ENM 3600: Data-driven Modeling and Probabilistic Scientific Computing

Lecture #11: Markov Chain Monte Carlo

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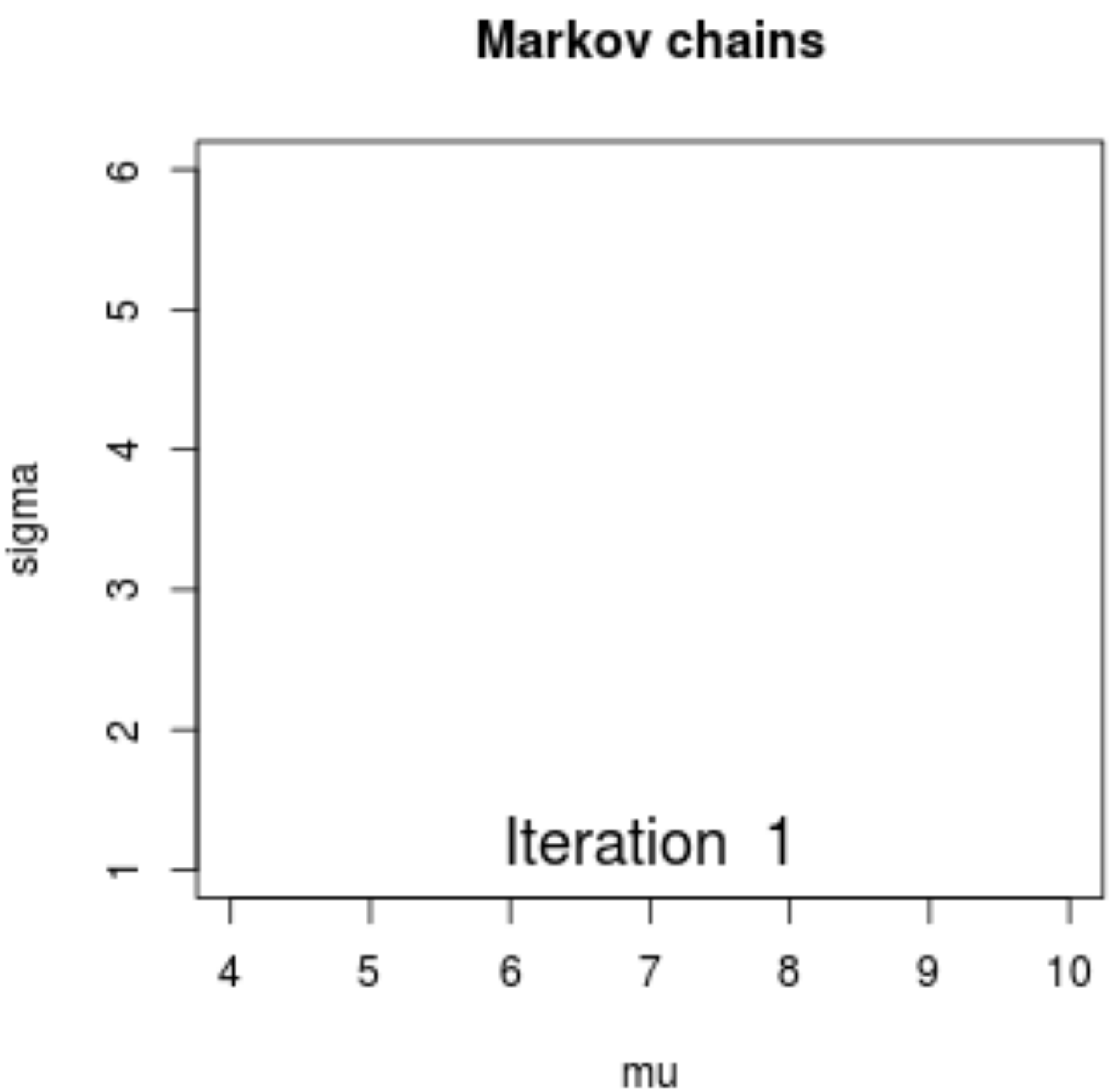
The Metropolis algorithm

