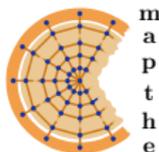


# $M$ -matrices and Randow Walks



M. J. Jiménez

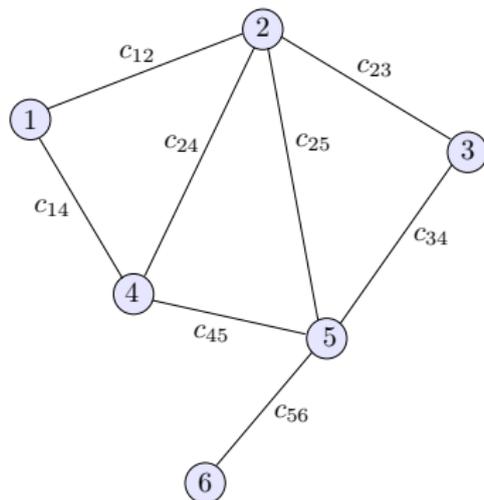
## IV Jornadas ALAMA: Laplacian and $M$ -matrices in graphs



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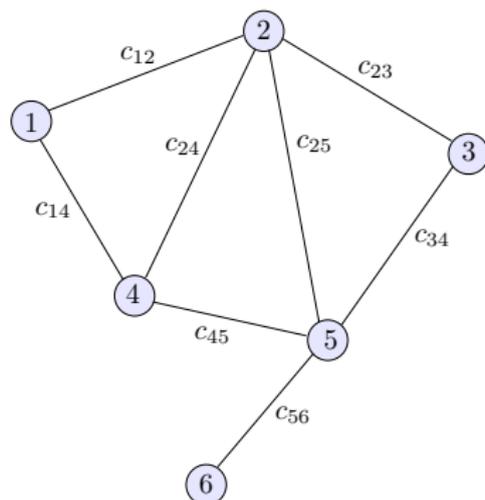
# Take me for a (simple) random walk

- Let  $\Gamma = (V, E, c)$  be a **connected network**,  $|V| = n$  ( $n=6$ ) and  $|E| = m$  ( $m=8$ ).



# Take me for a (simple) random walk

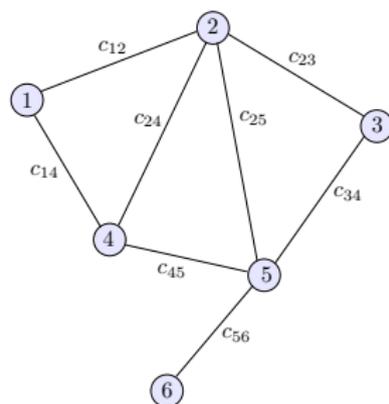
- Let  $\Gamma = (V, E, c)$  be a **connected network**,  $|V| = n$  and  $|E| = m$ .



- Given an initial vertex  $s_0$ , select *at random* an adjacent vertex  $s_1$ , and move to this neighbour, and after to  $s_2$  neighbour of  $s_1$  and so on.

# Take me for a (simple) random walk

- The sequence of vertices  $s_0, s_1, s_2, \dots, s_k, \dots$  is a **simple RW on  $\Gamma$** .

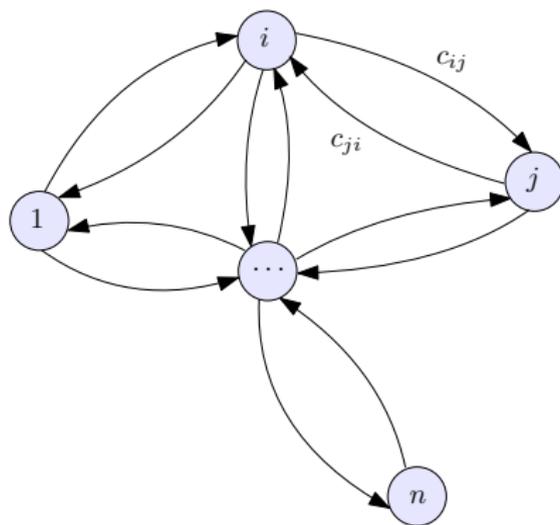


- At each step  $k$ , we have a random variable  $X_k$  taking values on  $V$ .
- Discrete time stochastic process defined on the state space  $V$

$$X_0, X_1, X_2, \dots, X_k, \dots$$

# Random Walks & Markov chains: Just the same

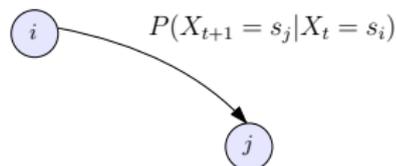
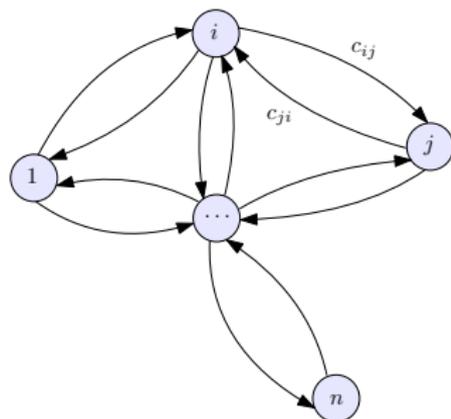
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► What does *at random* mean?

