Dynamic Temperature Markov Chain Monte Carlo Sampling Without Posterior Distribution Distortion

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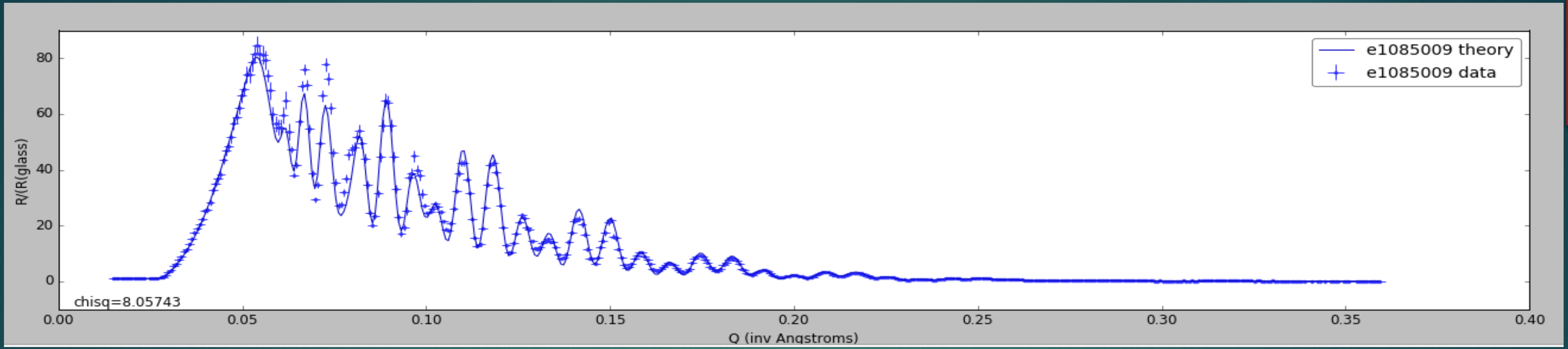
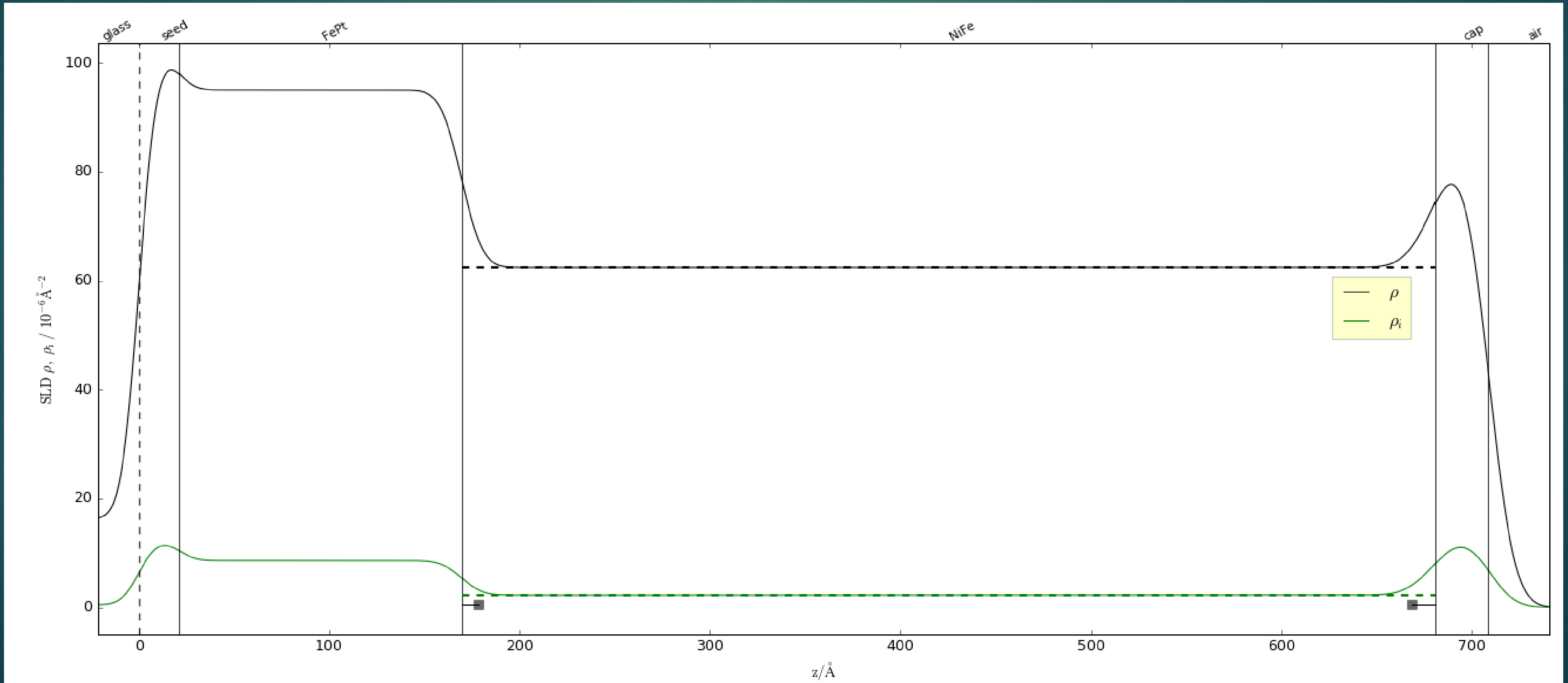
Fitting a Model

