Parameter Estimation for Network Processes

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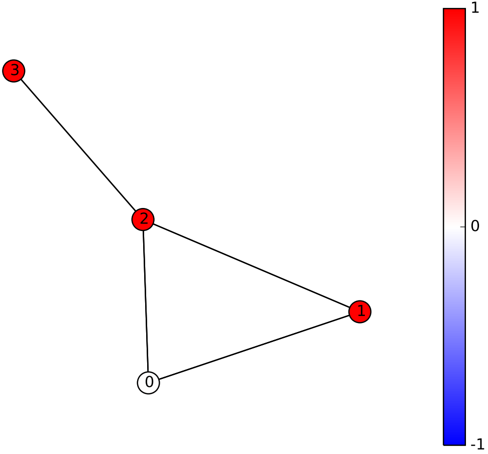
Overview

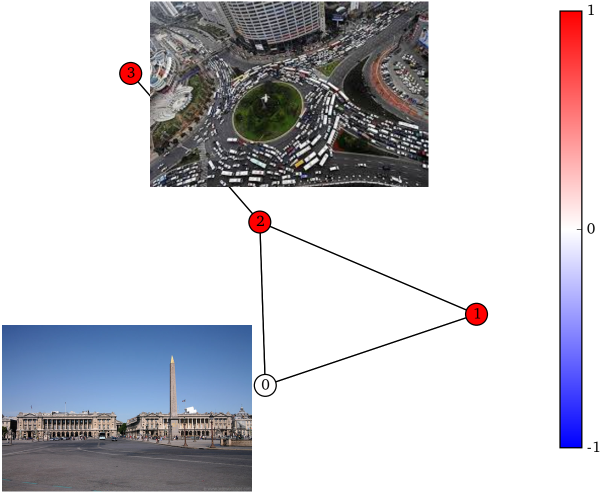
Section 1

Graph Attributes

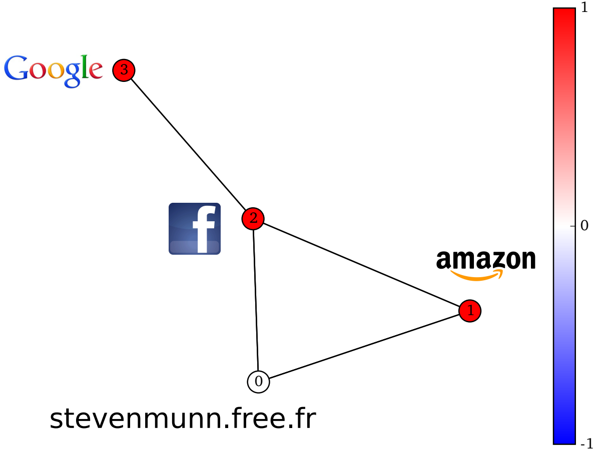
Attributed Graphs



Traffic Example



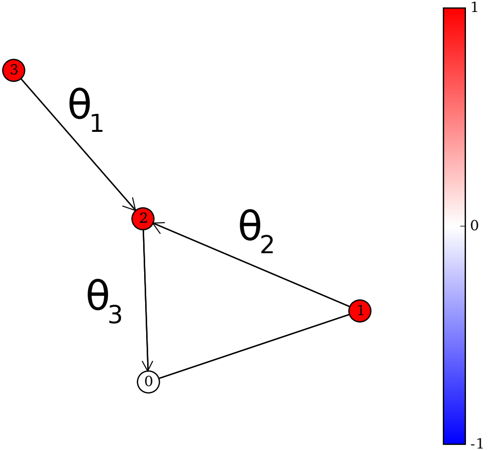
Website Visits Example



Section 2

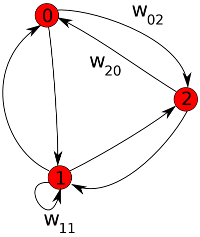
Reaction Networks

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

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

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,

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

Gibbs Sampling for Reaction Networks

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.

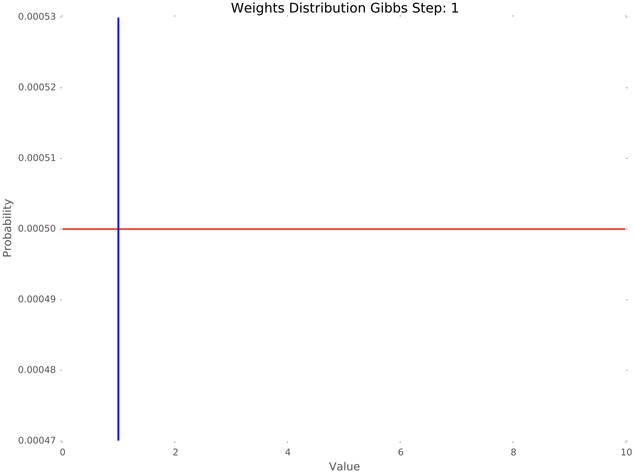
An example with two parameters

True parameters,

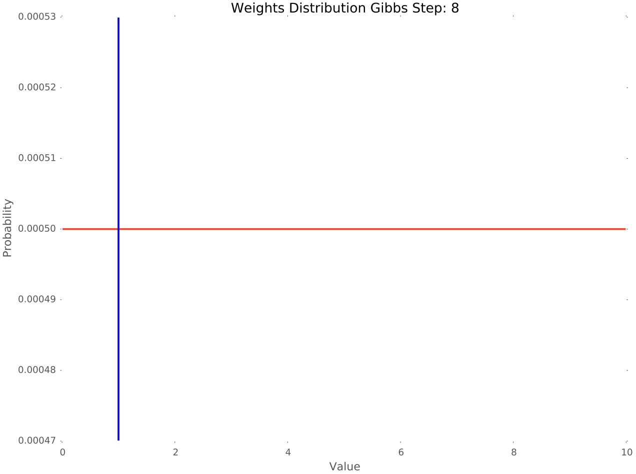
$$\mathbf{W} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & -1.45 & 0 \end{bmatrix}$$

