SA/UQ Practicum

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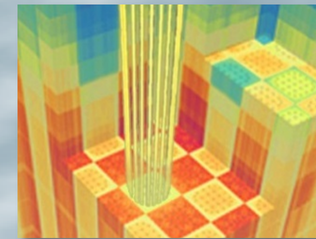

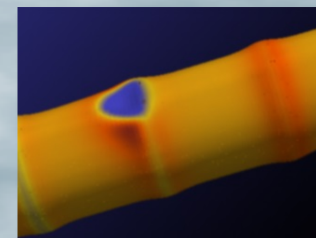

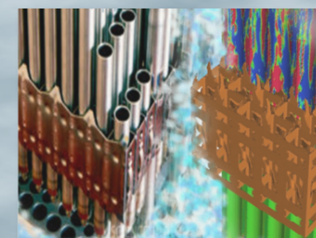

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Objectives

Two Primary Objectives:

- Use MATLAB to investigate SA and UQ for the Dittus—Boelter relation
  - Employ the Delayed Rejection Adaptive Metropolis (DRAM) algorithm
- Investigate sensitivity analysis for CTF: William Dawn

Delayed Rejection Adaptive Metropolis

Websites:

- https://rsmith.math.ncsu.edu/CASL_INSTITUTE19
- https://rsmith.math.ncsu.edu/UQ_TIA/CHAPTER8/index_chapter8.html
- https://mjlaine.github.io/mcmcstat/

Delayed Rejection Adaptive Metropolis

We fit the Monod model

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

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

Input parameters

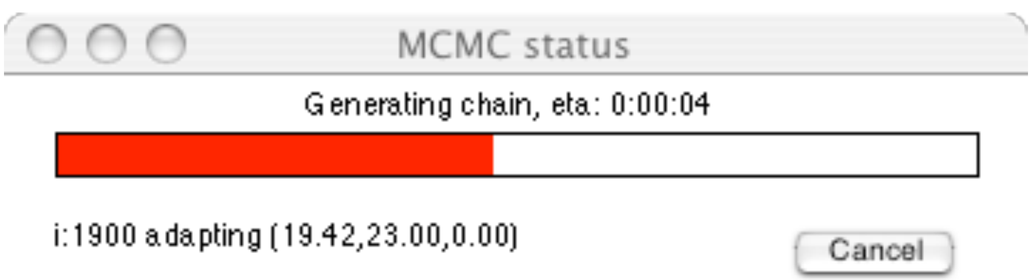
```
params = {
    {'theta1', tmin(1), 0}
    {'theta2', tmin(2), 0} };
```

and set options

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

Run code

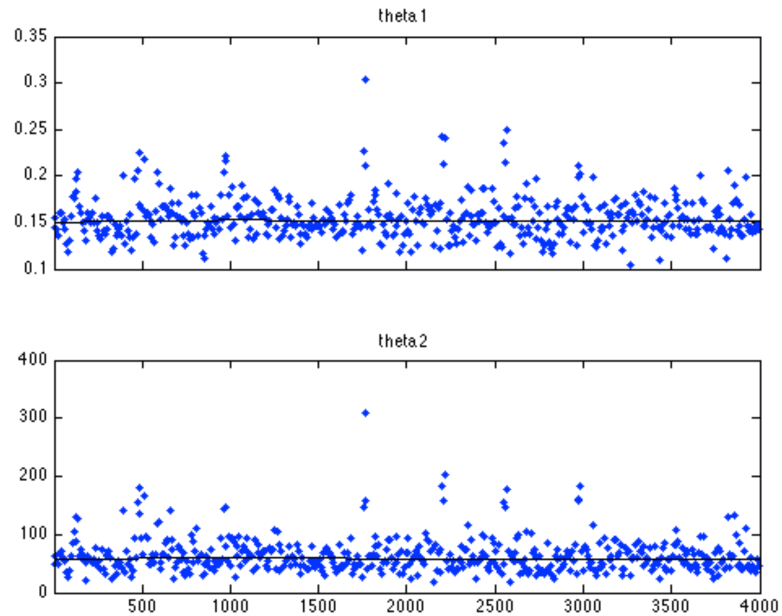
```
[res,chain,s2chain] = mcmcrun(model,data,params,options);
```