- Given data and some set of parameters **P** with a function f(**P**) meant to fit the data, Markov Chain Monte Carlo Sampling attempts to do importance sampling of the parameter space to

1) Find particular set $\mathbf{P}_i$ to fit data
2) Find confidence intervals for all parameter values



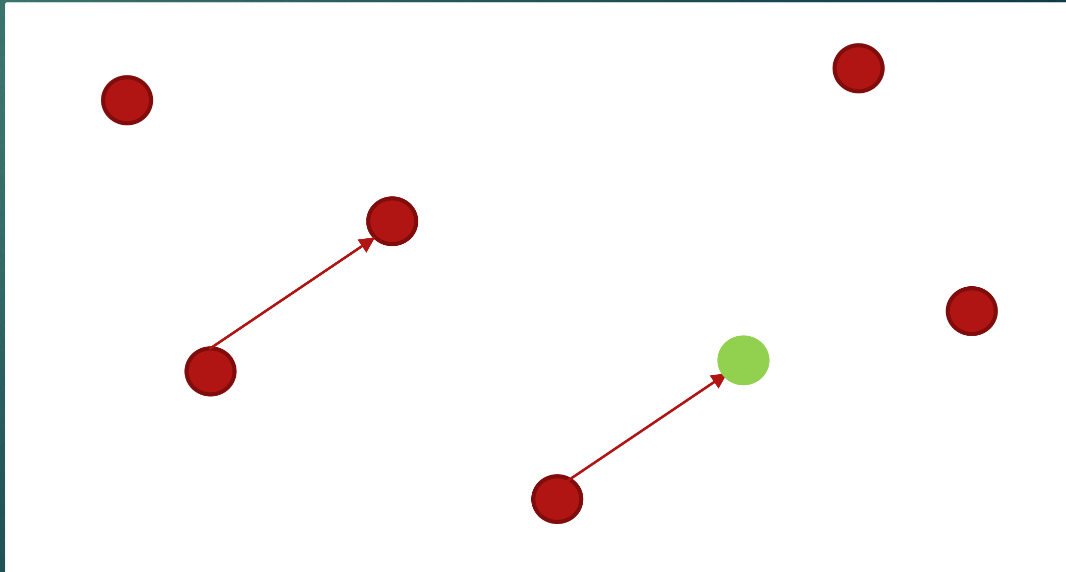
e1085009 theory
e1085009 data
R/(R(glass)
chisq=8.05743
Q (inv Angstroms)



glass
seed
FePt
NiFe
cap
air
SLD ρ, ρ_i / 10^{-6}Å^{-2}
ρ
ρ_i
z/Å

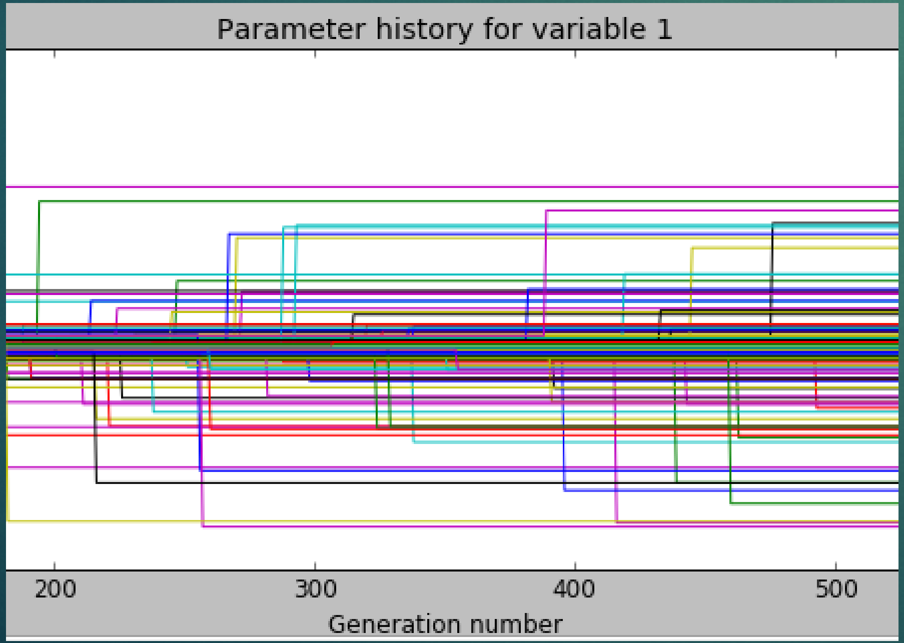
Introduction to MCMC Sampling Using Dream Algorithm

