Parameter Estimation for Network Processes

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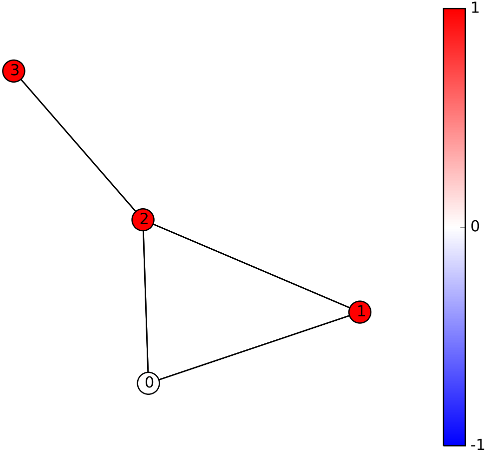
Overview

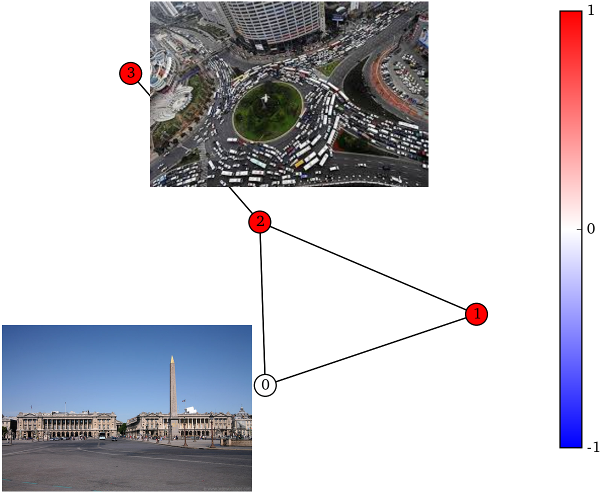
Section 1

Graph Attributes

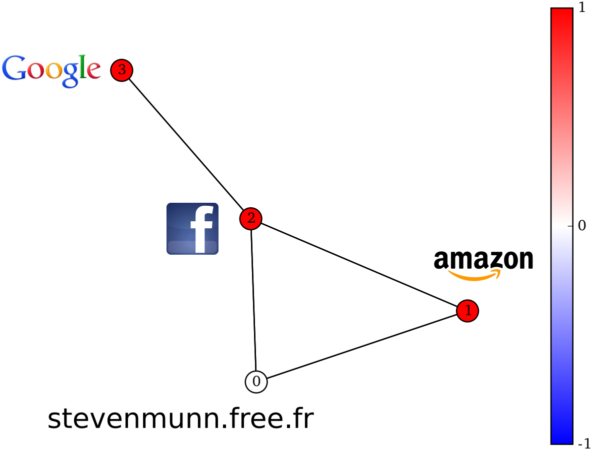
Attributed Graphs



Traffic Example



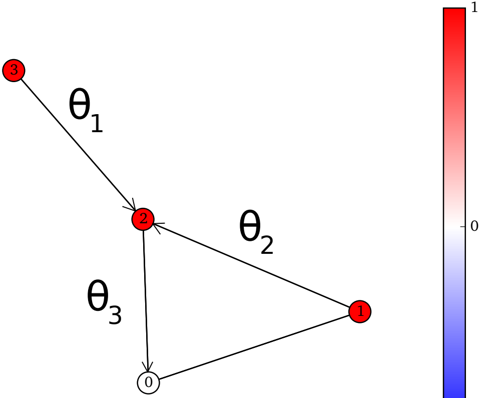
Website Visits Example



Section 2

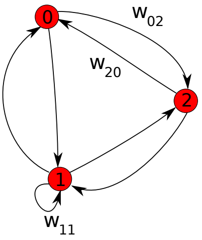
Reaction Networks

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

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

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,

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

Step 3

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.