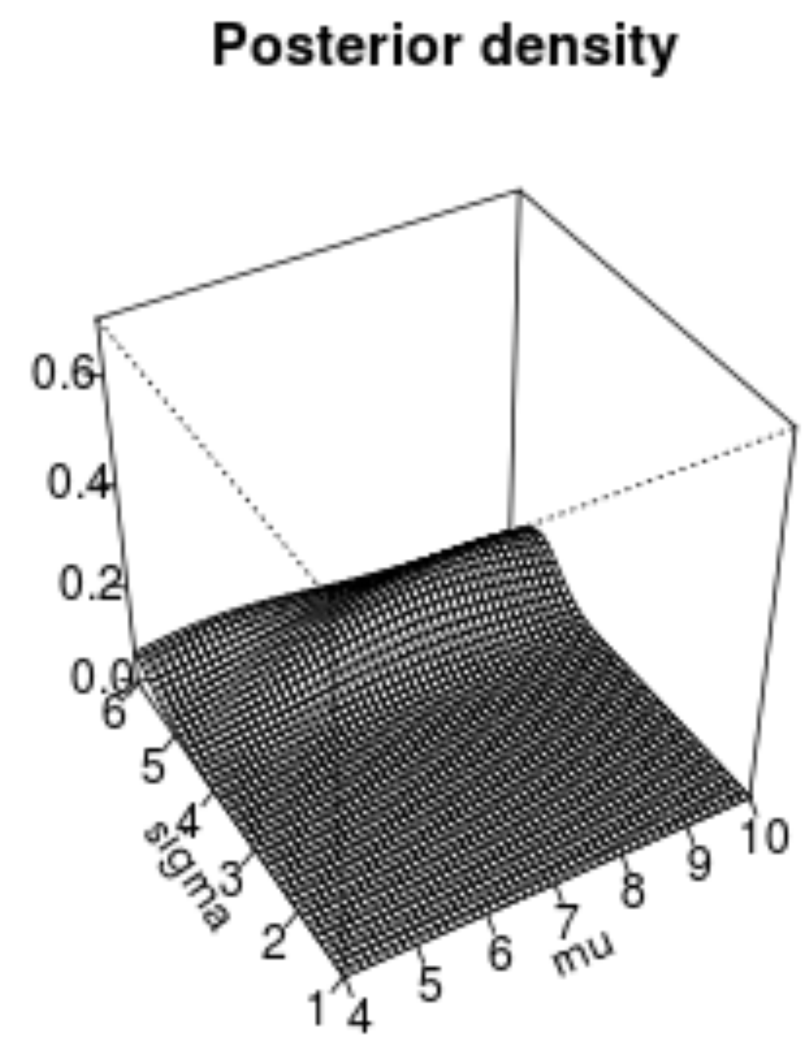
- Choose a symmetric proposal matrix Q. So, $Q_{ab} = Q_{ba}$.
- Initialize $x_o \in X$.
- for $i \in 0, 1, 2, \ldots, n-1$:
  - Sample proposal x from $Q(x_i, x)$ if x is discrete, otherwise, $p(x \mid x_i)$.
  - Sample r from Uniform$(0, 1)$.
  - If
    $$r < \frac{\tilde{\pi}(x)}{\tilde{\pi}(x_i)},$$
    accept and $x_{i+1} = x$.
  - Otherwise, reject and $x_{i+1} = x_i$.

Output: $x_o, x_1, \ldots, x_n$

- Symmetric proposals include:
  $$J(\theta^* \mid \theta^{(s)}) = \text{Uniform}(\theta^{(s)} - \delta, \theta^{(s)} + \delta)$$
  and
  $$J(\theta^* \mid \theta^{(s)}) = \text{Normal}(\theta^{(s)}, \delta^2).$$

The Metropolis algorithm





The Metropolis algorithm for Bayesian inference

Goal: We want to sample from

$$p(\theta \mid y) = \frac{f(y \mid \theta)\pi(\theta)}{m(y)}.$$

Typically, we don't know $m(y)$.

The notation is a bit more complicated, but the set up is the same.

We'll approach it a bit differently, but the idea is exactly the same.

We know $\pi(\theta)$ and $f(y \mid \theta)$, so we can can draw samples from these.

Our notation here will be that we assume parameter values $\theta_1, \theta_2, \ldots, \theta_s$ which are drawn from $\pi(\theta)$.

We assume a new parameter value comes in that is θ^*.

