Improving the Robustness of Bumps using Parallel Tempering

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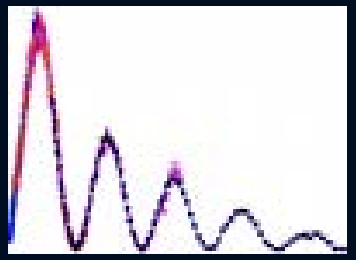
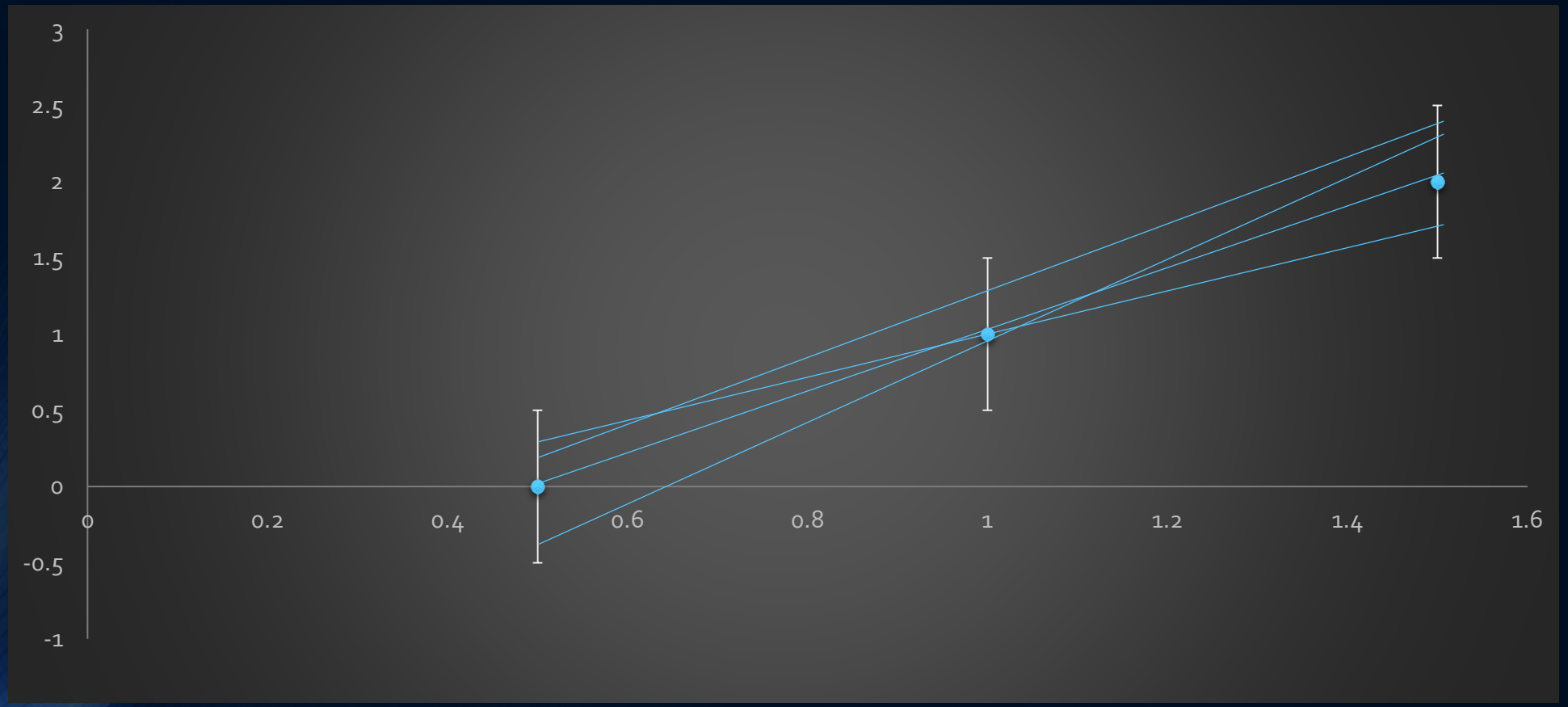
Bumps

- Data fitting and uncertainty analysis package for Python
- Takes in a set of data and an equation format
- Searches for the best parameters that will fit
- Utilized for reflectometry, small angle neutron scattering, and crystallography analysis