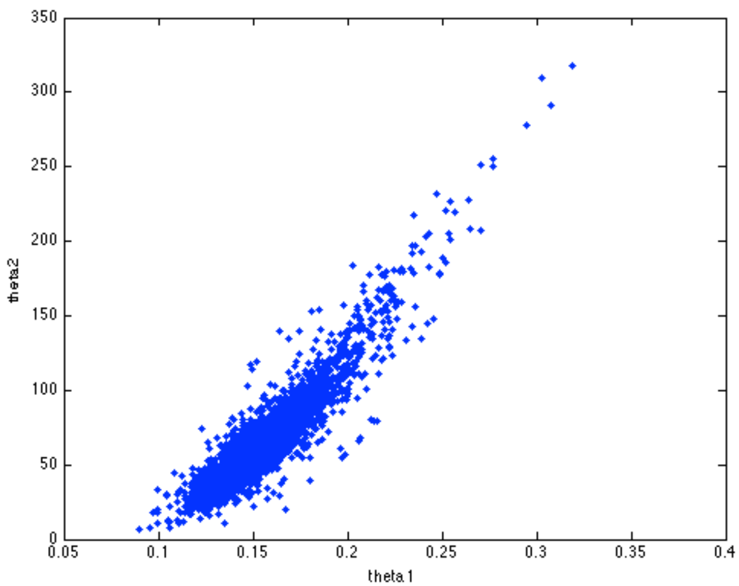


Delayed Rejection Adaptive Metropolis

Plot results

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





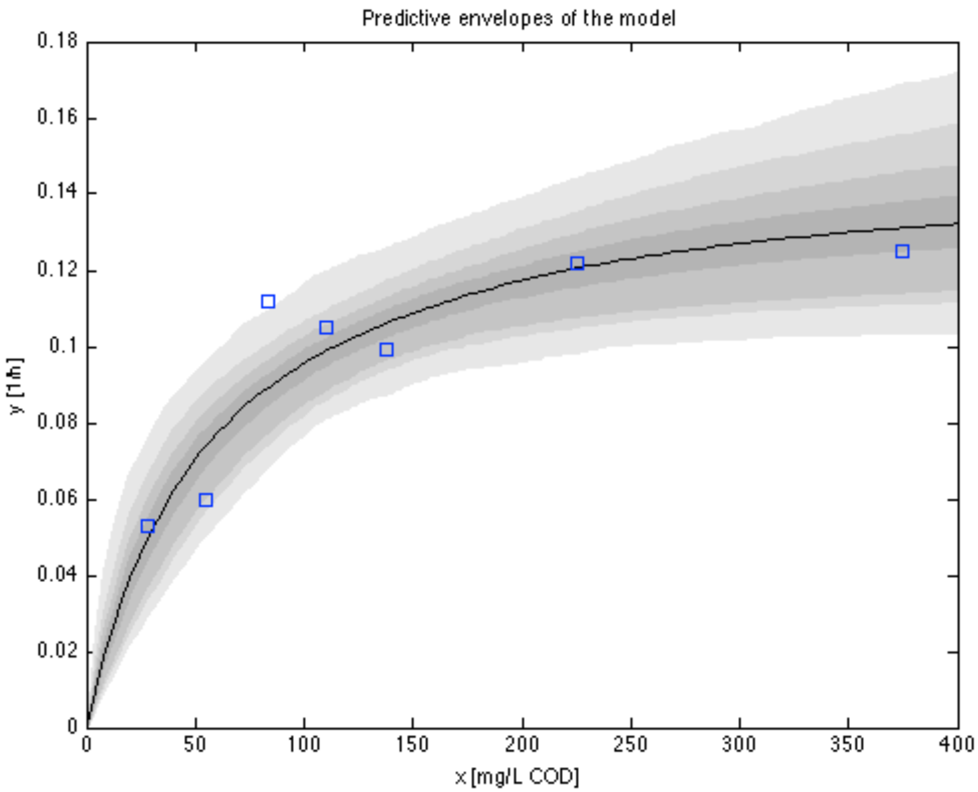
Examples:

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

Delayed Rejection Adaptive Metropolis

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')
```



SA/UQ for Dittus-Boelter Relation

Dittus-Boelter Relation:

$$Nu = 0.023 Re^{0.8} Pr^{0.4}$$

Nu: Nusselt number
Re: Reynolds number
Pr: Prandtl number

Recall: Sensitivity and Fisher matrices

$$\chi(q^*) = \begin{bmatrix} \frac{\partial Nu}{\partial q_1}(Re_1, Pr_1, q^*) & & \frac{\partial Nu}{\partial q_3}(Re_1, Pr_1, q^*) \\ \vdots & \cdots & \vdots \\ \frac{\partial Nu}{\partial q_1}(Re_N, Pr_N, q^*) & & \frac{\partial Nu}{\partial q_3}(Re_N, Pr_N, q^*) \end{bmatrix}$$

$$F = \chi^T \chi$$

Note: Can analytically compute sensitivities

$$\frac{\partial Nu}{\partial q_1} = Re^{q_2} Pr^{q_3}$$

$$\frac{\partial Nu}{\partial q_2} = q_1 Re^{q_2} Pr^{q_3} \ln(Re)$$

$$\frac{\partial Nu}{\partial q_3} = q_1 Re^{q_2} Pr^{q_3} \ln(Pr).$$

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$$F = \chi^T \chi$$

MATLAB Codes:

- DB_dram.m
- dbss.m
- Codes in MCMC_STAT

Step 0: Set Path in MATLAB subdirectory to include MCMC_STAT

SA/UQ for Dittus-Boelter Relation

Step 1: Open DB_dram.m in editor and familiarize yourself with following:

- Data structures for inputs
- Construction of Fisher information and covariance matrix
- Parameter representations and specification of MCMC inputs

Step 2:

- Run DB_dram with default values including the optimized parameter values q = [0.0045, 0.98, 0.4]
- Are the three parameters correlated and are any of the pairwise plots single-valued?
- Use the command *eig(Fisher)* to compute the eigenvalues of the Fisher information to determine if all there parameters are identifiable.
- Compare the histogram and kernel density estimate (KDE) for the Nusselt number at Re = 1000, Pr = 300. Specify approximately 2 standard deviations which is approximately 95% confidence.

SA/UQ for Dittus-Boelter Relation

Step 3:

- Change the nominal values to q = [0.023, 0.8, 0.4] and plot the chains before burn-in using the command *mcmcplot(chain1,[],results1,'chainpanel').* What do you observe regarding burn-in? Are your final densities the same as before?

Step 4:

- Use the commands *Re = data(26:36,1), Pr = data(26:36,2), Nu = data(26:36,3)* to use only one of the several data sets and repeat Step 2. Are the three parameters identifiable? Fix q_1 at the optimized value and modify your code to only perform Bayesian inference on q_2 and q_3. How do your results compare to those in Step 2?

Sensitivity Analysis for CTF

Note: See William Dawn's slides

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