The Metropolis algorithm for Bayesian inference

The Metropolis algorithm proceeds as follows:

1. Sample $\theta^* \sim J(\theta \mid \theta^{(s)})$.
2. Compute the acceptance ratio (r):

$$r = \frac{p(\theta^*|y)}{p(\theta^{(s)}|y)} = \frac{p(y \mid \theta^*)p(\theta^*)}{p(y \mid \theta^{(s)})p(\theta^{(s)})}.$$

3. Let

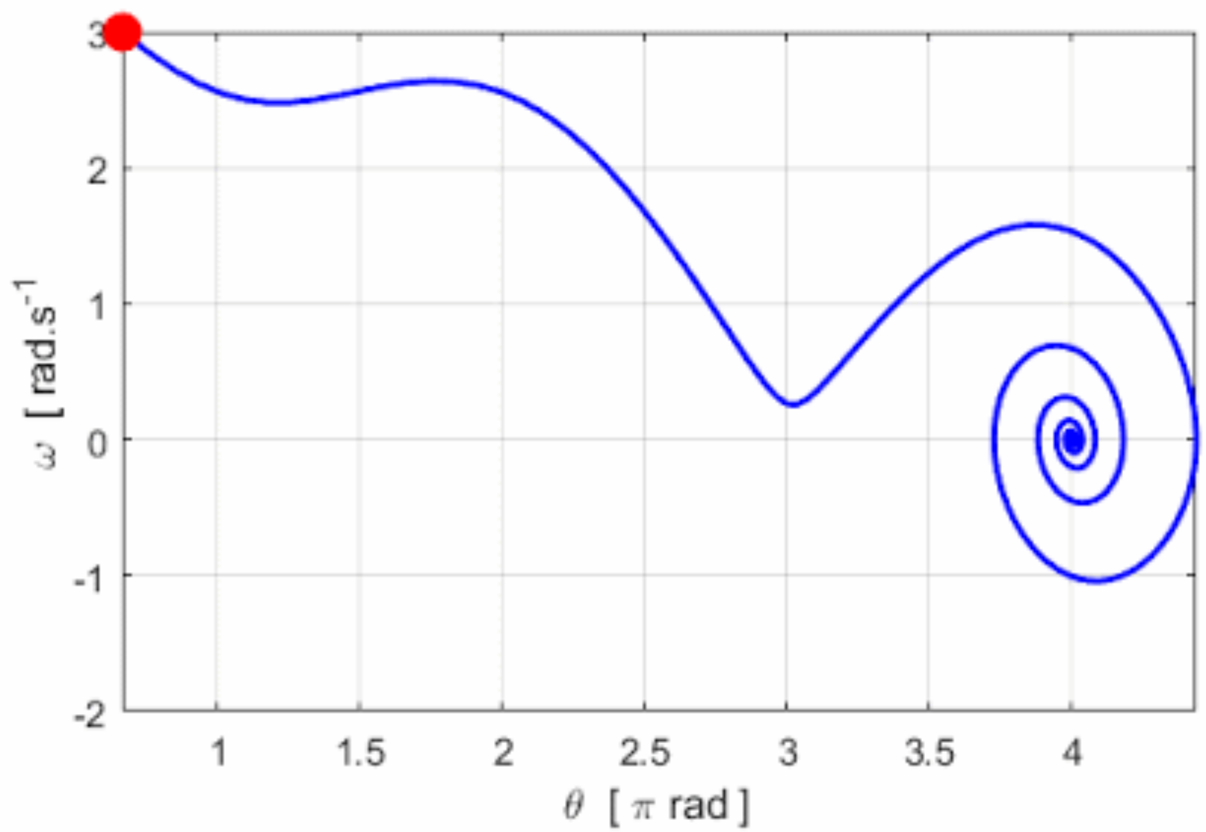
$$\theta^{(s+1)} = \begin{cases} \theta^* & \text{with prob min(r,1)} \\ \theta^{(s)} & \text{otherwise.} \end{cases}$$

Remark: Step 3 can be accomplished by sampling $u \sim \text{Uniform}(0, 1)$ and setting $\theta^{(s+1)} = \theta^*$ if $u < r$ and setting $\theta^{(s+1)} = \theta^{(s)}$ otherwise.