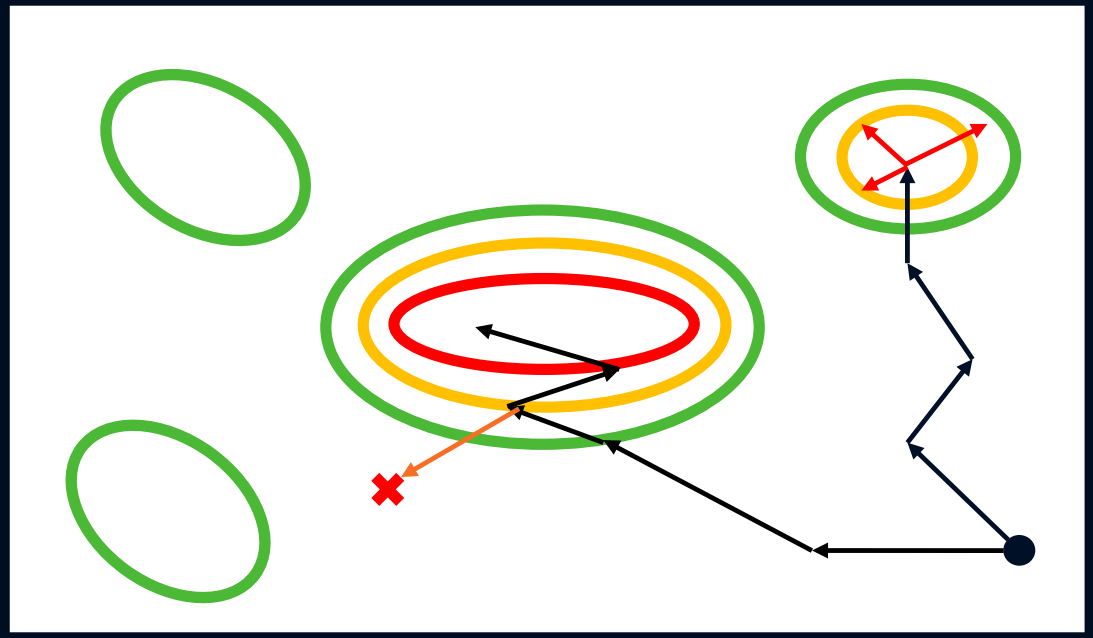
http://bumps.readthedocs.org/en/latest/_static/logo.png

Example



Markov Chain Monte Carlo

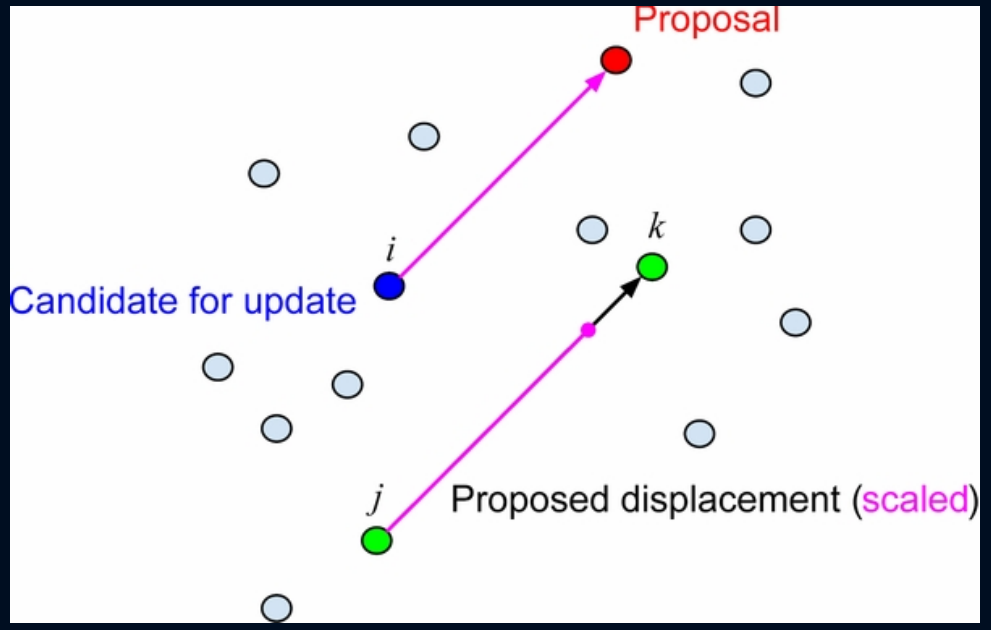
- Technique for sampling from the posterior distribution in very complex models
- **Acceptance:** $\mathrm{P} = e^{-\Delta E}$
- Problems
  - Determining step size and direction



