Convergence Diagnostics For Markov chain Monte Carlo

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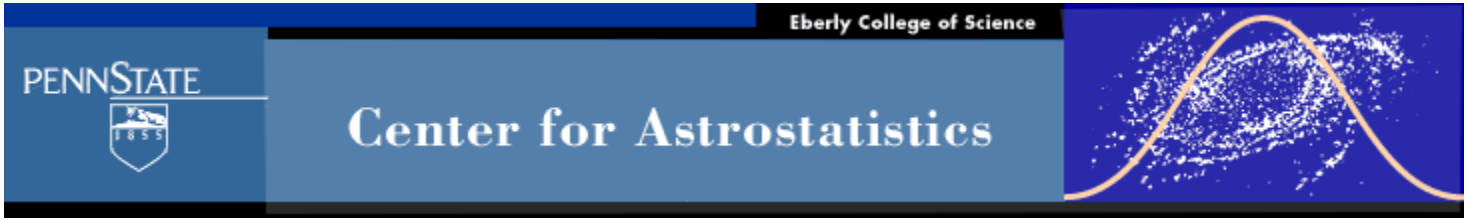
Bayesian Computing for Astronomical Data Analysis

June 5, 2015



MCMC: A Science & an Art

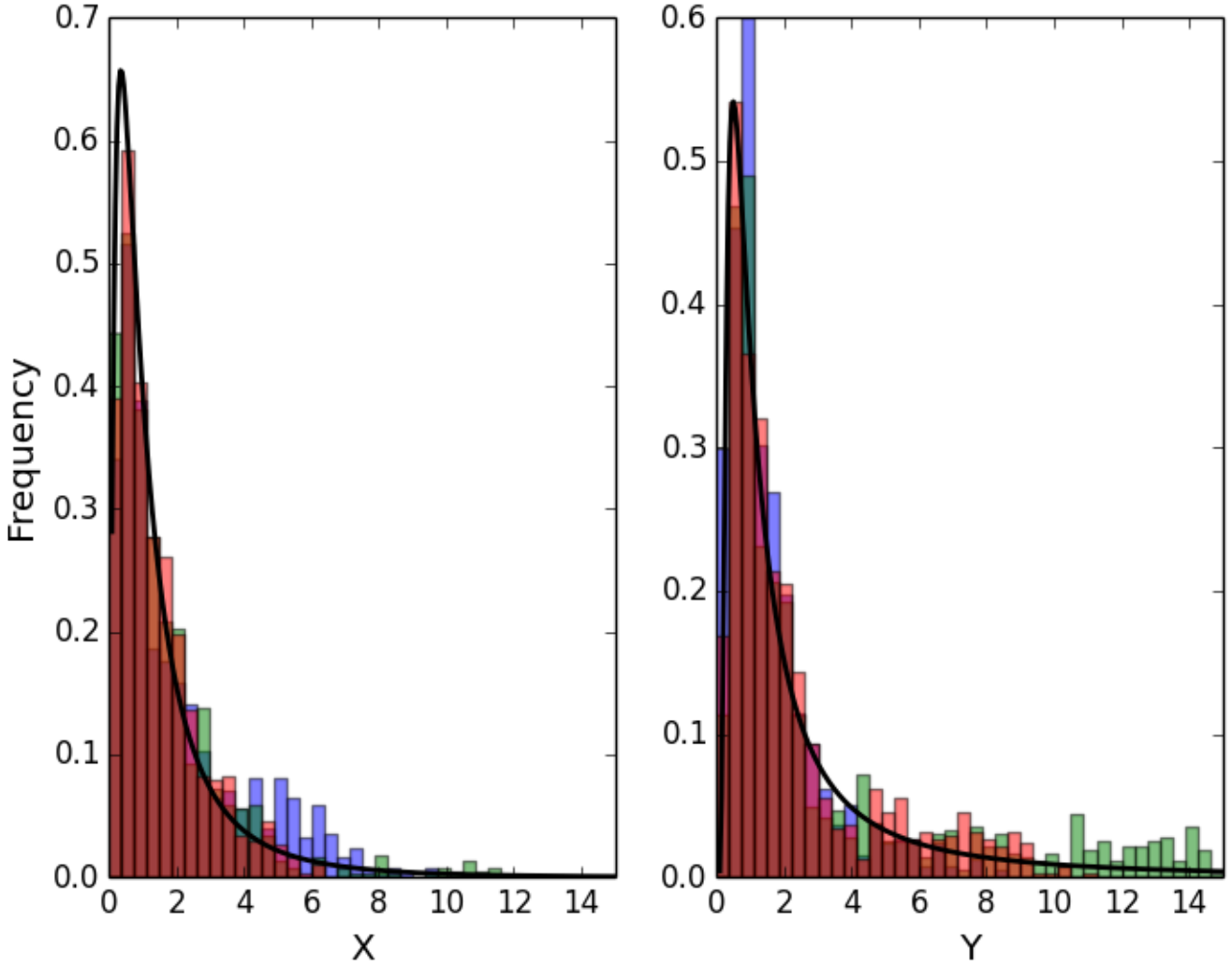
- Science:
  If your algorithm is designed properly, the Markov chain will converge to the target distribution… after infinite iterations
- Art:
  When is it wise to make inferences based on a finite Markov chain

Assessing Convergence is Essential

If you want to:

- Base your conclusions on posterior distributions
- Report accurate parameter estimates & uncertainties
- Avoid fooling yourself
- Avoid devoting resources (e.g., your effort, telescope time) to follow-up an “inference” that isn’t supported by data
- Avoid writing an erratum to your paper

Has this Chain Converged?



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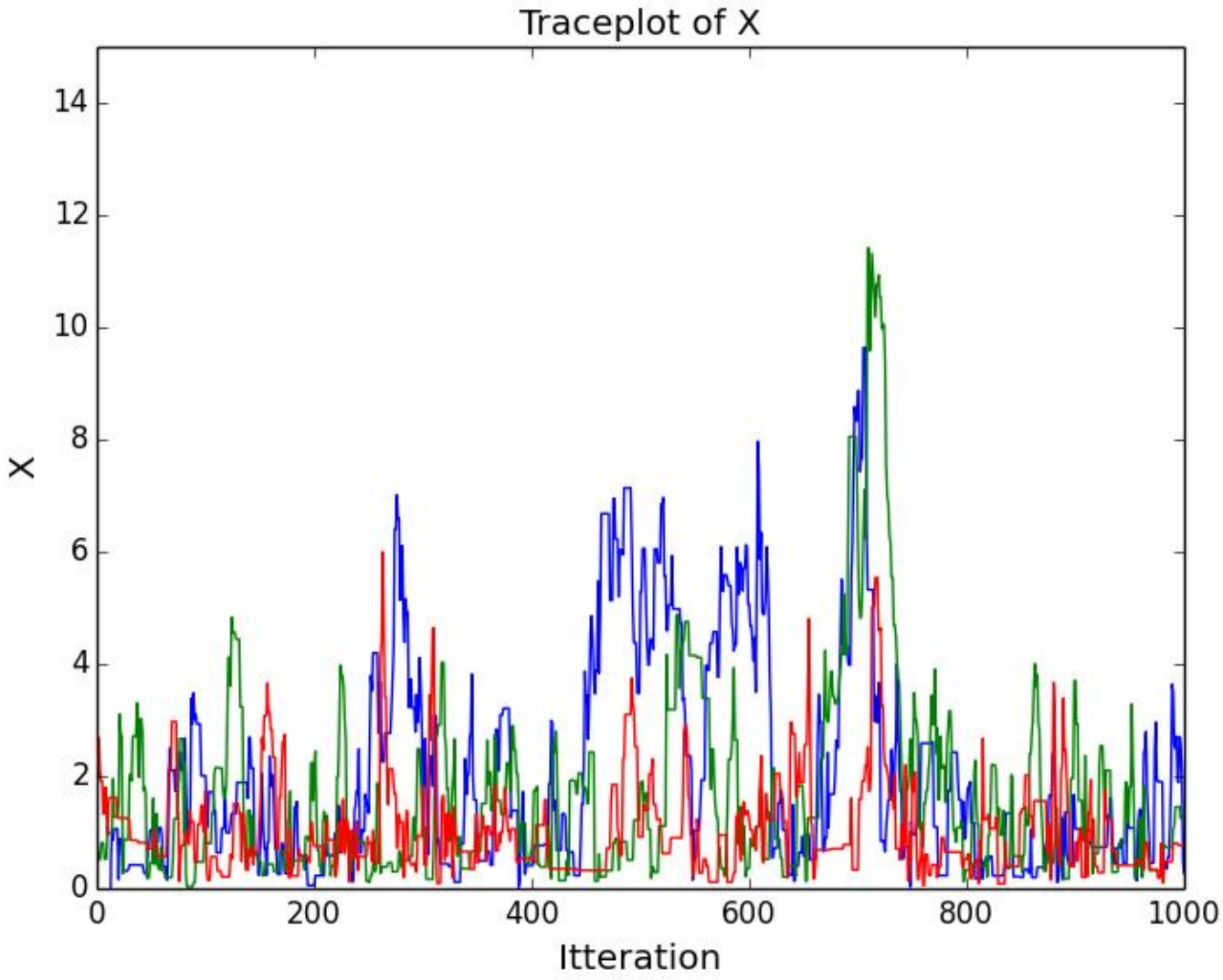

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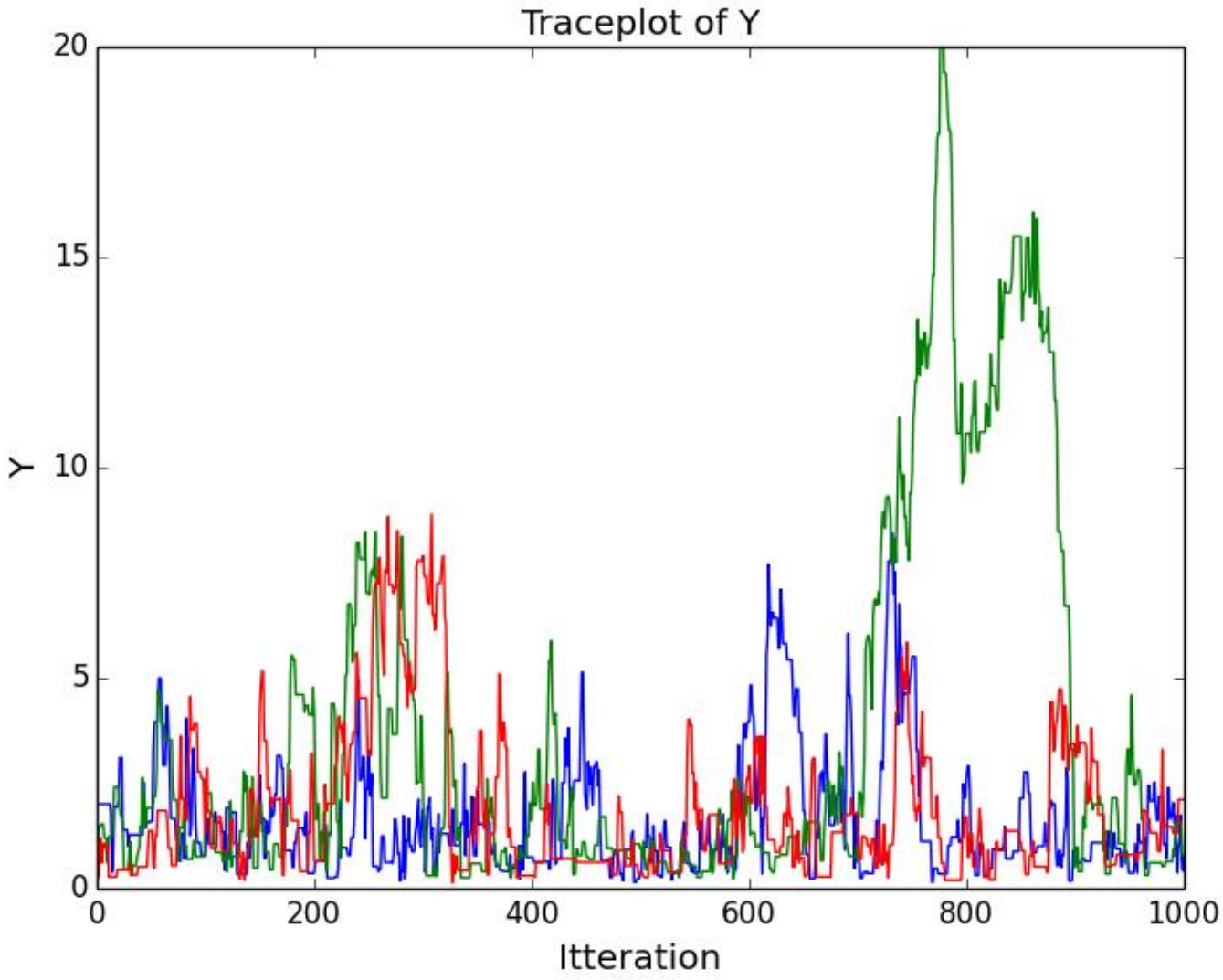

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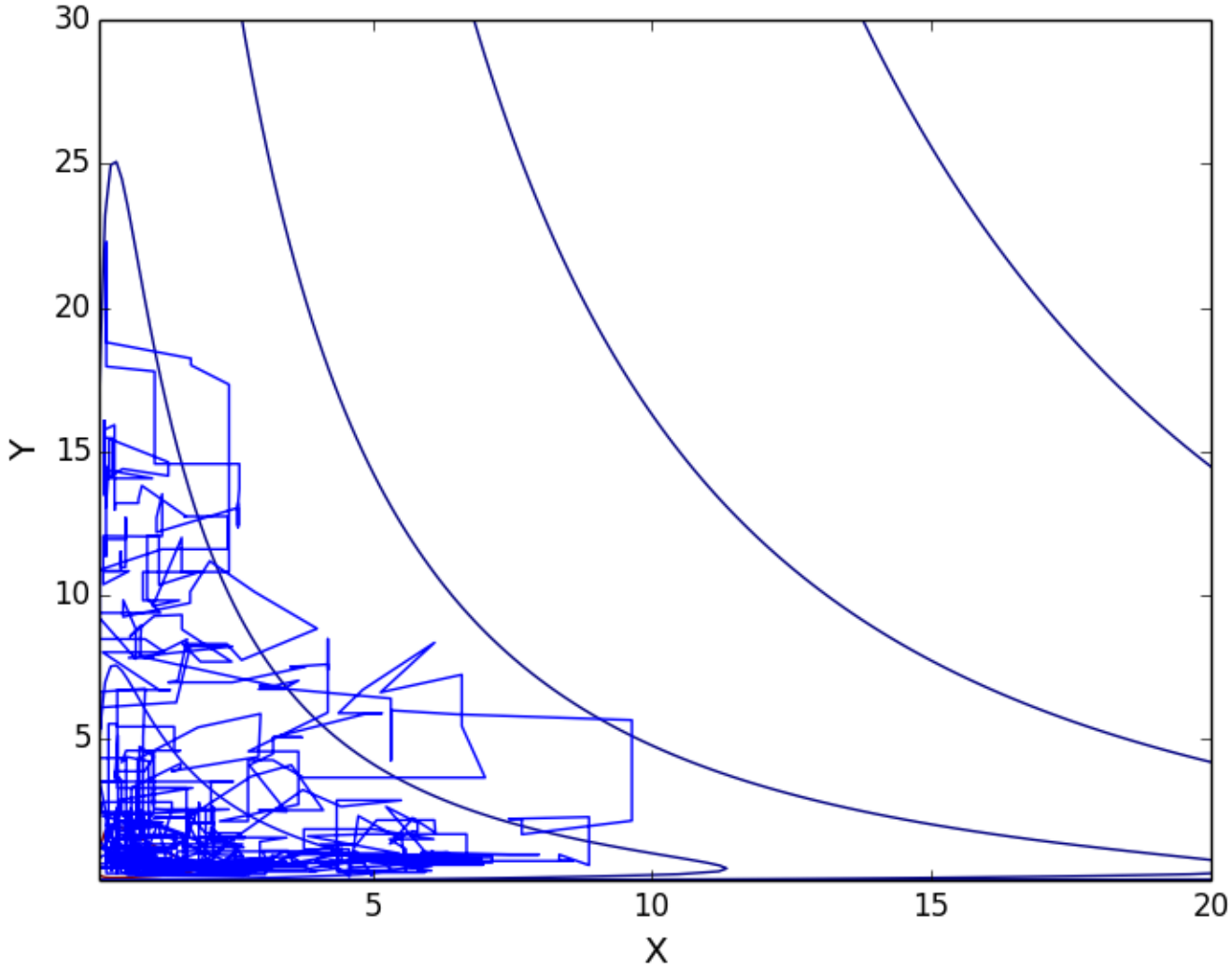

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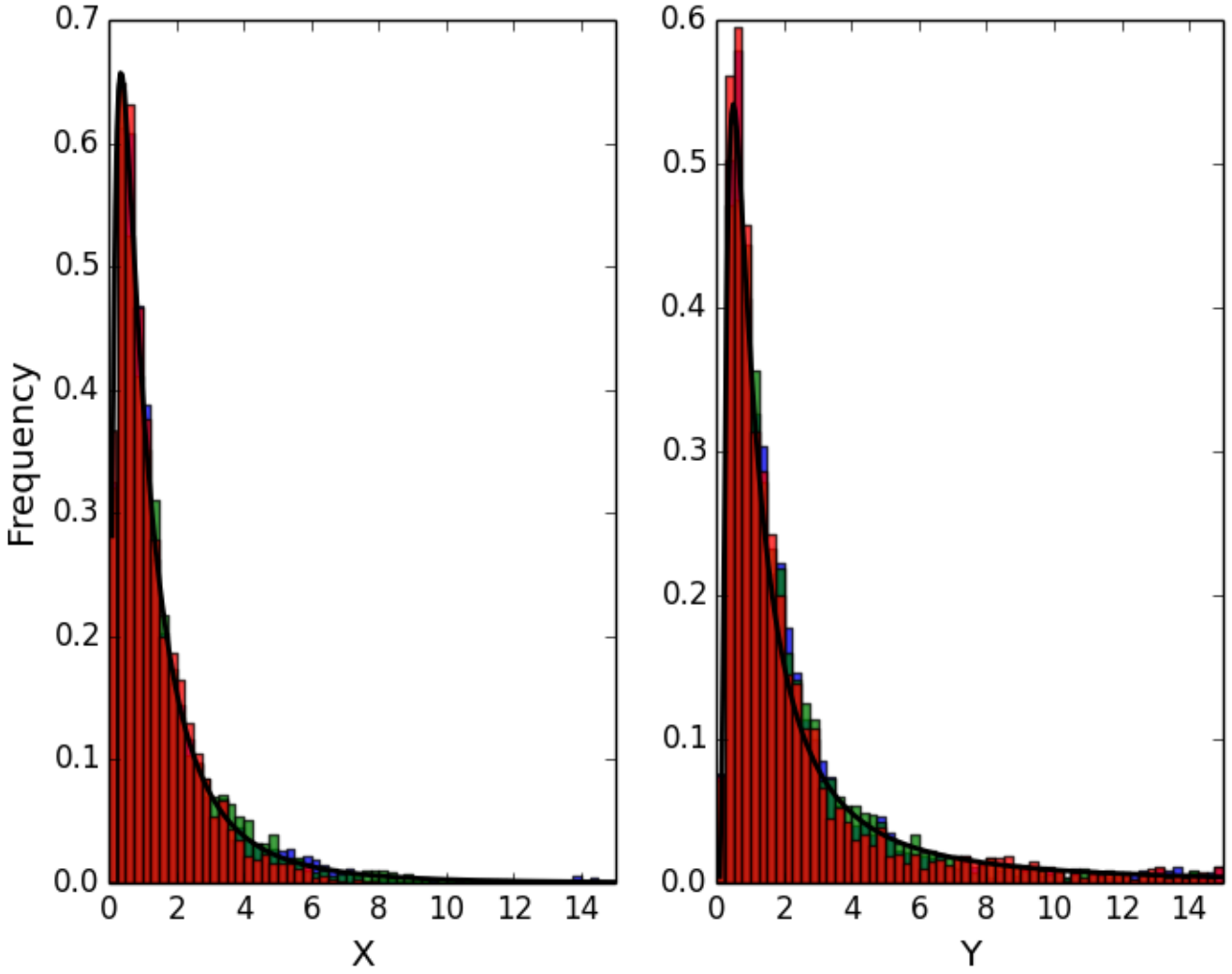