Bayesian calibration of dynamical systems

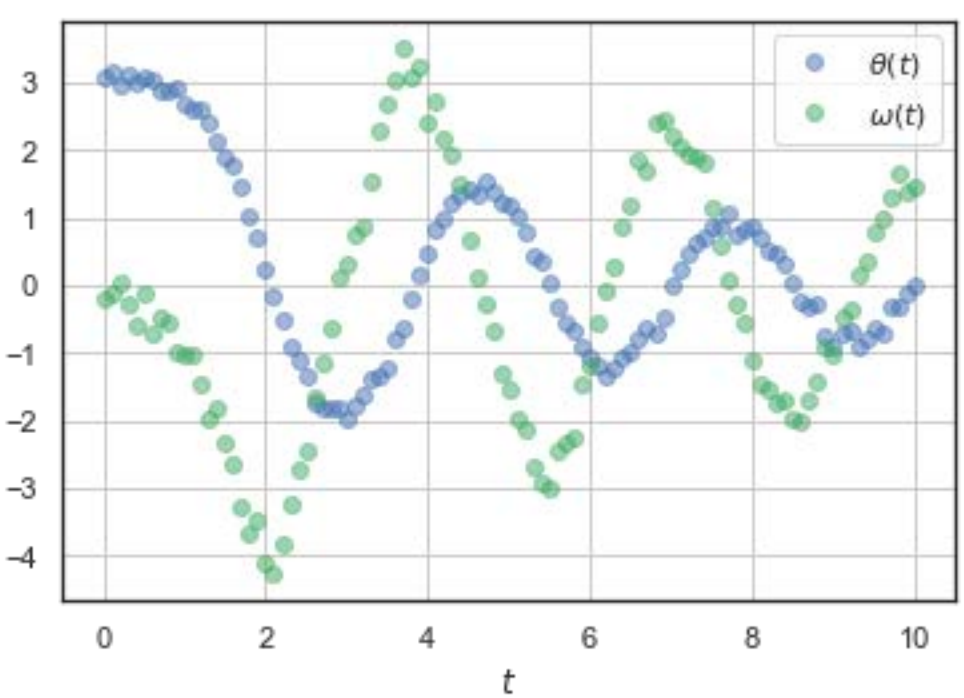
Example: Damped pendulum

$$\frac{d\theta}{dt} = \omega,$$
$$\frac{d\omega}{dt} = -b\omega - c\sin(\theta).$$



Given some noisy time-series data

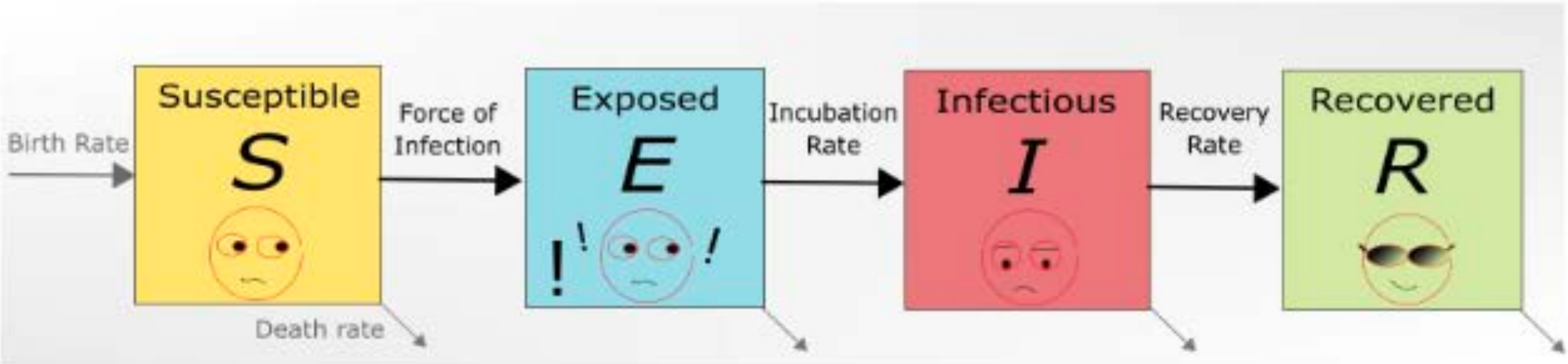
$$\mathcal{D} := \{\theta(t_i), \omega_i(t_i)\}, \quad i = 1, \ldots, n$$



