Work Log for November XXth-XXth

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November 13, 2014

1 Goals for the Week

1. RC example
2. Load external R packages, use them with RC

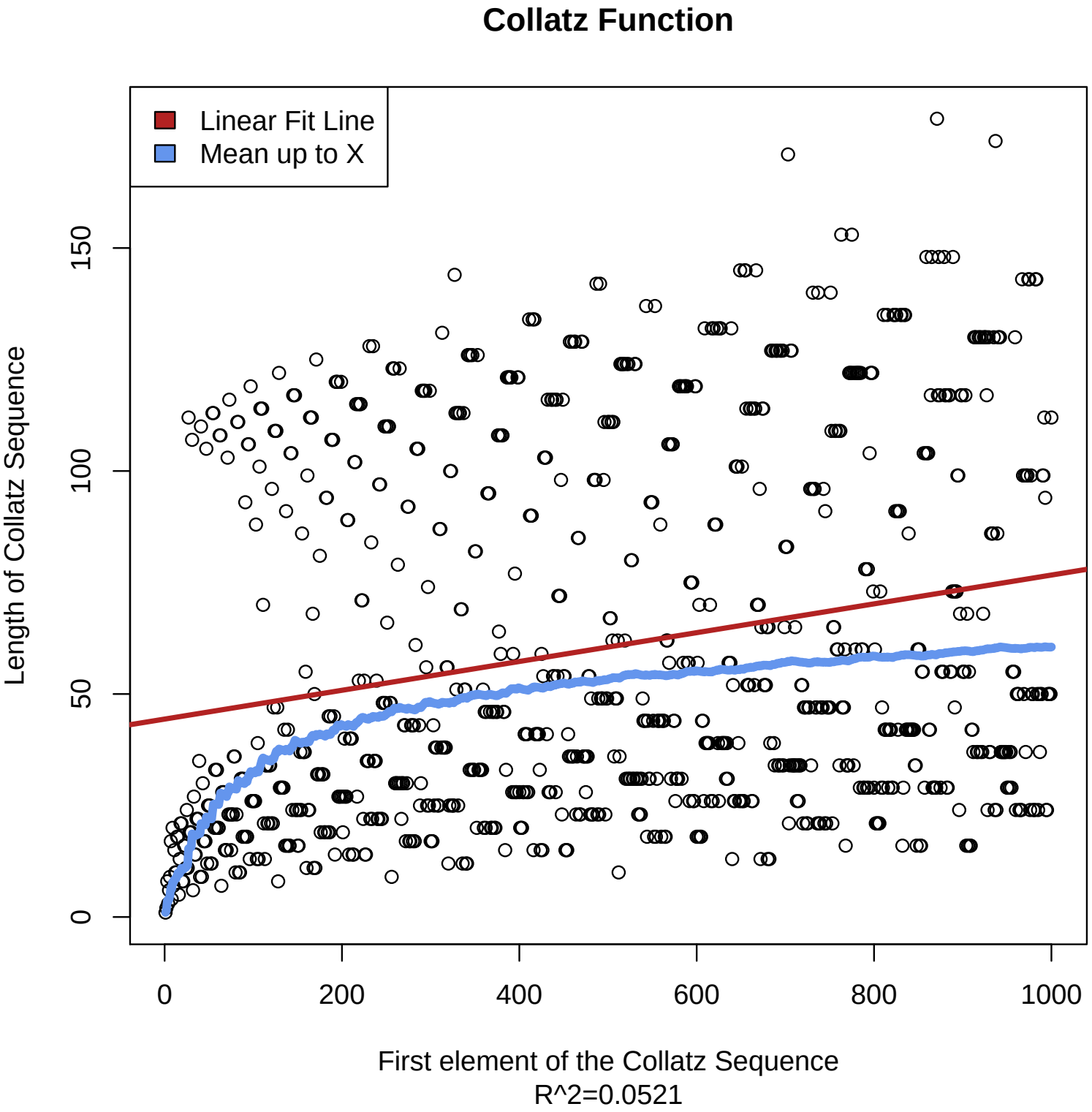
2 Progress/Notes

2.1 RC example

The RC example calculates the line of best fit for the collatz length of 1 to 1000. Here's how the output will typically look

```
[lbrown@star1 RC]$ make exec
../../EXTLIB/MPICH/mpich-shared/bin/mpirun -n 1 ./driver RCcar.cfg
Initializing the executive...
rank 0 going to statically run 'RC'
Executing --file=script.r
Line of Best Fit: y=0.0322921x + 44.3798
Standard Deviation = 40.87291
Graph written to CollatzGraph.pdf
Data written to CollatzData.csv
```

And here's CollatzGraph.pdf.


Collatz Function
Linear Fit Line
Mean up to X
Length of Collatz Sequence
0
50
100
150
0
200
400
600
800
1000
First element of the Collatz Sequence
R^2=0.0521

2.2 Load external R packages, use them with RC

2.3 Documentation

2.3.1 Document the RC car

Just comment the code

Added in a section at the beginning describing the code.

```
/*****************************************************************
 * Written by Logan Brown
 * NICS and UTK, 2014
 *
 * This code defines an IEL module function that executes 'script.r'
 * using the R language interpreter. Script.r must be placed in the
 * directory where the driver code is executed.
 *
 * iel-2.0/CASES/RC has an example using the Collatz Conjecture
 *
*****************************************************************/
```

And added a similar section to the R script

```
###############################################################################
# Script written by Logan Brown
# NICS and UT Knoxville, 2014
# This script finds the length the sequences generated by the following rule
#
#    Let a_0 be an integer. For all n > 0
#       a_(n+1) = (a_n)/2        if a_n is even;
#       a_(n+1) = 3(a_n) + 1     if a_n is odd and a_n != 1
#    When a_n = 1 the sequence stops (otherwise it cycles 1, 4, 2, 1, 4...)
#
# The script finds the length of these sequences for the first 1000 inputs
# by default, with the number of inputs determined by "number". It then
# finds a line of best fit for the increasing sequence length, and gets
# the standard deviation of the sequence lengths.
# It also writes out the calculated data to a file, and generates a graph.
###############################################################################
```

2.3.2 Ising Model

Write up a paragraph on the Ising Model – Done. See Ising.pdf

The Ising Model is basic thermodynamics model made up of 1-dimensional unit vectors calls "spins", existing on a 2 dimensional or 3 dimensional lattice. These spins (microstates) interact on each other in a quantifiable way which varies with temperature. We can measure the energy, magnetization, and heat capacity of the macrostate based on these interactions of the microstates. Our code evenly partitions the range of temperatures, then gives each process a temperature. Each process then uses Markov Chain Monte Carlo methods to approximate the distribution, using acceptance probability $\min\{1, e^{-\beta\Delta H}\}; \beta = \frac{1}{k_B T}$, where T is the temperature. The problem is that at low temperatures, the model is very likely to get stuck in an energy minimum. The solution is to use replica exchanges, to exchange data at high temperatures with data at lower temperatures.

http://jics.utk.edu/files/images/csure-reu/PDF-REPORT/Cheung-Zhao.pdf

2.4 Read through paper for Kwai

I made some notes. Do we want to talk about Kraken?

3 Goals for next Week

1. PSUADE
2. DAKOTA
3. Further documentation?