Differential Evolution Adaptive Metropolis (DREAM)

- Runs multiple chains in parallel
- Utilizes the differential evolution metaheuristic

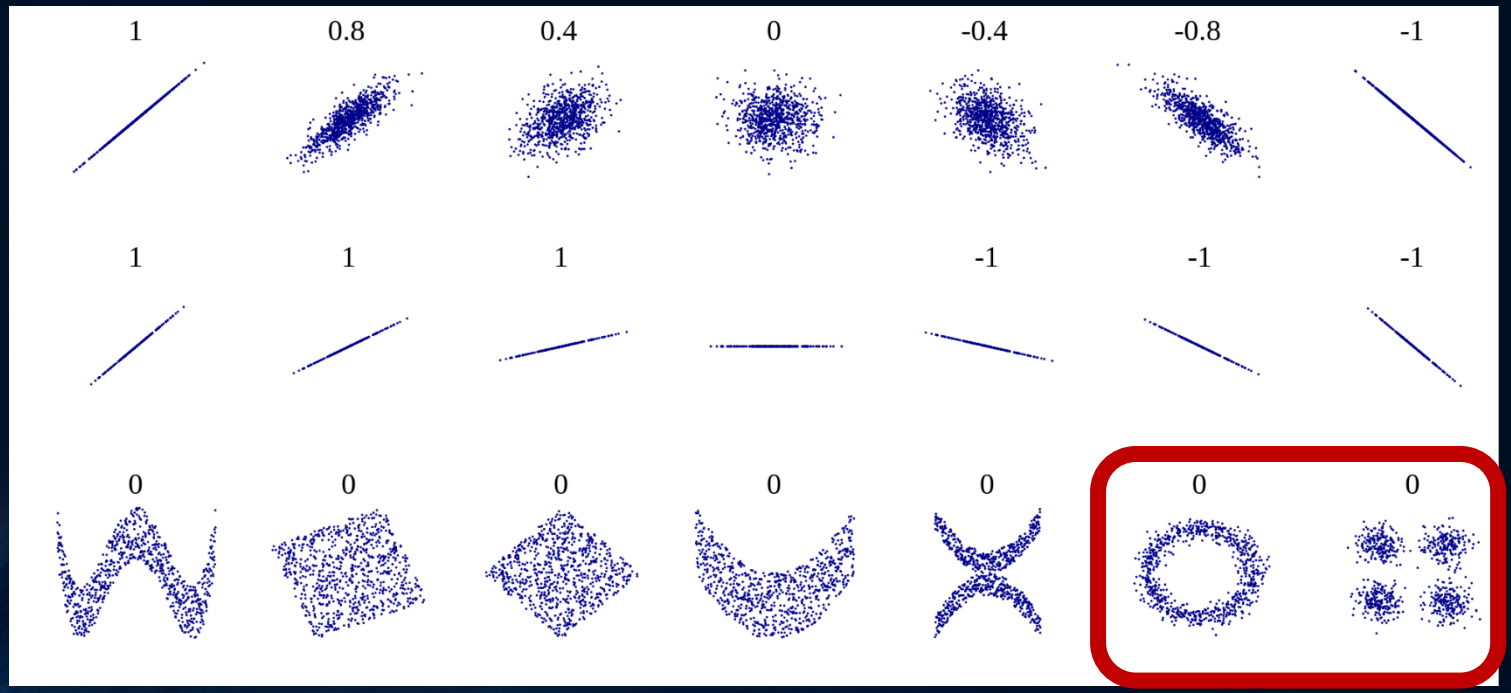
1. Take two points in the population
2. Use them to compute a vector
3. Use that vector to compute a step for a third point



