Using MCSim on Windows

Getting C compiler and command line shell MSYS

1. Download MinGW from: https://sourceforge.net/projects/mingw/files/latest/download?source=files
2. Run the setup file mingw-get-setup.exe
3. Select the default directory for installation C:\MinGW
4. In the Installation manager
    a. Mark the "basic setup" for installation (you can click all the packages, though ada, fortran, and objc are not used)
    b. Apply changes – this will take a while
5. Go to C:\MinGW\msys\1.0\etc
    a. Remove any existing "fstab" file
    b. Copy and rename fstab.sample as fstab (without any extension)
6. Go to C:\MinGW\msys\1.0
    a. Create a shortcut for the "msys.bat" Windows batch file and put on the desktop
    b. Double click this icon, and it will give you a "unix" shell command line. The "home" directory is C:\MinGW\msys\1.0\home\[USERNAME]\

Installing basic version of MCSim (WITHOUT any libraries, such as GSL)

1. Download latest version from http://ftp.gnu.org/gnu/mcsim/ (direct link: http://ftp.gnu.org/gnu/mcsim/mcsim-5.6.5.tar.gz)
2. Move to the "home" directory C:\MinGW\msys\1.0\home\[USERNAME]\
3. Open the MSYS command line (if you haven't already) and do the following (example with version 2.1):
    - `tar –xvzf mcsim-5.6.5.tar.gz`
    - `cd mcsim-5.6.5`
4. Need to edit one of the c files in the mcsim-5.6.5\sim directory to increase the step sizes. Specifically in "lsodes1.c" change
   ```
   static long mxstp0 = 500;
   ```
   to
   ```
   static long mxstp0 = 5000;
   ```
5. Then compile the program from the MSYS command line (the last one does some checks) [make sure you are in the directory ~\mcsim-5.6.5].
    - `./configure`
    - `make`
    - `make install`
    - `make check`

Testing simple digoxin model

6. Make a directory C:\MinGW\msys\1.0\home\[USERNAME]\digoxin and copy the digoxin.mcmc.model and digoxin.mcmc.*.in files to the directory
7. From the MSYS command line, go to the directory with the model file and compile the model

- `cd ~/digoxin`
- `makemcsim digoxin.mcmc.model`

8. The new file "mcsim.digoxin" is the executable. Now run the program with test "input" file
   - `./mcsim.digoxin.mcmc digoxin.mcmc.1.in`

   This should create the output file: digoxin.mcmc.1.out

   Do the same with the other three chains (they have a different random seed)

   - `./mcsim.digoxin.mcmc digoxin.mcmc.2.in`
   - `./mcsim.digoxin.mcmc digoxin.mcmc.3.in`
   - `./mcsim.digoxin.mcmc digoxin.mcmc.4.in`

   Now you have 4 ".out" files with which you can evaluate convergence and model fit!

9. Quick check of model fit – taking the last iteration from `digoxin.mcmc.1.out` and computing prediction vs. data
   - `./mcsim.digoxin.mcmc digoxin.mcmc.check.in`

   The resulting file `digoxin.mcmc.check.out` has a row for each data point along with its predicted value. The "in" file can be modified to take the last iteration from any "out" file.