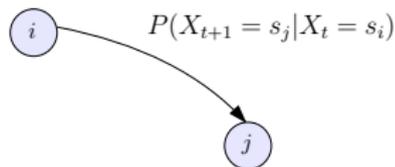
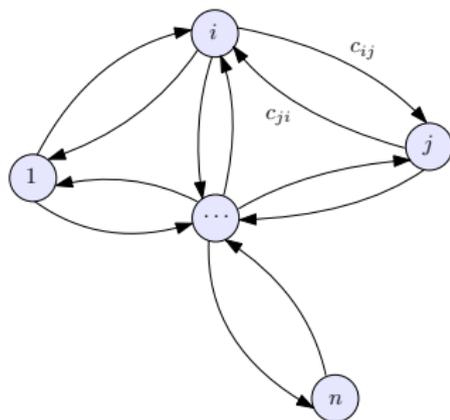


If at time  $k$  we are at vertex  $i$ , choose any neighbour to move to.

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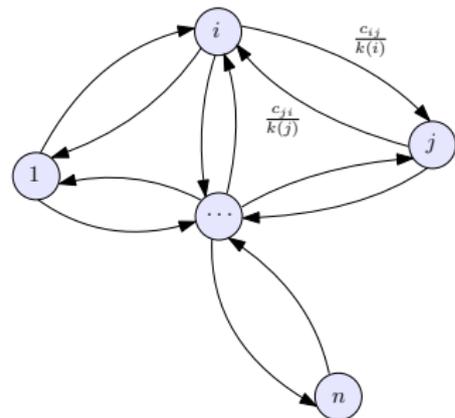


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Markov:  $P(X_{k+1} = j | X_k = i, X_{k-1} = i_{k-1}, \dots, X_0 = i_0) = P(X_{k+1} = j | X_k = i)$

# Take chances on the RW

- Let  $k_i = \sum_{j \sim i} c_{ij}$  denote the degree of vertex  $i$  then



$$p_{ij} = P(X_{k+1} = j | X_k = i) = \frac{c_{ij}}{k_i}$$

- Transition probability matrix: the stochastic matrix  $P = (p_{ij})_{i,j=1}^n$

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- The  $ij$ -th entry of  $P^k$  represents the probability of reaching state  $j$  after  $k$  steps if the walk starts at state  $i$ :

$$\mathbf{u}_k^T = \mathbf{u}_0^T P^k$$

$\mathbf{u}_t^T = (P(X_t = 1), P(X_t = 2), \dots, P(X_t = n))$  is the probability distribution vector at step  $t$ .

# Take chances on the RW

- Transition probability matrix: the stochastic matrix  $P = (p_{ij})_{i,j=1}^n$
- The Perron-Frobenius theorem for nonnegative irreducible matrices  $\equiv$  connected network implies the existence of a unique probability distribution  $\boldsymbol{\pi}$ , which is a positive left eigenvector associated to its dominant eigenvalue  $\lambda = 1$ .

$$\boldsymbol{\pi}^T = \boldsymbol{\pi}^T P, \quad \pi_i > 0, \quad \sum_{i \in V} \pi_i = 1$$

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- Stationary distribution,  $\pi$ :

$$P(X_0 = j) = \pi_j, \quad j = 1, \dots, n, \quad \text{then} \quad P(X_k = j) = \pi_j, \quad \text{for all } k.$$

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- Stationary distribution,  $\pi$ :

$$\pi_i = \frac{k_i}{\text{vol}(\Gamma)}, \text{ for all } i \in V, \text{ where } \text{vol}(\Gamma) = \sum_{i,j \in V} c_{ij} = \sum_{i \in V} k_i.$$

# Let's talk about the long term behavior of the RW

- Consider  $\Pi = \mathbf{1} \otimes \boldsymbol{\pi} = \mathbf{1} \cdot \boldsymbol{\pi}^T = \begin{bmatrix} \pi_1 & \pi_2 & \cdots & \pi_n \\ \vdots & \vdots & \dots & \vdots \\ \pi_1 & \pi_2 & \cdots & \pi_n \end{bmatrix}$ , then

# Let's talk about the long term behavior of the RW

- Consider  $\Pi = \mathbf{1} \otimes \boldsymbol{\pi} = \mathbf{1} \cdot \boldsymbol{\pi}^T$ , then

## Regular random walks

$$\Pi = \lim_{n \rightarrow +\infty} P^n$$

Some power  $n$  of  $P$  does not have zeros



It is possible for all  $i$  to go to all  $j$  in exactly  $n$  steps

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- Consider  $\Pi = 1 \otimes \pi = 1 \cdot \pi^T$ , then

