# Diffusion and random walks on graphs

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**Structural Analysis and Visualization of Networks**

# Module 4

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

# Lecture outline

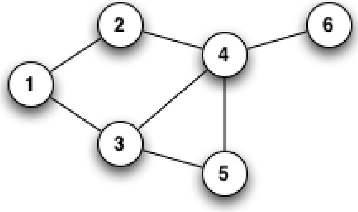
1. Random walks on graph
2. Diffusion on graph
   - Diffusion equation
   - Laplace operator
3. Spectral graph theory
   - Normalized laplacian

# Random walks on graph

- A random walk on graph on graph $G$ is a sequence of vertices $v_0, v_1, ...v_t..$, 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)

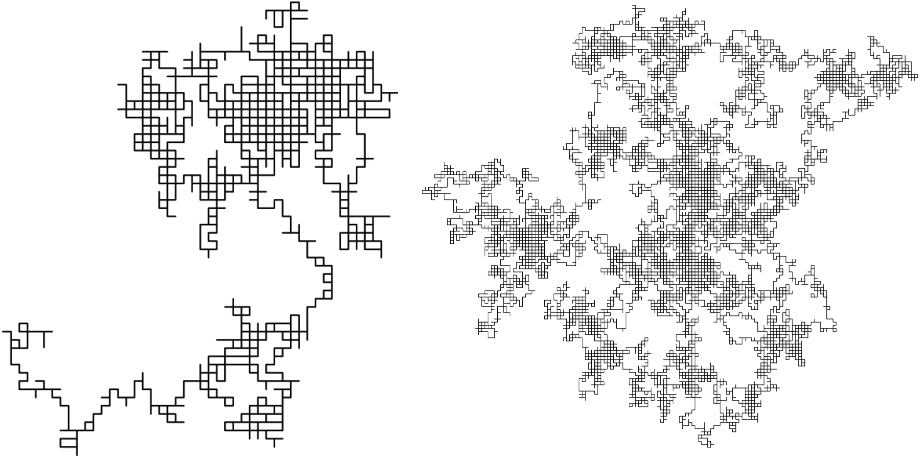


image from wikipedia.org

# 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

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

# Random walks on graph

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

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

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

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

- Limiting distribution = stationary distribution

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

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

- Left eigenvalue corresponding to $\lambda = 1$

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

# Random walks on graph

- Random walk is reversible if

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

- On undirected graph:

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

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

  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

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

- Converges (always!) to the same stationary distribution

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

# Random walks on graph

**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 $\mathbf{P}' = \frac{1}{2}(\mathbf{I} + \mathbf{D}^{-1}\mathbf{A})$, $\lambda_2' = \frac{1}{2}(1 + \lambda_2)$

# Physics of Diffusion

- 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)

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

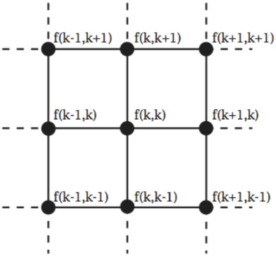
# Diffusion

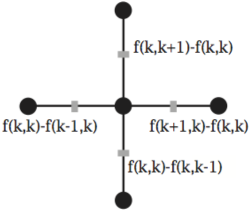
- Laplacian 2D

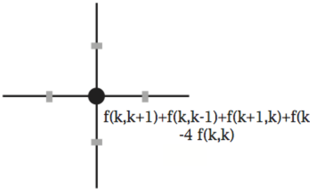
$$\Delta f = \nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

- 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

$$\begin{aligned}\phi_i(t+1) &= \phi_i(t) + \sum_j A_{ij}(\phi_j(t) - \phi_i(t))C\delta t \\ \frac{d\phi_i(t)}{dt} &= C\sum_j A_{ij}(\phi_j(t) - \phi_i(t))\end{aligned}$$

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

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

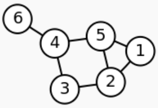
- Graph Laplacian

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

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

- 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

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

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

- 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

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

# Laplace matrix

- **L** - symmetric positive semidefinite

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

- 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 $\mathbf{v}_1 = \mathbf{e} = [1, 1, 1...1]^T$

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

- 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

# Diffusion on Graph

- Solution

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

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

$$\lim_{t\to\infty} \phi(t) = a_1(0)\mathbf{v_1}$$

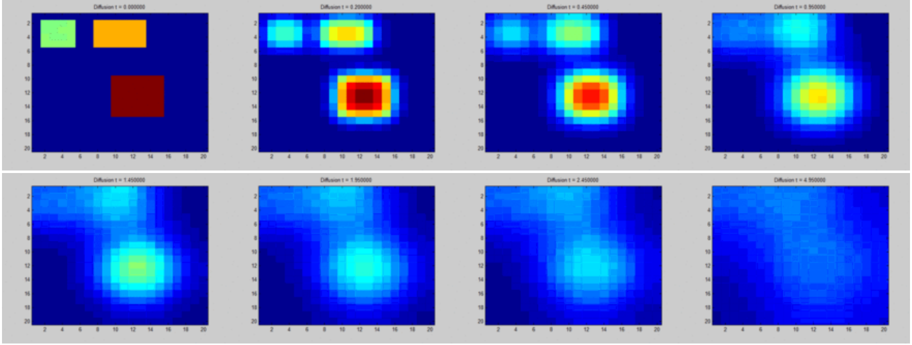
- Normalized solution $\mathbf{v}_1 = \frac{1}{\sqrt{N}}\mathbf{e}$

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

- Steady state

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

# Diffusion on Graph



# Smoothing operator

- 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

- 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: $\lambda_{max}(P) = 1$, $\lambda_1(\mathcal{L}) = 0$.

# Normalized Laplacian

- Conductance of a vertex set $S$

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

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

- Cheeger's inequality

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

# References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- Lovasz, L. (1993). Random walks on graphs: a survey. In Combinatorics, Paul Erdos is eighty (pp. 353 – 397). Budapest: Janos Bolyai Math. Soc.