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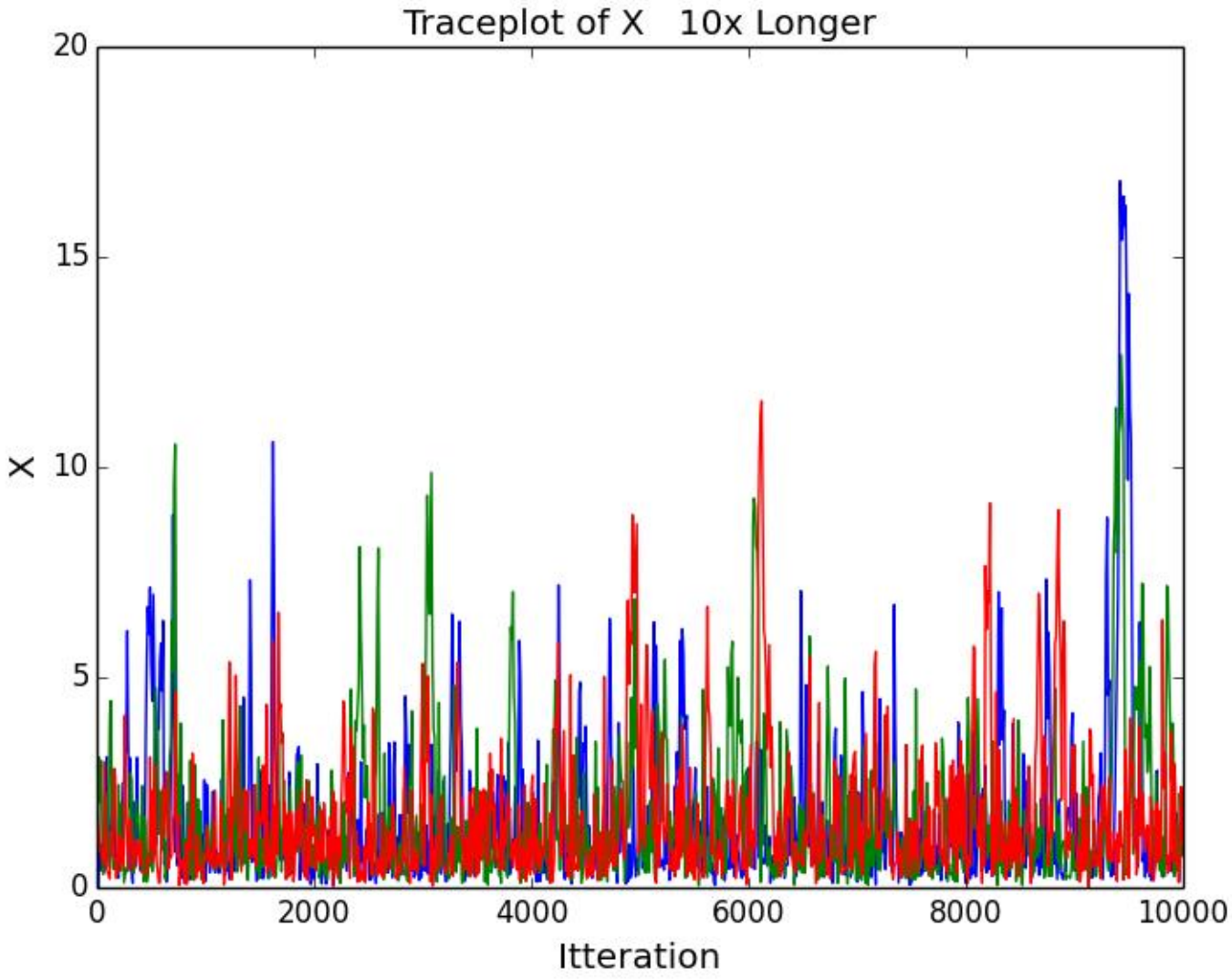

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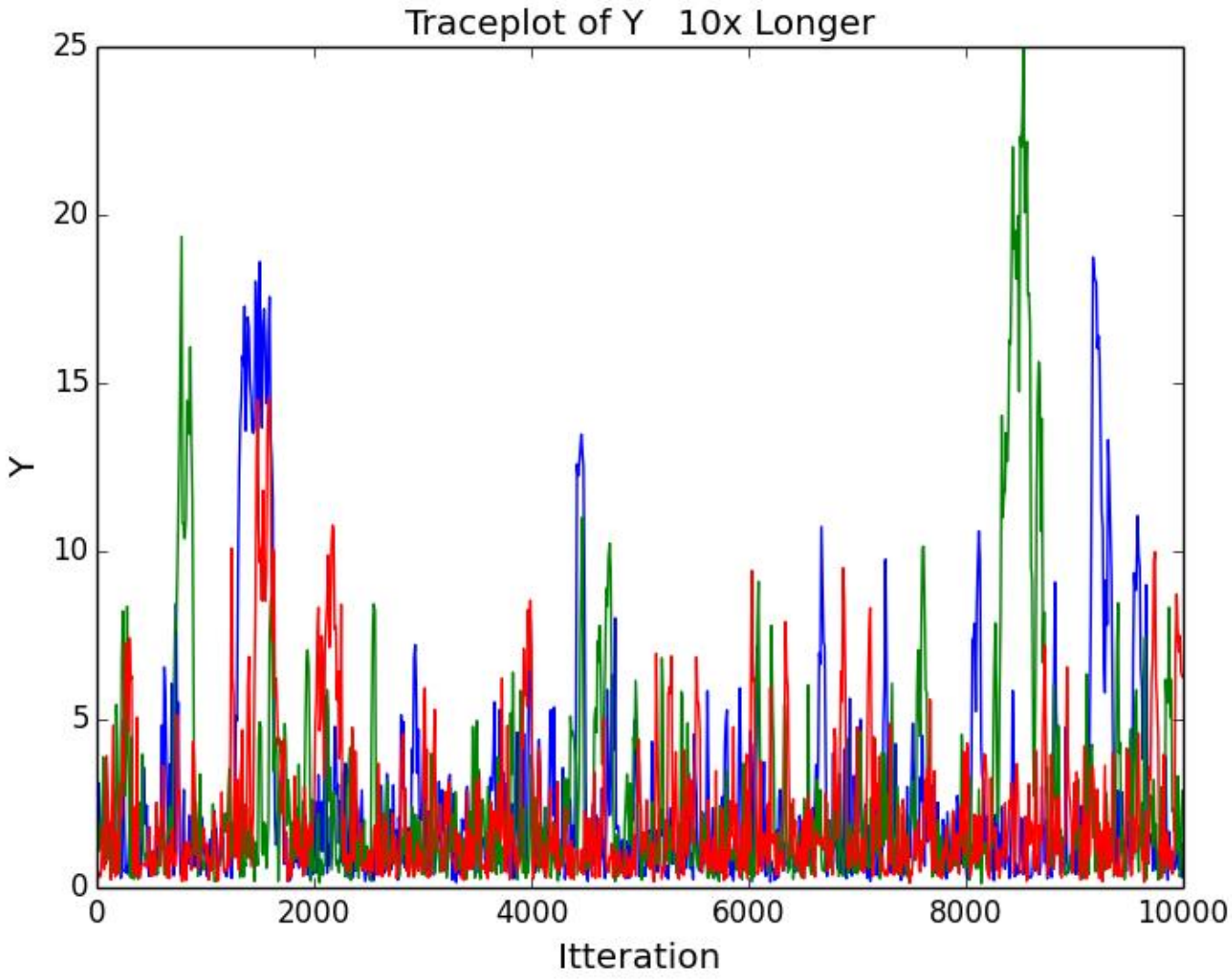

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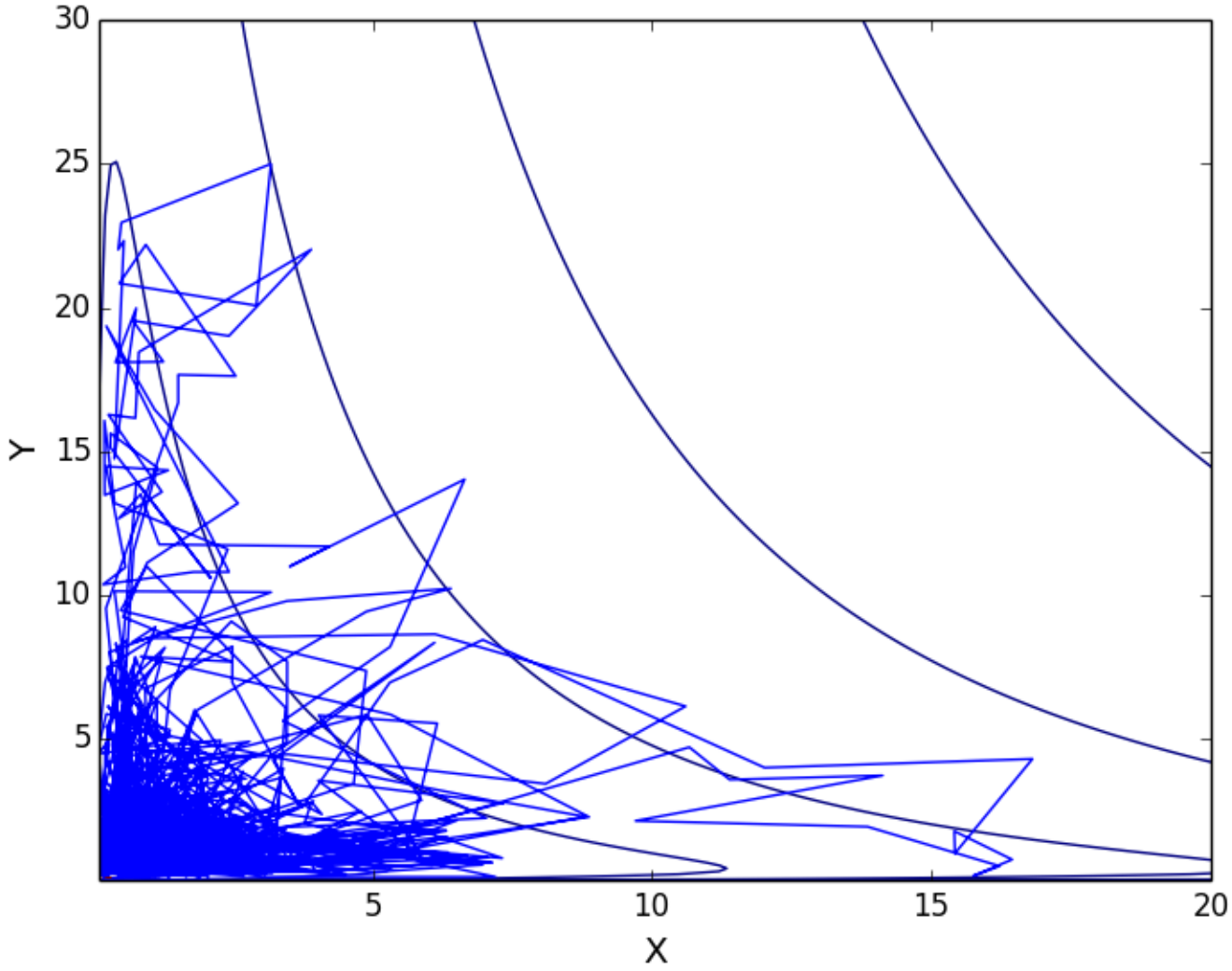

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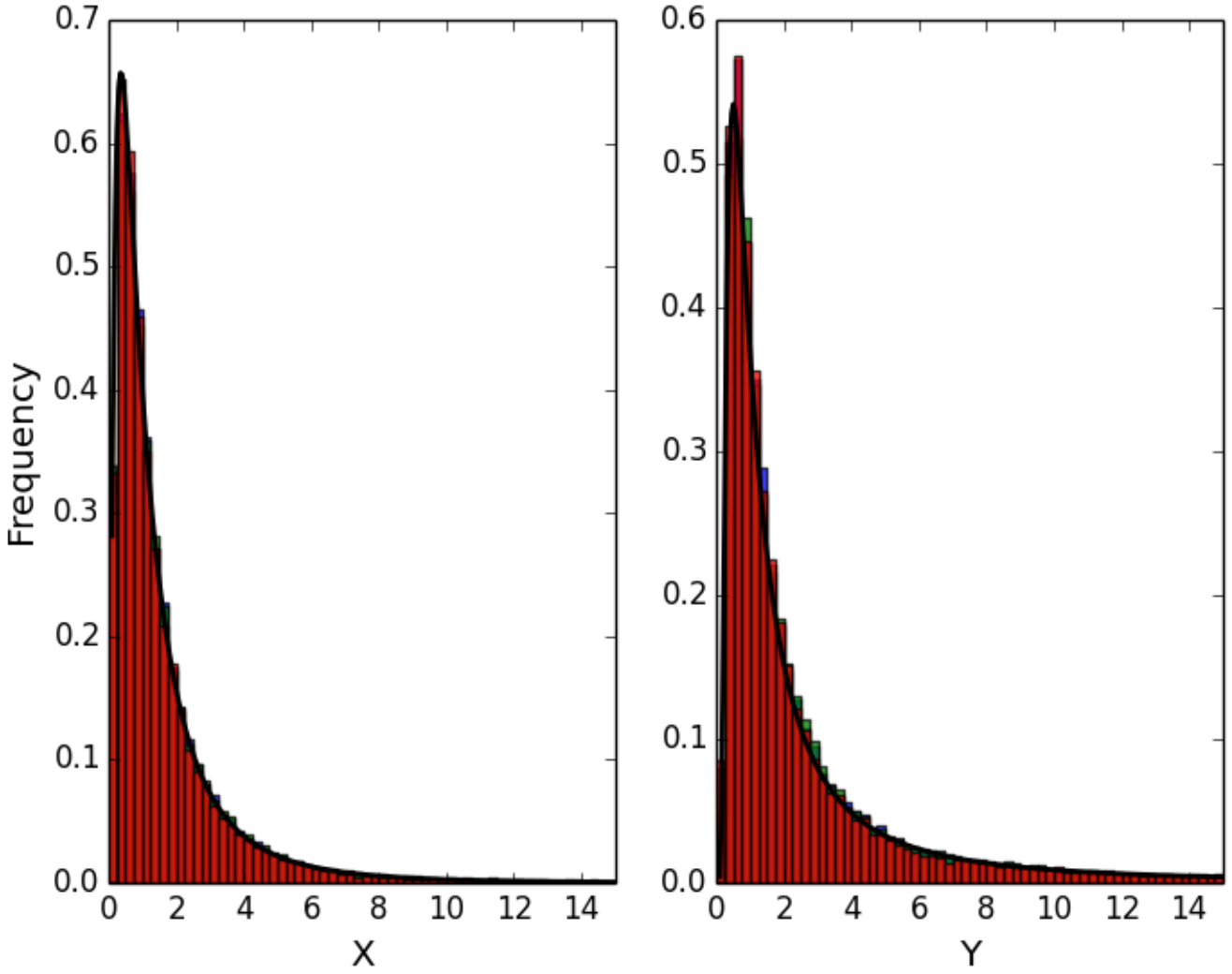