http://cdn.iopscience.com/images/0067-0049/210/1/11/Full/apjs488859f1_lr.jpg

The problem

- Problems with complex distributions are slow to converge



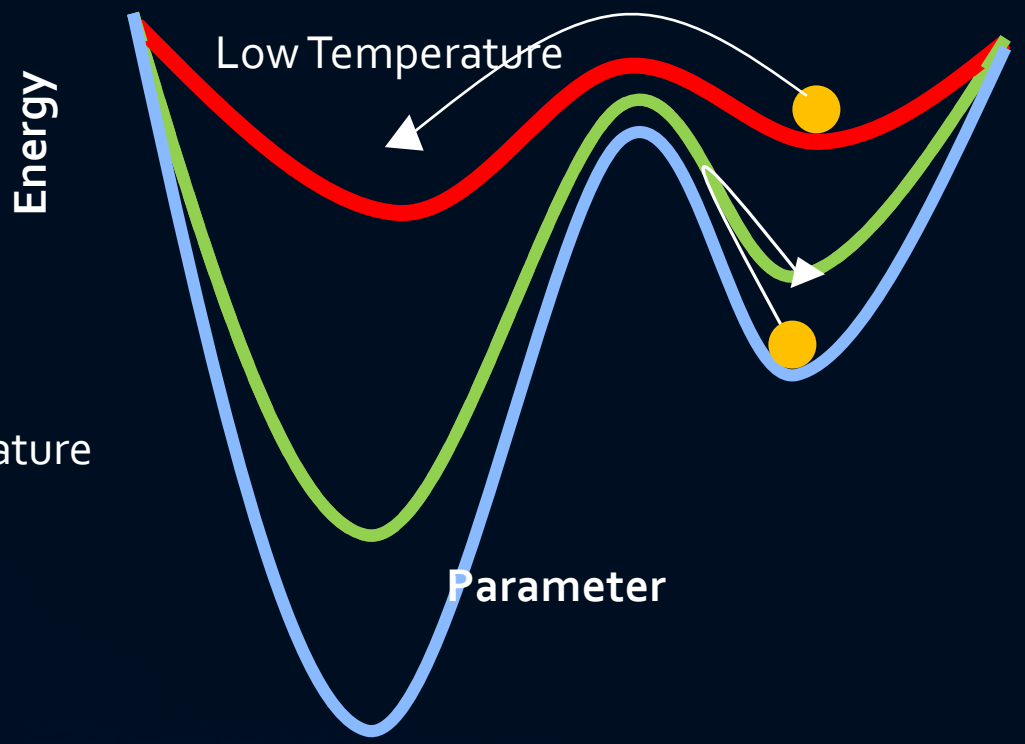
https://upload.wikimedia.org/wikipedia/commons/thumb/d/d4/Correlation_examples2.svg/2000px-Correlation_examples2.svg.png

