

# Diffusion and random walks on graphs

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## Network Science



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- 1 Diffusions and random walks on graphs
- 2 Epidemics
- 3 Epidemics on networks
- 4 Information flow
- 5 Diffusion of innovations
- 6 Social influence
- 7 Segregation model
- 8 Link prediction
- 9 Node labeling
- 10 Time evolution of networks

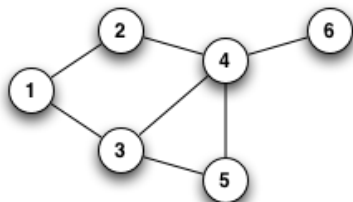
- 1 Random walks on graph
- 2 Diffusion on graph
  - Diffusion equation
  - Laplace operator
- 3 Spectral graph theory
  - Normalized laplacian

# Random walks on graph

- A random walk on graph  $G$  is a sequence of vertices  $v_0, v_1, \dots, v_t, \dots$ , where each  $v_{t+1}$  is chosen to be a random neighbor of  $v_t$ ,  $\{v_t, v_{t+1}\} \in E(G)$  and probability of the transition is given by

$$P_{ij} = P(x_{t+1} = v_j | x_t = v_i),$$

where  $\sum_j P_{ij} = 1$ , matrix  $P$  - row stochastic



# Random walks on graph

2D grid (k=2 regular graph)

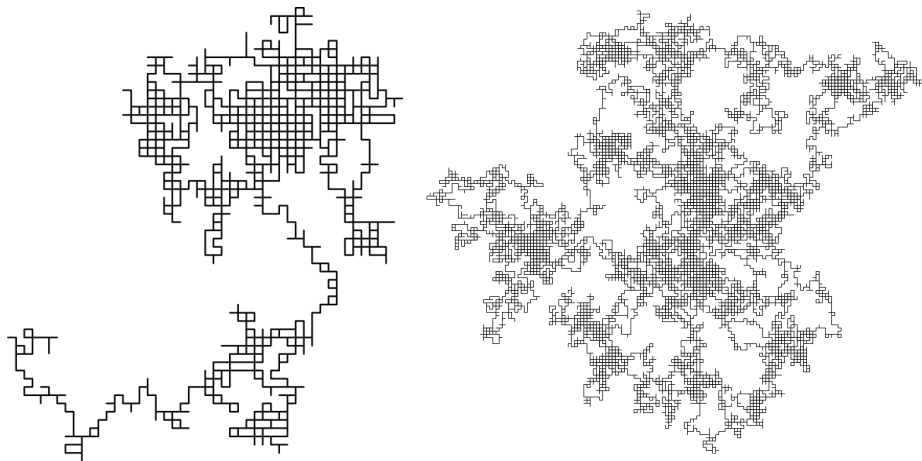


image from wikipedia.org

# Random walks on graph

- We will be considering undirected connected unweighted graphs
- Transition matrix

$$P_{ij} = \begin{cases} 1/d(i), & \text{if } \exists e(i,j), i \text{ and } j \text{ adjacent,} \\ 0 & \text{, otherwise} \end{cases}$$

- Using adjacency matrix

$$P_{ij} = \frac{A_{ij}}{d_i} = D_{ii}^{-1}A_{ij}, \text{ where } D_{ij} = d_i\delta_{ij}$$

- Let  $p_i(t)$  - probability, that a walk is at node  $i$  at moment  $t$  (probability distribution vector, value per node)
- Random walk

$$p_j(t+1) = \sum_i P_{ij}p_i(t) = \sum_i \frac{p_i(t)}{d_i}A_{ij}$$

- Matrix form

$$\vec{p}(t+1) = \vec{p}(t)\mathbf{P} = \vec{p}(t)(\mathbf{D}^{-1}\mathbf{A})$$

# Random walks on graph

- Starting from initial distribution  $\vec{p}(0)$  after  $t$  steps

$$\vec{p}(t) = \vec{p}(0)\mathbf{P}^t$$

- Random walk on connected non-bipartite graphs converges to limiting distribution

$$\lim_{t \rightarrow \infty} \vec{p}(t) = \lim_{t \rightarrow \infty} \vec{p}(0)\mathbf{P}^t = \vec{\pi}$$

