Uncertainty Propagation for Biological Models: Practicum

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Practicum Problem

SIR Model:

$$\begin{aligned}
\frac{dS}{dt} &= \delta N - \delta S - \underline{\gamma k} IS \quad &, \quad S(0) &= S_0 \\
\frac{dI}{dt} &= \underline{\gamma k} IS - (r + \delta) I \quad &, \quad I(0) &= I_0 \\
\frac{dR}{dt} &= rI - \delta R \quad &, \quad R(0) &= R_0
\end{aligned}$$

Note:

- Run either the 3 or 4 parameter model and compute the prediction intervals.

Monte Carlo Quadrature:

- Run rand_points.m to observe uniformly sampled and Sobol' points.
- Run pi_approx.m with different values of N to see if you observe convergence rate of $1/\sqrt{N}$

Website:

- http://www4.ncsu.edu/~rsmith/RTG_BIOMATH18/

Delayed Rejection Adaptive Metropolis (DRAM)

Websites:

- http://www4.ncsu.edu/~rsmith/UQ_TIA/CHAPTER8/index_chapter8.html
- http://helios.fmi.fi/~lainema/mcmc/

Delayed Rejection Adaptive Metropolis (DRAM)

We fit the Monod model

$$y = \theta_1 \frac{1}{\theta_2 + 1} + \epsilon \quad , \quad \epsilon \sim N(0, I\sigma^2)$$

to observations

x (mg / L COD): 28 55 83 110 138 225 375

y (1 / h): 0.053 0.060 0.112 0.105 0.099 0.122 0.125

First clear some variables from possible previous runs.

```
clear data model options
```

Next, create a data structure for the observations and control variables. Typically one could make a structure data that contains fields xdata and ydata.

```
data.xdata = [28    55    83    110   138   225   375]';   % x (mg / L COD)
data.ydata = [0.053 0.060 0.112 0.105 0.099 0.122 0.125]'; % y (1 / h)
```

Construct model

```
modelfun = @(x,theta) theta(1)*x./(theta(2)+x);
ssfun = @(theta,data) sum((data.ydata-modelfun(data.xdata,theta)).^2);
model.ssfun = ssfun;
model.sigma2 = 0.01^2;
```

Delayed Rejection Adaptive Metropolis (DRAM)

Input parameters

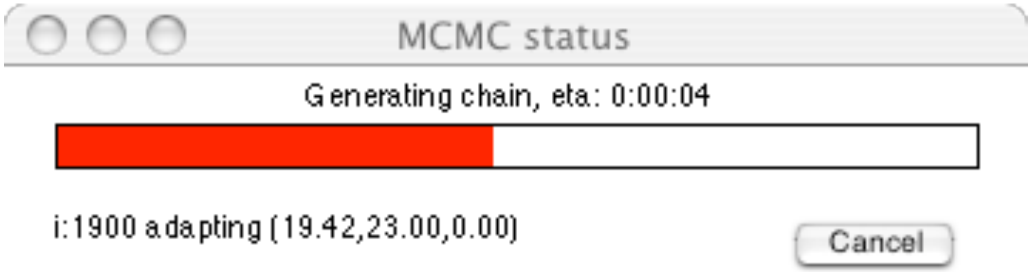
```
 params = {
     {'theta1', tmin(1), 0}
     {'theta2', tmin(2), 0} };
```

and set options

```
options.nsimu = 4000;
options.updatesigma = 1;
options.qcov = tcov;
```