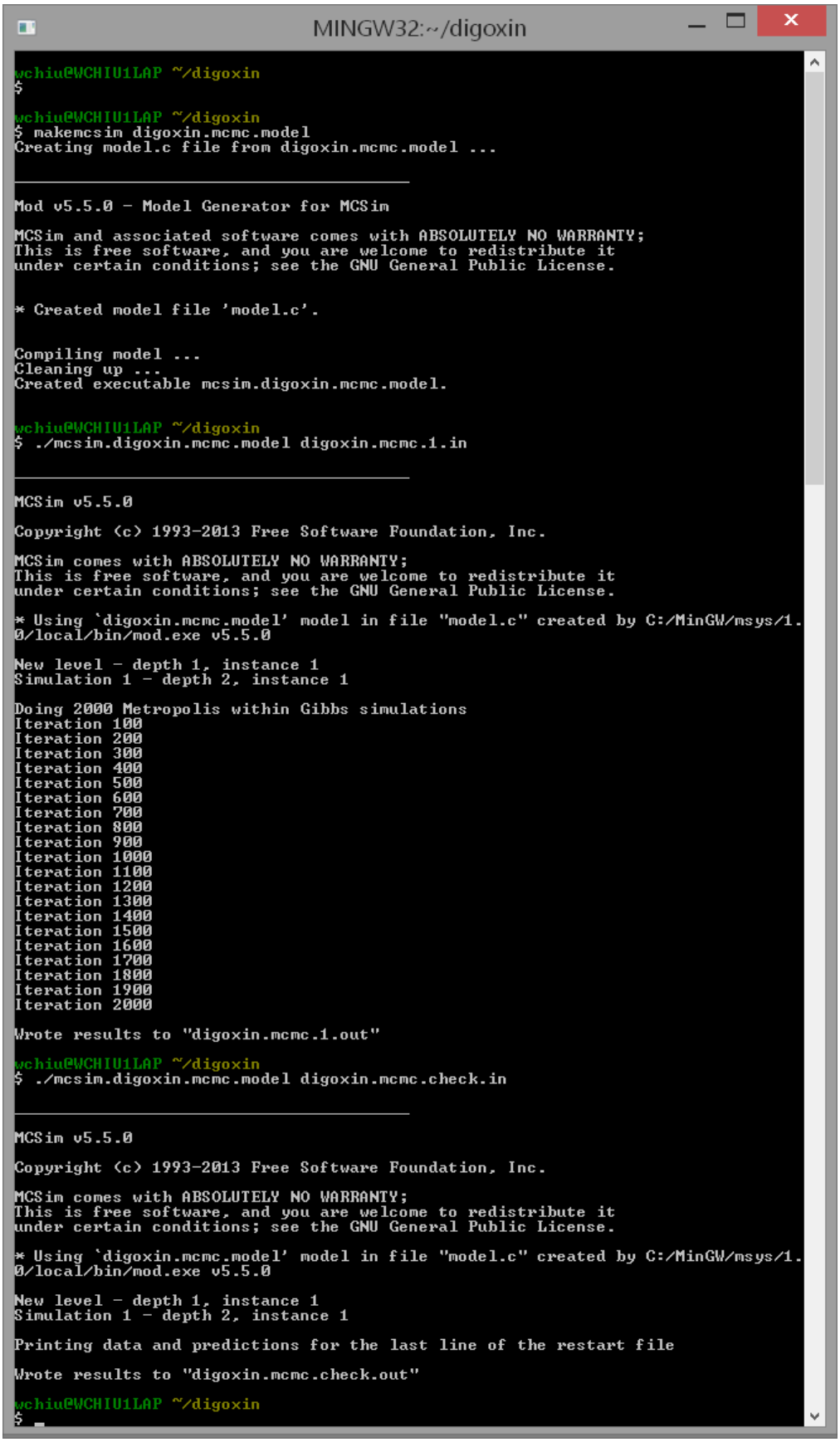
   - `./mcsim.digoxin.mcmc.1.out digoxin.mcmc.check.in`