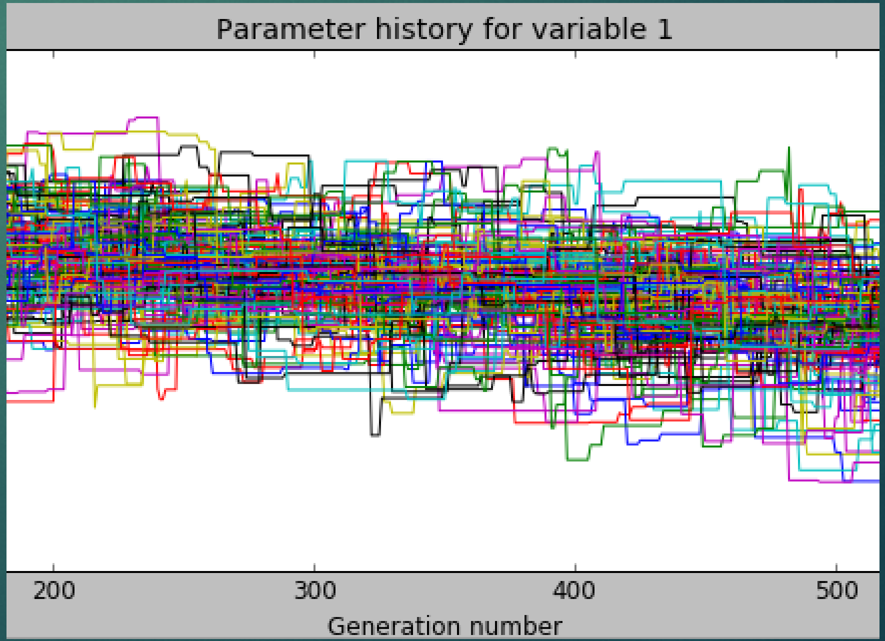
- Choose n different starting points in the parameter space
- For each point, through the DREAM algorithm a new possible point is picked
- The news points are either accepted and become the new current value for their chains. Or are rejected and then the chain value stays the same.



Problem

- Current DREAM Algorithm sometimes gets “stuck” exploring parameter space
  - No new points are accepted





Idea of Temperature: Possible Solution

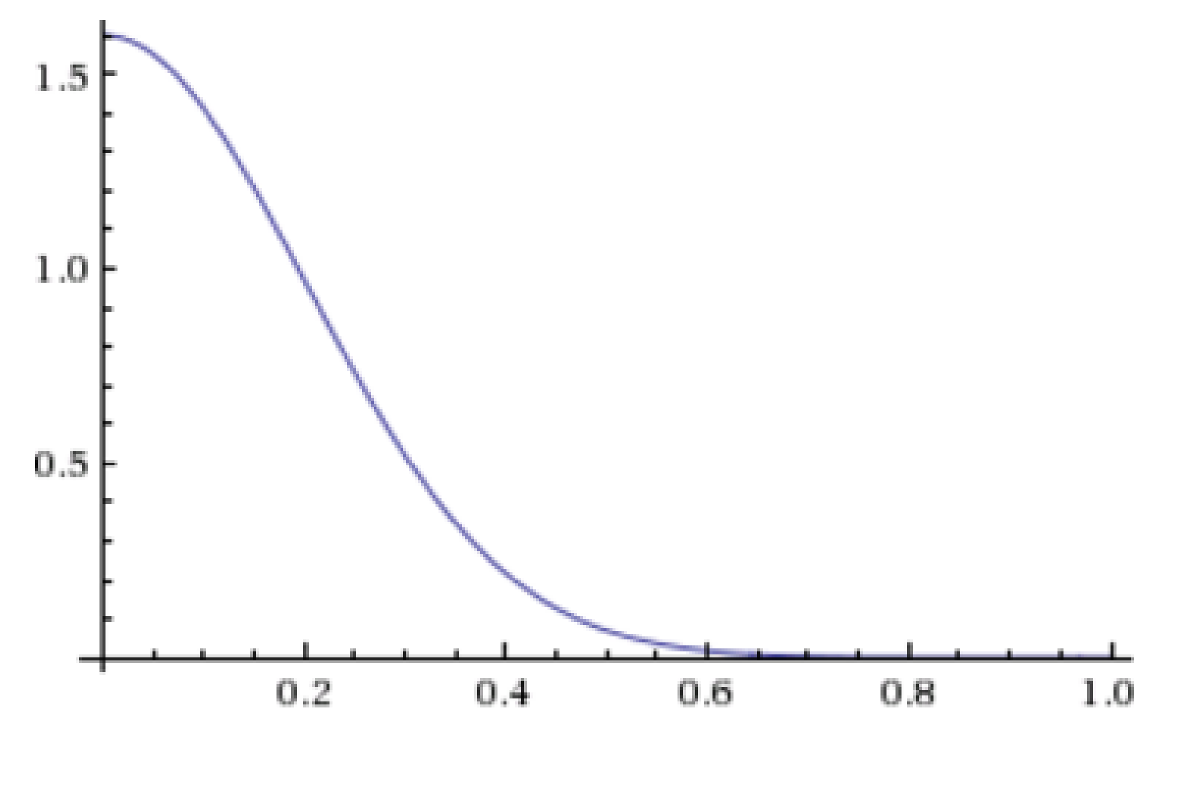
- When exploring parameter space accepts new points with probability:

$$\frac{\text{Likelihood New Point}}{\text{Likelihood Old Point}}$$

- Can multiply this by value T. High values of T will lead to more expansive exploration of the parameter space.
  - Note this is not the canonical definition of temperature for MCMC methods

