Diffusion and random walks on graphs

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Lecture outline

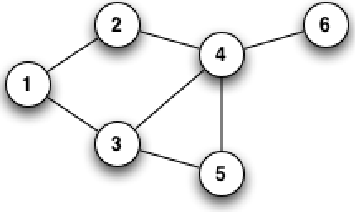
1. Random walks on graph
2. Diffusion on graph
   - Diffusion equation
   - Laplace operator
3. Spectral graph theory
   - Normalized laplacian

Random walks on graph

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

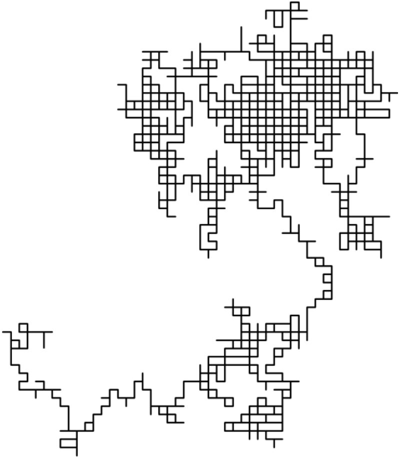
$$P_{ij} = P(x_{t+1} = v_j | x_t = v_i),$$

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



Random walks on graph

2D grid (k=2 regular graph)



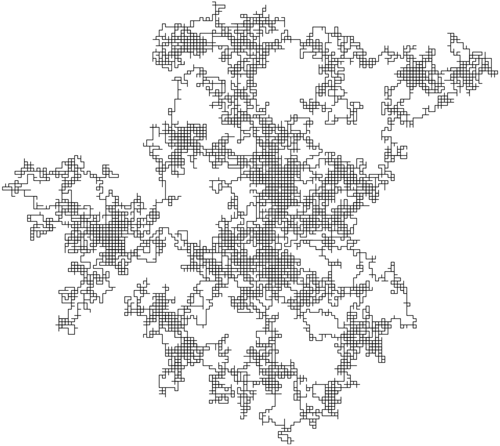


image from wikipedia.org

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 λ_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

Diffusion is the movement of a substance down a concentration gradient.
"to diffuse" = "to spread out"

- Let $\Phi(r, t)$ -concentration
- Fick'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)

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

Δ - Laplacian operator

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

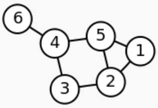
- Graph Laplacian

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

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

- 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

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

- 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

- $\mathbf{L}$ - 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

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

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

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

- 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 $i > 1$, $\lambda_1 = 0$:

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

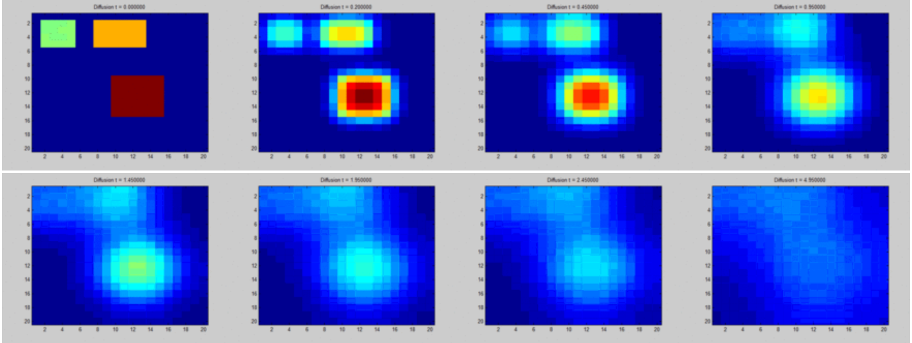
- Normalized solution $\mathbf{v_1} = \frac{1}{\sqrt{N}}\mathbf{e}$

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

- 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 $\nabla\phi = 0$, $\quad (L\phi)_i = 0$, 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 represents the same linear transformations in different basis and 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.