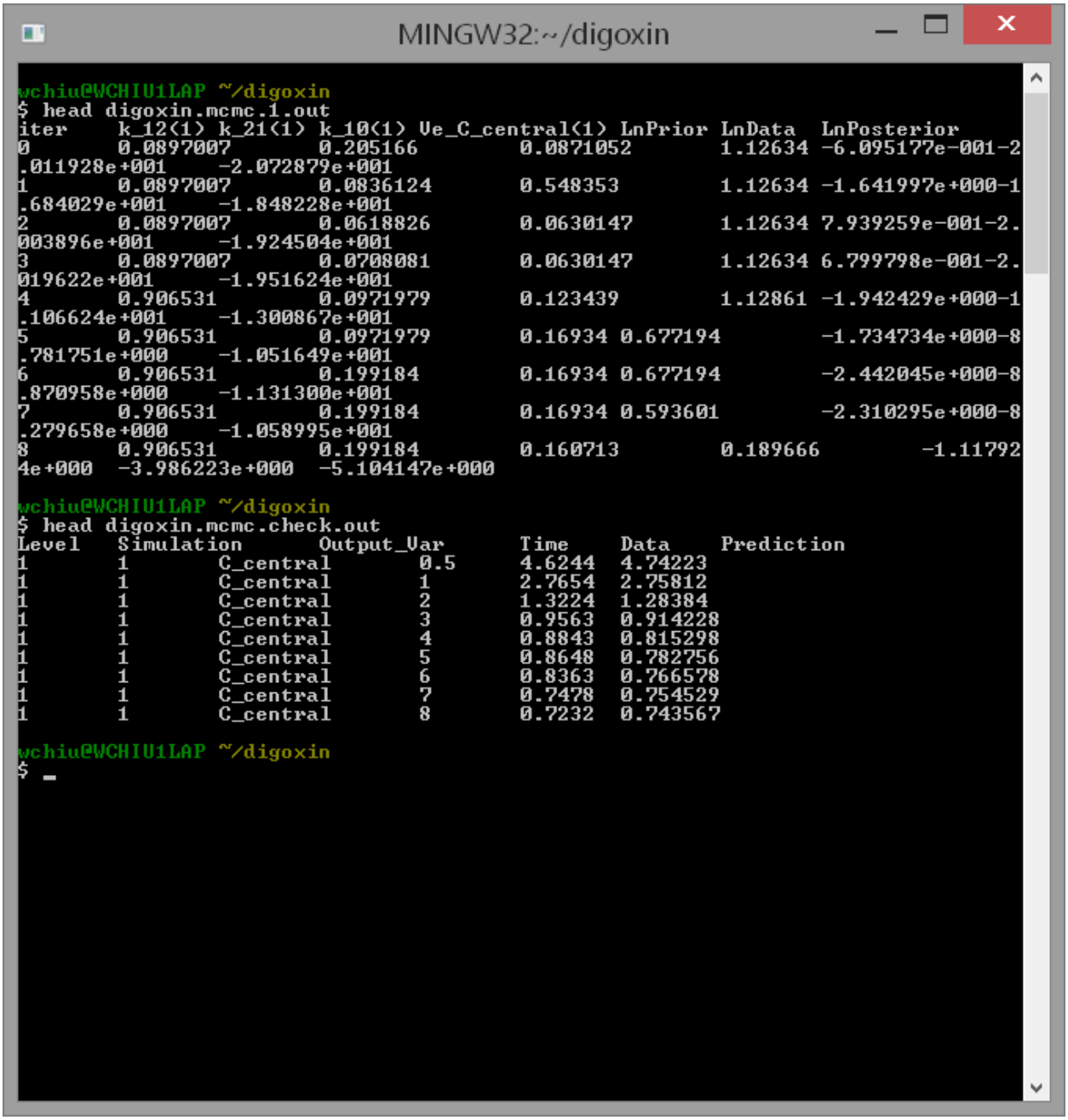
10. Calculate distribution of model predictions – taking all the iterations from `digoxin.mcmc.1.out` and computing prediction
    - `./mcsim.digoxin digoxin.mcmc.setpoints.in`