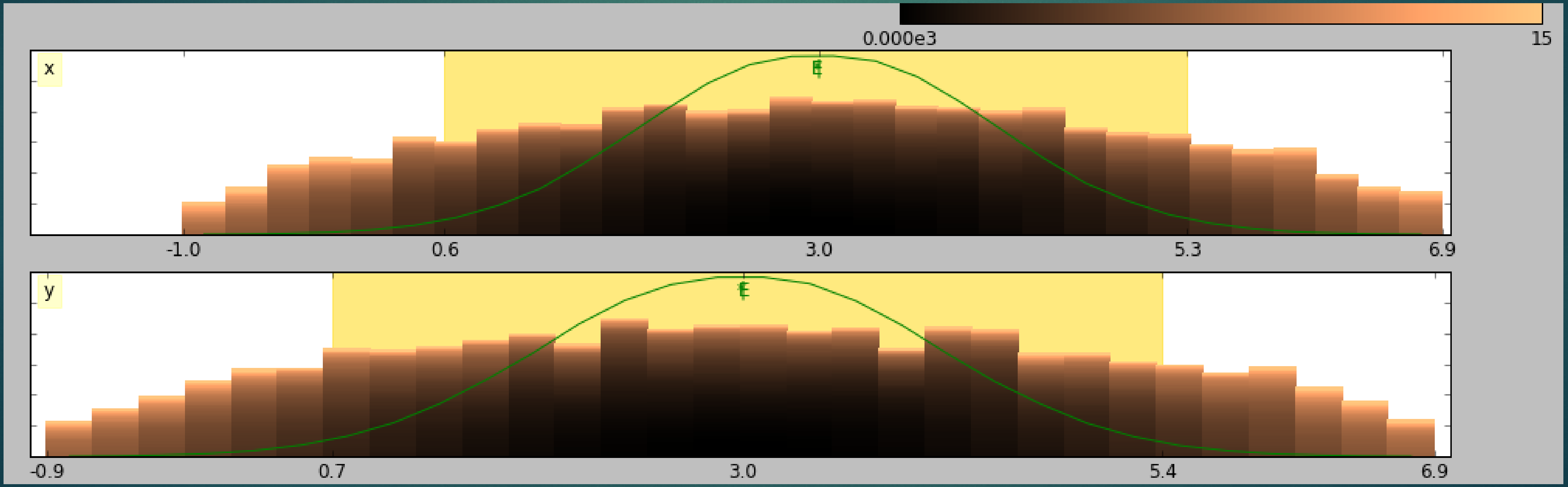
Dynamic Temperature Methods (Finding the Ideal Temperature for a Model)

- Ideal acceptance rate is around 20%
- Have stuckness multiplier to alter temperature based on the previous acceptance rate
  - Solve $M = Ae^{-B\,accept^2}$ given $M(.2) = 1\ and\ M''(.2) = -1$
  - Current function: $M = 1.6e^{-12.5\,accept^2}$



Innate Problems With High Temperature Sampling

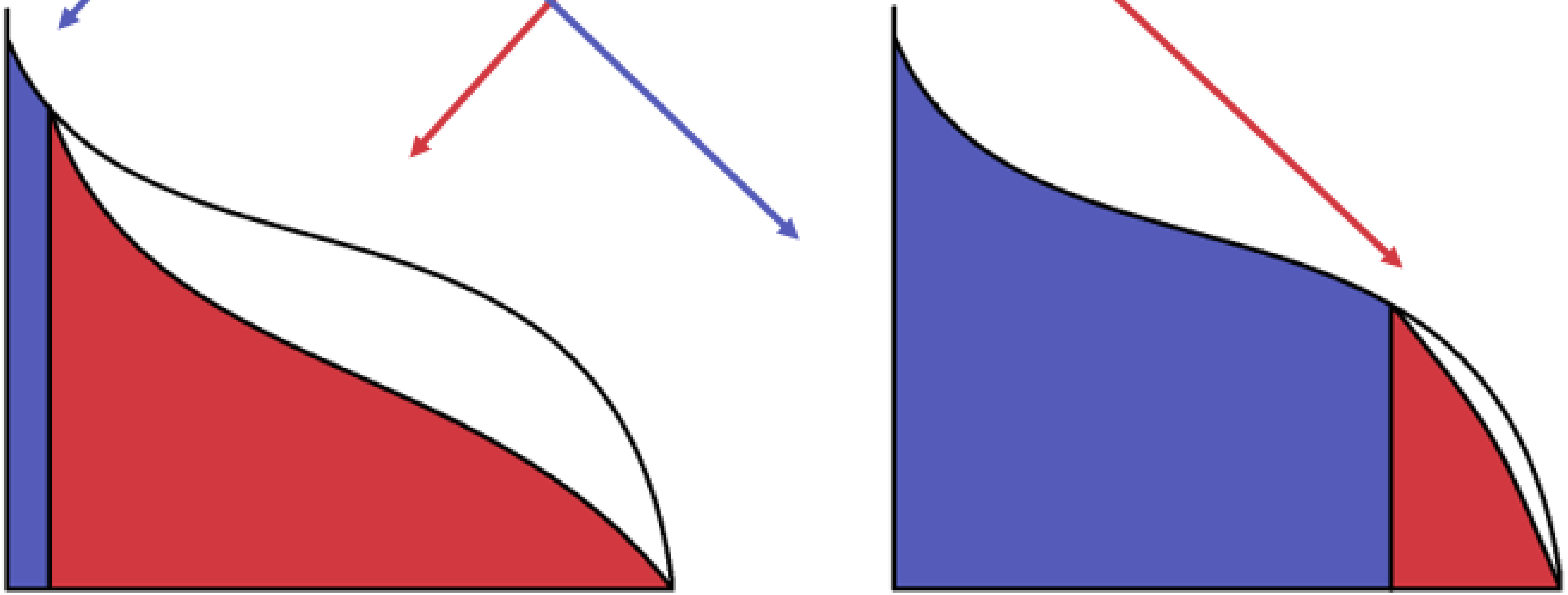
- By its very nature sampling at high temperature will distort the posterior