## Regular random walks

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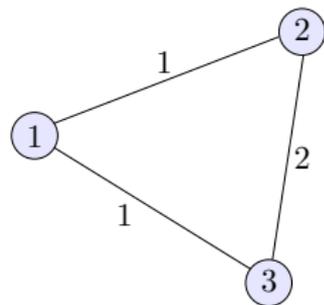
but FOR JUST

## Irreducible random walks

$$\Pi = \lim_{n \rightarrow +\infty} \frac{I + P + \dots + P^{n-1}}{n}$$

# Let's talk about the long term behavior of the RW

Example regular random walk:

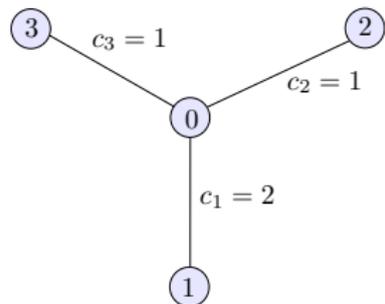


$$P = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ \frac{1}{3} & \frac{2}{3} & 0 \end{bmatrix} \quad P^{20} = \begin{bmatrix} 0.25 & 0.375 & 0.375 \\ 0.25 & 0.375 & 0.375 \\ 0.25 & 0.375 & 0.375 \end{bmatrix}$$

$$\begin{aligned} \lim_{n \rightarrow \infty} P^n &= \Pi = \mathbf{1} \otimes \boldsymbol{\pi} = \mathbf{1} \cdot \begin{bmatrix} \frac{1}{4} & \frac{3}{8} & \frac{3}{8} \end{bmatrix} \\ &= \mathbf{1} \otimes \frac{1}{\sum_{i \in V} k_i} \mathbf{k} = \mathbf{1} \cdot \frac{1}{8} \begin{bmatrix} 2 & 3 & 3 \end{bmatrix} \end{aligned}$$

# Let's talk about the long term behavior of the RW

Example JUST irreducible random walk, not regular:

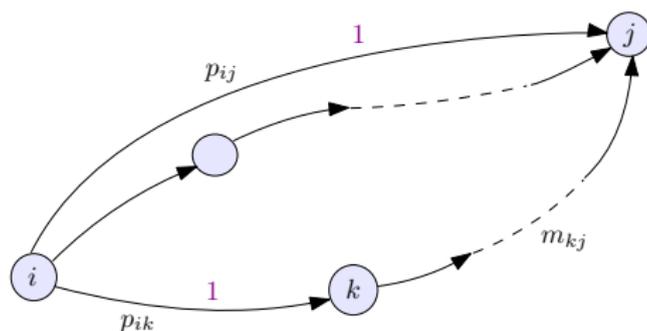


$$P = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{4} \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$\Pi = \lim_{n \rightarrow +\infty} \frac{I + P + \dots + P^{n-1}}{n} \quad \text{and} \quad \boldsymbol{\pi} = \frac{1}{\sum_{i \in V} k_i} \mathbf{k} = \frac{1}{8} \begin{bmatrix} 4 \\ 2 \\ 1 \\ 1 \end{bmatrix}$$

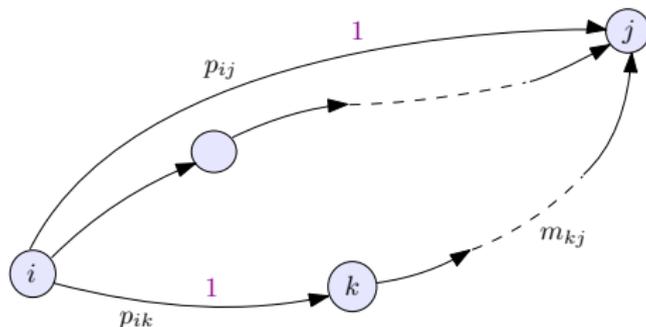
# What about short term behavior?

- If a random walk starts in state  $s_i$ , the **expected number of steps to reach state  $s_j$  for the first time** is called the **Mean First Passage Time** or the **hitting time from  $s_i$  to  $s_j$** . It is denoted by  $m_{ij}$ .