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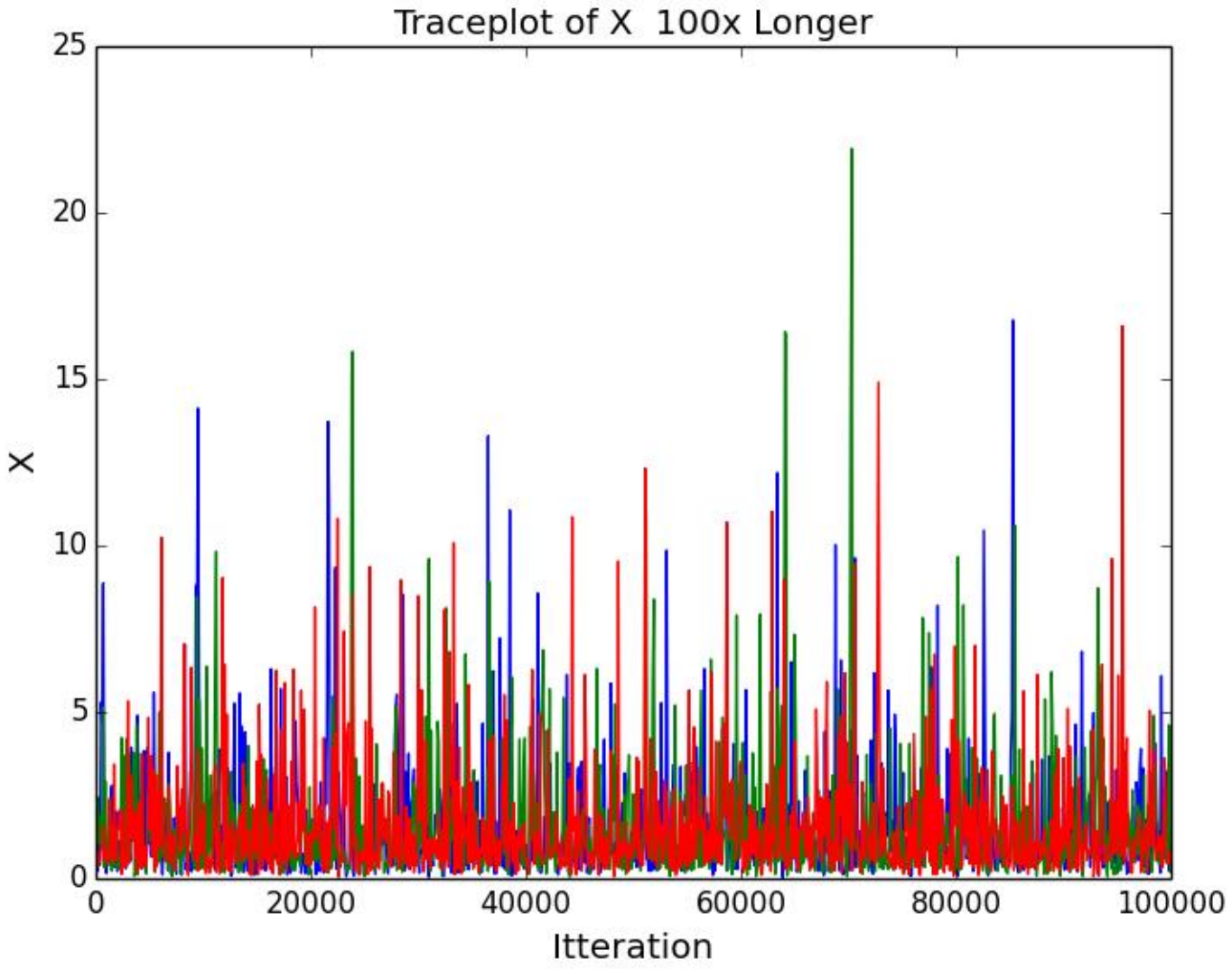

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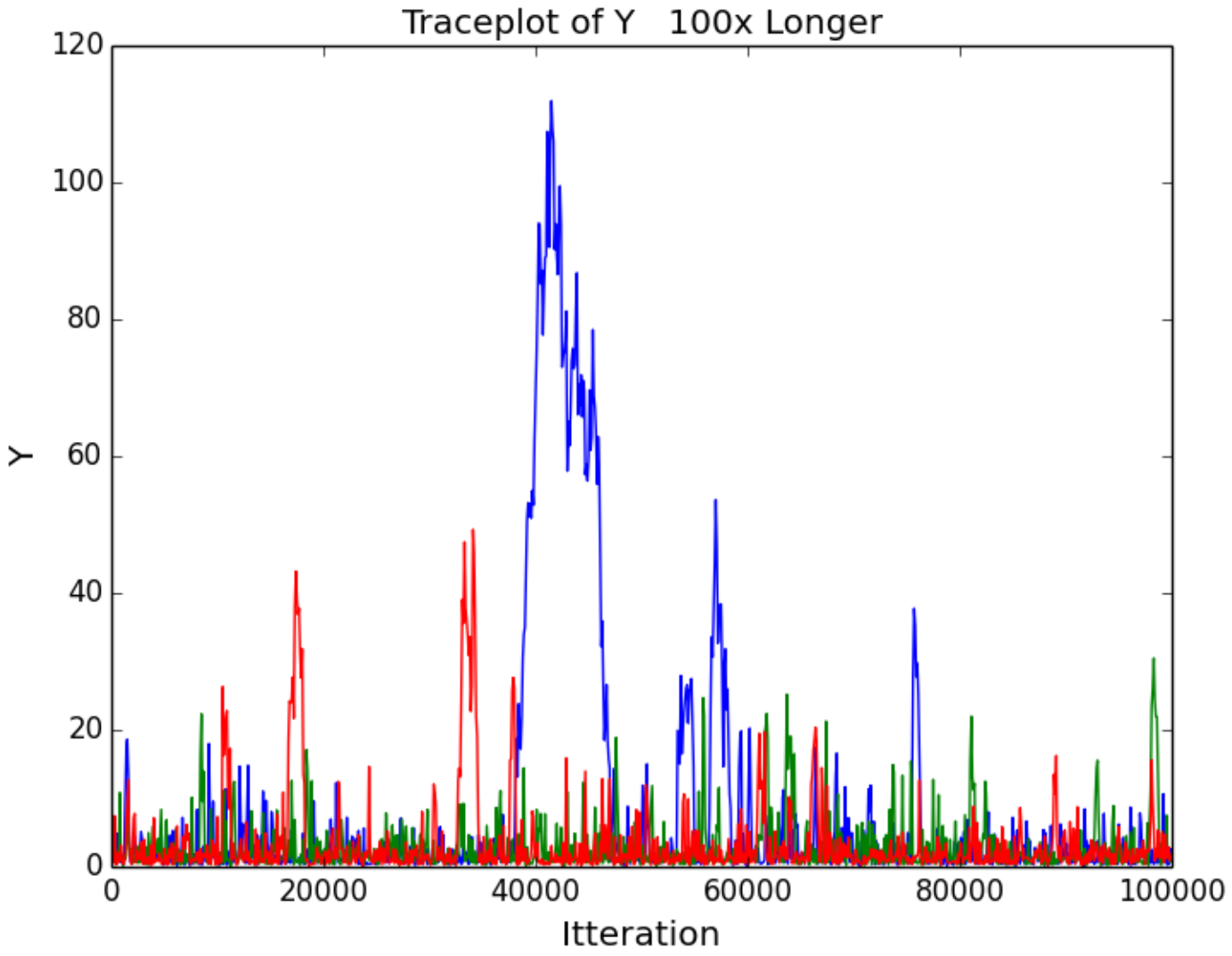

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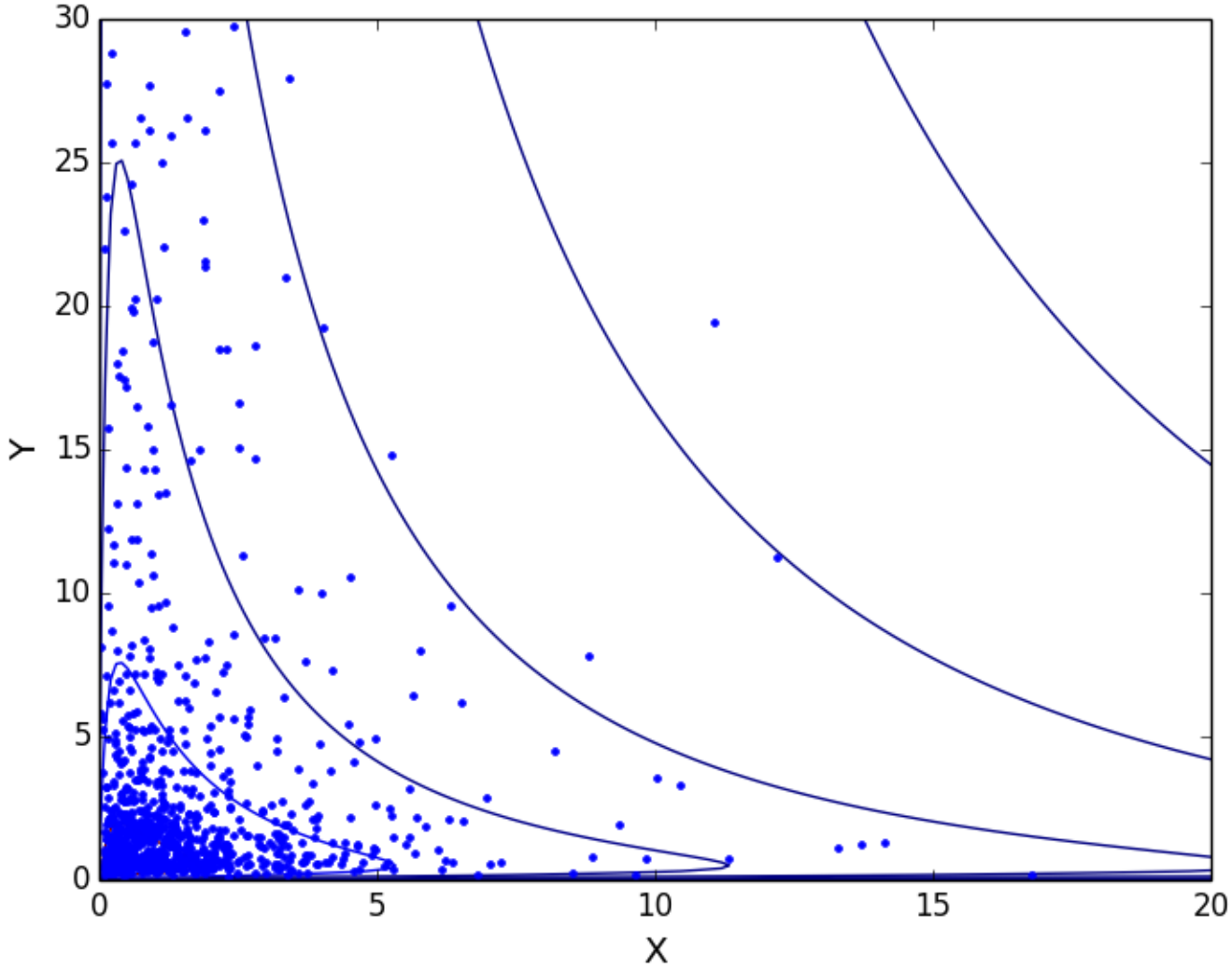


Good Signs

- Any sufficiently large segment of Markov chain would give similar results
- Desirable acceptance rate of proposed steps
- Chain “mixes well”. (i.e., chain has run much longer than any observed timescale for correlation between samples)
- Multiple chains initialized from different initial conditions give similar results
- MCMC analysis of similar problem using simulated data give accurate results, even with significantly fewer iterations

Why Only “Maybe”?

- You can’t prove convergence
  - At best, you fail to prove a failure to converge
- Convergence rate can be exponentially sensitive to barriers between local modes.
- What if there’s a narrow bottleneck between two regions of high probability?
- What if there’s another posterior mode that we’ve completely overlooked?

What should I do?

- Be paranoid
- Run chains longer than you think you need to
- Compute several Markov chains
  - initialized with significantly different initial states
- Look at your Markov chains yourself
  - Trace plots
  - Marginal joint densities

What warning signs should I be looking for?

- Differences within or across Markov chains
- “Poor mixing”
- Low/high acceptance rates
- Autocorrelation between states of Markov chain
- Strongly correlated parameters
- Suspicious tails or posterior shapes

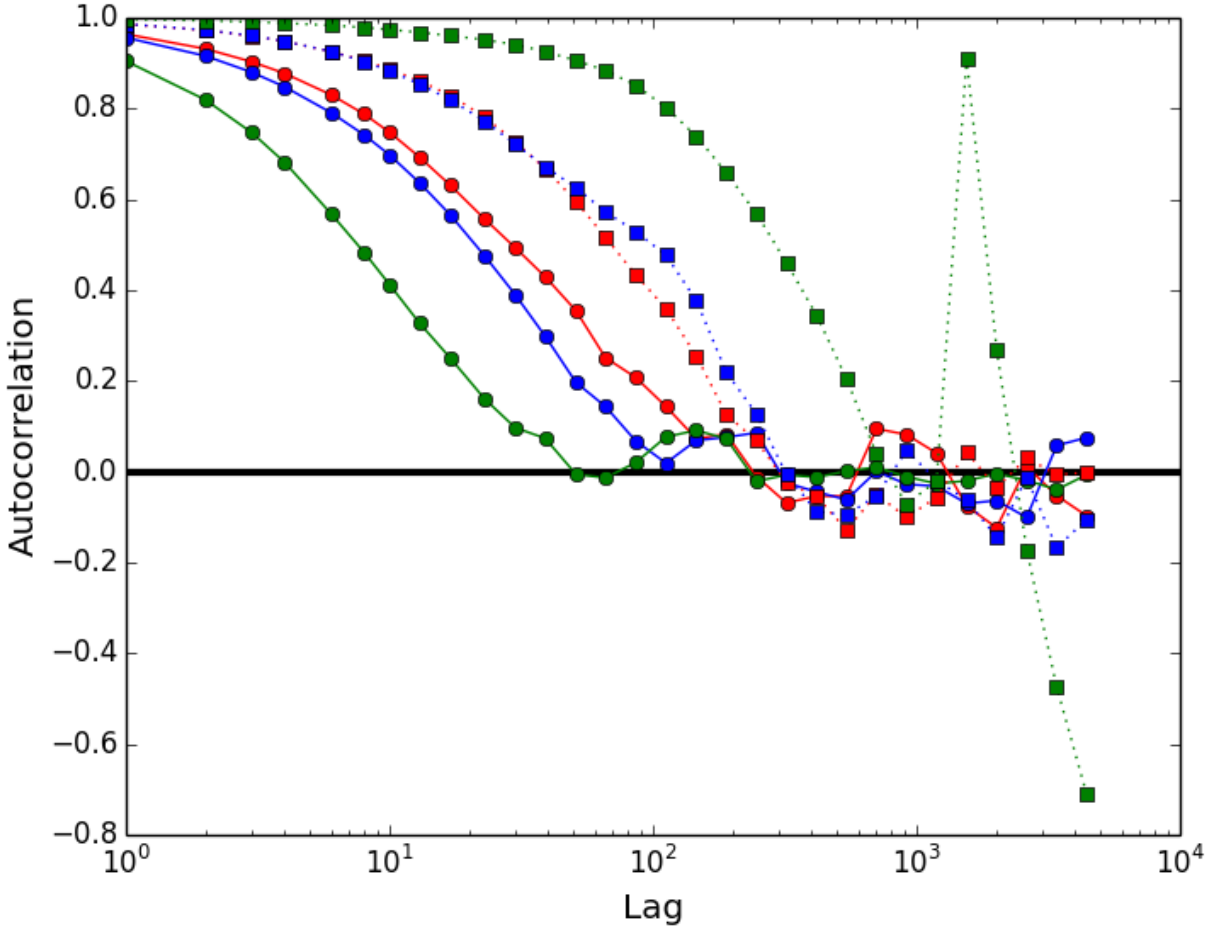
Check Autocorrelation of Markov chain

- Autocorrelation as a function of lag

$$\rho_{lag} = \frac{\sum_i^{N-lag}(\theta_i - \bar{\theta})(\theta_{i+lag} - \bar{\theta})}{\sum_i^{N}(\theta_i - \bar{\theta})^2}$$

- What is smallest lag to give an $\rho_{lag} \approx 0$?
- One of several methods for estimating how many iterations of Markov chain are needed for *effectively* independent samples

Checking Autocorrelation Function



Getting More Quantitative

Calculate convergence diagnostics

- Geweke (1992): Compares means calculated from distinct segments of Markov chain
- Raftery & Lewis (1992): Estimates the *minimum* chain length needed to estimate a percentile to some precision

- Gelman & Rubin (1992): $\hat{R}$ compares variances between chains
- Brooks & Gelman (1998): Several generalizations of $\hat{R}$
  - Account for covariances
  - Can apply to higher moments
  - Scale reduction for arbitrary credible intervals

Estimate Potential Scale Reduction Factor

Gelman-Rubin diagnostic ($\hat{R}$)

- Compute *m* independent Markov chains
- Compares variance of each chain to pooled variance
- If initial states (θ_{1j}) are overdispersed, then $\hat{R}$ approaches unity from above
- Provides estimate of how much variance could be reduced by running chains longer
- It is an *estimate!*

$$W = \frac{1}{m}\sum_{j=1}^{m} s_j^2 \qquad \bar{\bar{\theta}} = \frac{1}{m}\sum_{j=1}^{m} \bar{\theta}_j$$

$$B = \frac{n}{m-1}\sum_{j=1}^{m}(\bar{\theta}_j - \bar{\bar{\theta}})^2 \qquad s_j^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\theta_{ij} - \bar{\theta}_j)^2$$

$$\hat{\mathrm{Var}}(\theta) = (1 - \frac{1}{n})W + \frac{1}{n}B \qquad \hat{R} = \sqrt{\frac{\hat{\mathrm{Var}}(\theta)}{W}}$$

Estimate Potential Scale Reduction Factor

Bare Minimum:

- Check $\hat{R}$ for each model parameter
- Check $\hat{R}$ for any important functions of model parameters

Better:

- Consider applying a generalization that checks for covariances, moments or intervals of interest

Estimate Potential Scale Reduction Factor

Returning to previous example:

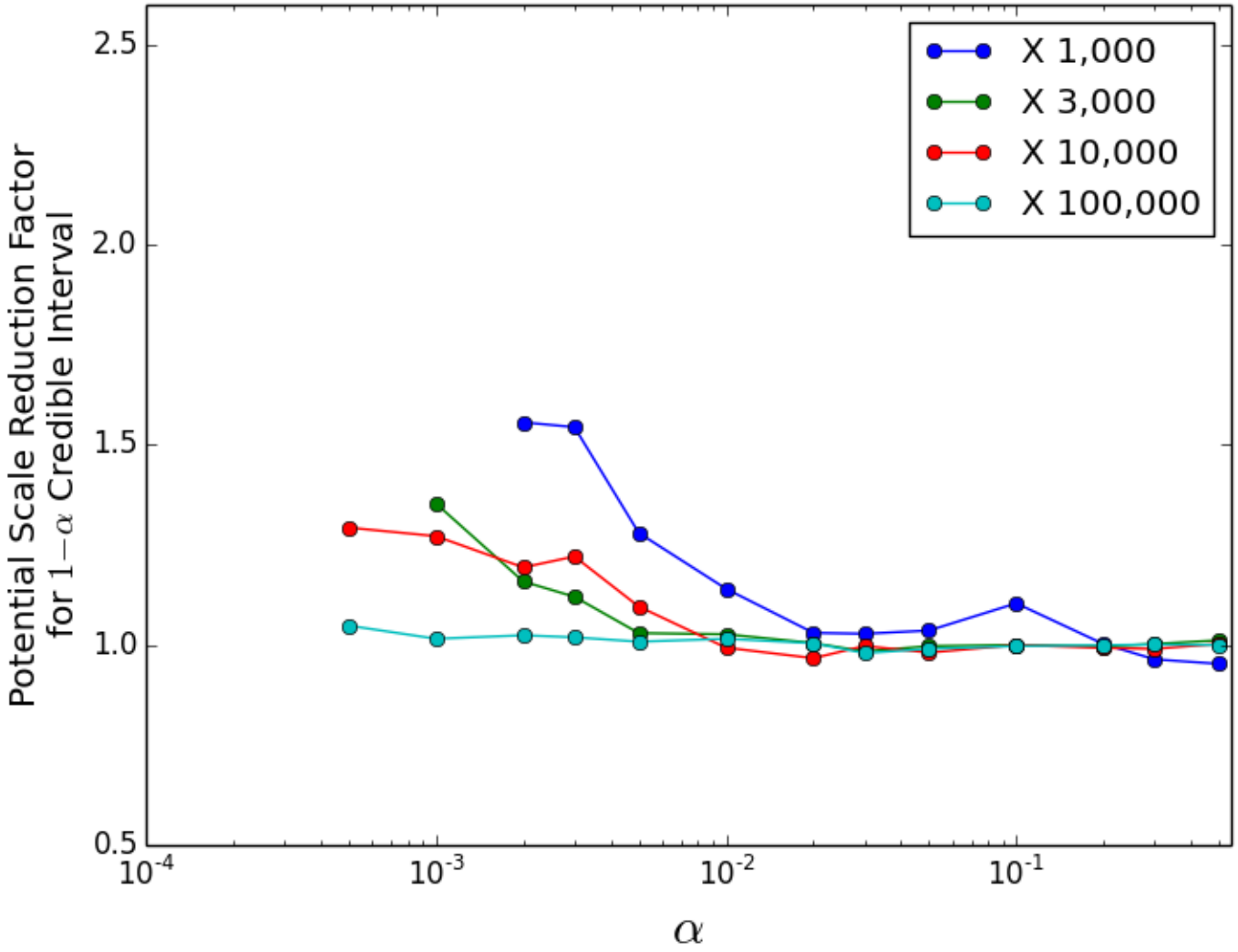
- Gelman-Rubin diagnostic ($\hat{R}$) is <1.001
- Consider generalized statistic

$$\widehat{R}_{\text{interval}} = \frac{\text{length of total-sequence interval}}{\text{mean length of the within-sequence intervals}}$$

for central (1-α) credible interval

- Plot as function of α

Estimate Potential Scale Reduction Factor



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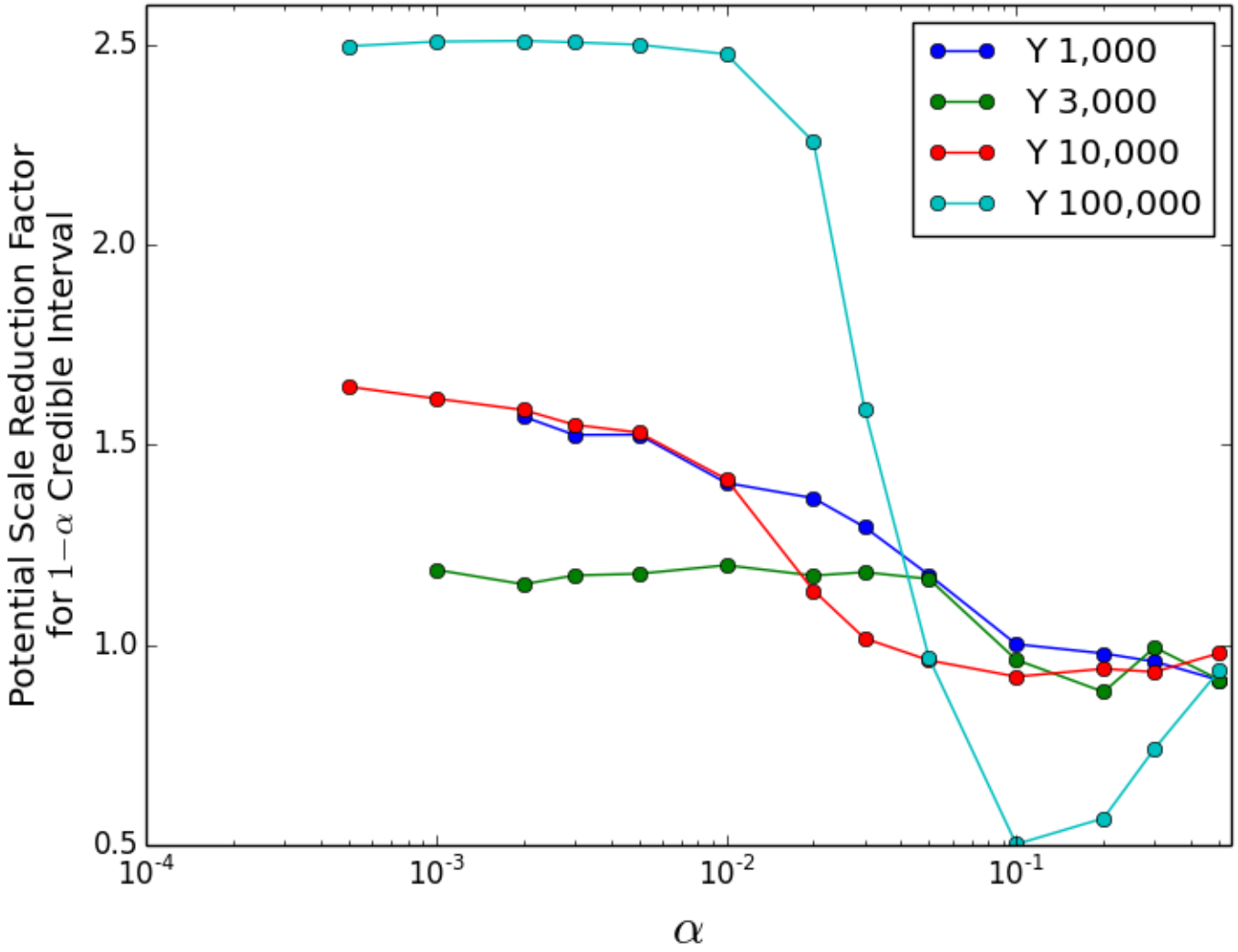


Test using Simplified Problems where You Can Compare to Target Density

This target distribution for the first example was:

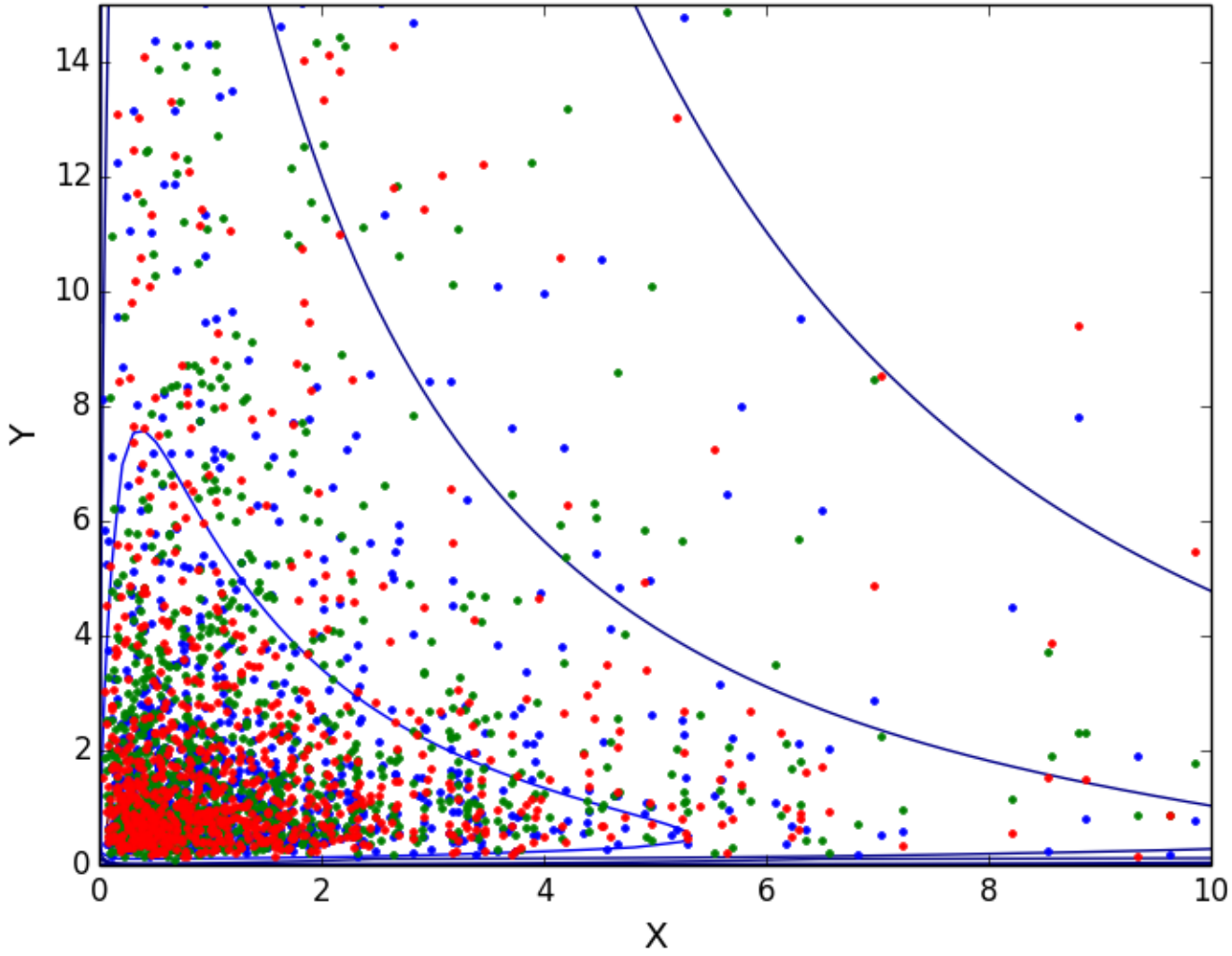
- p(x,y) = p(x) p(y)
- p(x) is LogNormal (zero mean, unit scale)

$$f_X(x;\mu,\sigma) = \frac{1}{x\sigma\sqrt{2\pi}}\, e^{-\frac{(\ln x-\mu)^2}{2\sigma^2}}, \quad x > 0$$

- p(y) is InverseGamma (unit shape, unit scale)

$$f(x;\alpha,\beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{-\alpha-1} \exp\left(-\frac{\beta}{x}\right)$$

Test using Simplified Problems where You Can Compare to Target Density



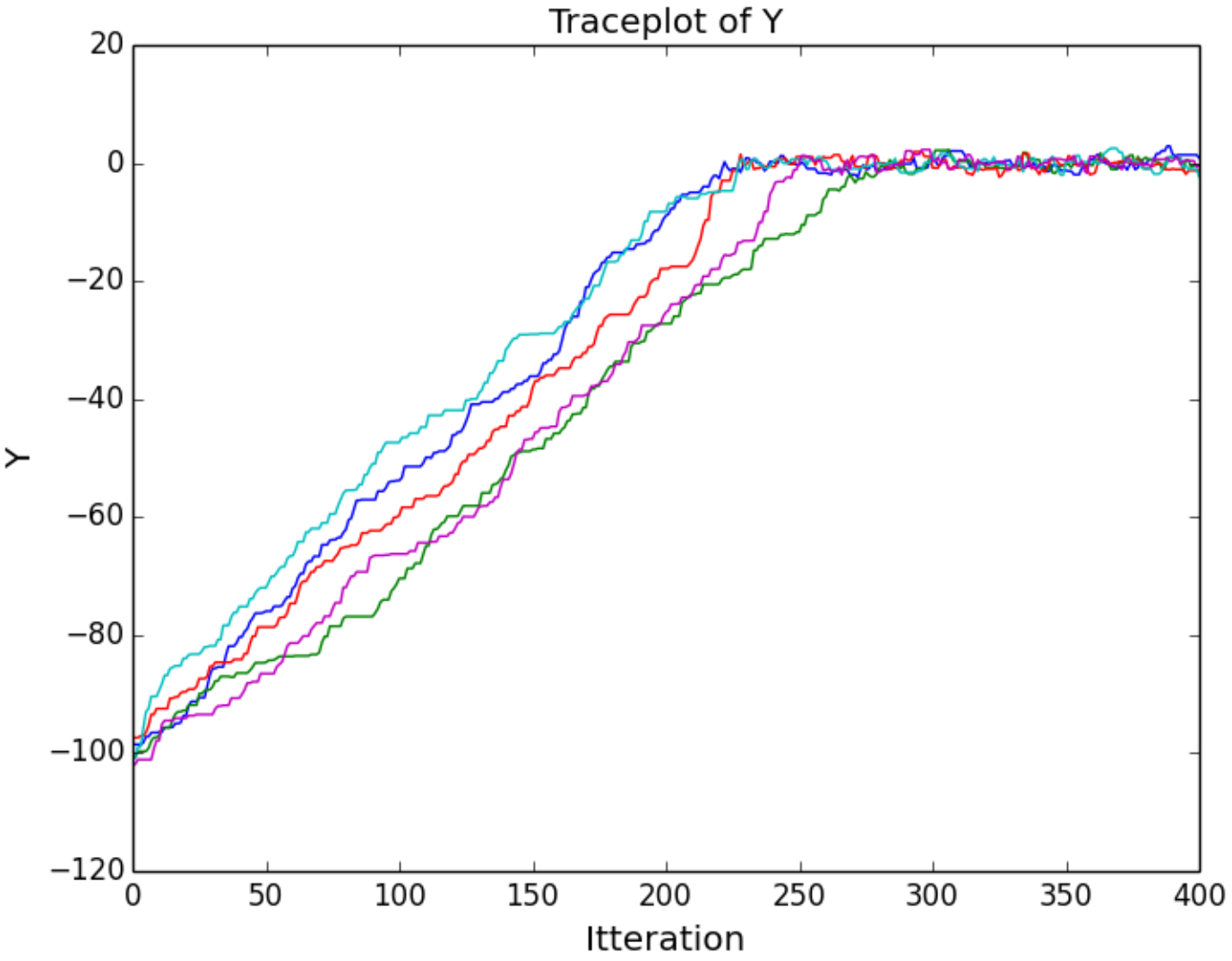
Use Problematic Runs to Improve Your Algorithm

- Why did our Markov chains struggle on a relatively simple target distribution?
- How could we change our algorithm to accelerate convergence?

Has this Chain Converged?

- Let’s try this game again…

Has this Chain Converged?



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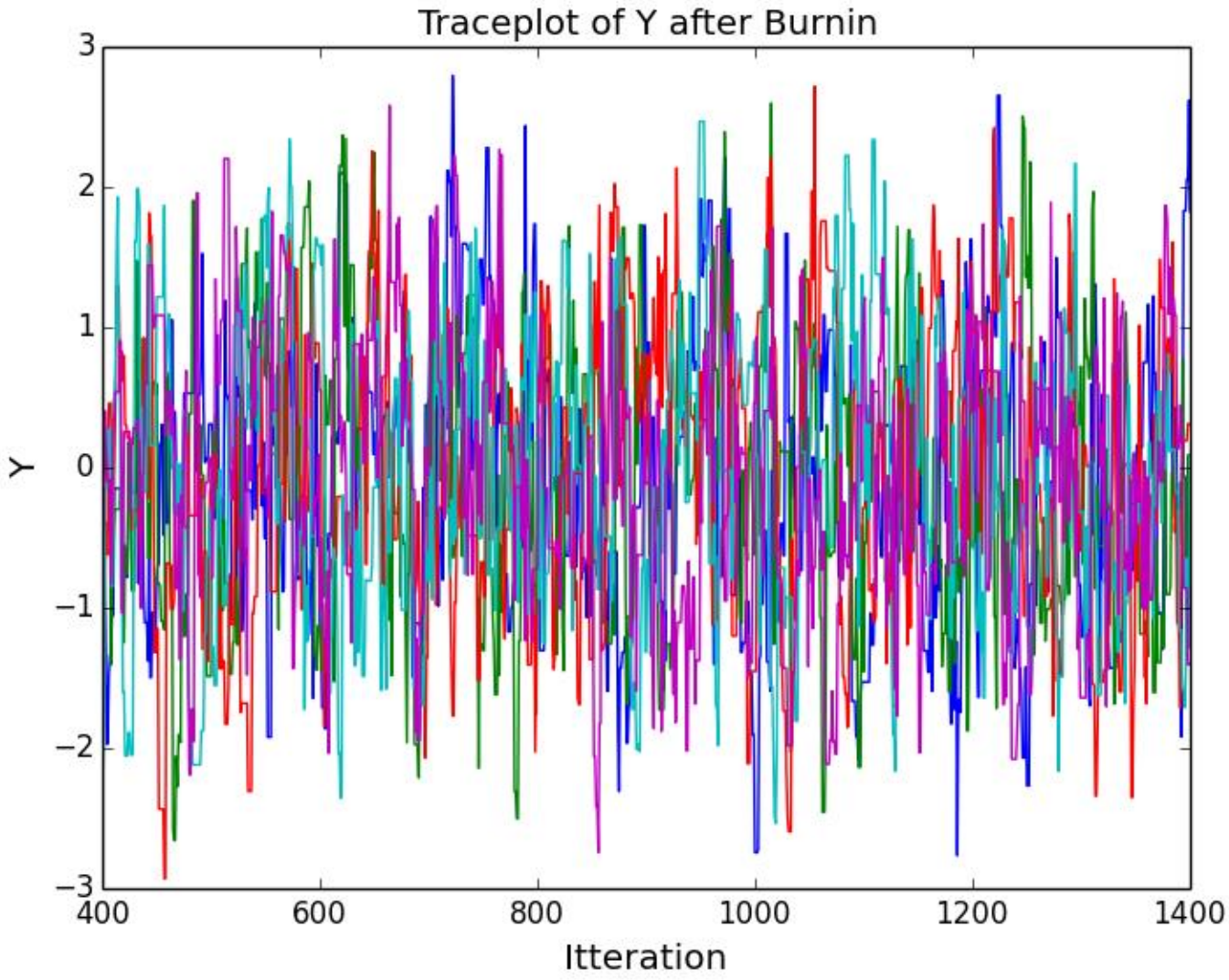

