Paths and Random Walks on Graphs

Based on materials by Lala Adamic and Purnamrita Sarkar
Motivation: Link prediction in social networks
Motivation: Basis for recommendation

These recommendations are based on items you own and more.

1. **One Thousand Exercises in Probability**
   by Geoffrey R. Grimmett, David R. Stirzaker
   Average Customer Review: ★★★★★
   In Stock:
   Publication Date: August 2, 2001
   *Our Price: $53.95*
   Used & new from $42.74
   
   I Own It  Not interested  ★★★★★  Rate it
   Recommended because you purchased *Probability and Random Processes* (edit)

2. **The Elements of Statistical Learning**
   by T. Hastie, et al.
   Average Customer Review: ★★★★★
   In Stock:
   Publication Date: July 30, 2003
   *Our Price: $64.76*
   Used & new from $55.00
   
   I Own It  Not interested  ★★★★★  Rate it
Motivation: Personalized search

Where Are My Car Keys?
Why graphs?

• The underlying data is naturally a graph
  – Papers linked by citation
  – Authors linked by co-authorship
  – Bipartite graph of customers and products
  – Web-graph
  – Friendship networks: who knows whom
What are we looking for

- Rank nodes for a particular query
  - Top k matches for “Random Walks” from Citeseer
  - Who are the most likely co-authors of “Manuel Blum”.
  - Top k book recommendations for Jen from Amazon
  - Top k websites matching “Sound of Music”
  - Top k friend recommendations for Bob when he joins “Facebook”
History: Graph theory

- Euler’s **Seven Bridges of Königsberg** – one of the first problems in graph theory
- Is there a route that crosses each bridge only once and returns to the starting point?


Eulerian paths

- If starting point and end point are the same:
  - only possible if no nodes have an odd degree
  - each path must visit and leave each shore
- If don’t need to return to starting point
  - can have 0 or 2 nodes with an odd degree

- Eulerian path: traverse each edge exactly once
- Hamiltonian path: visit each vertex exactly once
Node degree from matrix values

- Outdegree = \( \sum_{j=1}^{n} A_{ij} \)
  
  - Example: outdegree for node 3 is 2, which we obtain by summing the number of non-zero entries in the 3rd row.

- Indegree = \( \sum_{i=1}^{n} A_{ij} \)
  
  - Example: the indegree for node 3 is 1, which we obtain by summing the number of non-zero entries in the 3rd column.

\[
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 \\
0 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 \\
0 & 1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0
\end{bmatrix}
\]
Definitions

• **n x n Adjacency matrix A.**
  – A(i,j) = weight on edge from i to j
  – If the graph is undirected A(i,j)=A(j,i), i.e. A is symmetric

• **n x n Transition matrix P.**
  – P is row stochastic
  – P(i,j) = probability of stepping on node j from node i
    = A(i,j)/∑iA(i,j)

• **n x n Laplacian Matrix L.**
  – L(i,j)=∑iA(i,j)-A(i,j)
  – Symmetric positive semi-definite for undirected graphs
  – Singular
Definitions

Adjacency Matrix

\[
A = \begin{bmatrix}
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
\end{bmatrix}
\]

Transition Matrix

\[
P = \begin{bmatrix}
1/3 & 1/3 & 1/3 \\
1/2 & 1/2 & \cdot \\
1/4 & 1/4 & 1/4 & 1/4 \\
1/3 & 1/3 & 1/3 & \cdot \\
1/2 & 1/2 & \cdot & \cdot \\
\end{bmatrix}
\]

Definitions

Graph Laplacian

\[ L = D - A \]

\[ D = \text{diag}(d) \]
Spectral Graph Analysis

Graph Laplacian

\[
L = D - A \\
D = \text{diag}(d)
\]

Take the eigendecomposition of \( L \)

\[
L = Q \Lambda Q^T
\]
Eigenvectors

• Intuitive definition: An eigenvector is a direction for a matrix

• An eigenvector of an $n \times n$ matrix $A$ is a vector such that $Av = \lambda v$, where $v$ is the eigenvector and $\lambda$ is the corresponding eigenvalue
  – Multiplying vector $v$ by the scalar $\lambda$ effectively stretches or shrinks the vector

• An $n \times n$ matrix should have $n$ linearly independent eigenvectors
Eigenvectors Illustrated

- Consider an elliptical data cloud. The eigenvectors are then the major and minor axes of the ellipse.
### Spectral Graph Analysis

\[ L = Q \Lambda Q^T \]

**Eigenvalue** $\lambda_1 = 0$

**Eigenvector** $q_1$ is constant

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Spectral Graph Analysis

\[ L = Q \Lambda Q^T \]

\( Q = \begin{bmatrix} q_1 & q_2 & q_3 & q_4 & q_5 \end{bmatrix} \)

\( \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\
0 & \lambda_2 & 0 & 0 & 0 \\
0 & 0 & \lambda_3 & 0 & 0 \\
0 & 0 & 0 & \lambda_4 & 0 \\
0 & 0 & 0 & 0 & \lambda_5 \end{bmatrix} \)

\( Q^T = \begin{bmatrix} q_1^T \\
q_2^T \\
q_3^T \\
q_4^T \\
q_5^T \end{bmatrix} \)
Random Walks

Adjacency matrix $A$

\[
\begin{pmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 1 & 0 \\
\end{pmatrix}
\]