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- If  $i = j$ , the expected number of steps to return to  $s_i$  for the first time is the **mean recurrence time for  $s_i$** .

$$m_{ii} = \frac{1}{\pi_i}$$

# Random Walks meet $M$ -matrices

- Probabilistic Laplacian and combinatorial Laplacian

$$\Delta = I - P \quad L = D_k - A = D_k(I - P)$$

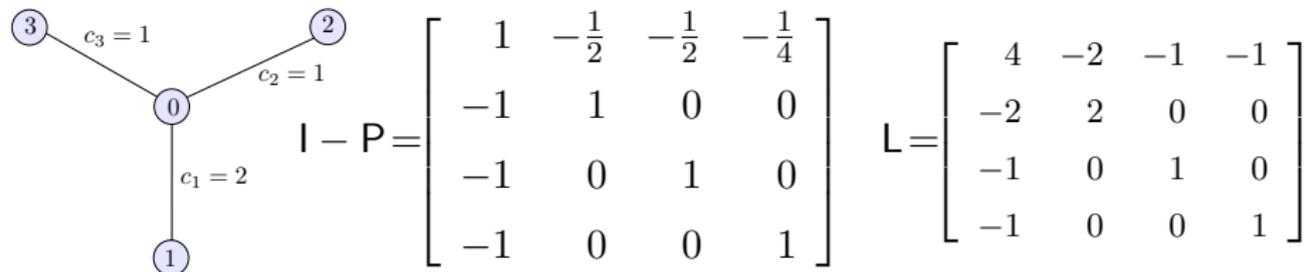
where  $D_k$  is diagonal of degrees and  $A = (c_{ij})_{i,j=1}^n$  is the adjacency matrix.

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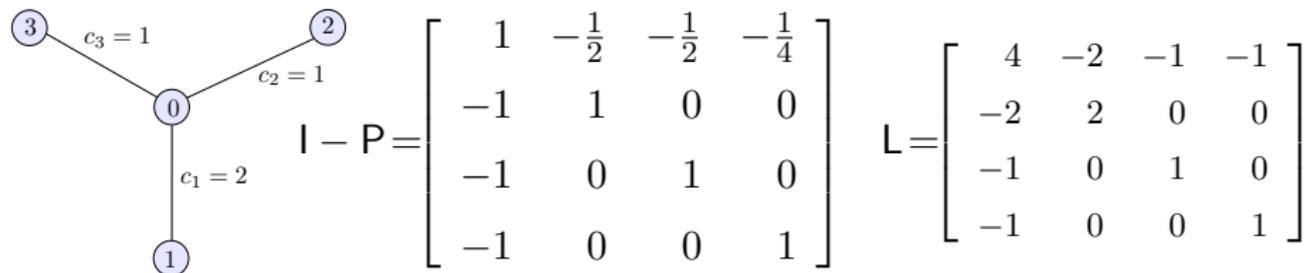
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# Random Walks meet $M$ -matrices



## o Properties

$$\Delta \mathbf{1} = (I - P) \mathbf{1} = \mathbf{0} \quad \text{and} \quad L \mathbf{1} = \mathbf{0}$$

$L$  is a symmetric **positive (semi)-definite**  $Z$ -matrix  $\Rightarrow L$  is an  **$M$ -matrix**

## Back to Mean First Passage Time

$$m_{ij} = p_{ij} + \sum_{k \neq j} p_{ik}(m_{kj} + 1) = 1 + \sum_{k \neq j} p_{ik}m_{kj} \quad \text{and} \quad m_{ii} = \frac{1}{\pi_i}$$

- The mean first passage time matrix,  $M = (m_{ij})$ :

$$M = PM + J - PD_{\pi}^{-1} \iff (I - P)M = J - PD_{\pi}^{-1}$$

# Back to Mean First Passage Time

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- Properties of the system
  - $I - P$  is singular
  - The system is compatible
  - $(I - P) \cdot \mathbf{1} = 0 \Rightarrow \mathbf{1} \in \text{Ker}(I - P)$

# Back to Mean First Passage Time

- The mean first passage time matrix,  $M = (m_{ij})$ :

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$$M = H(J - PD_{\pi}^{-1}) + 1\alpha^T$$

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- Imposing the condition  $m_{ii} = \frac{1}{\pi_i}$  ( $M_d = D_{\pi}^{-1}$ ):

$$M = (H\Pi - J(H\Pi)_d + I - H + JH_d)D_{\pi}^{-1}$$

# The matrices that we use to know

$$D_k(I - P)M = D_k(J - PD_{\pi}^{-1}) \iff LM = D_kJ - \text{vol}(\Gamma)AD_k^{-1}$$

- Consider  $G$  any 1-inverse of  $L$

$$M = GD_kJ - J(GD_kJ)_d + \text{vol}(\Gamma)(D_k^{-1} - G + JG_d)$$

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and for  $g = 1$ ,  $G = Z_L$  is invertible and called **Fundamental matrix** for  $L$

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- If  $L^\#$  is the group inverse for  $L$  then,

$$M = \text{vol}(\Gamma) \left( D_k^{-1} - L^\# + JL_d^\# + \Pi L^\# + L^\# \Pi^T - 2JD_{L^\# \pi} \right)$$

# The notorious constant

- The **Kemeny's constant** is

$$K = \sum_{j \in V} m_{ij} \pi_j \quad \text{or in matrix form} \quad M\pi = K\mathbf{1}$$

the expected time to get any randomly chosen vertex from vertex  $i$ .

- It is constant and independent of the starting vertex.

