Parameter Estimation for Networks Processes

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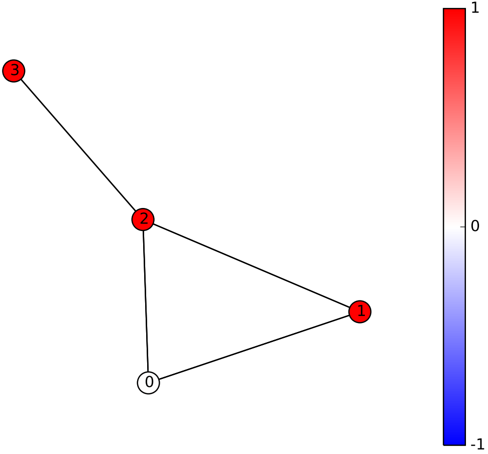
Overview

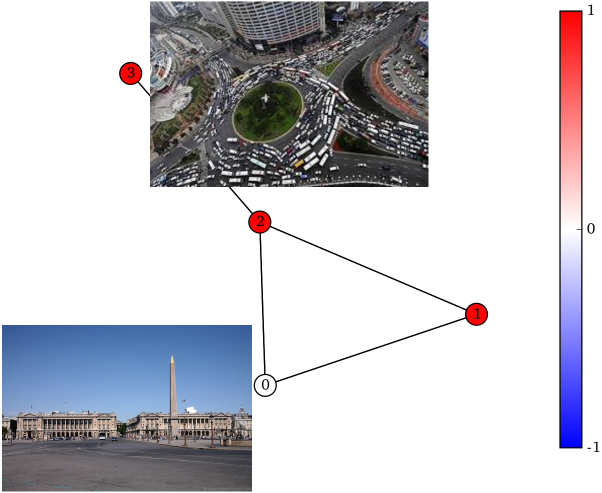
Section 1

Graph Attributes

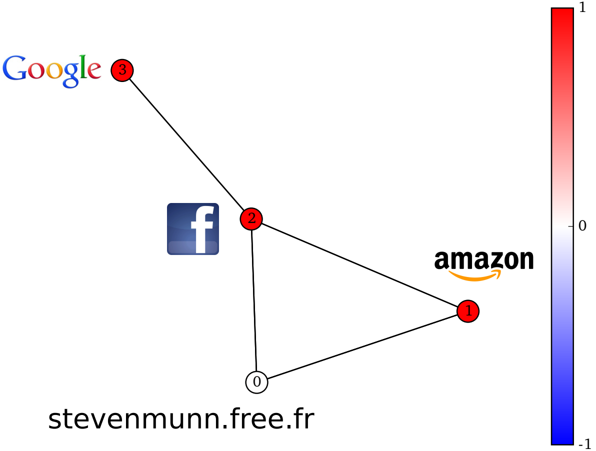
Attributed Graphs



Traffic Example



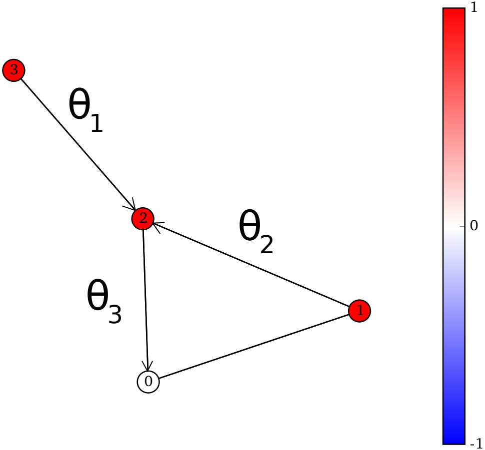
Website Visits Example



Section 2

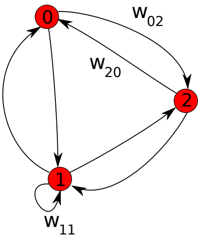
Reaction Networks

Reaction Attributes



Graph Weights

$$\mathbf{W} = \begin{bmatrix} w_{00} & w_{01} & w_{02} \\ w_{10} & w_{11} & w_{12} \\ w_{20} & w_{21} & w_{22} \end{bmatrix}$$



Reaction ODE

$$dM^T = \begin{bmatrix} 1 & 1 & 1 & \dots \end{bmatrix} \times \begin{bmatrix} w_{00} & w_{01} & w_{02} & \dots \\ w_{10} & w_{11} & w_{12} & \dots \\ w_{20} & w_{21} & w_{22} & \dots \\ \dots & & & \dots \end{bmatrix} \otimes \begin{bmatrix} 1 & M_0 & M_0 & \dots \\ M_1 & 1 & M_1 & \dots \\ M_2 & M_2 & 1 & \dots \\ \dots & & & \dots \end{bmatrix}$$

Example: Homework One

$$
\begin{aligned}
dM^T &= \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & \theta_1 \\ 0 & 0 & \theta_1 \\ 0 & \theta_2 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & M_0 & M_0 \\ M_1 & 1 & M_1 \\ M_2 & M_2 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & \theta_1 M_0 \\ 0 & 0 & \theta_1 M_1 \\ 0 & \theta_2 M_2 & 0 \end{bmatrix} \\
&= \begin{bmatrix} 1 & \theta_2 M_2 & \theta_1 (M_0 + M_1) \end{bmatrix}
\end{aligned}
$$

Section 3

Gibbs Sampling

Multiple Parameters Estimation

Start with parameters $\boldsymbol{\theta}^{(t)}$ (e.g. sampled from a uniform distribution)
Update each component one after the other as follows:

- Sample $\theta_1^{(t+1)}$ from $p\left(\theta_1 | \text{data}, \theta_2, \theta_3, \ldots\right)$
- Sample $\theta_2^{(t+1)}$ from $p\left(\theta_2 | \text{data}, \theta_1, \theta_3, \ldots\right)$
- ...

Gibbs Sampling for Reaction Networks

Step 1

Define an upper and lower bound ($\boldsymbol{W}_{up}$ and $\boldsymbol{W}_{low}$) on the graph weights.

Step 2

Initialize the probability for each parameter as a uniform distribution between the upper and lower bounds,

$$p\left(w_{ij}\right) = u\left(\left(\boldsymbol{W}_{up}\right)_{ij}, \left(\boldsymbol{W}_{low}\right)_{ij}\right)$$

We now have an initial guess for the weights matrix $\boldsymbol{W}$. Next, we will update each component one at a time.

Gibbs Update for first component

We need to compute,

$$p\left(w_{00} \middle| \text{data}, w_{01}, w_{02}, w_{10}, w_{11}, \ldots\right)$$

to sample a new value for w_{00}. Currently, we do this using the same Bayesian inference method from homework one.

Problems with Gibbs Sampling

Probability Distribution is not Helpful

Unfortunately, if the weight matrix is not close to the ground truth then,

$$p\left(w_{00} \middle| \text{data}, w_{01}, w_{02}, w_{10}, w_{11}, \ldots\right)$$

yields a distribution that converges on meaningless values and Gibbs sampling gets stuck.