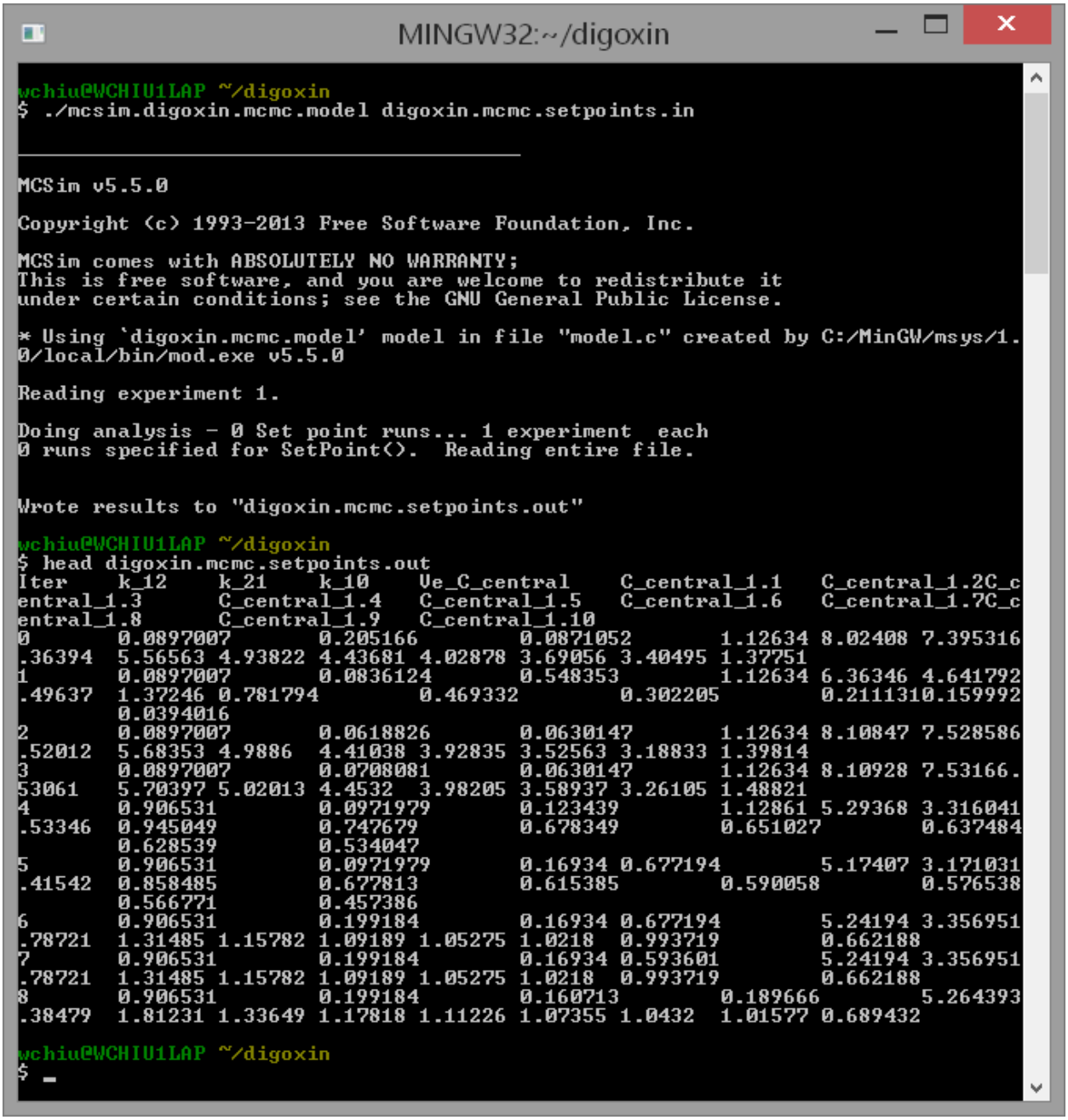
    The resulting file `digoxin.mcmc.setpoints.out` has a row for each iteration. Each row contains the parameters and all the predictions specified. For instance, C_central_1.1 is the prediction for the first timepoint, whereas C_central_1.10 is the prediction for the 10^{th} timepoint.