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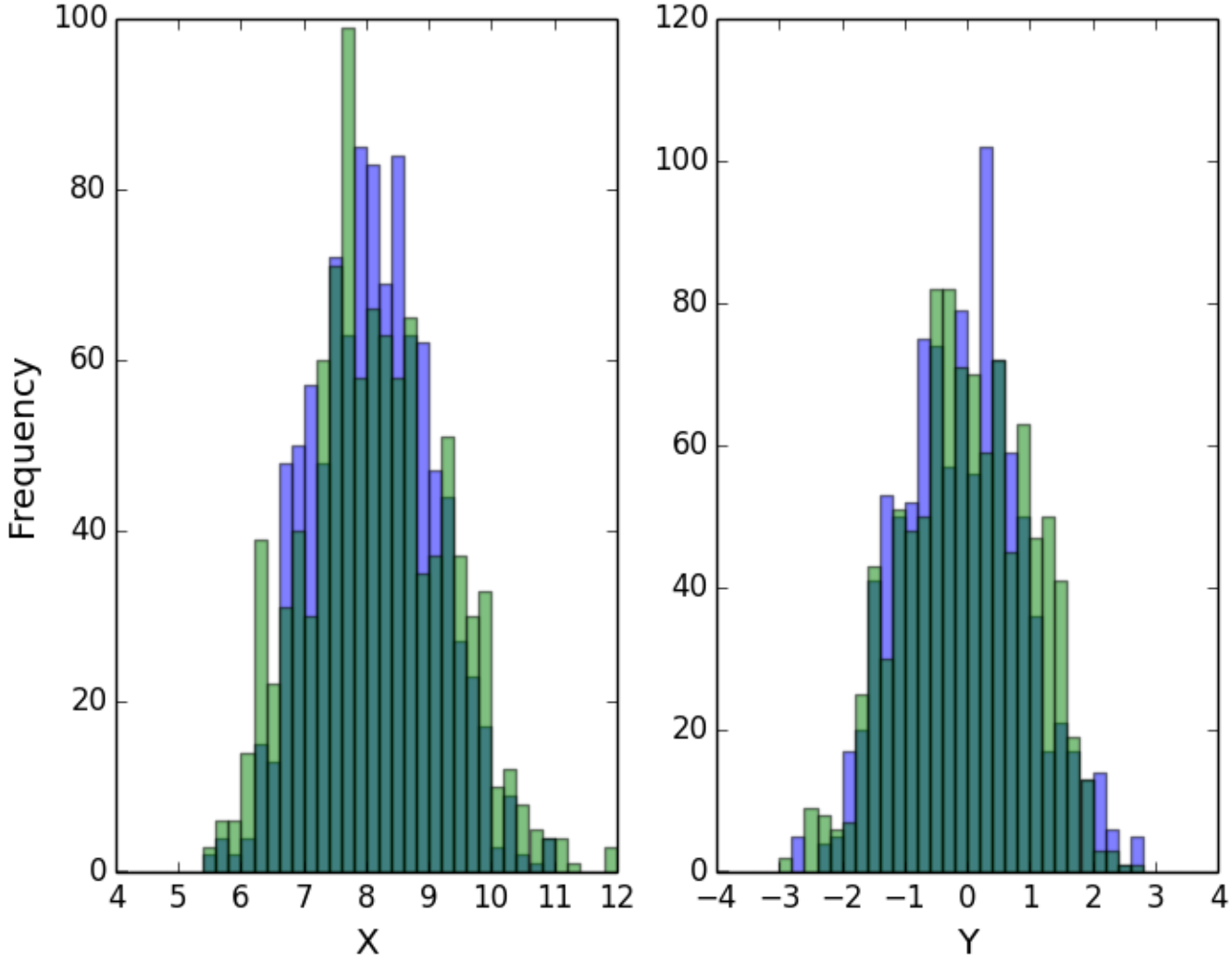

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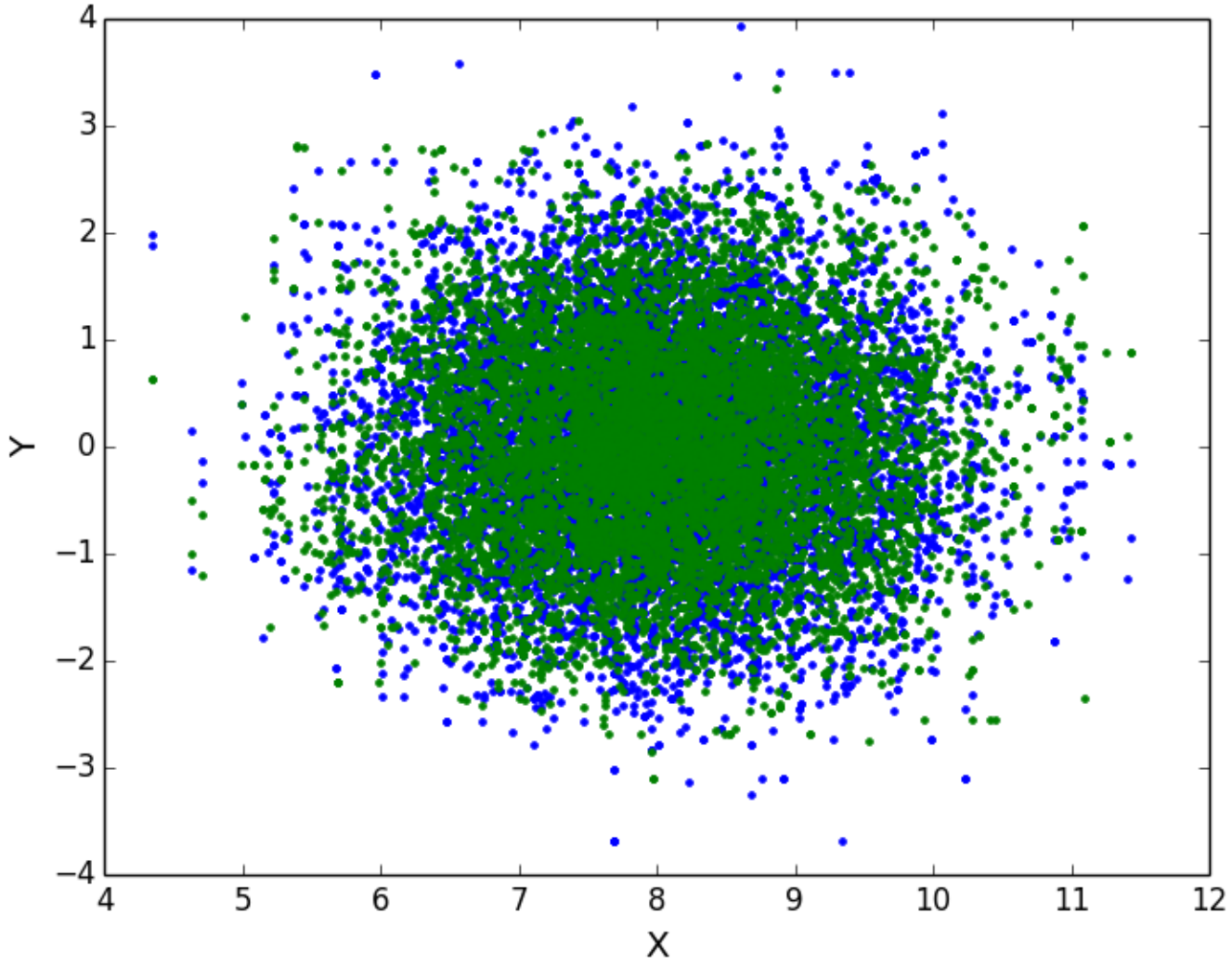

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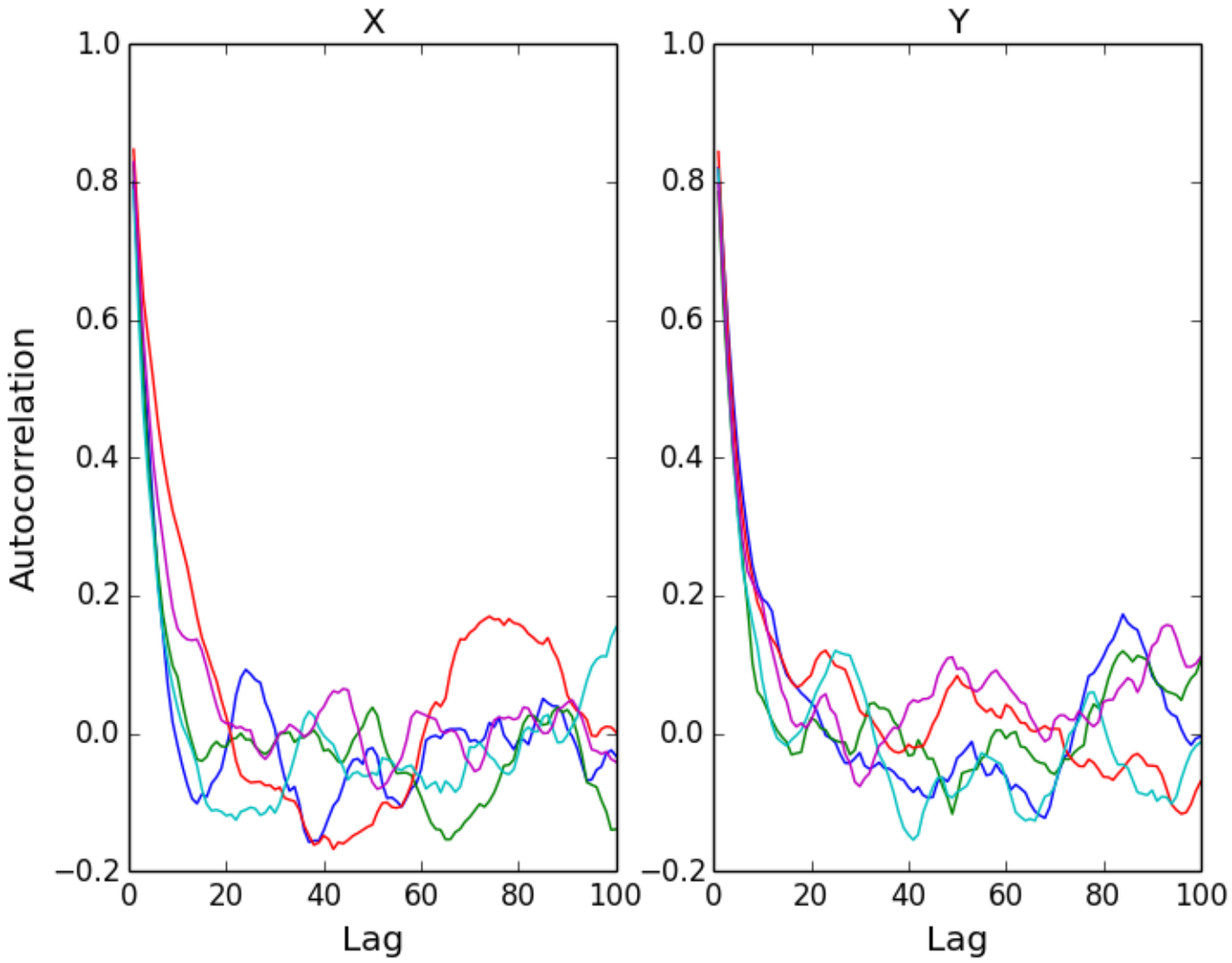

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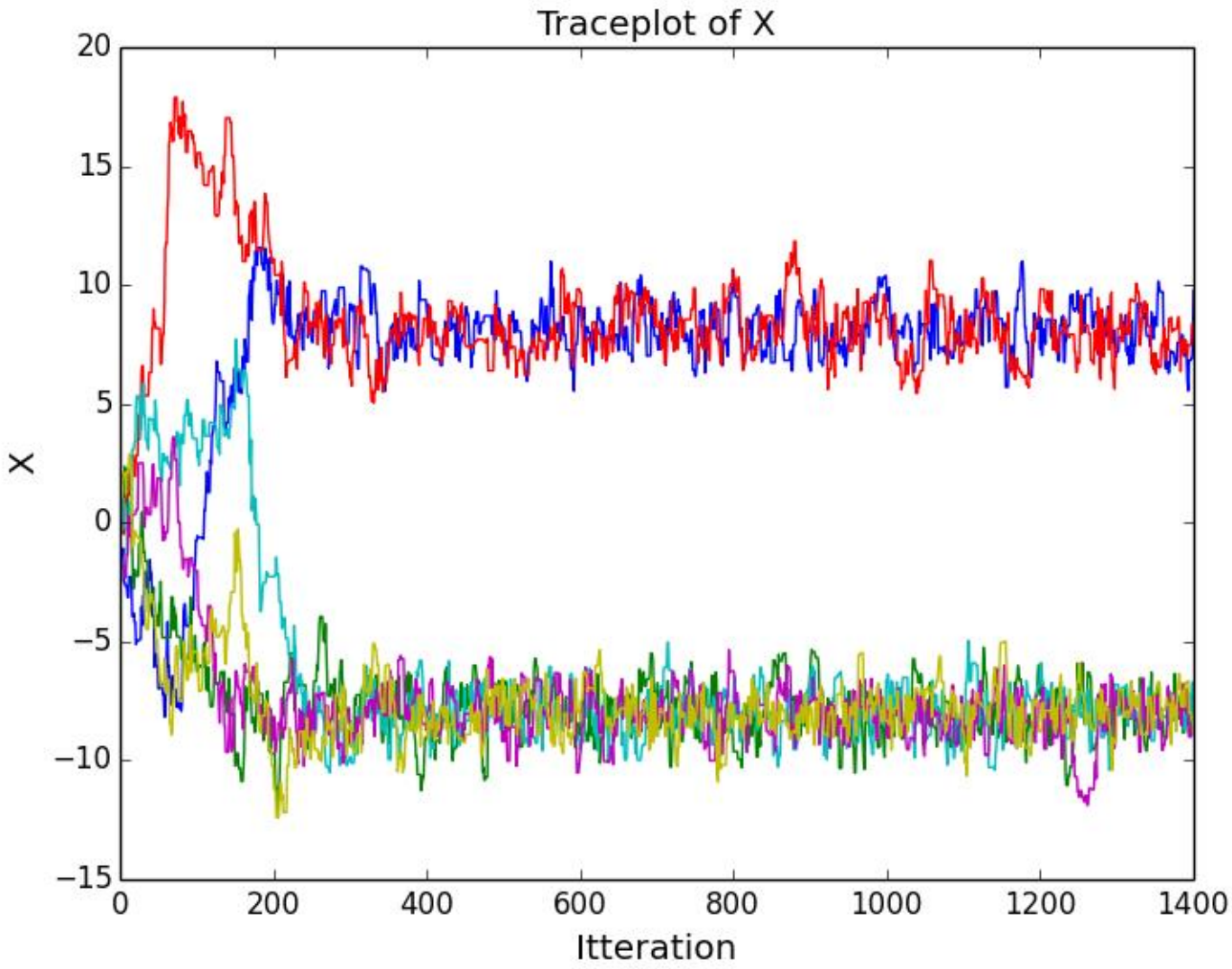

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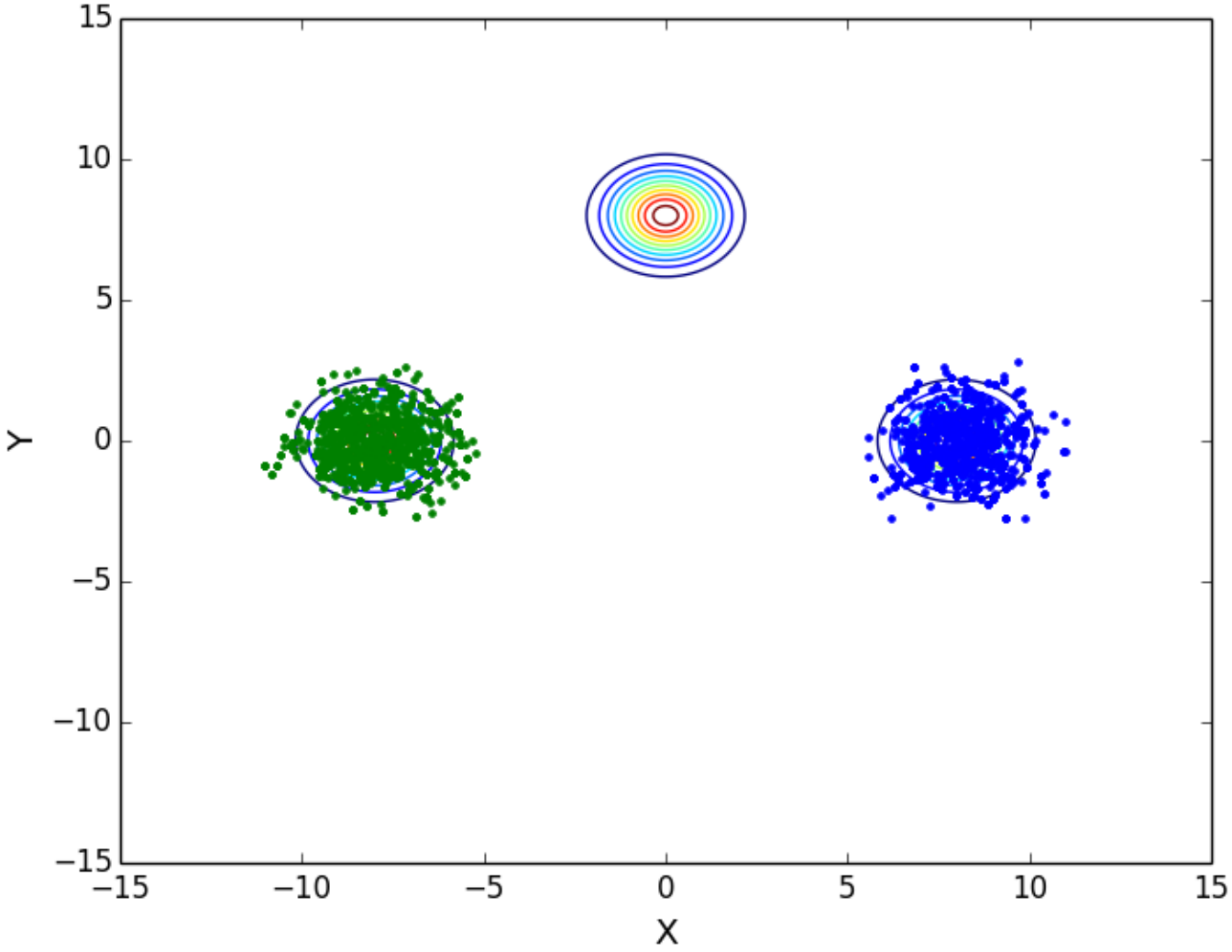


My chain isn't perfect… Now what?