- Limiting distribution = stationary distribution

$$\lim_{t \rightarrow \infty} \vec{p}(t+1) = \lim_{t \rightarrow \infty} \vec{p}(t)\mathbf{P}$$

$$\vec{\pi} = \vec{\pi}\mathbf{P}$$

- Left eigenvalue corresponding to  $\lambda = 1$

$$\lambda \vec{\pi} = \vec{\pi}\mathbf{P}$$

# Random walks on graph

- Random walk is reversible if

$$\pi_i P_{ij} = \pi_j P_{ji}$$

- On undirected graph:

$$\pi_i \frac{A_{ij}}{d_i} = \pi_j \frac{A_{ji}}{d_j}$$

$$\frac{\pi_i}{d_i} = \frac{\pi_j}{d_j} = \text{const}$$

and  $\sum_i \pi_i = 1$

- Stationary (stable) distribution

$$\pi_i = \frac{d_i}{\sum_j d_j} = \frac{d_i}{2|E|}$$



# Random walks on graph

- Lazy random walk

$$p_j(t+1) = \frac{1}{2}p_j(t) + \frac{1}{2} \sum_i \frac{p_i(t)}{d_i} A_{ij}$$

- Matrix form

$$\vec{p}(t+1) = \frac{1}{2}\vec{p}(t)(\mathbf{I} + \mathbf{D}^{-1}\mathbf{A})$$

- Converges (always!) to the same stationary distribution

$$(2\lambda - 1)\vec{\pi} = \vec{\pi}(\mathbf{D}^{-1}\mathbf{A})$$

## Theorem

Let  $\lambda_2$  denote second largest eigenvalue of transition matrix  $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$ ,  $\mathbf{p}(\mathbf{t})$  probability distribution vector and  $\boldsymbol{\pi}$  stationary distribution. If walk starts from the vertex  $i$ ,  $p_i(0) = 1$ , then after  $t$  steps for every vertex:

$$|p_j(t) - \pi_j| \leq \sqrt{\frac{d_j}{d_i}} \lambda_2^t$$

- For  $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$ ,  $\lambda_1 = 1$ ,  $\lambda_2 < 1$
- For  $\mathbf{P}' = \frac{1}{2}(\mathbf{I} + \mathbf{D}^{-1}\mathbf{A})$ ,  $\lambda'_2 = \frac{1}{2}(1 + \lambda_2)$

- Let  $\Phi(r, t)$  -concentration
- Fik's Law

$$J = -C \frac{\partial \Phi}{\partial r} = -C \nabla \Phi$$

- Continuity equation (conserved quantity)

$$\frac{\partial \Phi}{\partial t} + \nabla J = 0$$

- Diffusion equation ( heat equation)

$$\frac{\partial \Phi(r, t)}{\partial t} = C \Delta \Phi(r, t)$$

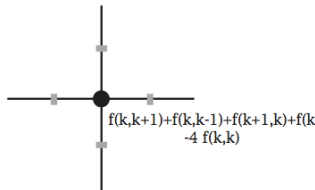
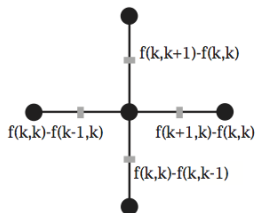
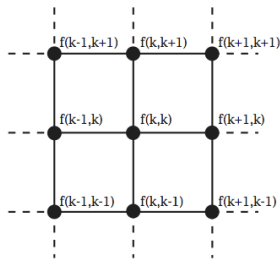
# Diffusion

- Laplacian 2D

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

- Discretized Laplacian in 2D

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



# Diffusion on network

- Some substance that occupy vertices, on each time step diffuses out  $\phi_i(t)$  - quantity per node

$$\phi_i(t+1) = \phi_i(t) + \sum_j A_{ij}(\phi_j(t) - \phi_i(t))C\delta t$$

$$\frac{d\phi_i(t)}{dt} = C \sum_j A_{ij}(\phi_j(t) - \phi_i(t))$$

$$\frac{d\phi_i}{dt} = C\left(\sum_j A_{ij}\phi_j - \sum_j A_{ij}\phi_i\right) = C\left(\sum_j A_{ij}\phi_j - d_i\phi_i\right) = C \sum_j (A_{ij} - \delta_{ij}d_j)\phi_j$$

$$\frac{d\phi_i}{dt} = -C \sum_j L_{ij}\phi_j$$

# Graph Laplacian

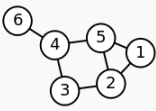
- Graph Laplacian

$$L_{ij} = d_j \delta_{ij} - A_{ij} = D_{ij} - A_{ij}, \quad D_{ij} = d_j \delta_{ij}$$

$$L_{ij} = \begin{cases} d(i), & \text{if } i = j, \\ -1, & \text{if } \exists e(i, j) - i \text{ and } j \text{ adjacent,} \\ 0, & \text{otherwise} \end{cases}$$