Solution: Create a Transform

- First create function f(x) which is a pdf of the likelihoods of all selected points
- Transform (Weighting Function): $W(x) = \dfrac{\int_0^x f(t)dt + x\int_x^1 \frac{f(t)}{t}dt}{\int_0^{Tx} f(t)dt + Tx\int_{Tx}^1 \frac{f(t)}{t}dt}$
  - Every sampled point is given a weight based on its likelihood

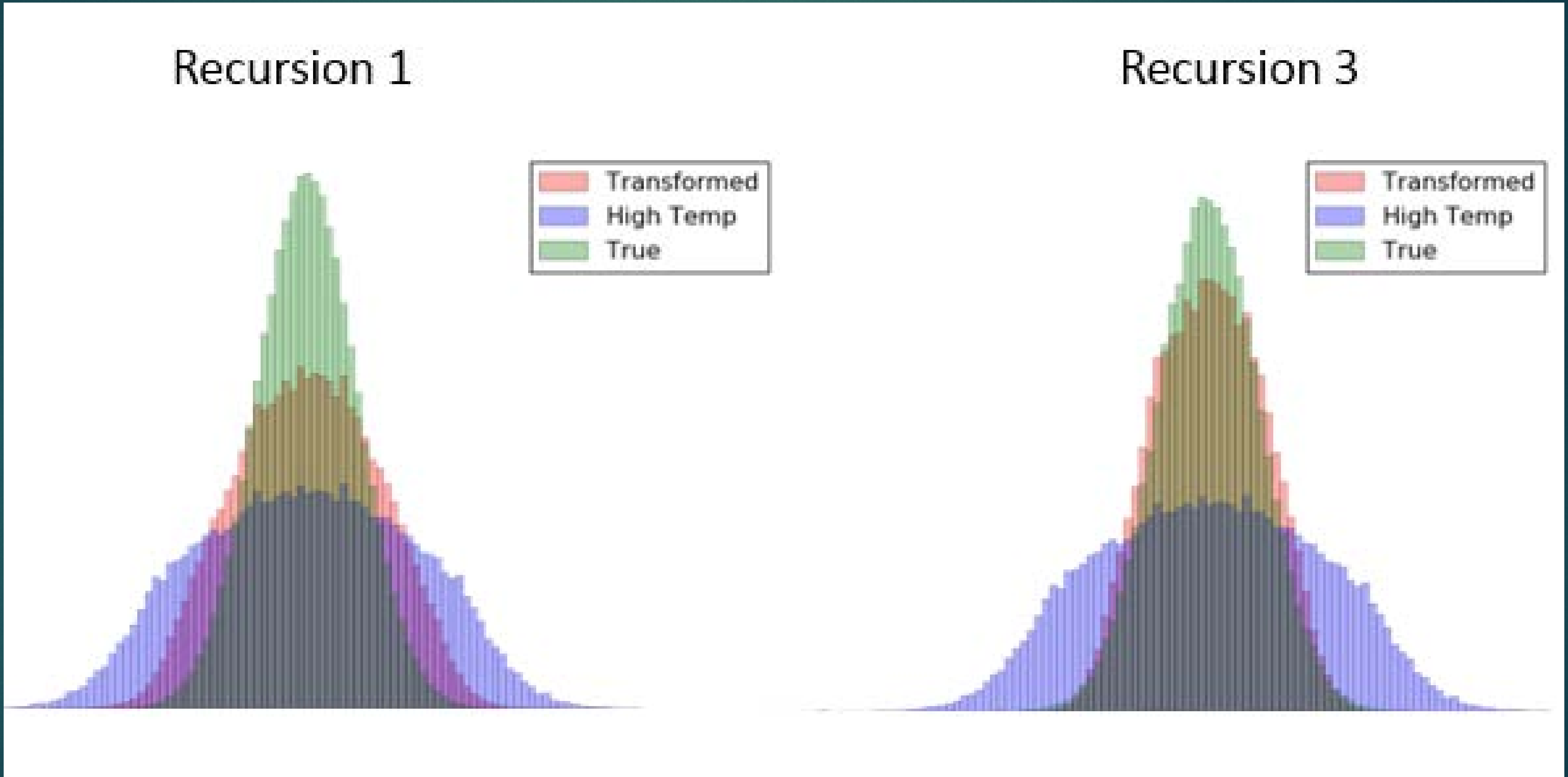
$$W(x) = \frac{\int_0^x f(t)dt + x\int_x^1 \frac{f(t)}{t}dt}{\int_0^{Tx} f(t)dt + Tx\int_{Tx}^1 \frac{f(t)}{t}dt}$$