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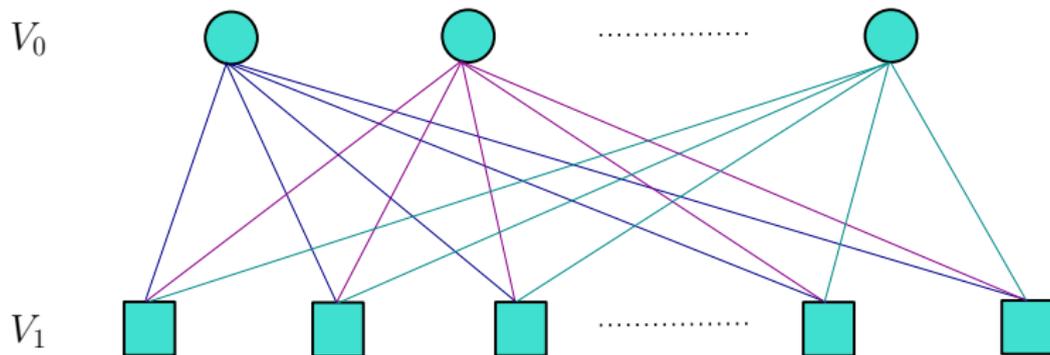
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the expected time to get any randomly chosen vertex from vertex  $i$ .

- It is constant and independent of the starting vertex.
- In terms of  $L^\#$ , the group inverse for  $L$ ,

$$K = \mathbf{1} + \text{tr}(L^\# D_k) - \frac{1}{\text{vol}(\Gamma)} \mathbf{k}^\top L^\# \mathbf{k}.$$

# Let's dance with a complete bipartite graph



$$\mathbf{L}^\# = \begin{array}{c} V_0 \\ \hline V_1 \end{array} \left[ \begin{array}{c|c} V_0 & V_1 \\ \hline \frac{1}{k_0} \left( 1 - \frac{n + k_0}{n^2} \mathbf{J} \right) & -\frac{1}{n^2} \\ \hline -\frac{1}{n^2} & \frac{1}{k_1} \left( 1 - \frac{n + k_1}{n^2} \mathbf{J} \right) \end{array} \right] \quad n = k_0 + k_1$$

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$$M = L^\# D_k J - J (L^\# D_k J)_d + \text{vol}(\Gamma) \left( D_k^{-1} - L^\# + J L_d^\# \right)$$

$$M = \begin{array}{c} V_0 \\ \hline V_1 \end{array} \left[ \begin{array}{c|c} V_0 & V_1 \\ \hline 2k_1 & 2k_0 - 1 \\ \hline 2k_1 - 1 & 2k_0 \end{array} \right]$$

# Let's dance with a complete bipartite graph

$$K = 1 + 1^T L_d^{\#} k - \pi^T L^{\#} k$$

Complete bipartite with  $n$  vertices then  $K = n - \frac{1}{2}$

$$K = 1 + 1^T \left[ \begin{array}{c|c} \frac{1}{k_0} \left( 1 - \frac{n + k_0}{n^2} J \right) & 0 \\ \hline 0 & \frac{1}{k_1} \left( 1 - \frac{n + k_1}{n^2} J \right) \end{array} \right] \begin{bmatrix} k_0 \\ k_1 \end{bmatrix}$$

$$-\frac{1}{2k_0k_1} [k_0 \mid k_1] \left[ \begin{array}{c|c} \frac{1}{k_0} \left( 1 - \frac{n + k_0}{n^2} J \right) & -\frac{1}{n^2} \\ \hline -\frac{1}{n^2} & \frac{1}{k_1} \left( 1 - \frac{n + k_1}{n^2} J \right) \end{array} \right] \begin{bmatrix} k_0 \\ k_1 \end{bmatrix} = n - \frac{1}{2}$$

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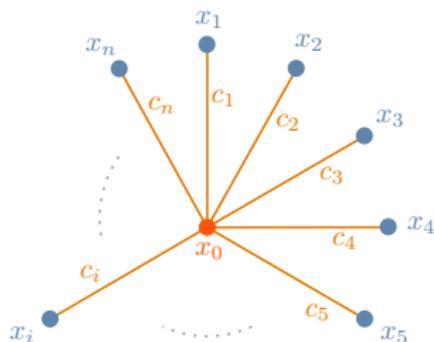
$$K = \sum_{j \in V} m_{ij} \pi_j \quad \text{or in matrix form} \quad K\mathbf{1} = M\boldsymbol{\pi}$$

$$K\mathbf{1} = M\boldsymbol{\pi} = \left[ \begin{array}{c|c} 2k_1 & 2k_0 - 1 \\ \hline 2k_1 - 1 & 2k_0 \end{array} \right] \frac{1}{2k_0 k_1} \left[ \begin{array}{c} k_0 \\ \hline k_1 \end{array} \right] = \left( n - \frac{1}{2} \right) \mathbf{1}$$