Parallel Tempering

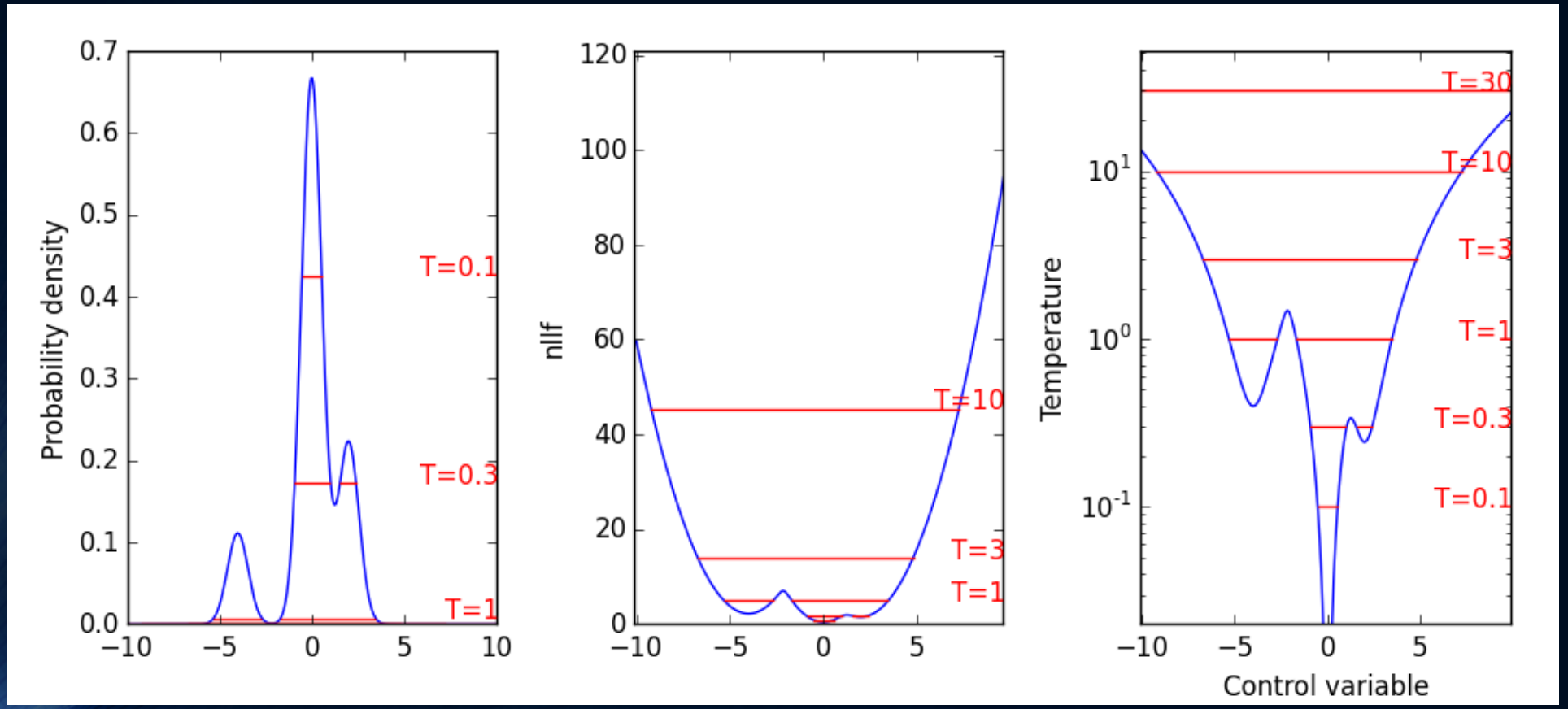
- Temperature Parameter

$$P = e^{\frac{-\Delta E}{T}}$$

- High temperatures – cover large areas
- Low temperatures – explore local minima