- What is your goal?
  - Ball park estimate of the median value of a parameter
  - Precisely define the boundary of a 99.9% credible region
- What are the consequences?
- Different goals merit different levels of paranoia

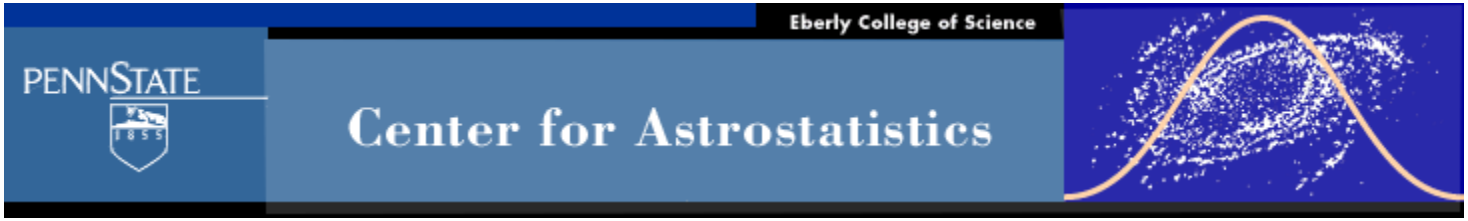
My chain isn’t perfect… Now what?

- Run Markov chains for many more iterations
- Change problem and/or algorithm to accelerate convergence

How a non Non-Converged Markov chain be Useful?

- Even if your chains haven't converged, have they allowed you to learn something about your target density?
- Can you change your algorithm so it will converge more quickly?
  - Change step sizes?
  - Alternative parameterization of problem?
  - Change proposal distribution of MCMC?
  - Solve problem via Importance Sampling?

Pause for Questions



Ensemble MCMC: A Great Tool for Target Densities with Correlations Between Parameters

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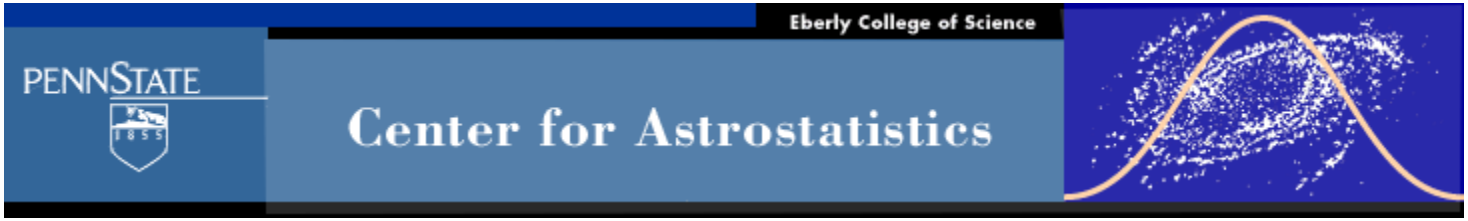
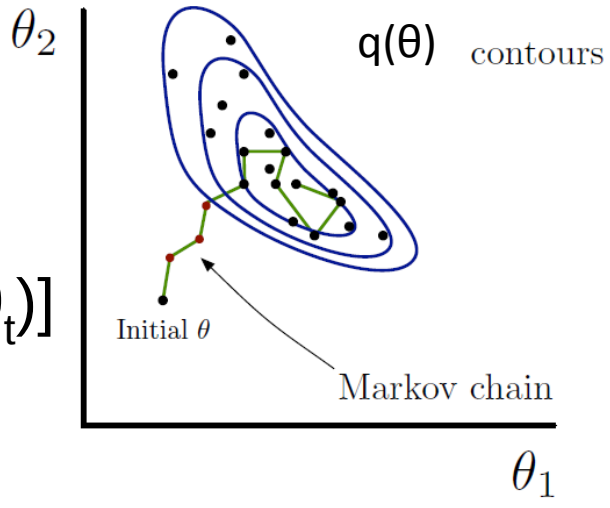


Simple Markov Chain Monte Carlo

- Initialise chain with θ_0 (initial guess)
- Loop (iterate over t)
  1. Propose trail state, θ', according to $k(\theta'|\theta_t)$.
  2. Calculate unnormazlized posterior probability for trial state, $q(\theta') \sim p(\theta'|\text{Data,Model})$.
  3. Accept or reject trial state
     - Draw random number, u ~ U[0,1)
     - $\alpha(\theta'|\theta_t) = [q(\theta')\, k(\theta_t|\theta')] / [q(\theta_t)\, k(\theta'|\theta_t)]$
     - If $u \le \alpha(\theta'|\theta_t)$, then set $\theta_{t+1} = \theta'$ (accept)
     - If $u > \alpha(\theta'|\theta_t)$, then set $\theta_{t+1} = \theta_t$ (reject)
- Test for non-convergence



Why Go Beyond Simple MCMC?

- Standard MCMC converges extremely slowly if the proposal distribution is not well chosen
  - It's hard to find a good proposal distribution for complex problems (e.g., many parameters)
  - Want a way to automatically choose good proposal distribution
- Standard MCMC evaluates 1 model at a time
  - Parallelizing standard MCMC requires parallelizing the model evaluation (may be impractical)

What is Ensemble/Population MCMC?

- Instead of updating one set of model parameters at a time, update an ensemble/population of model parameters each “generation”

- Technically, the Markov chain is now over a product space of your model parameters

Advantages of Ensemble MCMC

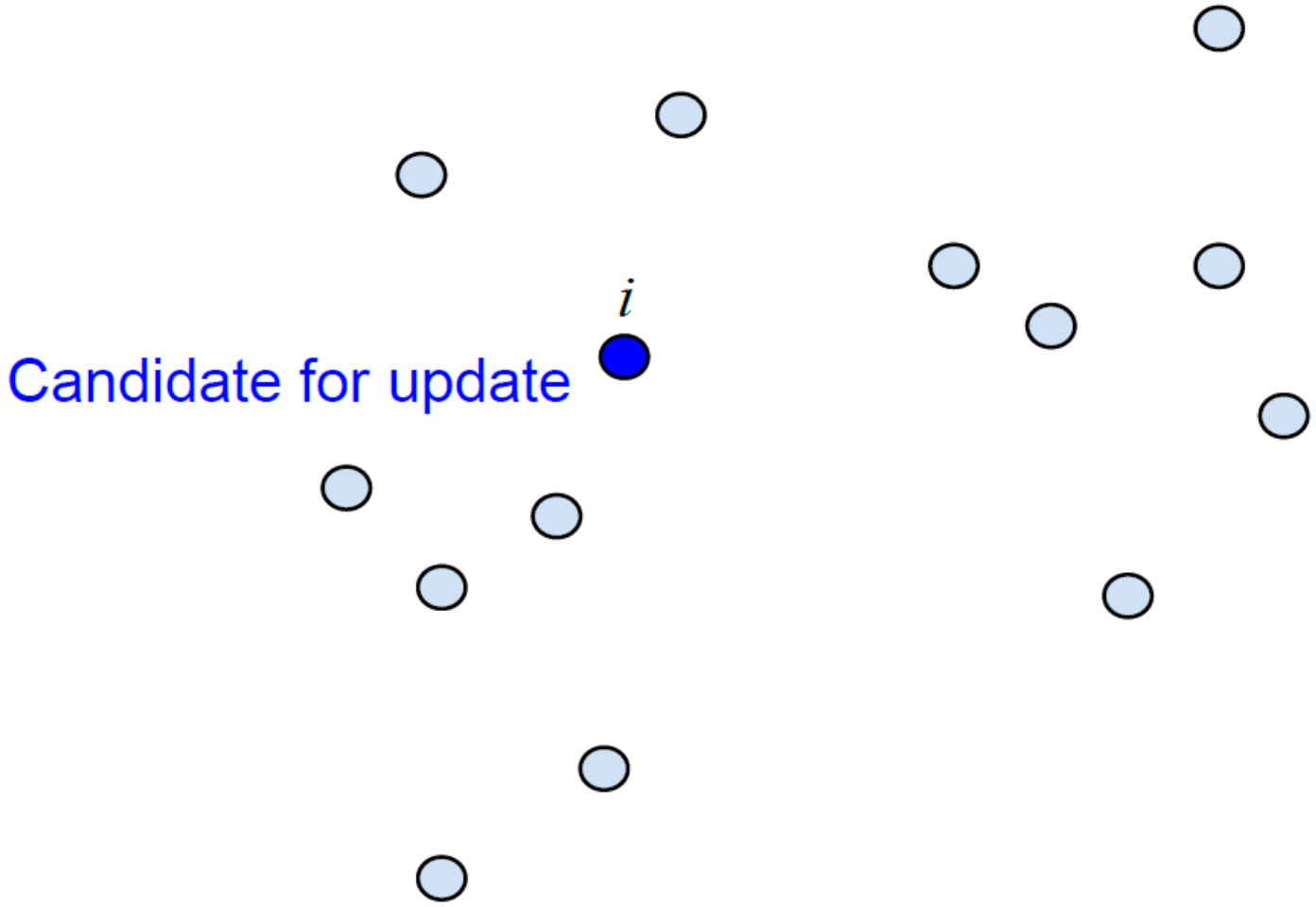
Ensemble MCMC:

- Can take advantage of having a population of model parameters when proposing each trial set of model parameters
- Makes it easy to parallelize over each set of model parameters within a generation

Two Specific Ensemble MCMC Algorithms

- Differential Evolution MCMC
  (ter Braak 2006; ter Braak & Vgurt 2008; Nelson et al. 2014)
  - Combines three states from previous generation for each trial state
- Affine-Invariant Ensemble MCMC
  (Goodman & Weare 2010; Foreman-Mackey et al. 2013)
  - Combines two states from previous generation for each trial state
- Both algorithms
  - Automatically infer shape & scale for proposals
  - Require only a few new parameters (and performance is typically insensitive to their choice)

Affine-Invariant Ensemble MCMC



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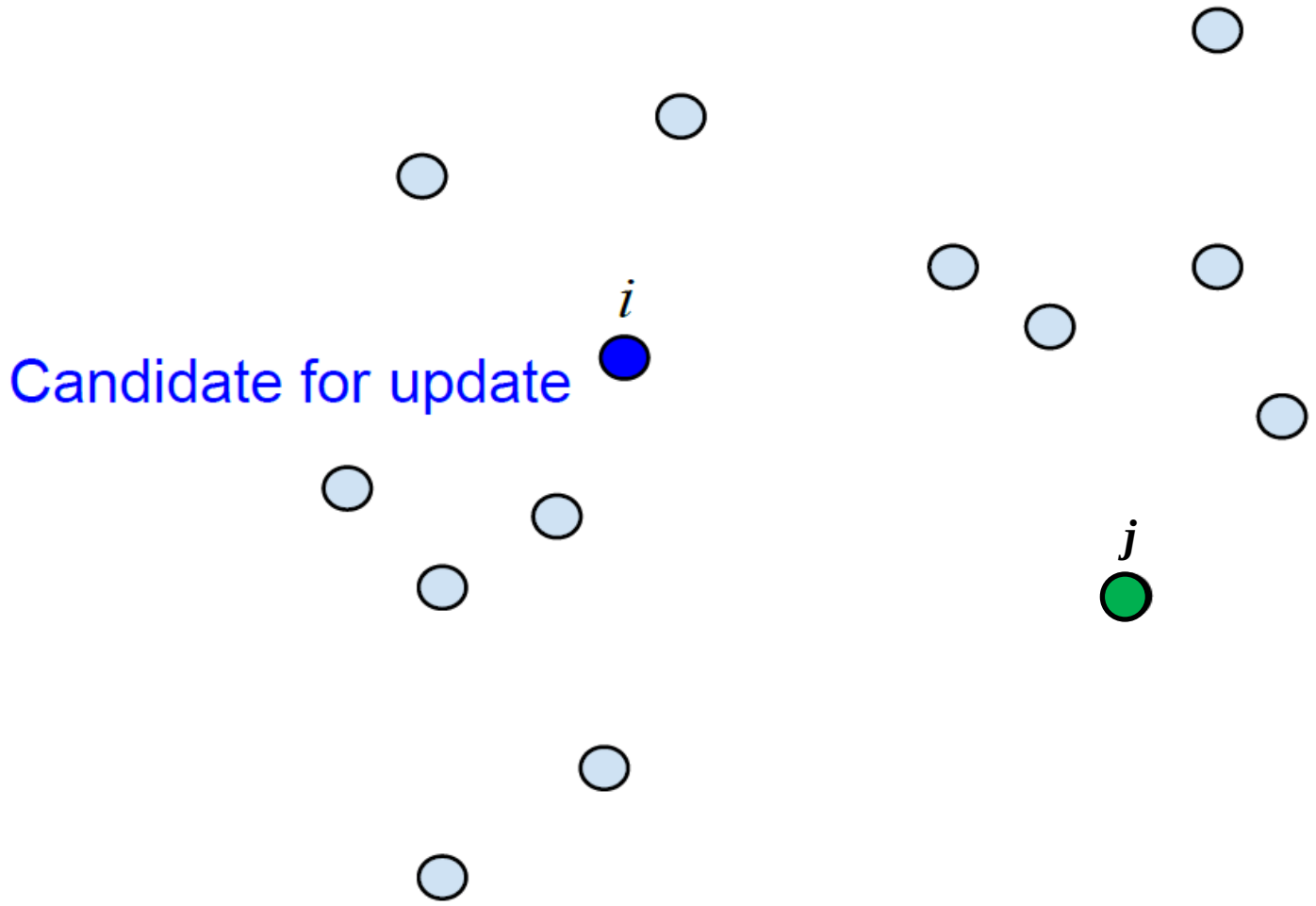

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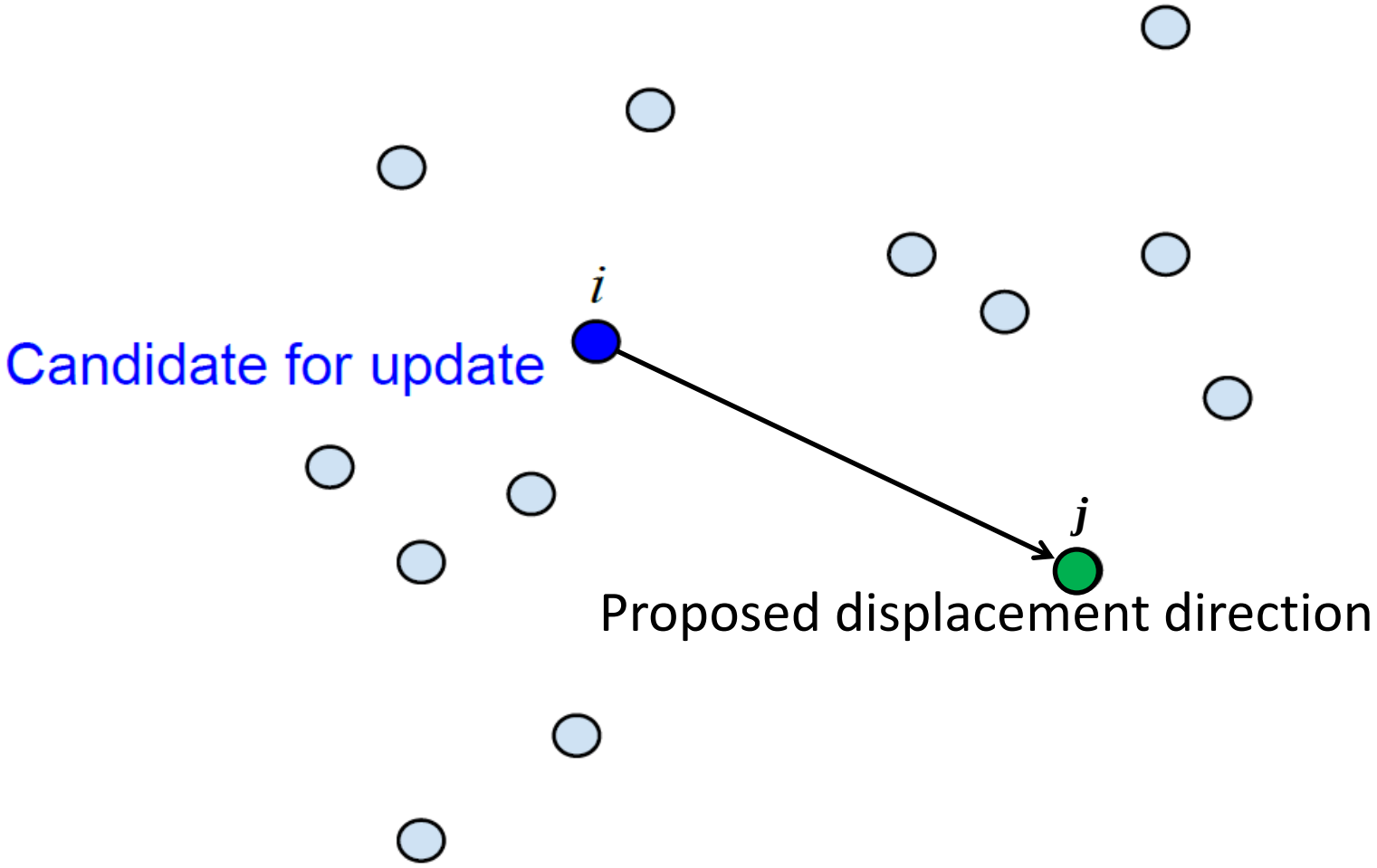

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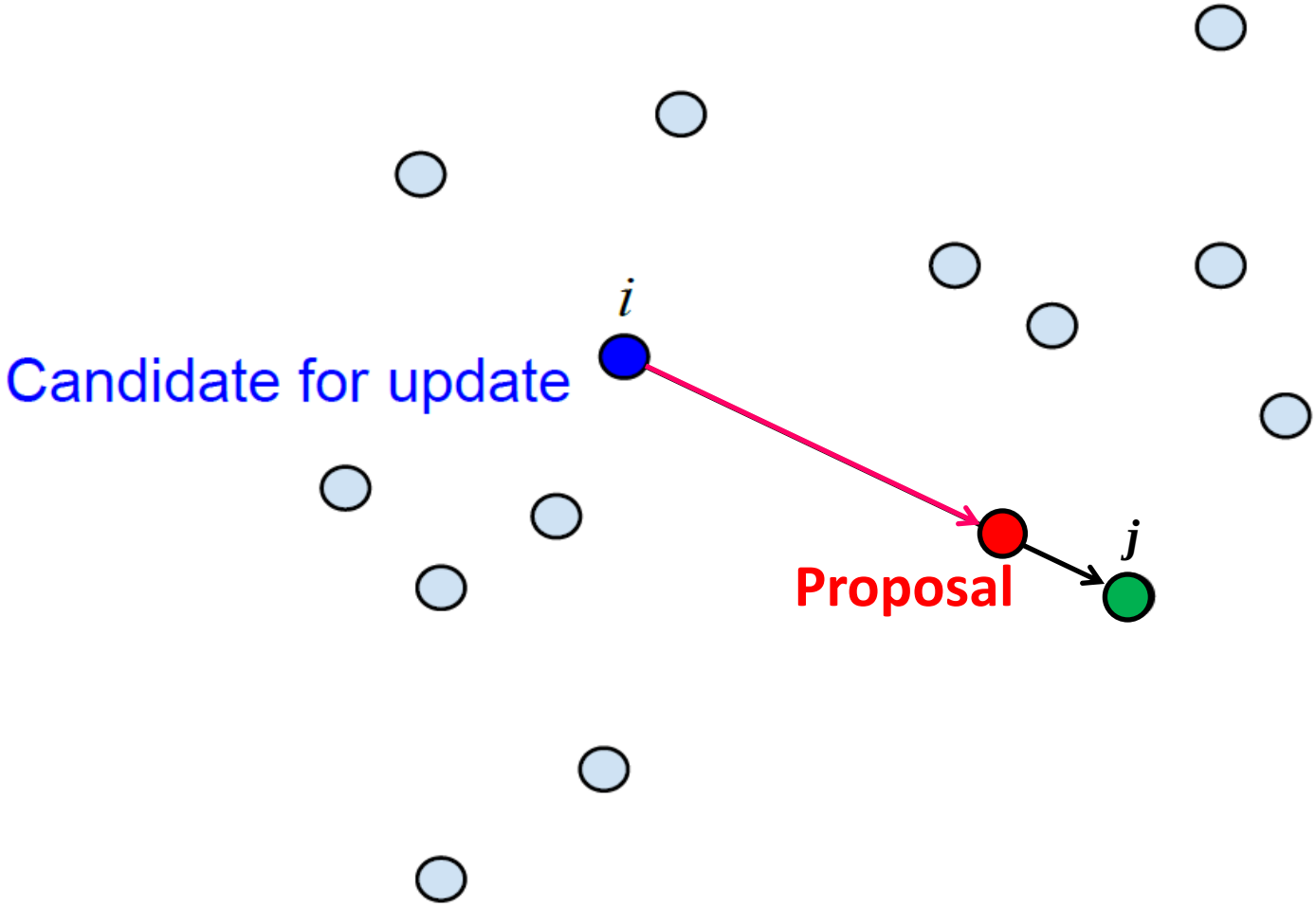