$\Downarrow$

$$K = n - \frac{1}{2}$$

# Here comes the network



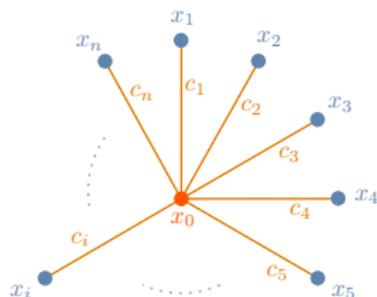
$$\mathbf{L}^\#(x_0, x_0) = \frac{1}{(n+1)^2} \sum_{k=1}^n \frac{1}{c_k} \equiv \alpha$$

$$\mathbf{L}^\#(x_0, x_j) = \alpha - \frac{1}{n+1} \frac{1}{c_j}, \quad j = 1, \dots, n$$

$$\mathbf{L}^\#(x_j, x_j) = \alpha - \frac{n-1}{n+1} \frac{1}{c_j}, \quad j = 1, \dots, n$$

$$\mathbf{L}^\#(x_i, x_j) = \alpha - \frac{1}{n+1} \left( \frac{1}{c_i} + \frac{1}{c_j} \right), \quad i, j = 1, \dots, n, i \neq j$$

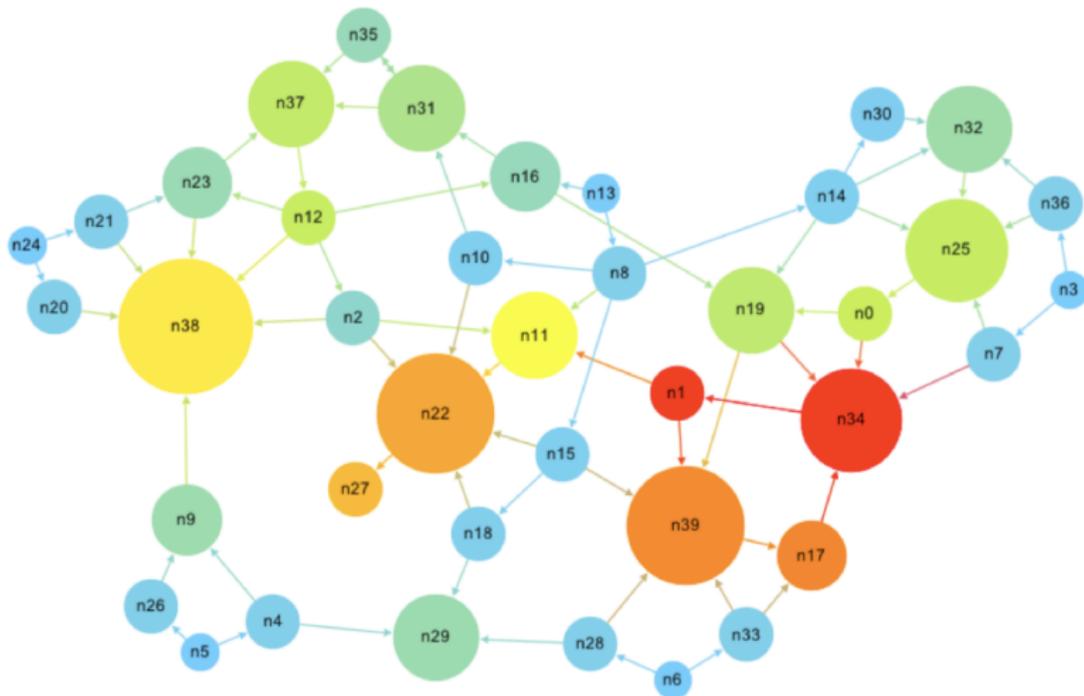
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$$M = L\#D_kJ - J(L\#D_kJ)_d + \text{vol}(\Gamma)\left(D_k^{-1} - L\# + JL\#_d\right)$$

$$M = \left[ \begin{array}{c|c} \frac{1}{\pi_0} & \frac{2k_0}{c_j} - 1 \\ \hline 1 & \frac{1}{\pi_j} \end{array} \right]$$

# Everybody is looking for something

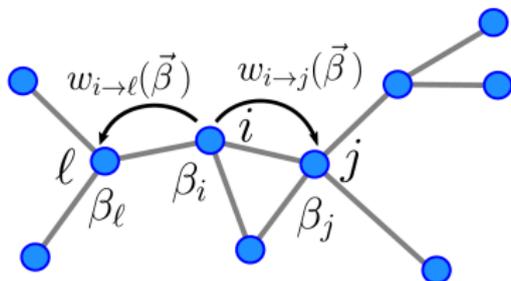


**PageRank:** Mesure of quantity and quality of websites' links for engine searchers

# We do need another models

- Degree-biased random walks describe a dynamics where a walker in a particular network's node uses the **degree information of neighbors** to choose randomly a new node to visit