Run code

```
[res,chain,s2chain] = mcmcrun(model,data,params,options);
```

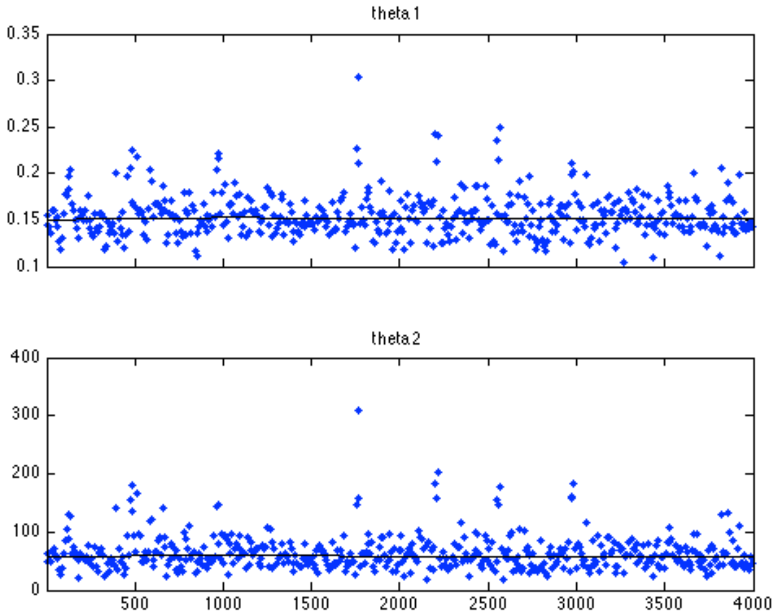


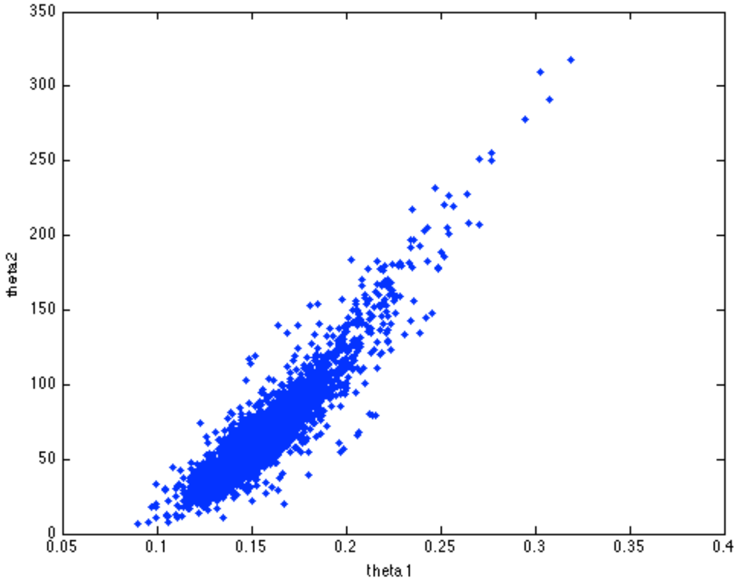
```
Generating chain, eta: 0:00:04
i:1900 adapting (19.42,23.00,0.00)
```

Delayed Rejection Adaptive Metropolis (DRAM)

Plot results

```
figure(2); clf
mcmcplot(chain,[],res,'chainpanel');
figure(3); clf
mcmcplot(chain,[],res,'pairs');
```





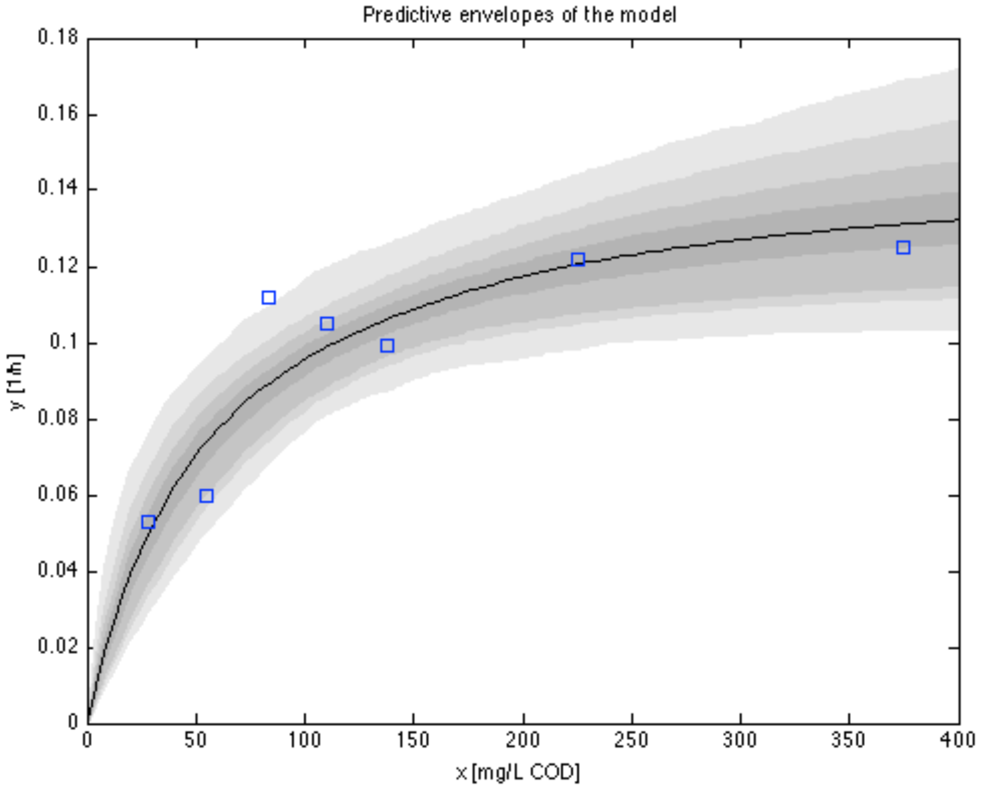
Examples:

- Several available in MCMC_EXAMPLES
- ODE solver illustrated in algae example

Delayed Rejection Adaptive Metropolis (DRAM)

Construct credible and prediction intervals

```
 figure(5); clf
 out = mcmcpred(res,chain,[],x,modelfun);
 mcmcpredplot(out);
 hold on
plot(data.xdata,data.ydata,'s');  % add data points to the plot
xlabel('x [mg/L COD]');
ylabel('y [1/h]');
hold off
title('Predictive envelopes of the model')
```



DRAM for SIR Example

SIR Model:

$$\frac{dS}{dt} = \delta N - \delta S - \underline{\gamma k} IS \quad , \; S(0) = S_0 \qquad \text{Susceptible}$$

$$\frac{dI}{dt} = \underline{\gamma k} IS - (r + \delta) I \quad , \; I(0) = I_0 \qquad \text{Infectious}$$

$$\frac{dR}{dt} = rI - \delta R \quad , \; R(0) = R_0 \qquad \text{Recovered}$$

Note: Parameter set $q = [\gamma, k, r, \delta]$ is not identifiable

Website

- http://helios.fmi.fi/~lainema/mcmc/
- http://www4.ncsu.edu/~rsmith/

DRAM for SIR Example: Results