentration
- Fik's Law
$$J = -D\frac{\partial \Phi}{\partial r} = -D\nabla\Phi$$
- Continuity equation (conserved quantity)
$$\frac{\partial \Phi}{\partial t} + \nabla J = 0$$
- Diffusion Equation
$$\frac{\partial \Phi(r, t)}{\partial t} = D\Delta\Phi(r, t)$$

Graph Laplacian

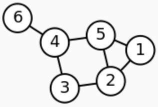
- $\Psi_i(t)$ - quantity per node

$$\Psi_i(t+1) = \Psi_i(t) + \sum_j A_{ij}(\Psi_j(t) - \Psi_i(t))C\delta t \quad (1)$$

$$\frac{d\Psi_i(t)}{dt} = C\sum_j A_{ij}(\Psi_j(t) - \Psi_i(t)) \quad (2)$$

$$\frac{d\Psi_i}{dt} = C\sum_j A_{ij}\Psi_j - C\sum_j A_{ij}\Psi_i = \quad (3)$$

$$= C\sum_j A_{ij}\Psi_j - Ck_i\Psi_i = C\sum_j (A_{ij} - \delta_{ij}k_j)\Psi_j = -C\sum_j L_{ij}\Psi_j \quad (4)$$

Labeled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2&0&0&0&0&0\\ 0&3&0&0&0&0\\ 0&0&2&0&0&0\\ 0&0&0&3&0&0\\ 0&0&0&0&3&0\\ 0&0&0&0&0&1 \end{pmatrix}$	$\begin{pmatrix} 0&1&0&0&1&0\\ 1&0&1&0&1&0\\ 0&1&0&1&0&0\\ 0&0&1&0&1&1\\ 1&1&0&1&0&0\\ 0&0&0&1&0&0 \end{pmatrix}$	$\begin{pmatrix} 2&-1&0&0&-1&0\\ -1&3&-1&0&-1&0\\ 0&-1&2&-1&0&0\\ 0&0&-1&3&-1&-1\\ -1&-1&0&-1&3&0\\ 0&0&0&-1&0&1 \end{pmatrix}$

Graph Laplacian

- Discrete Laplace operator

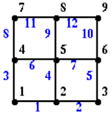
$$L_{ij} = k_j \delta_{ij} - A_{ij}$$
$$D_{ij} = k_j \delta_{ij}$$

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

- Laplacian

$$\Delta f = \nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial x^2}$$

$$\Delta f(x,y) = (f(x+h,y)+f(x-h,y)+f(x,y+h)+f(x,y-h)-4f(x,y))/h^2$$



	1	2	3	4	5	6	7	8	9
1	**2**	−1		−1					
2	−1	**3**	−1		−1				
3		−1	**2**			−1			
4	−1			**3**	−1		−1		
5		−1		−1	**4**	−1		−1	
6			−1		−1	**3**			−1
7				−1			**2**	−1	
8					−1		−1	**3**	−1
9						−1		−1	**2**

Diffusion on Graph

- Diffusion equation

$$\frac{d\mathbf{\Psi}}{dt} + C\mathbf{L}\mathbf{\Psi} = 0$$

- Eigenvector basis

$$\mathbf{L}\mathbf{v}_i = \lambda\mathbf{v}_i$$

$$\mathbf{\Psi}(t) = \sum a_i(t)\mathbf{v}_i$$

- ODE

$$\sum_i \left(\frac{da_i(t)}{dt} + c\lambda_i a_i(t) \right) \mathbf{v}_i = 0$$

$$\frac{da_i(t)}{dt} + c\lambda_i a_i(t) = 0$$

$$a_i(t) = a_i(0)e^{-C\lambda_i t}$$

- Solution

$$\mathbf{\Psi}(t) = \sum_i a_i(0)\mathbf{v}_i e^{-C\lambda_i t}$$

Laplace matrix

- Eigenvectors and eigenvalues

$$\mathbf{L}\mathbf{v}_i = \lambda \mathbf{v}_i, \lambda_i \geq 0$$

- smallest eigenvalue for $\mathbf{e} = [1, 1, 1...1]^T$

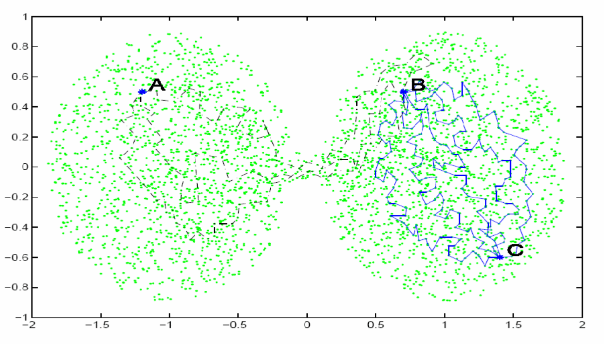
$$\mathbf{L}\mathbf{e} = (\mathbf{D} - \mathbf{A})\mathbf{e} = 0$$

- $\lambda_n \geq \lambda_{n-1} ... \geq \lambda_1 = 0$
- Solution $t \to \infty$

$$\mathbf{\Psi}(\infty) = a_1(0)\mathbf{v}_1 = const$$

Random walks on graph

- random walk - sequence of random steps, where on every node randomly select next to visit from nearest neighbours.
- directed and undirected graph
- can go along the same edge more then once
- visit nodes more then once



- Let $p_i(t)$ - probability, that a walk is at node i at moment t, $\sum_i p_i(t) = 1$
- $p_i(t)$ dependes on $p_j(t-1)$, where $j \in N(i)$
- Equation

$$p_i(t) = \sum_j p_j(t-1) A_{ji} \frac{1}{k_j}$$

- Let

$$D_{ij} = k_j \delta_{ij}$$

- Matrix form

$$\mathbf{p}(t) = (\mathbf{D}^{-1}\mathbf{A})^T \mathbf{p}(t-1)$$

- if $\lim_{t\to\infty} \mathbf{p}(t) = \pi$, then

$$\pi = (\mathbf{D}^{-1}\mathbf{A})^T \pi$$

Random walk on graphs

- Solution

$$(\mathbf{I} - \mathbf{D}^{-1}\mathbf{A})^T \pi = 0 \tag{5}$$
$$(\mathbf{D}^{-1}\mathbf{D} - \mathbf{D}^{-1}\mathbf{A})^T \pi = 0 \tag{6}$$
$$(\mathbf{D} - \mathbf{A})^T \mathbf{D}^{-1} \pi = 0 \tag{7}$$
$$\mathbf{L}^T \mathbf{D}^{-1} \pi = 0 \tag{8}$$

- if graph is undirected $\mathbf{L}^T = \mathbf{L}$, $\mathbf{L}\mathbf{v} = 0$, $\mathbf{v} = \mathbf{e}$, then

$$\mathbf{D}^{-1}\pi = \mathbf{e}$$

$$\pi = \mathbf{D}\mathbf{e}, \pi_i = k_i$$

- Stationary distribution (normalized $\sum_i \pi_i = 1$)

$$\pi_i = \frac{k_i}{2m}$$