Example – Gaussian Mixture Model

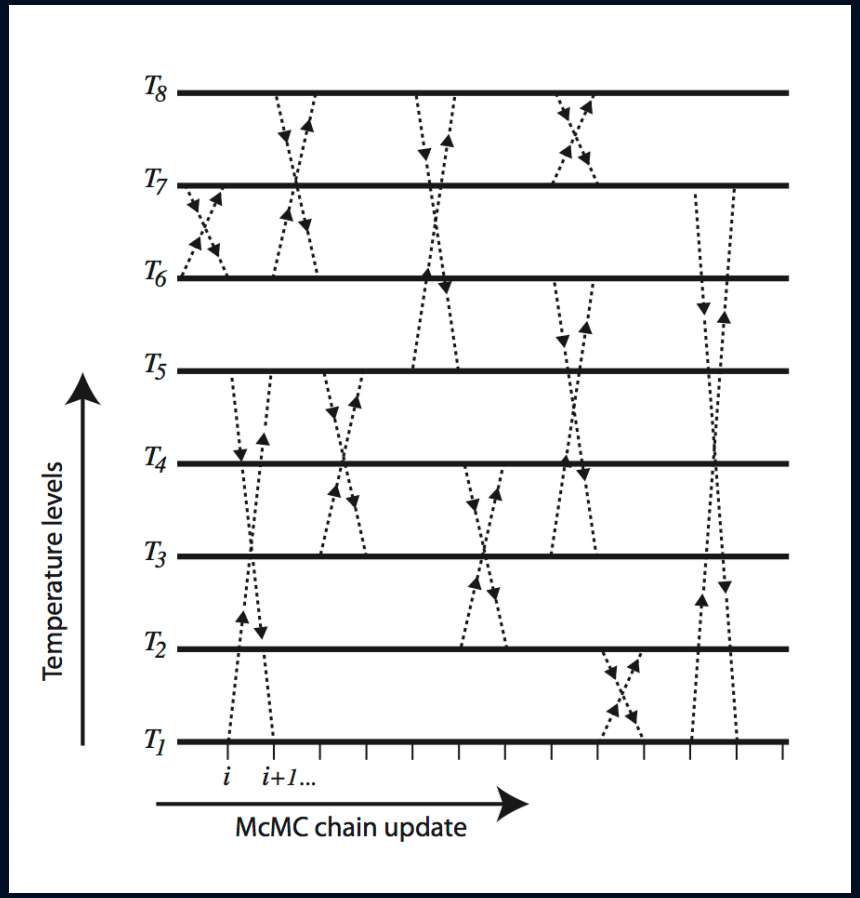


Parallel Tempering

- Multiple chains in parallel
- Chains are occasionally swapped

$$P = e^{\Delta E \Delta \beta}$$

$$\Delta\beta = \frac{1}{T_{i+1}} - \frac{1}{T_i}$$



http://www.iearth.org.au/images/PT-scheme.png

Optimizations

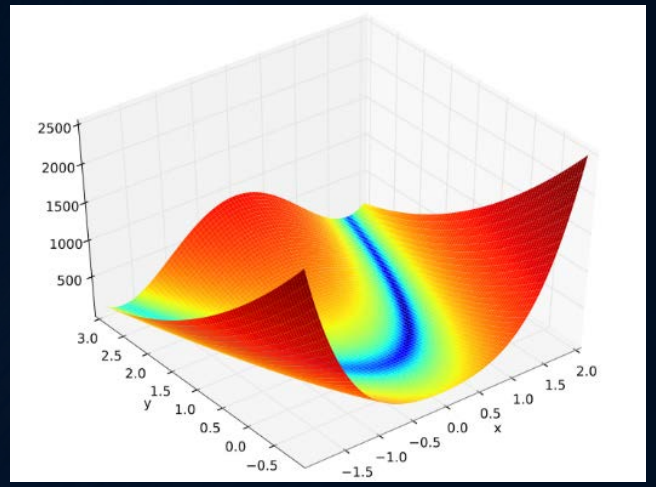
- Step Scaler
  - Holds average acceptance rate around 23.4%
  - Minimizes the step size issue
- Step Switcher
  - Switches between 3 steppers based on performance
    - DE
    - Jiggle (temperature-dependent)
    - Subspace jiggle (when chains are completely stuck)
- Dynamic Temperatures
  - Reallocate temperatures to critical levels

Tests

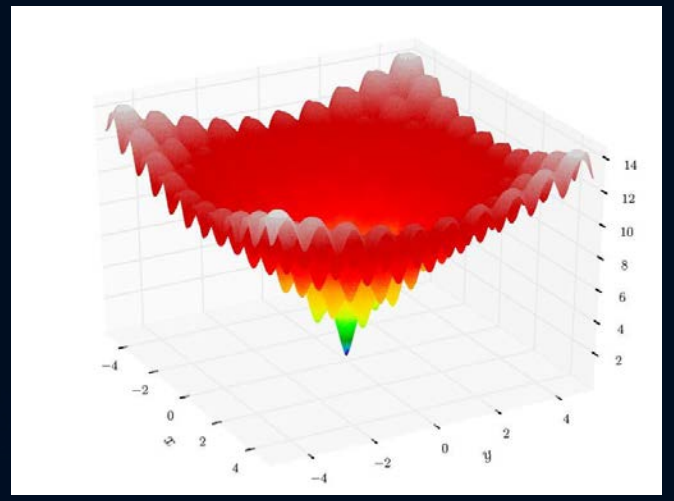
- 10 Runs
- Problems
  - Model Functions (40,000 steps)
  - Spinal Reconstruction Problems (40,000 steps)
  - Reflectivity Test Case (70,000 steps)