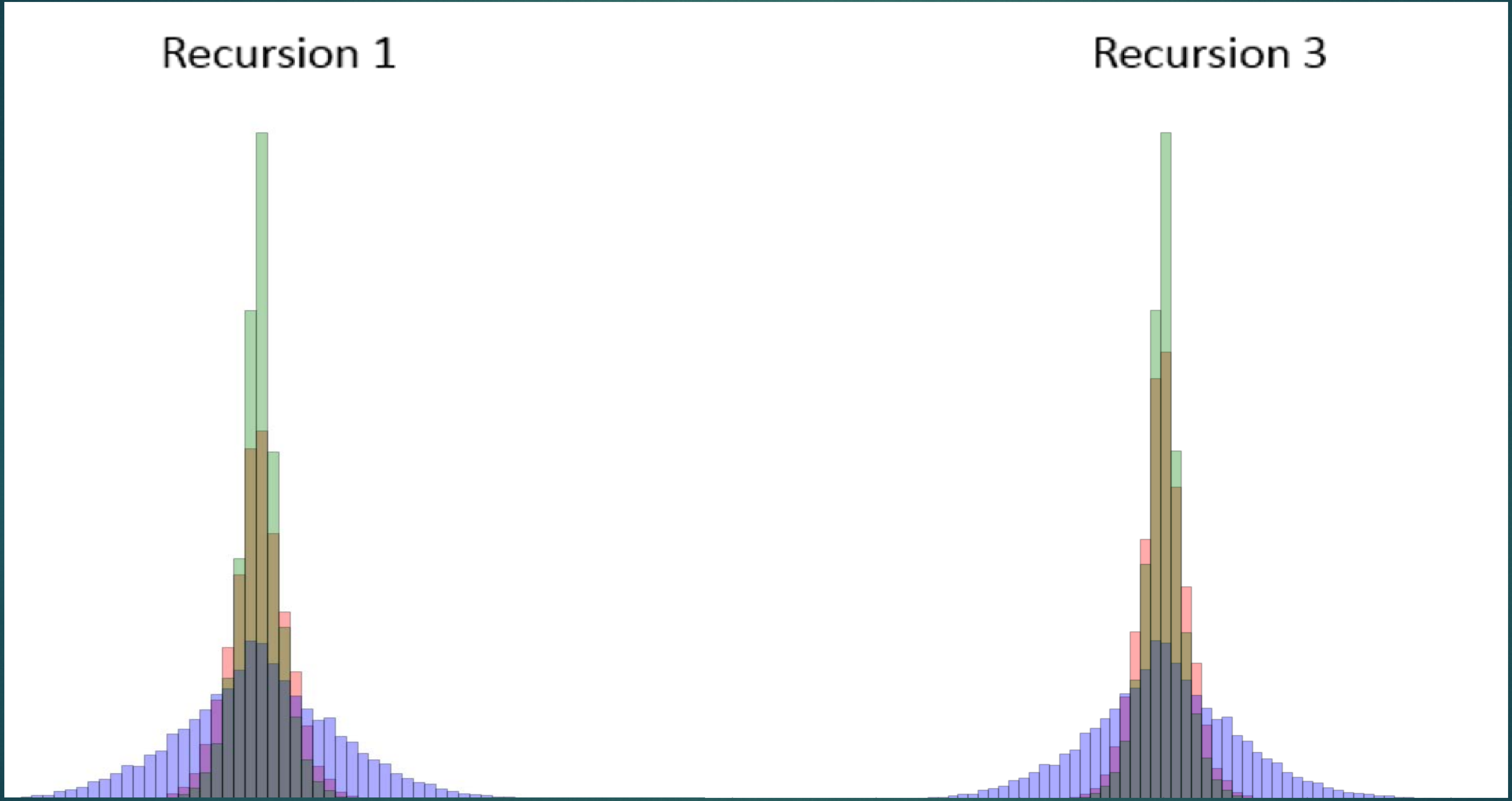
Recursion of Process

- In weighting function theoretically need likelihood distribution at low temperature
  - Approximate it with the high temperature distribution
  - Apply weighting function to create a more accurate likelihood pdf
  - Recursively create more and more accurate distributions until an equilibrium is reached