Exercises:

- Use R or some other appropriate software (NOT Excel) to compare the data with model predictions as a function of time.
  - A single prediction
  - The distribution of model predictions (e.g., median, inter-quartile, 95% CI).
- Currently, the setpoints file outputs the predictions at only at the time points where there are data. Typically, we want figures that show a "smooth curve" to compare with the data. Modify the setpoints file so that it outputs a "smoother" time course – and show both a single prediction as well as the distribution of predictions.


MINGW32:~/digoxin
wchiu@WCHIU1LAP ~/digoxin
$
wchiu@WCHIU1LAP ~/digoxin
$ makemcsim digoxin.mcmc.model
Creating model.c file from digoxin.mcmc.model ...
Mod v5.5.0 - Model Generator for MCSim
MCSim and associated software comes with ABSOLUTELY NO WARRANTY;
This is free software, and you are welcome to redistribute it
under certain conditions; see the GNU General Public License.
* Created model file 'model.c'.
Compiling model ...
Cleaning up ...
Created executable mcsim.digoxin.mcmc.model.
wchiu@WCHIU1LAP ~/digoxin
$ ./mcsim.digoxin.mcmc.model digoxin.mcmc.1.in
MCSim v5.5.0
Copyright (c) 1993-2013 Free Software Foundation, Inc.
MCSim comes with ABSOLUTELY NO WARRANTY;
This is free software, and you are welcome to redistribute it
under certain conditions; see the GNU General Public License.
* Using `digoxin.mcmc.model' model in file "model.c" created by C:/MinGW/msys/1.
0/local/bin/mod.exe v5.5.0
New level - depth 1, instance 1
Simulation 1 - depth 2, instance 1
Doing 2000 Metropolis within Gibbs simulations
Iteration 100
Iteration 200
Iteration 300
Iteration 400
Iteration 500
Iteration 600
Iteration 700
Iteration 800
Iteration 900
Iteration 1000
Iteration 1100
Iteration 1200
Iteration 1300
Iteration 1400
Iteration 1500
Iteration 1600
Iteration 1700
Iteration 1800
Iteration 1900
Iteration 2000
Wrote results to "digoxin.mcmc.1.out"
wchiu@WCHIU1LAP ~/digoxin
$ ./mcsim.digoxin.mcmc.model digoxin.mcmc.check.in
MCSim v5.5.0
Copyright (c) 1993-2013 Free Software Foundation, Inc.
MCSim comes with ABSOLUTELY NO WARRANTY;
This is free software, and you are welcome to redistribute it
under certain conditions; see the GNU General Public License.
* Using `digoxin.mcmc.model' model in file "model.c" created by C:/MinGW/msys/1.
0/local/bin/mod.exe v5.5.0
New level - depth 1, instance 1
Simulation 1 - depth 2, instance 1
Printing data and predictions for the last line of the restart file
Wrote results to "digoxin.mcmc.check.out"
wchiu@WCHIU1LAP ~/digoxin
$