- Matrix form

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

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

# Diffusion on Graph

- Diffusion equation

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

- Eigenvector basis

$$\mathbf{L}\mathbf{v}_k = \lambda_k\mathbf{v}_k$$

$$\phi(t) = \sum_k a_k(t)\mathbf{v}_k, \quad a_k(t) = \phi(t)^T \mathbf{v}_k$$

- ODE

$$\sum_k \left( \frac{da_k(t)}{dt} + C\lambda_k a_k(t) \right) \mathbf{v}_k = 0$$

$$\frac{da_k(t)}{dt} + C\lambda_k a_k(t) = 0$$

$$a_k(t) = a_k(0)e^{-C\lambda_k t}$$

- Solution

$$\phi(t) = \sum_k a_k(0)\mathbf{v}_k e^{-C\lambda_k t}$$

- $\mathbf{L}$  - symmetric positive semidefinite

$$\phi^T \mathbf{L} \phi = \sum_{ij} L_{ij} \phi_i \phi_j = \sum_{ij} (d_i \delta_{ij} - A_{ij}) \phi_i \phi_j = \frac{1}{2} \sum_{ij} A_{ij} (\phi_i - \phi_j)^2$$

- Spectral properties

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

- real non-negative eigenvalues  $\lambda_i \geq 0$  and orthogonal eigenvectors  $\mathbf{v}_i$
- smallest eigenvalue always  $\lambda_1 = 0$  for  $\mathbf{v}_1 = \mathbf{e} = [1, 1, 1, \dots, 1]^T$

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

- Number of zero eigenvalues = number of connected components
- In connected graph  $\lambda_2 \neq 0$  - algebraic connectivity of a graph (spectral gap),  $\mathbf{v}_2$  - Fiedler vector



- Solution

$$\phi(t) = \sum_k a_k(0) \mathbf{v}_k e^{-C\lambda_k t}$$

- all  $\lambda_i > 0$  for  $i > 1$ ,  $\lambda_1 = 0$ :

$$\lim_{t \rightarrow \infty} \phi(t) = a_1(0) \mathbf{v}_1$$

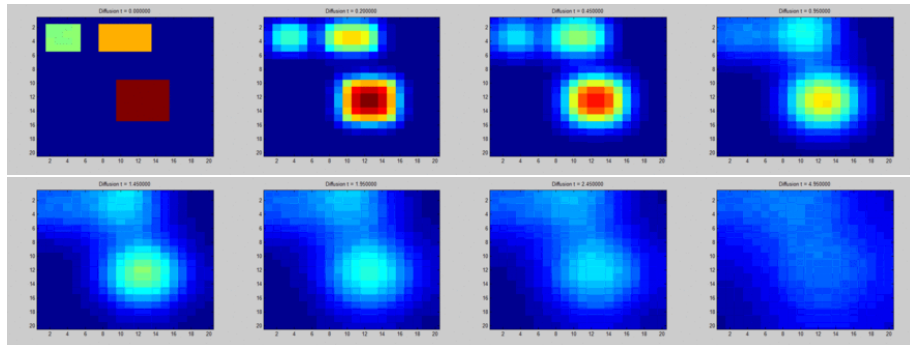
- Normalized solution  $\mathbf{v}_1 = \frac{1}{\sqrt{N}} \mathbf{e}$

$$a_1(0) = \phi(0)^T \mathbf{v}_1 = \frac{1}{\sqrt{N}} \sum_j \phi_j(0)$$

- Steady state

$$\lim_{t \rightarrow \infty} \phi(t) = \left( \frac{1}{N} \sum_j \phi_j(0) \right) \mathbf{e} = \text{const}$$

# Diffusion on Graph



- Smoothing operator

$$(L\phi)_i = \sum_j (D_{ij} - A_{ij})\phi_j = \sum_j (d_i\delta_{ij}\phi_j - A_{ij}\phi_j) = d_i(\phi_i - \frac{1}{d_i} \sum_j A_{ij}\phi_j)$$

- Laplace equation  $\nabla\phi = 0$ ,  $(L\phi)_i = 0$ , solution - harmonic function

$$\phi_i = \frac{1}{d_i} \sum_j A_{ij}\phi_j$$

- Regression on graphs

- Normalized Laplacian

$$\mathcal{L} = D^{-1/2} L D^{-1/2}$$

$$\mathcal{L}_{ij} = \begin{cases} 1 & , \text{ if } i = j, \\ -\frac{1}{\sqrt{d_i d_j}} & , \text{ if } \exists e(i, j) - i \text{ and } j \text{ adjacent,} \\ 0 & , \text{ otherwise} \end{cases}$$

- Connection to random walks:

$$P = D^{-1} A = D^{-1/2} (I - \mathcal{L}) D^{1/2}$$

Similar matrices, share properties of represented linear operators, i.e. eigenvalues:  $\lambda_{\max}(P) = 1$ ,  $\lambda_1(\mathcal{L}) = 0$ .

- Conductance of a vertex set  $S$

$$\phi(S) = \frac{\text{cut}(S, V \setminus S)}{\min(\text{vol}(S), \text{vol}(V \setminus S))}$$

where  $\text{vol}(S) = \sum_{i \in S} k_i$  - sum of all node degrees in the set

- Cheeger's inequality

$$\lambda_2(\mathcal{L})/2 \leq \min_S \phi(S) \leq \sqrt{2\lambda_2(\mathcal{L})}$$

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