Markov Chain Monte Carlo

One of the first topics we studied in this course was fitting parameters using a general least squares method. However, the algorithms we developed are applicable to only systems in which the parameters appear linearly. In addition, once the number of parameters increases even for linear systems, the matrices become computationally expensive to handle.

With this next project you will non-linear parameter fitting[1] using the Metropolis[2] algorithm to implement a Markov Chain Monte Carlo[3] fitting of parameters to models. This project will consist of two parts. In the first section, each team will be given unique set of discrete data obtained from a physical system that is modeled in a particular way. I will assign the data/model to each group. You are to use the Metropolis algorithm to estimate the parameters along with the uncertainties in those parameters. In the second part, you will read the article and write a 2–5 sentence reflection focusing on the question of whether randomness can serve to mitigate a moral decision.

The delivarables for this project are:

(1) A basic description of the physical system, if any.

(2) The `MatLab` code for each section.

(3) A PowerPoint presentation in which results are presented. All results should include any associated estimates of the goodness of fits, etc.

(4) A short narrative reflecting on

  (i) What were the key concepts you learned from this project

  (ii) What were the most difficult obstacles to overcome

  (iii) What parts of the project were most completely addressed, which were not, and why you felt that.

  (iv) What more would you like to learn about this topic.

  (v) A 2–5 sentence reflection on the article on randomness and moral decisions.

The following rubric will be used to assess your presentatiion

Content :

4. **Expert** Clear articulation and use of all the key concepts, synthesis of all results, conclusion supported by results
3. **Proficient** A general sense and use of key concepts, synthesis of key results, conclusion supported by results
2. **Almost Proficient** Some key results or synthesis omitted, conclusion not entirely supported by results
1. **Developing** Most of the key results not included, little to no synthesis, conclusion not supported by results

Communication and Organization :

4. **Expert** Oral presentation had clear organization, and each part was effectively and concisely delivered
3. **Proficient** Oral presentation had clear organization, was easy to follow, and included relevant information
2. **Almost Proficient** Oral presentation had some organization but was somewhat difficult to follow (e.g., too detailed, too general, missing important sections)
1. **Developing** Oral presentation was disorganized or unclear

Visuals :

4. **Expert** Tables/graphs summarize data and/or conclusions, figures and images explained and described well, axes labled and units listed.
3. **Proficient** Most figures and images explained and described well,
2. **Almost Proficient** Visuals were of uneven quality; Labels and legends somewhat unclear, relation to conclusions not clear or not drawn from figures
1. **Developing** Visuals were confusing, unprofessional, and/or not clearly relevant

References:

[1]Haario H., Saksman E. and Tamminen J., 2005. Componentwise adaptation for high dimensional MCMC. Comput. Stat., 20(2), pages 265273.

[2]Metropolis N., Rosenbluth A.W., Rosenbluth M.N., Teller A.H. and Teller E., 1953. *Equations of State Calculations by Fast Computing Machines.* Journal of Chemical Physics, 21(6), pages 1087–1092.

[3]Brooks S., Gelman A., Jones G.L., Meng X., 2011. Handbook of Markov Chain Monte Carlo. Chapman & Hall / CRC, USA.