Infer a posterior distribution over the unknown parameters

$$p(b, c|\mathcal{D})$$

Example: Epidemiology models



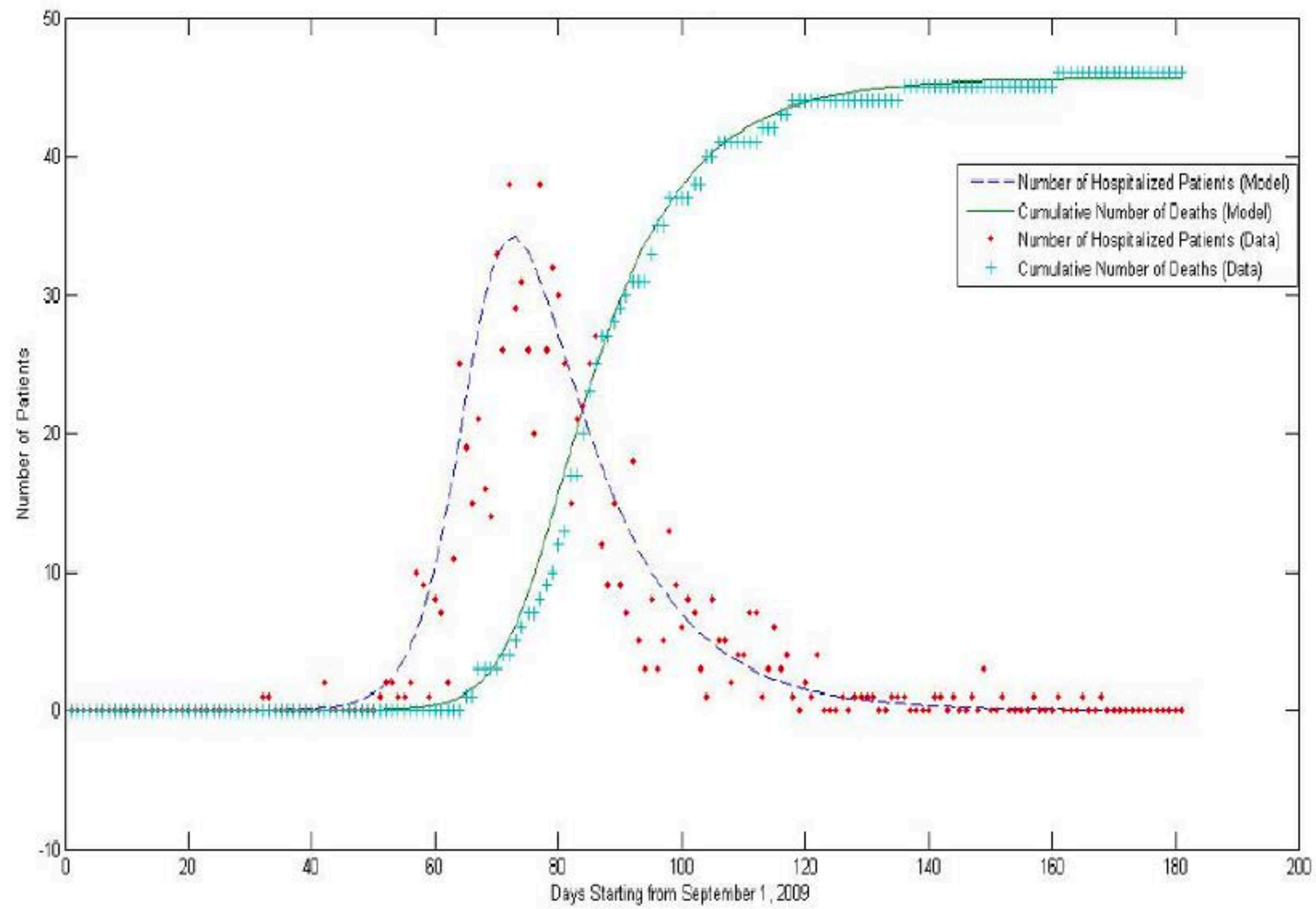
$$\frac{dS}{dt} = -\frac{\beta S I}{N}$$

$$\frac{dE}{dt} = \frac{\beta S I}{N} - \sigma E$$

$$\frac{dI}{dt} = \sigma E - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

$$N = S + E + I + R$$



Probabilistic programming

Stan

http://mc-stan.org/

PyMC3

https://github.com/pymc-devs/pymc3

Edward

http://edwardlib.org/

https://github.com/uber/pyro