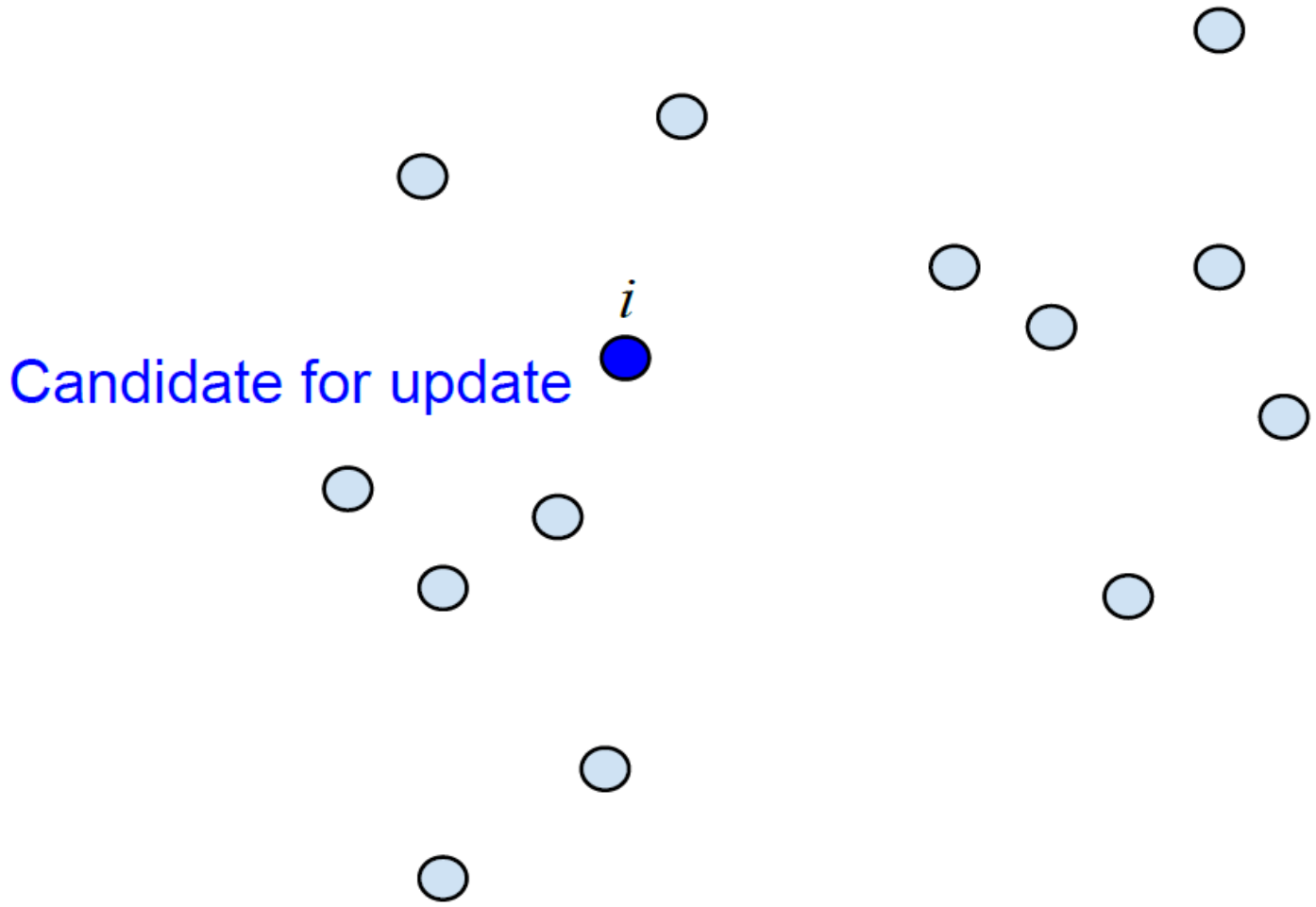
Affine-Invariant Ensemble MCMC

Implementation details

- Proposal step: $\theta_i' = \theta_{t,j} + z\,[\theta_{t,i} - \theta_{t,j}]$
  - z: random variable drawn from distribution $g(z) = z\,g(z)$
  - Update parameters for each "chain" in blocks
- Acceptance probability $\alpha = \min[1, z^{N_d-1}\, q(\theta')/q(\theta_{t,i})\,]$
  - N_d = dimension of parameter space
  - Target distribution: $q(\theta) \sim p(\theta' | \text{Data,Model})$
- Tunable parameters: a, $g(z)$ and N_{chains} (population size)
- Suggestions
  - $g(z) = z^{-1/2}$, $z \in [a^{-1}, a]$,
    0, else
  - $a = 2$
  - $N_{chains} > \text{few} \times N_d$

Goodman & Weare 2010
Foreman-Mackey et al. 2013

Differential Evolution MCMC



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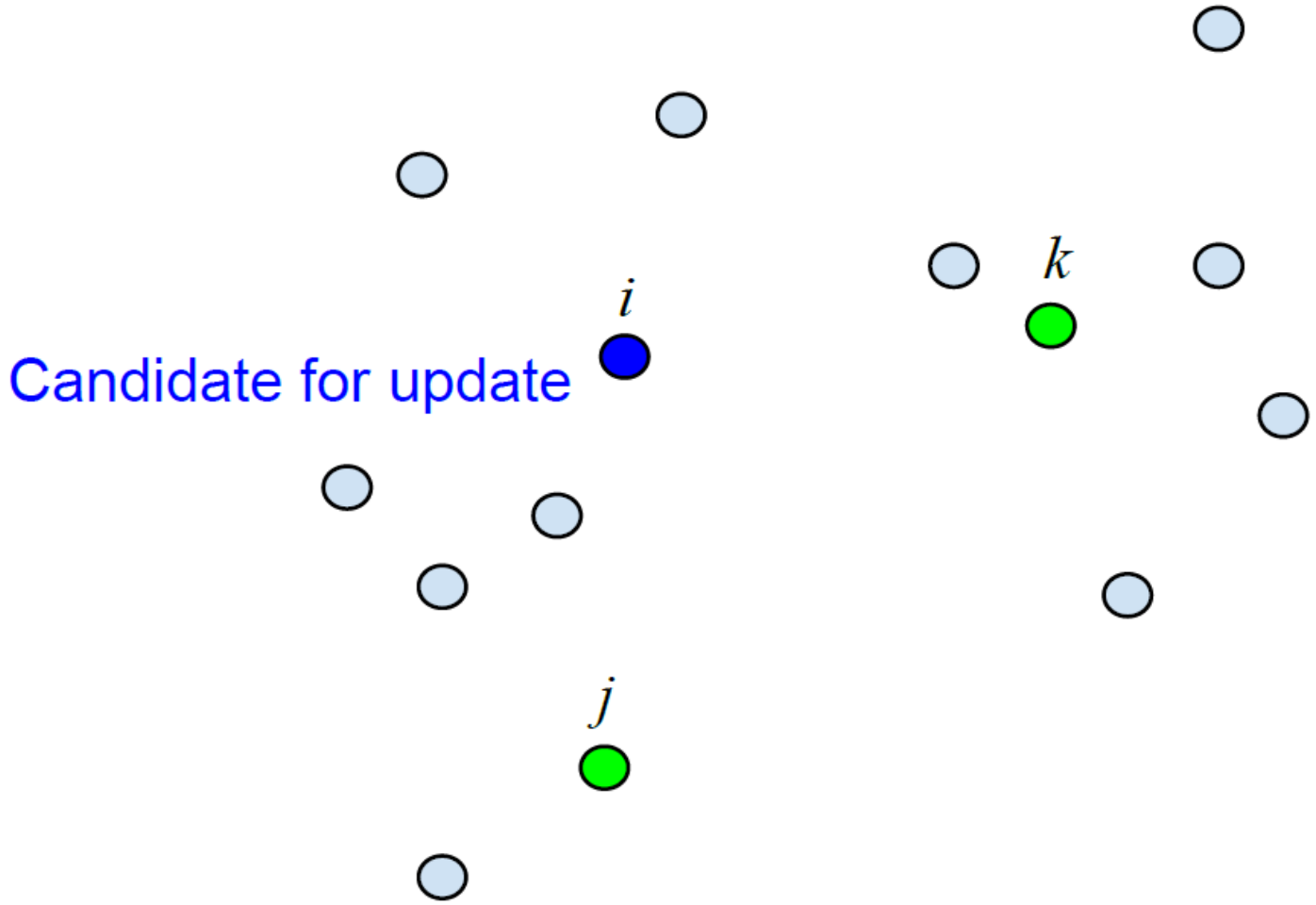

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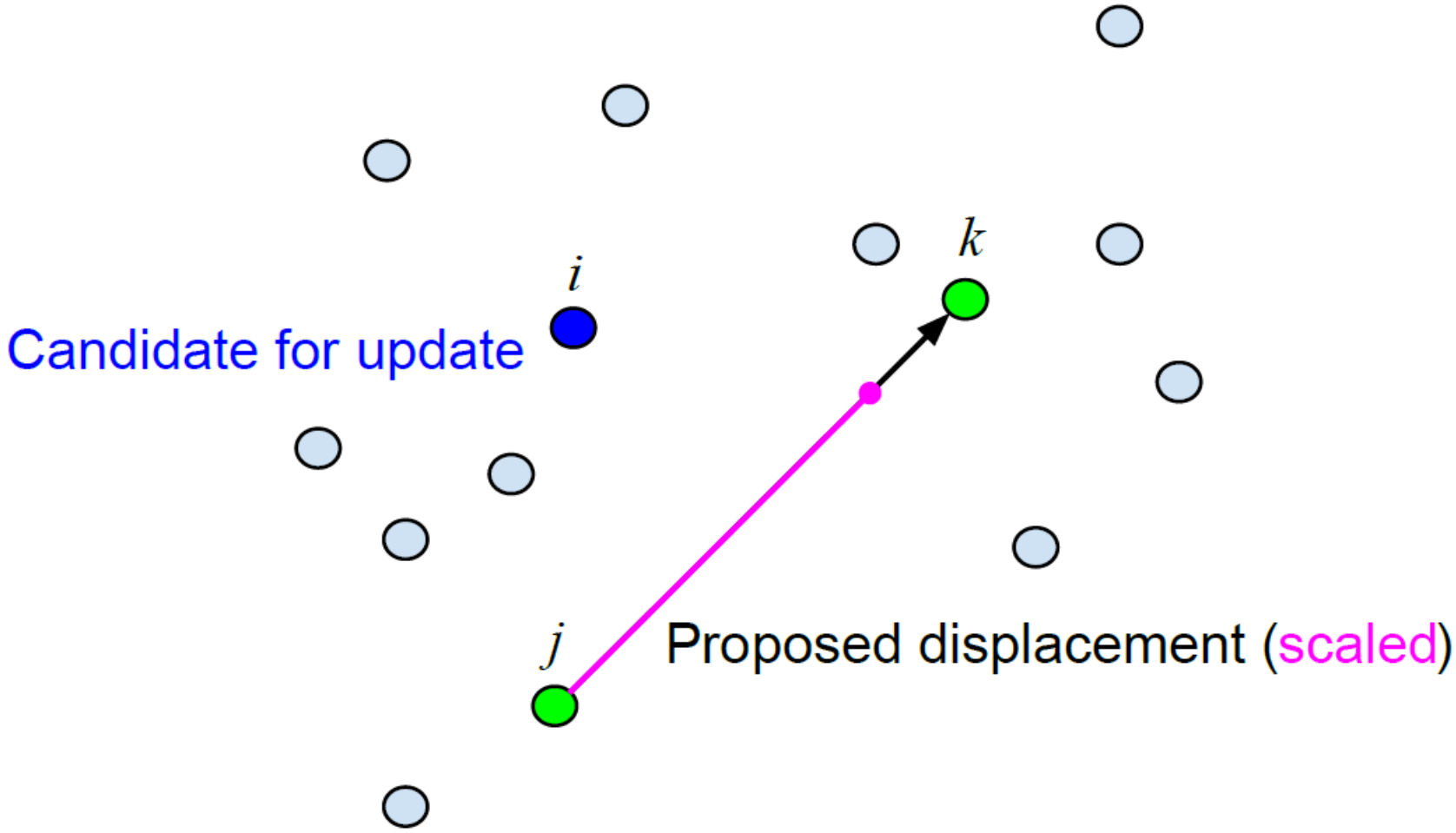

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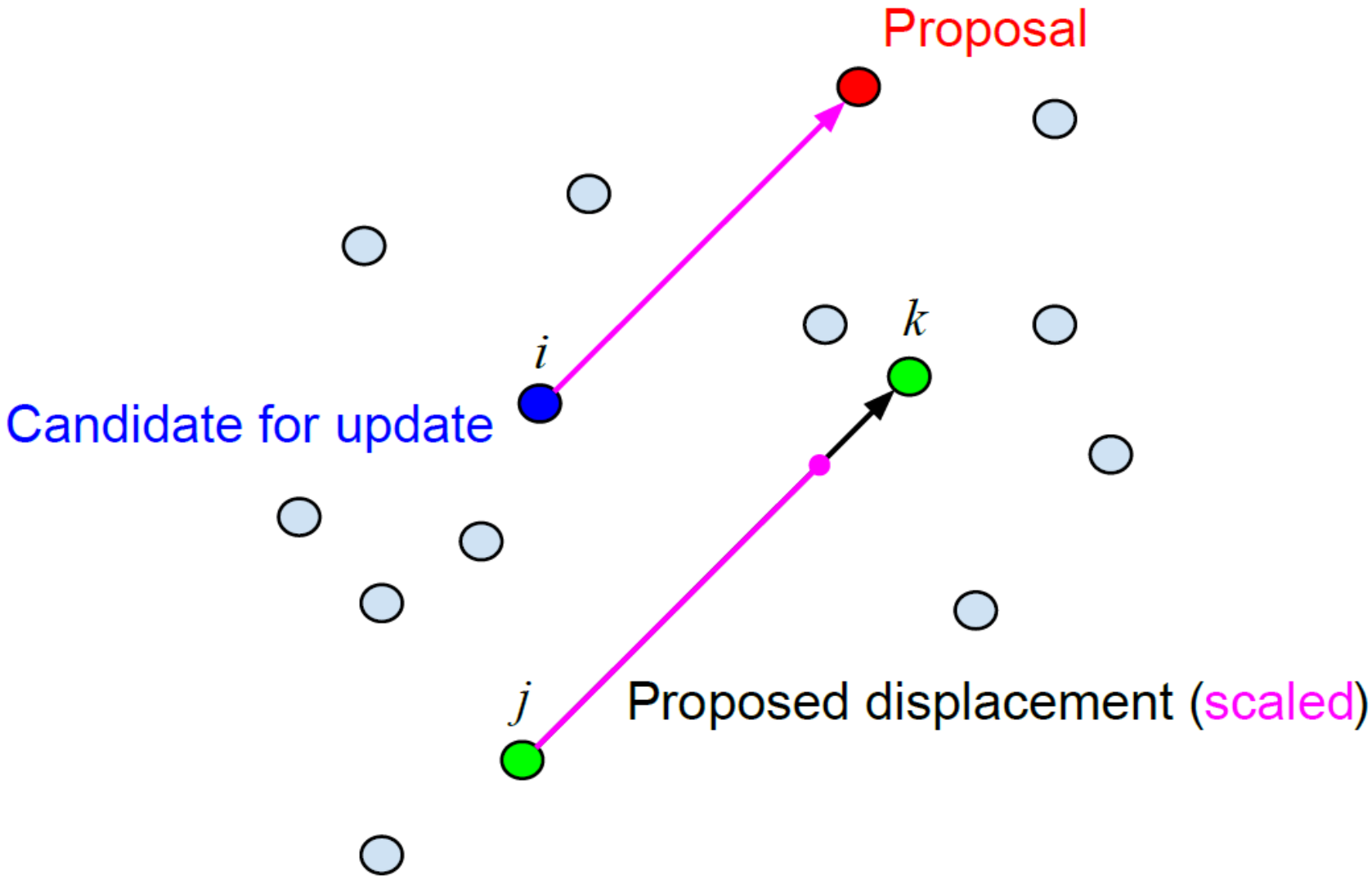


Differential Evolution MCMC

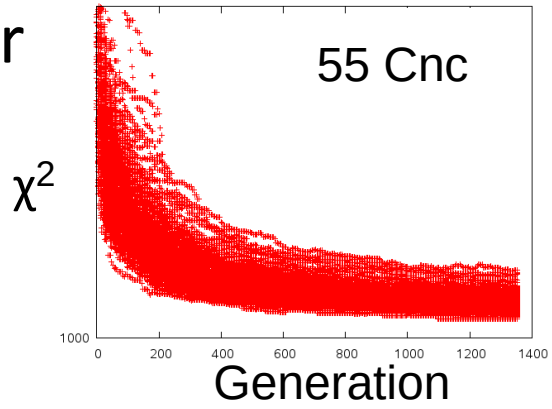
Implementation details

- Proposal step: $\theta' = \theta_{t,i} + \gamma\,[\theta_{t,k} - \theta_{t,j}]$ (most of the time)
  - $\gamma = \gamma_o\,(1 + z)$
  - $z \sim N(0, \sigma_\gamma^2)$
  - $\gamma_o = 2.38 / (2N_{dim})^{1/2}$, (initially, can adjust to improve acceptance rate)
  - Update parameters for each "chain" in blocks
- Optionally, occasionally use large proposal steps
  - $\gamma = (1 + z)$ $z \sim N(0, \sigma_\gamma^2)$
- Acceptance probability: same as standard MCMC
- Tunable parameters: σ_γ, and N_{chains} (population size)
- Suggestions:
  - $N_{chains} >$ few $\times N_d$
  - $0.001 < \sigma_\gamma < 0.1$ (quite insensitive in our tests; Nelson et al 2014)
  - Adapt γ_o to achieve good acceptance rate (~0.25)

ter Braak 2006
Nelson et al. 2014

Choosing Initial Population

- Generate initial population from prior
  - Great… if it works
  - But often get stuck in local maxima, resulting in unreasonable number of generations to complete burn-in



- Generate initial population close to posterior
  - Dramatically reduces burn-in time
  - But what if you missed another important posterior maxima?
- Compromise: Generate initial population to be near posterior, but more dispersed than posterior

How Can Things Still Go Wrong?