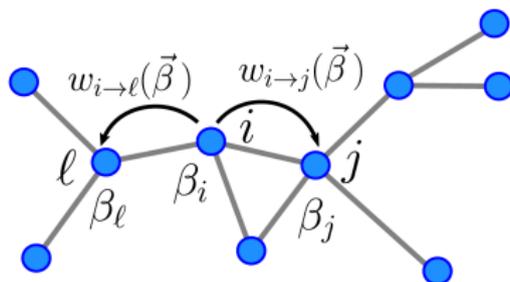
$$p_{ij}^{\beta} = \frac{c_{ij}k_j^{\beta}}{\sum_{\ell=1}^n c_{i\ell}k_{\ell}^{\beta}}$$



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- Degree-biased random walks describe a dynamics where a walker in a particular network's node uses the **degree information of neighbors** to choose randomly a new node to visit

$$p_{ij}^{\beta} = \frac{c_{ij}k_j^{\beta}}{\sum_{\ell=1}^n c_{i\ell}k_{\ell}^{\beta}}$$



- Lazy random walks describe a dynamics where **there is a constant positive probability**  $(1 - \alpha)$  of remaining in each node

$$\bar{P} = (1 - \alpha)I + \alpha P, \alpha \in (0, 1)$$

# We're maniacs of $M$ -matrices

- In the standard case  $P$  is associated with  $L$ , which is an irreducible, symmetric **diagonally dominant** irreducible, symmetric  $M$ -matrix,  $\lambda = 0$  is the lowest eigenvalue and  $\omega = 1$  is the associated eigenvector.

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- What about considering a generalized  $P$  associated with a **general irreducible, symmetric  $M$ -matrix**?
- The lowest eigenvalue is simple and  $\lambda \geq 0$ . Moreover, the associated eigenvector is positive.

# All we want, all we need, is here in our Schrödinger operator

- Positive Semidefinite Schrödinger matrix

$$L_q = L + D_q$$

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- If  $\lambda$  is the lowest eigenvalue of  $L_q$  and  $\omega$  is the associated eigenvector

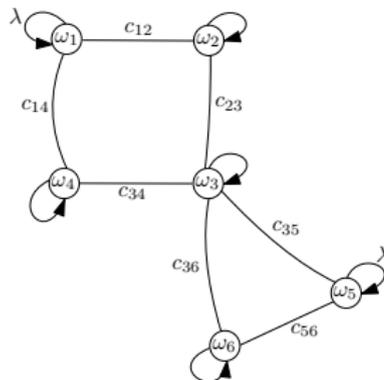
$$q = q_\omega + \lambda, \quad q_\omega = -\frac{1}{\omega} L\omega$$

and  $\lambda \geq 0$ ,  $\omega_i > 0$ , for all  $i \in V$ .

# All we want, all we need, is here in our Schrödinger operator

- Schrödinger Transition probability matrix

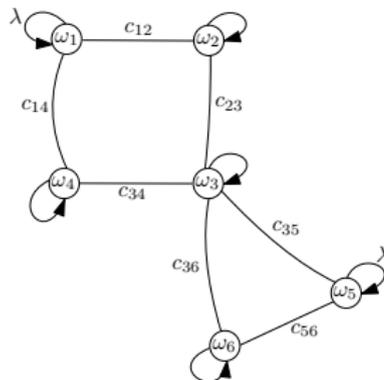
$$p_{ij}^{\lambda, \omega} = \frac{(c_{ij} + \lambda \omega_i \omega_j) \omega_j}{(k_i + q_i) \omega_i}$$



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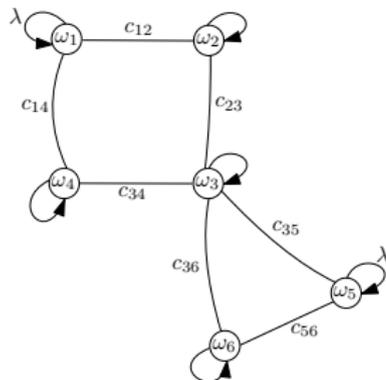
- There is a non-negative probability of remaining at vertex  $i$

$$p_{ii}^{\lambda, \omega} = \frac{\lambda \omega_i^2}{k_i + q_i}$$

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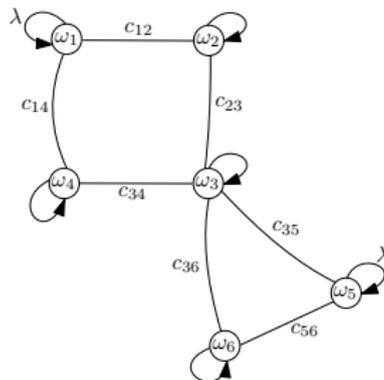
- Stationary distribution

$$\pi_i^{\lambda, \omega} = \frac{k_i + q_i \omega_i^2}{\text{vol}(\Gamma)} = \frac{(k_i + q_i) \omega_i^2}{\lambda + \sum_{i,j} c_{ij} \omega_i \omega_j}$$