Testing - Model functions

- 10 parameters
- Find the global minima



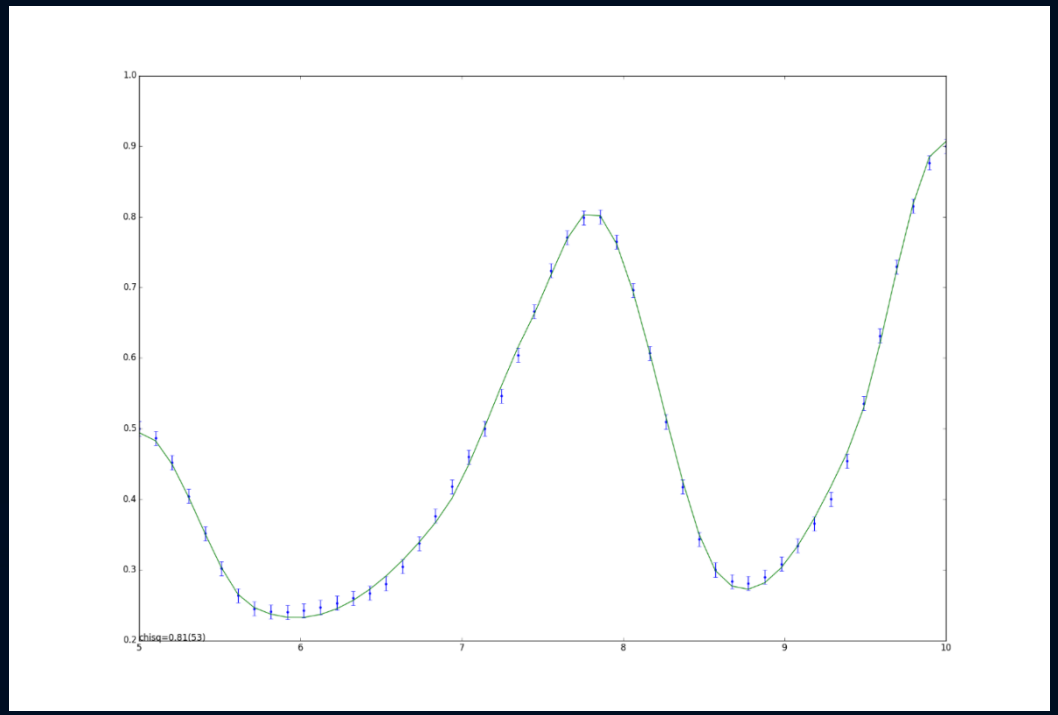
Rosenbrock Function



Ackley Function

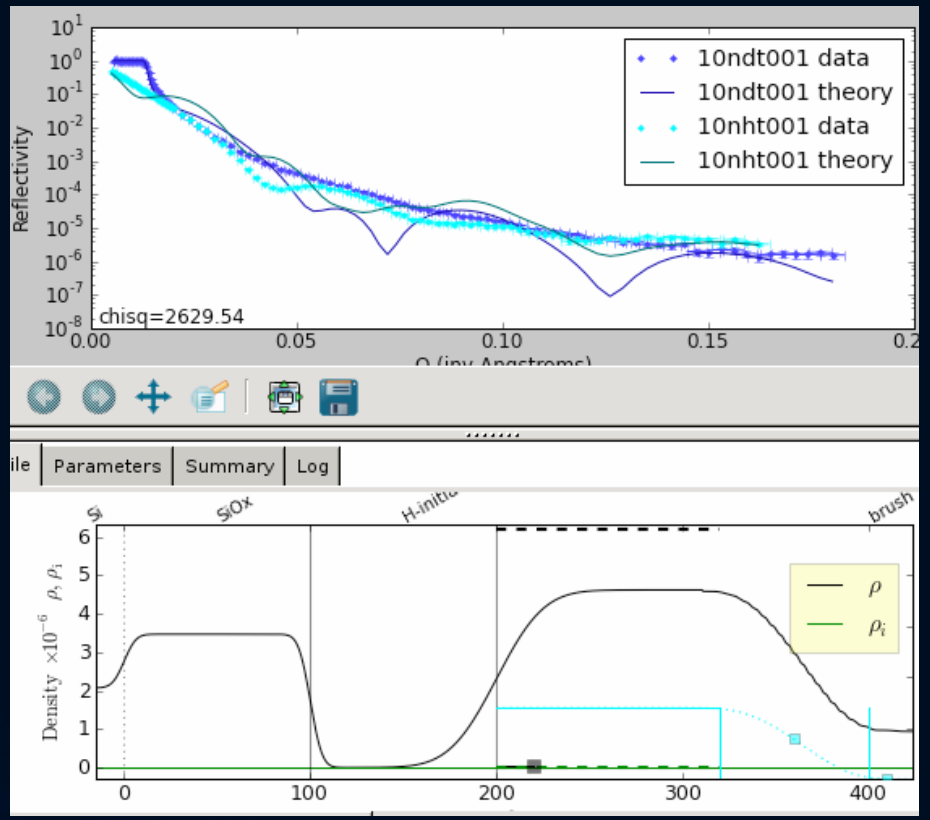
Testing - Spline Reconstruction

- 16 parameters
- Find the control points for a B-spline
- Data is randomly generated each run