$$\mathbf{W}_{\mathbf{lower}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -1.45 & 0 \end{bmatrix} \qquad \mathbf{W}_{\mathbf{upper}} = \begin{bmatrix} 1 & 0 & 2 \\ 0 & 0 & 2 \\ 0 & -1.45 & 0 \end{bmatrix}$$

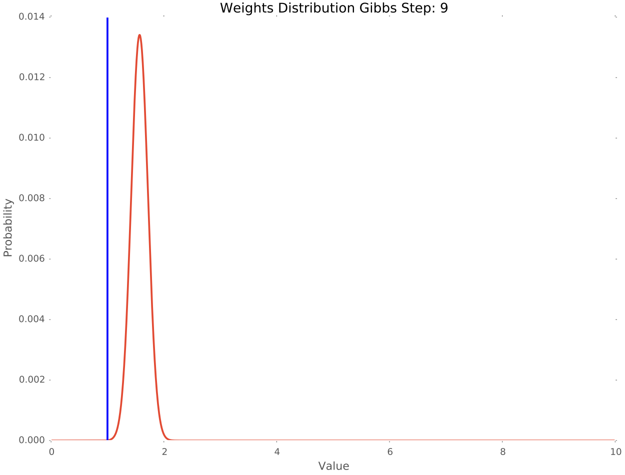
w_{02} Estimate at step 1



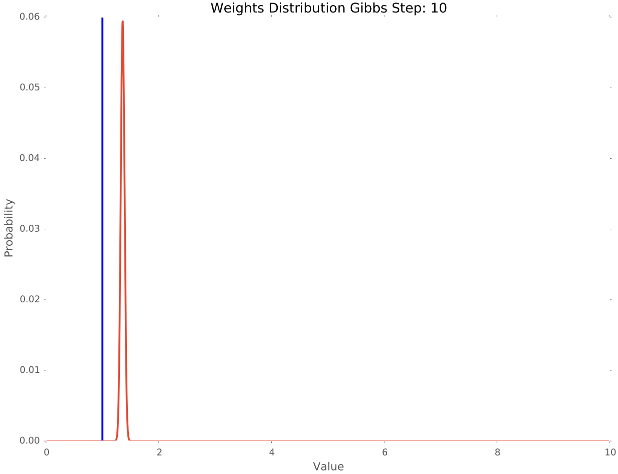
w_{02} Estimate at step 8



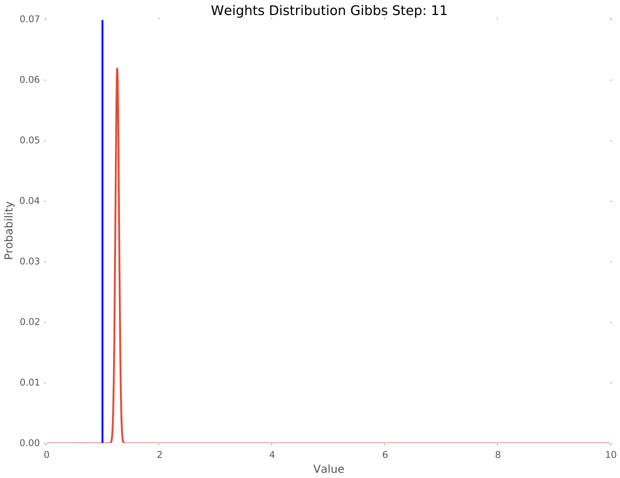
w_{02} Estimate at step 9



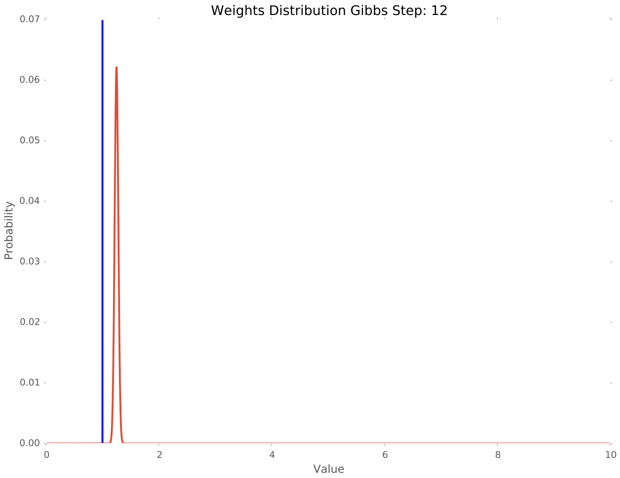
w_{02} Estimate at step 10



w_{02} Estimate at step 11



w_{02} Estimate at step 12



Gibbs Sampling Problems

Probability density in parameter space is too focused

Most of the parameter space has near-zero probability. The space over plausible parameters is very small. This is espcially true for runaway reactions (where the rates are all positive).