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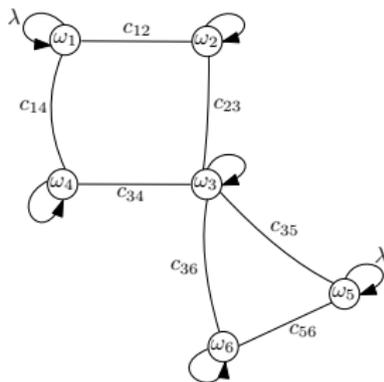
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- The matrix  $P^{\lambda, \omega}$  is markovian and has  $\pi^{\lambda, \omega}$  as stationary distribution

# Oops! We do it again

- The mean first passage time matrix,  $M^{\lambda,\omega} = (m_{ij}^{\lambda,\omega})_{i \neq j}$

$$p_{ij}^{\lambda,\omega} = \frac{(c_{ij} + \lambda\omega_i\omega_j)\omega_j}{(k_i + q_i)\omega_i}$$



$$M^{\lambda,\omega} = P^{\lambda,\omega} M^{\lambda,\omega} + J - P^{\lambda,\omega} D_{\pi^{\lambda,\omega}}^{-1} \iff (I - P^{\lambda,\omega}) M^{\lambda,\omega} = J - P^{\lambda,\omega} D_{\pi^{\lambda,\omega}}^{-1}$$

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- Any 1-inverse or *system solving* inverse,  $H^{\lambda,\omega}$ , provide a solution

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- Relation between  $L_q$  and  $I - P^{\lambda,\omega}$

$$I - P^{\lambda,\omega} = D_{\bar{k}}^{-1} [L_q - \lambda\omega\omega^T] D_\omega$$

where  $\bar{k}_i = (k_i + q_i)\omega_i$ .

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$$M^{\lambda,\omega} = \text{vol}(\Gamma) D_{\omega}^{-1} (D_{\bar{k}}^{-1} - G^{\lambda,\omega} + J G_d^{\lambda,\omega}) D_{\omega}^{-1}$$

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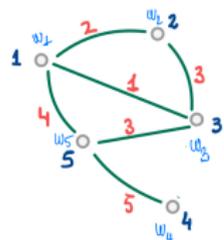
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$$K(M^{\lambda, \omega}) = 1 - g + \text{tr}(G^{\lambda, \omega} D_{q+k})$$

# A little bit of it



$$\lambda = 1.458$$

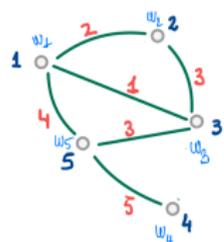
$$\omega = [0.992, 0.0619, 0.0508, 0.0201, 0.0907]$$

$$L_q = L + D_q, \quad q = q_\omega + \lambda, \quad q_\omega = -\frac{1}{\omega}L\omega$$

$$q_\omega = [-6.4584, 29.5416, 21.5416, 17.5416, 34.5416] \text{ and } q = q_\omega + \lambda$$

$$\underbrace{\begin{bmatrix} 2 & -2 & -1 & 0 & -4 \\ -2 & 36 & -3 & 0 & 0 \\ -1 & -3 & 30 & 0 & -3 \\ 0 & 0 & 0 & 24 & -5 \\ -4 & 0 & -3 & -5 & 48 \end{bmatrix}}_{L_q} = \underbrace{\begin{bmatrix} 7 & -2 & -1 & 0 & -4 \\ -2 & 5 & -3 & 0 & 0 \\ -1 & -3 & 7 & 0 & -3 \\ 0 & 0 & 0 & 5 & -5 \\ -4 & 0 & -3 & -5 & 12 \end{bmatrix}}_L + \underbrace{\begin{bmatrix} -5 & 0 & 0 & 0 & 0 \\ 0 & 31 & 0 & 0 & 0 \\ 0 & 0 & 23 & 0 & 0 \\ 0 & 0 & 0 & 19 & 0 \\ 0 & 0 & 0 & 0 & 36 \end{bmatrix}}_{D_q = D_{q_\omega + \lambda}}$$

# A little bit of it



$$\lambda = 1.458$$

$$\omega = [0.992, 0.0619, 0.0508, 0.0201, 0.0907]$$

- Stationary probability distribution

$$\pi^{\lambda, \omega} = \begin{bmatrix} 0.4714 \\ 0.1169 \\ 0.0651 \\ 0.0081 \\ 0.3386 \end{bmatrix} \quad \pi = \begin{bmatrix} 0.01620 \\ 0.01157 \\ 0.01620 \\ 0.01157 \\ 0.02778 \end{bmatrix}$$

- “importance” w.r.t.  $\lambda, \omega$ : **1, 5, 2, 3, 4**
- “importance” **1=3, 5, 2=4**

**It's friday,**



**we're (almost) done!**