MINGW32:~/digoxin
wchiu@WCHIU1LAP ~/digoxin
$ head digoxin.mcmc.1.out
iter k_12(1) k_21(1) k_10(1) Ve_C_central(1) LnPrior LnData LnPosterior
0 0.0897007 0.205166 0.0871052 1.12634 -6.095177e-001-2
.011928e+001 -2.072879e+001
1 0.0897007 0.0836124 0.548353 1.12634 -1.641997e+000-1
.684029e+001 -1.848228e+001
2 0.0897007 0.0618826 0.0630147 1.12634 7.939259e-001-2.
003896e+001 -1.924504e+001
3 0.0897007 0.0708081 0.0630147 1.12634 6.799798e-001-2.
019622e+001 -1.951624e+001
4 0.906531 0.0971979 0.123439 1.12861 -1.942429e+000-1
.106624e+001 -1.300867e+001
5 0.906531 0.0971979 0.16934 0.677194 -1.734734e+000-8
.781751e+000 -1.051649e+001
6 0.906531 0.199184 0.16934 0.677194 -2.442045e+000-8
.870958e+000 -1.131300e+001
7 0.906531 0.199184 0.16934 0.593601 -2.310295e+000-8
.279658e+000 -1.058995e+001
8 0.906531 0.199184 0.160713 0.189666 -1.11792
4e+000 -3.986223e+000 -5.104147e+000
wchiu@WCHIU1LAP ~/digoxin
$ head digoxin.mcmc.check.out
Level Simulation Output_Var Time Data Prediction
1 1 C_central 0.5 4.6244 4.74223
1 1 C_central 1 2.7654 2.75812
1 1 C_central 2 1.3224 1.28384
1 1 C_central 3 0.9563 0.914228
1 1 C_central 4 0.8843 0.815298
1 1 C_central 5 0.8648 0.782756
1 1 C_central 6 0.8363 0.766578
1 1 C_central 7 0.7478 0.754529
1 1 C_central 8 0.7232 0.743567
wchiu@WCHIU1LAP ~/digoxin
$


MINGW32:~/digoxin
wchiu@WCHIU1LAP ~/digoxin
$ ./mcsim.digoxin.mcmc.model digoxin.mcmc.setpoints.in
MCSim v5.5.0
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MCSim comes with ABSOLUTELY NO WARRANTY;
This is free software, and you are welcome to redistribute it
under certain conditions; see the GNU General Public License.
* Using `digoxin.mcmc.model' model in file "model.c" created by C:/MinGW/msys/1.0/local/bin/mod.exe v5.5.0
Reading experiment 1.
Doing analysis - 0 Set point runs... 1 experiment each
0 runs specified for SetPoint(). Reading entire file.
Wrote results to "digoxin.mcmc.setpoints.out"
wchiu@WCHIU1LAP ~/digoxin
$ head digoxin.mcmc.setpoints.out
Iter k_12 k_21 k_10 Ve_C_central C_central_1.1 C_central_1.2C_central_1.3 C_central_1.4 C_central_1.5 C_central_1.6 C_central_1.7C_central_1.8 C_central_1.9 C_central_1.10
0 0.0897007 0.205166 0.0871052 1.12634 8.02408 7.39531 6.36394 5.56563 4.93822 4.43681 4.02878 3.69056 3.40495 1.37751
1 0.0897007 0.0836124 0.548353 1.12634 6.36346 4.64179 2.49637 1.37246 0.781794 0.469332 0.302205 0.211131 0.159992 0.0394016
2 0.0897007 0.0618826 0.0630147 1.12634 8.10847 7.52858 6.52012 5.68353 4.9886 4.41038 3.92835 3.52563 3.18833 1.39814
3 0.0897007 0.0708081 0.0630147 1.12634 8.10928 7.53166. 6.53061 5.70397 5.02013 4.4532 3.98205 3.58937 3.26105 1.48821
4 0.906531 0.0971979 0.123439 1.12861 5.29368 3.31604 1.53346 0.945049 0.747679 0.678349 0.651027 0.637484 0.628539 0.534047
5 0.906531 0.0971979 0.16934 0.677194 5.17407 3.17103 1.41542 0.858485 0.677813 0.615385 0.590058 0.576538 0.566771 0.457386
6 0.906531 0.199184 0.16934 0.677194 5.24194 3.35695 1.78721 1.31485 1.15782 1.09189 1.05275 1.0218 0.993719 0.662188
7 0.906531 0.199184 0.16934 0.593601 5.24194 3.35695 1.78721 1.31485 1.15782 1.09189 1.05275 1.0218 0.993719 0.662188
8 0.906531 0.199184 0.160713 0.189666 5.26439 3.38479 1.81231 1.33649 1.17818 1.11226 1.07355 1.0432 1.01577 0.689432
wchiu@WCHIU1LAP ~/digoxin
$