Transition matrix $P$

\[
\begin{pmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1/2 & 1/2 & 0 \\
\end{pmatrix}
\]
What is a random walk

$t=0$
What is a random walk

t=0

1/2 1 1
1 1/2

1/2

1/2 1
1 1/2

1

1/2

1/2 1
1 1/2

1

1/2
What is a random walk

$t=0$

$t=1$

$t=2$
What is a random walk
Probability Distributions

• \( \phi_i^{(t)} = \) probability that the surfer is at node \( i \) at time \( t \)

• \( \phi_i^{(t+1)} = \sum_j \phi_i^{(t)} \times \Pr(j \rightarrow i) \)

• \( \phi_i^{(t+1)} = \phi_i^{(t)} \times P \)
  = \( \phi_i^{(t-1)} \times P \times P \)
  = \( \phi_i^{(t-2)} \times P \times P \times P \)
  \( \vdots \)
  = \( \phi_i^{(0)} \times P^t \)

• What happens when the surfer walks for a long time?
Stationary Distribution

• When the surfer keeps walking for a long time

• When the distribution does not change anymore – i.e. \( \phi(t+1) = \phi(t) \)

• For “well-behaved” graphs this does not depend on the start distribution!!
What is a stationary distribution?
Intuitively and Mathematically
What is a stationary distribution?

**Intuitively** and Mathematically

- The stationary distribution at a node is related to the amount of time a random walker spends visiting that node.
What is a stationary distribution? Intuitively and Mathematically

• The stationary distribution at a node is related to the amount of time a random walker spends visiting that node.

• Remember that we can write the probability distribution as

\[
\phi^{(t+1)} = \phi^{(t)} \times P
\]
What is a stationary distribution? Intuitively and Mathematically

• The stationary distribution at a node is related to the amount of time a random walker spends visiting that node.

• Remember that we can write the probability distribution as

\[ \phi^{(t+1)} = \phi^{(t)} \times P \]

• For the stationary distribution \( \phi^{(\infty)} \) we have

\[ \phi^{(\infty)} = \phi^{(\infty)} \times P \]
What is a stationary distribution? Intuitively and Mathematically

• The stationary distribution at a node is related to the amount of time a random walker spends visiting that node.

• Remember that we can write the probability distribution as
  \[ \phi(t+1) = \phi(t) \times P \]

• For the stationary distribution \( \phi(\infty) \) we have
  \[ \phi(\infty) = \phi(\infty) \times P \]

• Whoa! that’s just the left eigenvector of the transition matrix!
Power Method
(Horn & Johnson, 1985)

• P has a unique left eigenvector $\phi^{(\infty)}$
  – Called the Perron vector

Power method to compute $\phi^{(\infty)}$

1: set $\phi^{(0)}$ to be a normalized nonnegative random vector
2: set $i = 0$
3: loop until $\phi^{(0)}, \phi^{(1)}, \ldots, \phi^{(i-1)}, \phi^{(i)}$ converges
4: set $\phi^{(i+1)} = P\phi^{(i)}$
5: normalize $\phi^{(i+1)}$
6: $i++$
7: end loop
8: return $\phi^{(i)}$
Interesting Questions

• Does a stationary distribution always exist? Is it unique?
  – Yes, if the graph is “well-behaved”.
Well-behaved graphs

- **Irreducible**: There is a path from every node to every other node.
Well-behaved graphs

- **Aperiodic**: The GCD of all cycle lengths is 1. The GCD is also called period.

Periodicity is 3  Aperiodic
Implications of the Perron Frobenius Theorem

• If a Markov chain is irreducible and aperiodic then the **largest eigenvalue of the transition matrix** will be equal to **1** and all the other eigenvalues will be **strictly less than 1**.

  – Let the eigenvalues of P be \( \{ \sigma_i \mid i=0:n-1 \} \) in non-increasing order of \( \sigma_i \).

  – \( \sigma_0 = 1 > \sigma_1 > \sigma_2 \geq \ldots \geq \sigma_n \)
Implications of the Perron Frobenius Theorem

• If a Markov chain is irreducible and aperiodic then the largest eigenvalue of the transition matrix will be equal to $1$ and all the other eigenvalues will be strictly less than $1$.
  – Let the eigenvalues of $P$ be $\{\sigma_i| i=0:n-1\}$ in non-increasing order of $\sigma_i$.
  – $\sigma_0 = 1 > \sigma_1 > \sigma_2 >= \ldots >= \sigma_n$

• These results imply that for a well-behaved graph there exists an unique stationary distribution.
Google’s PageRank

• PageRank is a “vote” by all other webpages about the importance of a page
• A link to a page counts as a vote of support
• PageRank uses a random surfer model
  – Occasionally, the surfer gets bored and jumps to a random other page

• “The 25,000,000,000 Eigenvector: the Linear Algebra Behind Google”
Random Walk on Web Graph

• Probability transition matrix given by

\[ P_{u,v} = \frac{A_{u,v}}{d_u^{\text{out}}} = \frac{A_{u,v}}{\sum_{v=1}^{n} A_{u,v}} \]

\[ P = D^{-1} A \]

• Use a teleporting random walk (Page et al., 1998) to ensure that the graph is strongly connected and aperiodic:

\[ P_{\text{teleport}} = \eta P + (1 - \eta) \frac{11^T - I}{|V|} \]