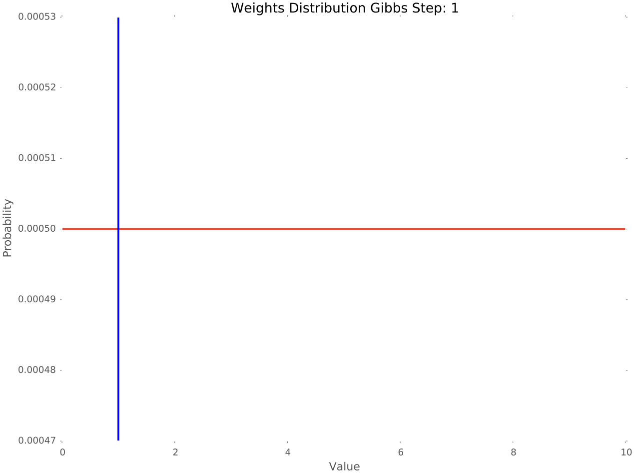
An example with two parameters

True parameters,

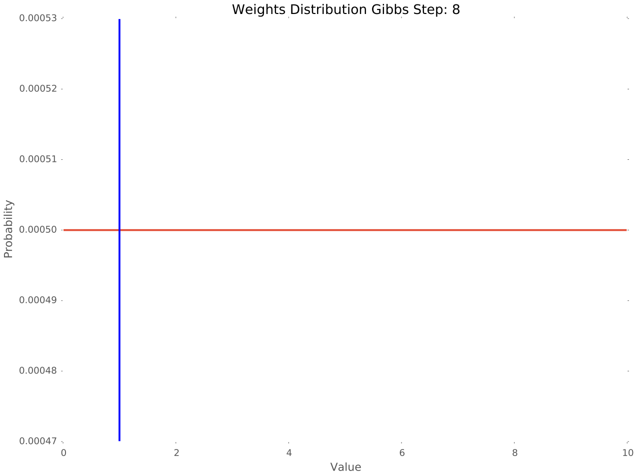
$$\mathbf{W} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & -1.45 & 0 \end{bmatrix}$$

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

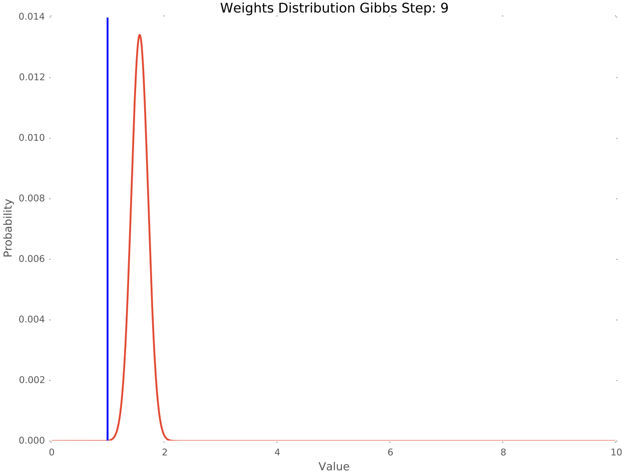
w_{02} Estimate at step 1



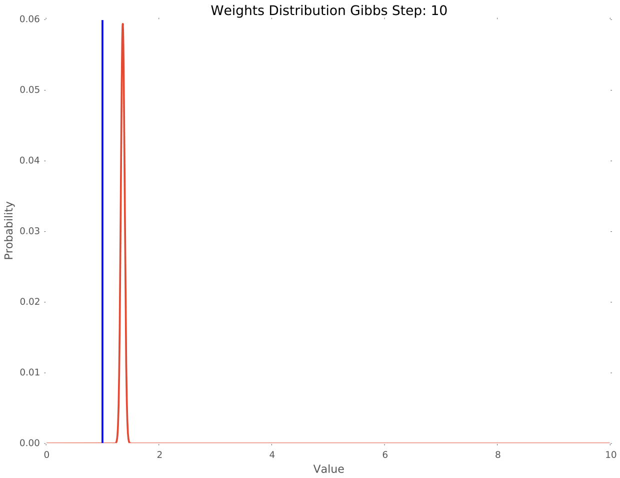
w_{02} Estimate at step 8



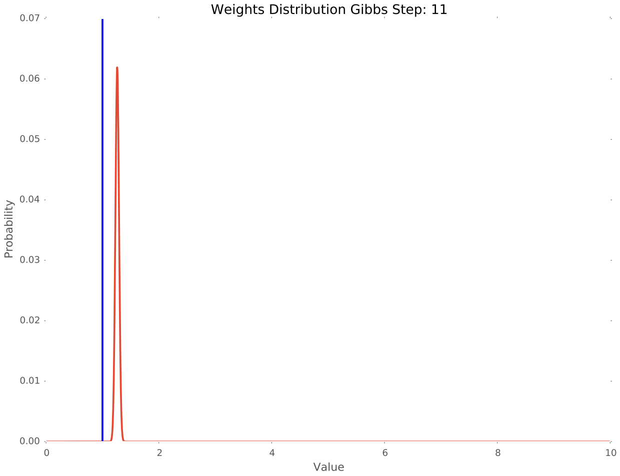
w_{02} Estimate at step 9



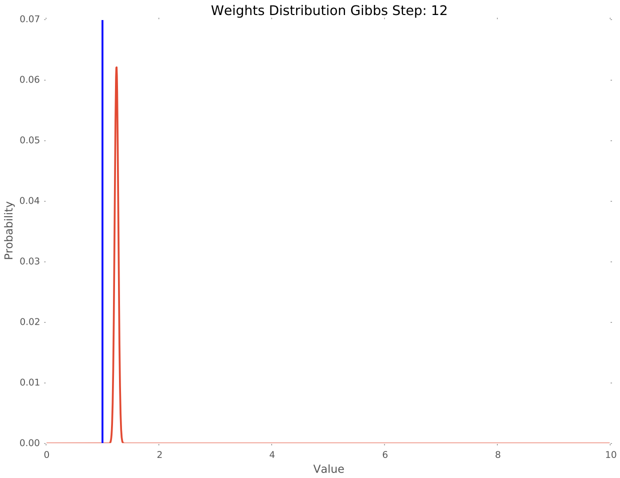
w_{02} Estimate at step 10



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).

Particle Filters

My bootstrap method probably has bugs

Perhaps a regularized particle filter would be effective?