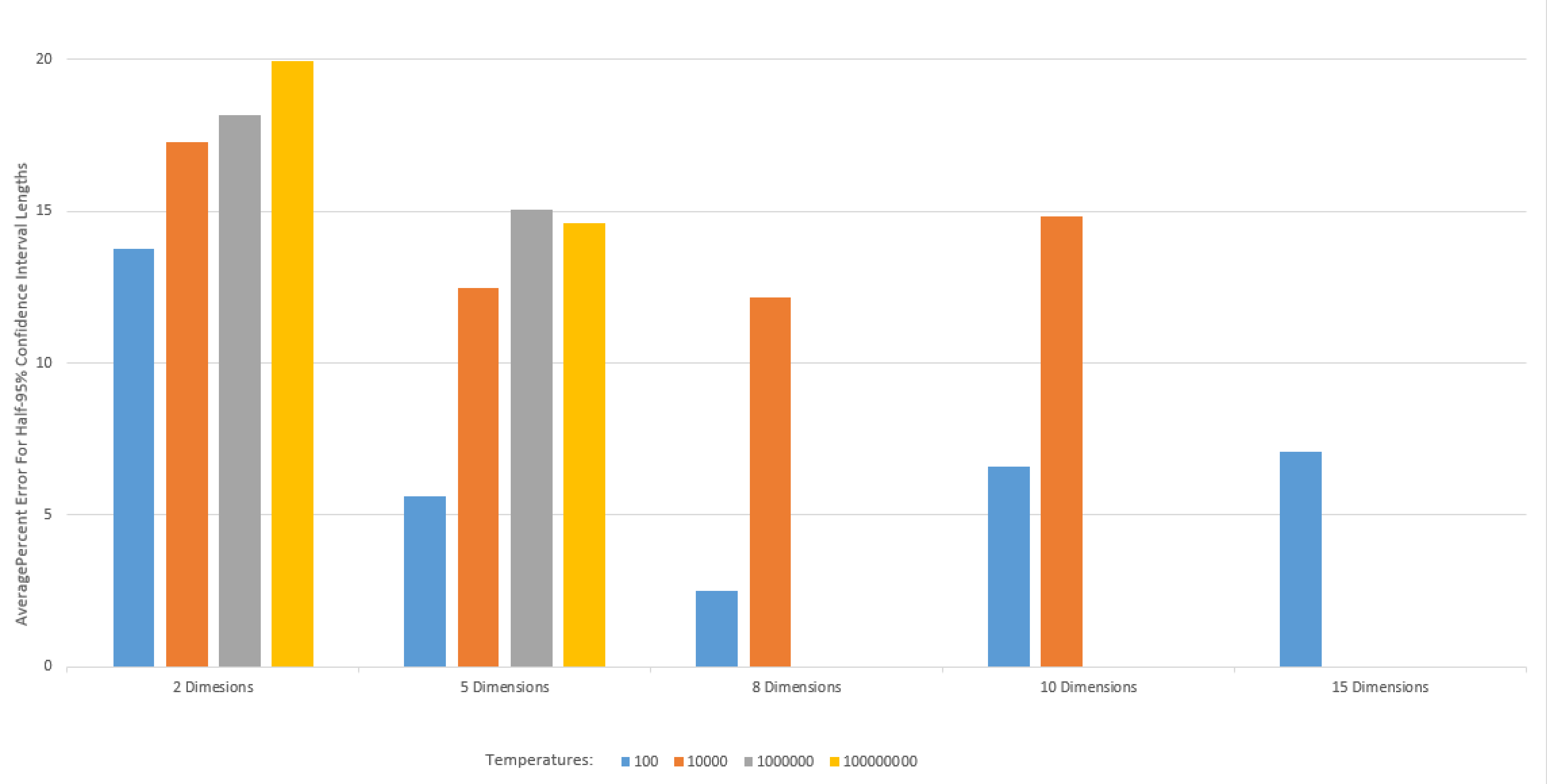
Findings on a Gaussian



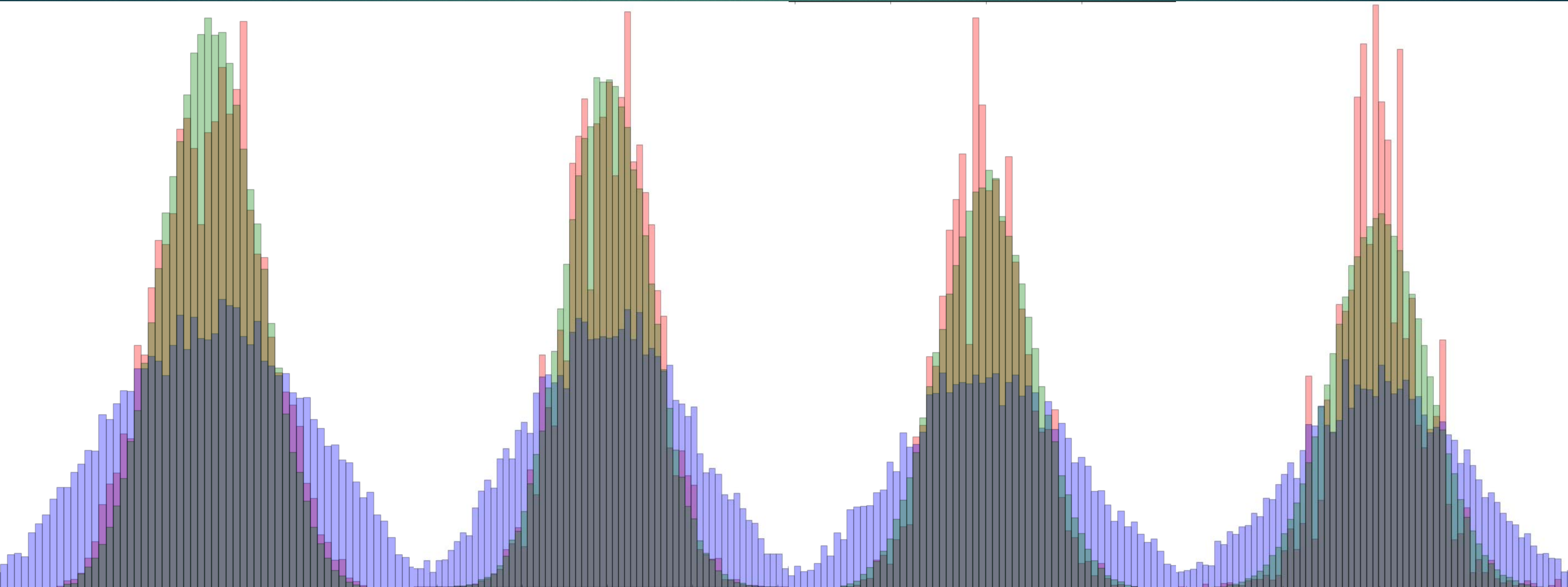
Findings On a Laplace Distribution



Analysis On Gaussians with 100,000 Samples

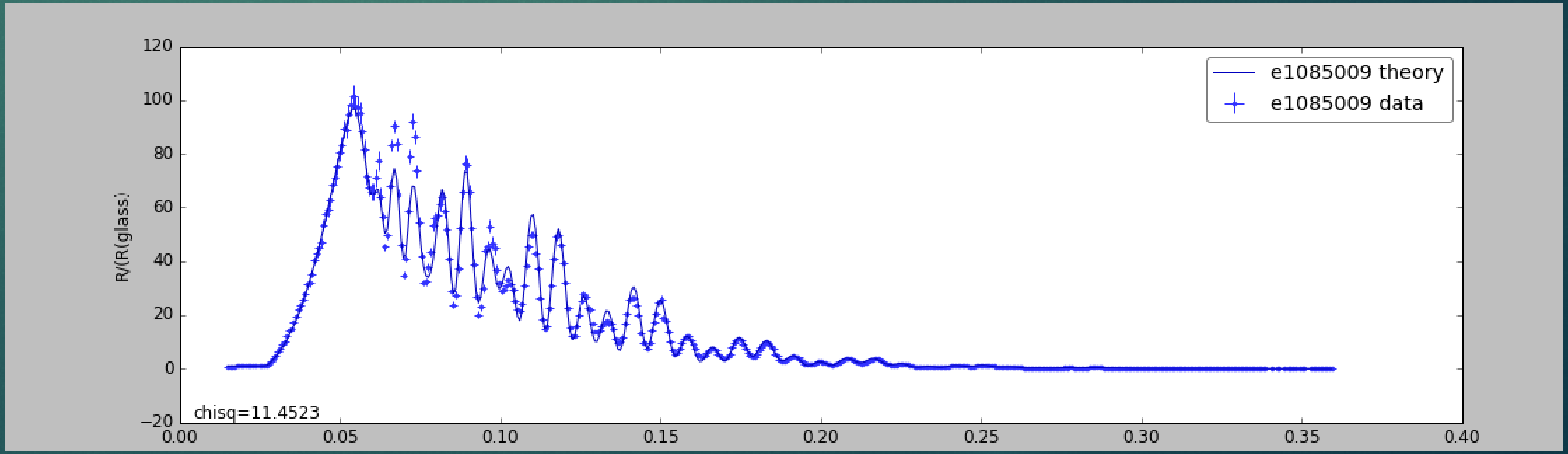


5 Dimensions 8 Dimensions 10 Dimensions 15 Dimensions



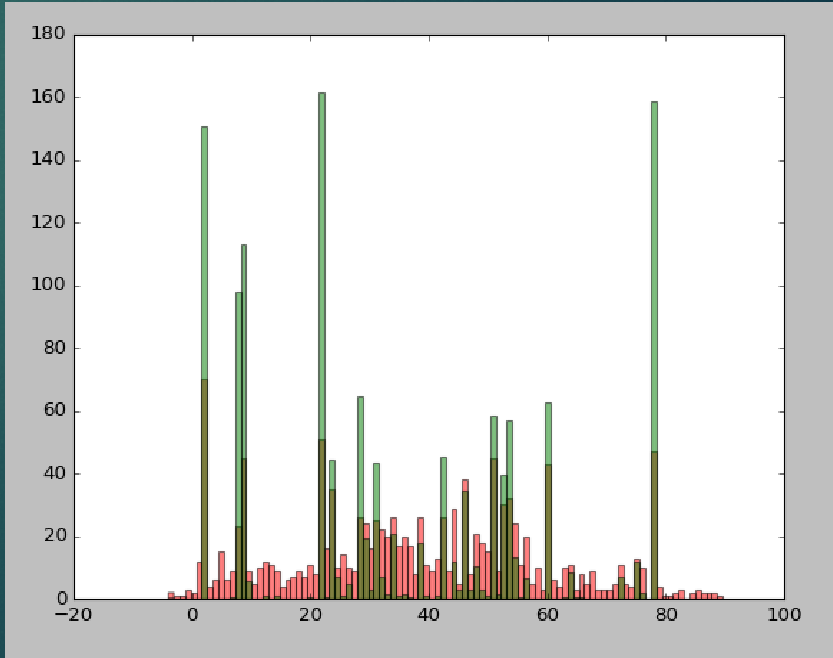
Applications

- Neutron Reflectometry
  - MCMC Sampling used to solve for parameters in transfer-matrix
- Use method to resolve stuck problems
  - Such as the orientation of the HIV Gag protein in the lipid bilayer based on 3 angles of axial revolution



Future Work

- Solve loss of accuracy and reliability at high temperatures and dimensionalities
  - Problem of quantization of proposed posterior
- Give mathematical proof that method should theoretically converge onto the true posterior



Acknowledgements

- Dr. Julie Borchers
- Dr. Yamali Hernandez
- Mr. Paul Kienzle
- Dr. Frank Heinrich
- SURF Student Aaron Schankler