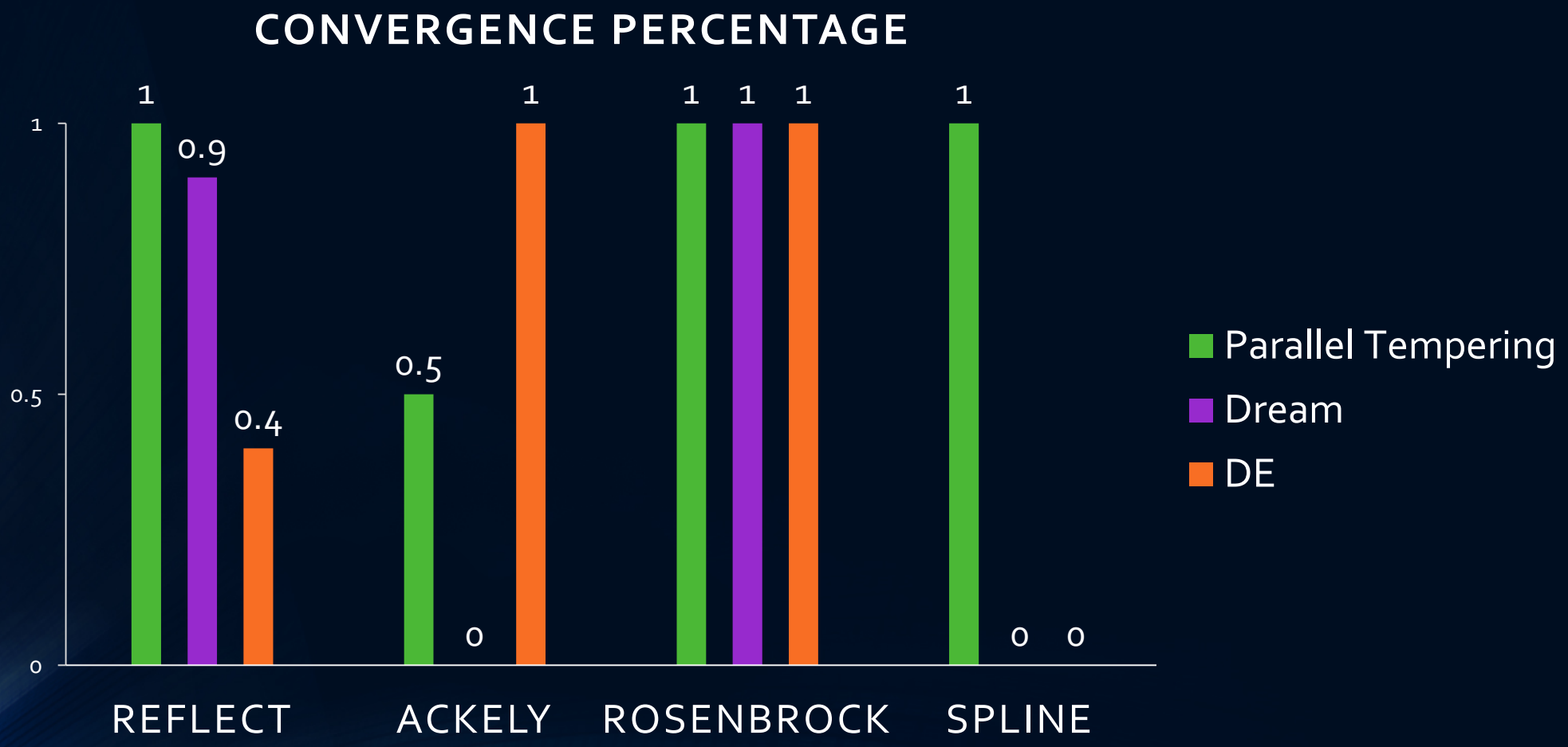


Testing – Reflectivity Analysis

- 18 parameters
- Density and Thickness of each layer



Data


CONVERGENCE PERCENTAGE
1
0.5
0
1
0.9
0.4
0.5
0
1
1
1
1
1
0
0
REFLECT
ACKELY
ROSENBROCK
SPLINE
Parallel Tempering
Dream
DE

Discussion

- Parallel Tempering performed very well in three out of the four tests
- Faltered on the Ackley Function
  - Due to large amount of local minima
- Adaptive Stepper seemed to perform well on other reflectivity problems
- No Free Lunch Theorem
  - Not one algorithm will be able to solve every problem

Future Work

- Maximum and minimum temperature adjuster
  - Increase exploration if needed
- Reweighted histograms/full implementation of MCMC
- Implementing an adaptive stepper in DREAM

Acknowledgements

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