- Initial population too far from target density
  - Choose initial population close to target density
  - Test that results insensitive to choice
- Non-linear correlations between parameters
  - Results in long auto-correlation times
  - Increasingly problematic with higher-dimensional parameter spaces
- Multi-modal target density
  - DEMCMC can deal with a few viable modes, but autocorrelation time increases

Example Application of DEMCMC

Measuring planet masses & orbits from Doppler observations of Exoplanet Systems

- Physical Model
  - Non-Interacting: Linear superposition of Keplerian orbits $v_{\star,\vec{\theta}}(t,j) = \sum_i K_i \left\{\cos\left[\omega_i + f_i(t)\right] + e_i \cos\omega_i\right\} + C_j$
  - Interacting: Full n-body model $\frac{d^2\vec{r_i}}{dt^2} = -\sum_{j=1}^{N} \frac{Gm_j(\vec{r_i} - \vec{r_j})}{|\vec{r_i} - \vec{r_j}|^3}$
- Likelihood assumes observations with uncorrelated, Gaussian uncertainties

$$\chi^2 = \sum_k \frac{\left[v_{\star,obs}(t_k,j_k) - v_{\star,\vec{\theta}}(t_k,j_k)\right]^2}{(\sigma_{\star,obs}(t_k,j_k)^2 + \sigma_{jit}^2)}$$

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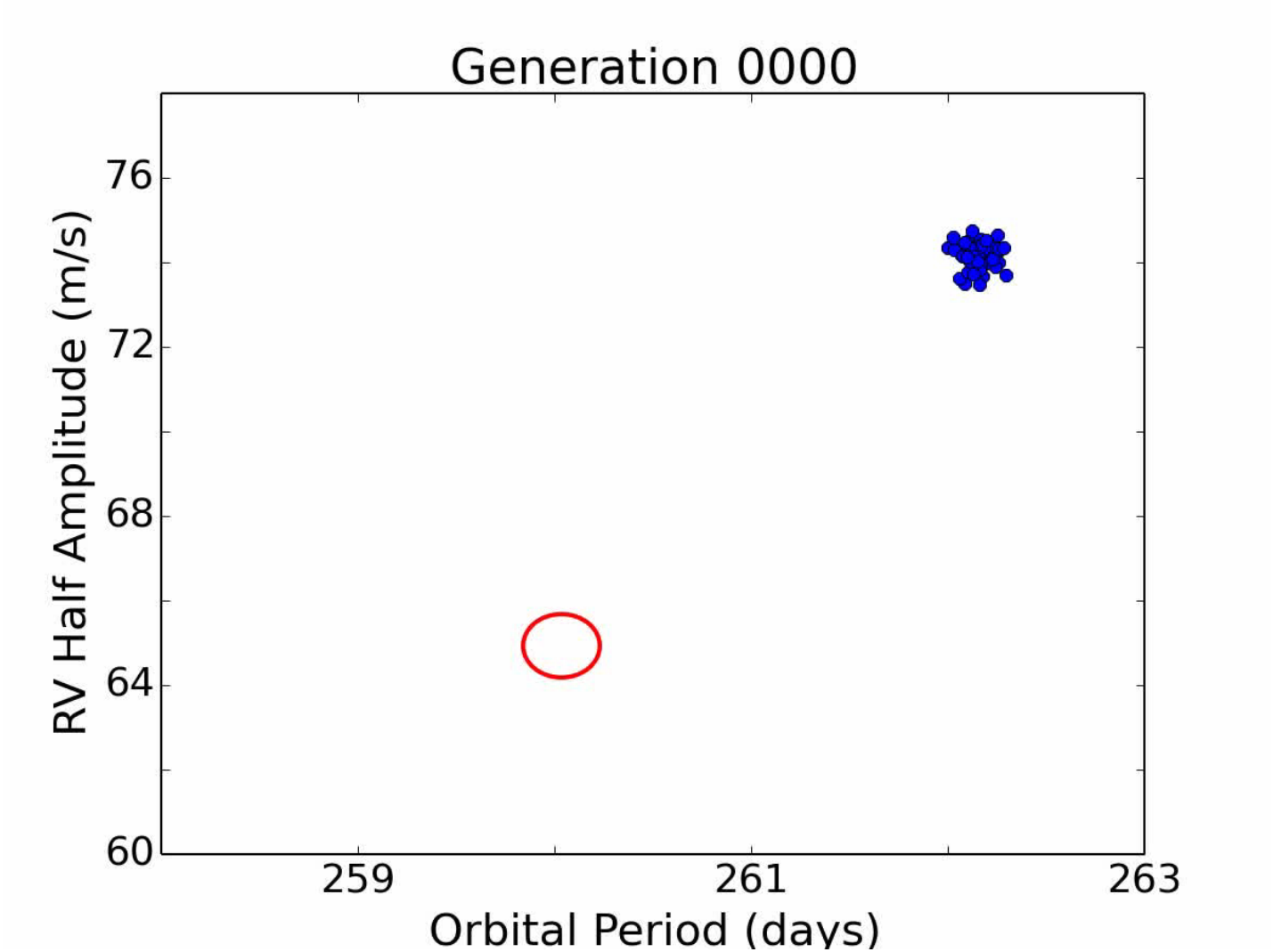
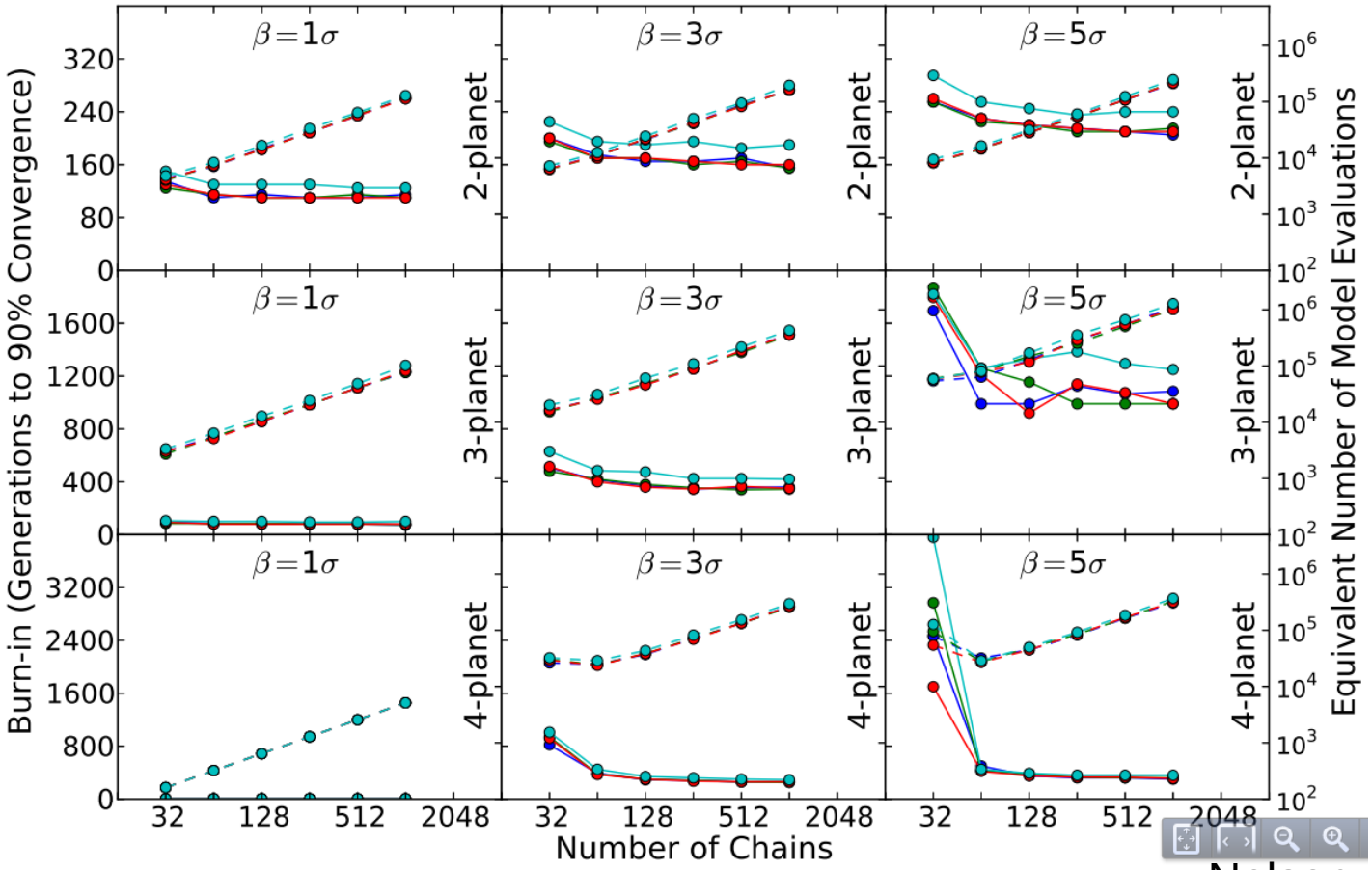
What if Poor Initial Population?



Nelson

Test Burn-In Required using Synthetic Data

- For initial population, take posterior sample and increase dispersion about mean



Nelson et al. 2014

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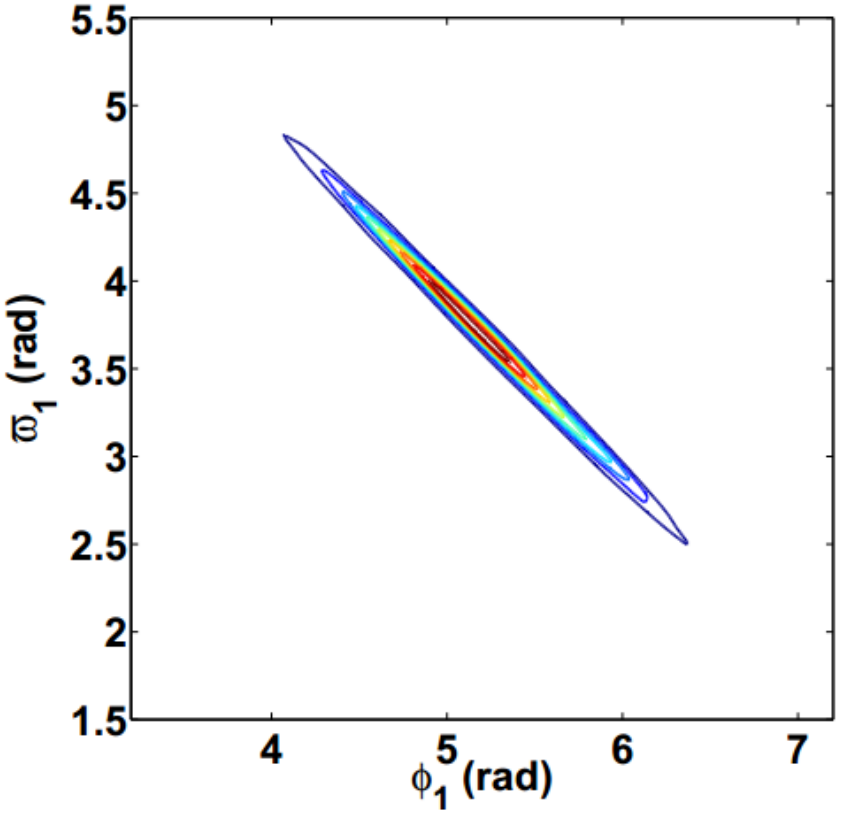
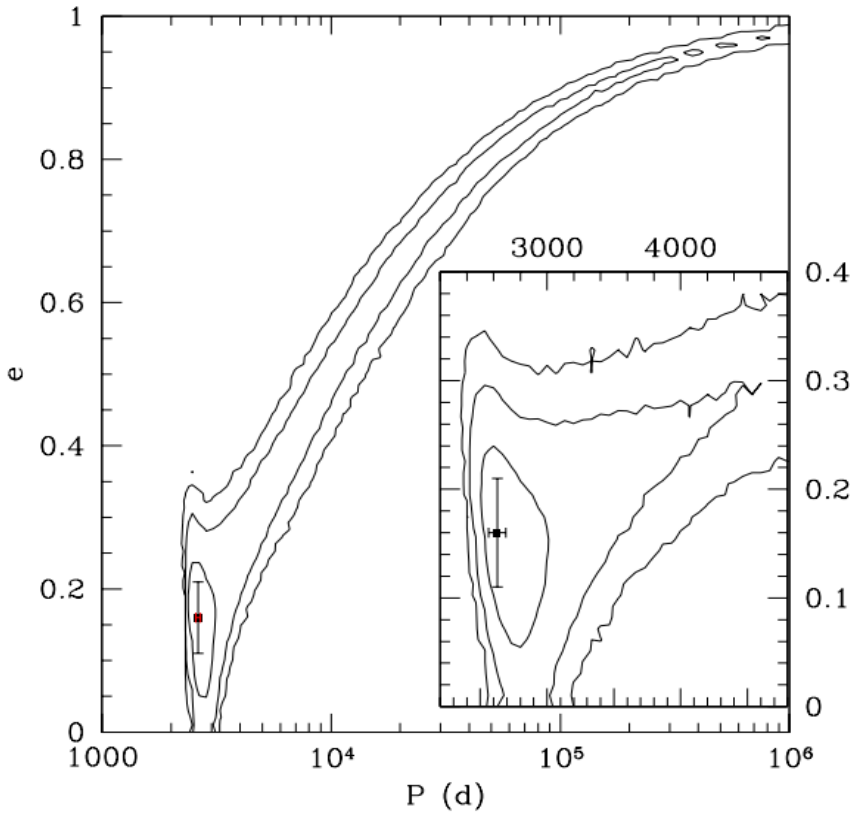
Non-Linear Parameter Correlations

Linear Correlations
(still efficient)



Non-Linear Correlations
(reduce efficiency)



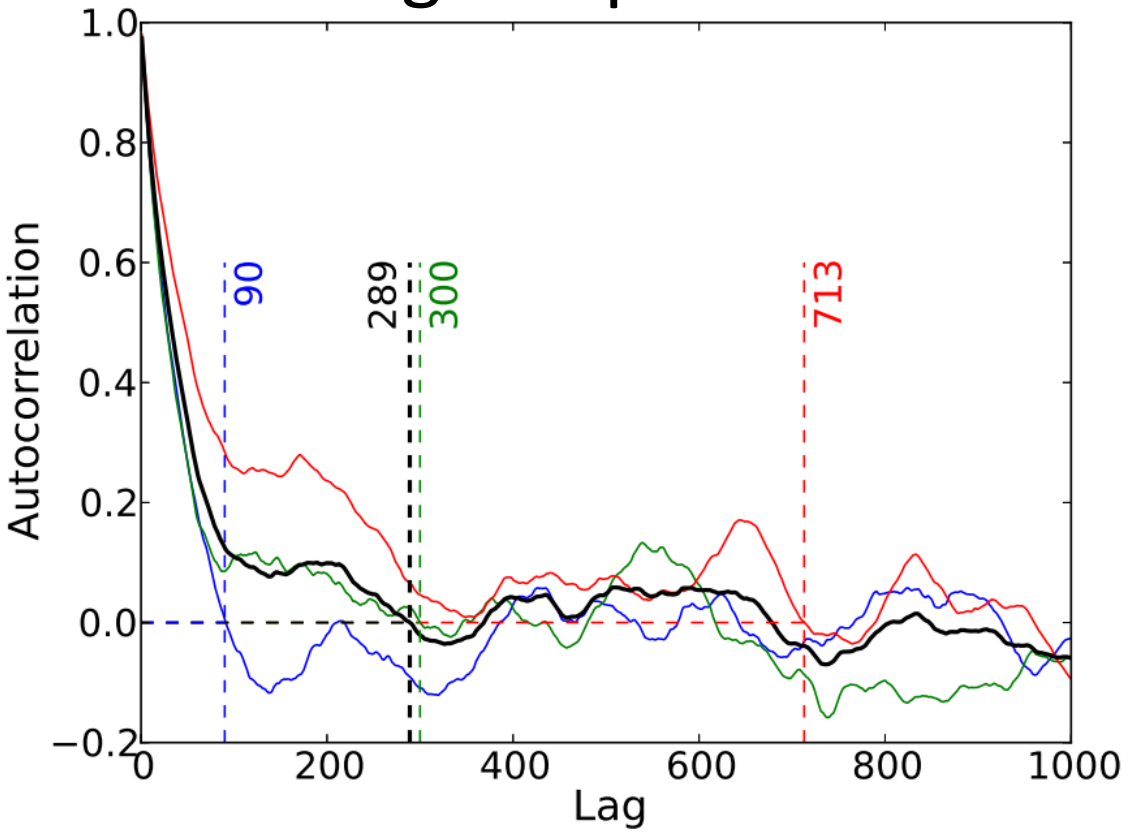
Hou et al. 2012

Ford 2006

Check Sufficient Effective Sample Size

Often, it is practical to run DEMCMC longer to make up for correlations among samples

- Check autocorrelation and other MCMC diagnostics for *all* parameters of interest



Nelson et al. 2014

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  - DEMCMC can deal with a few viable modes, but autocorrelation time increases

Dealing with Multiple Modes

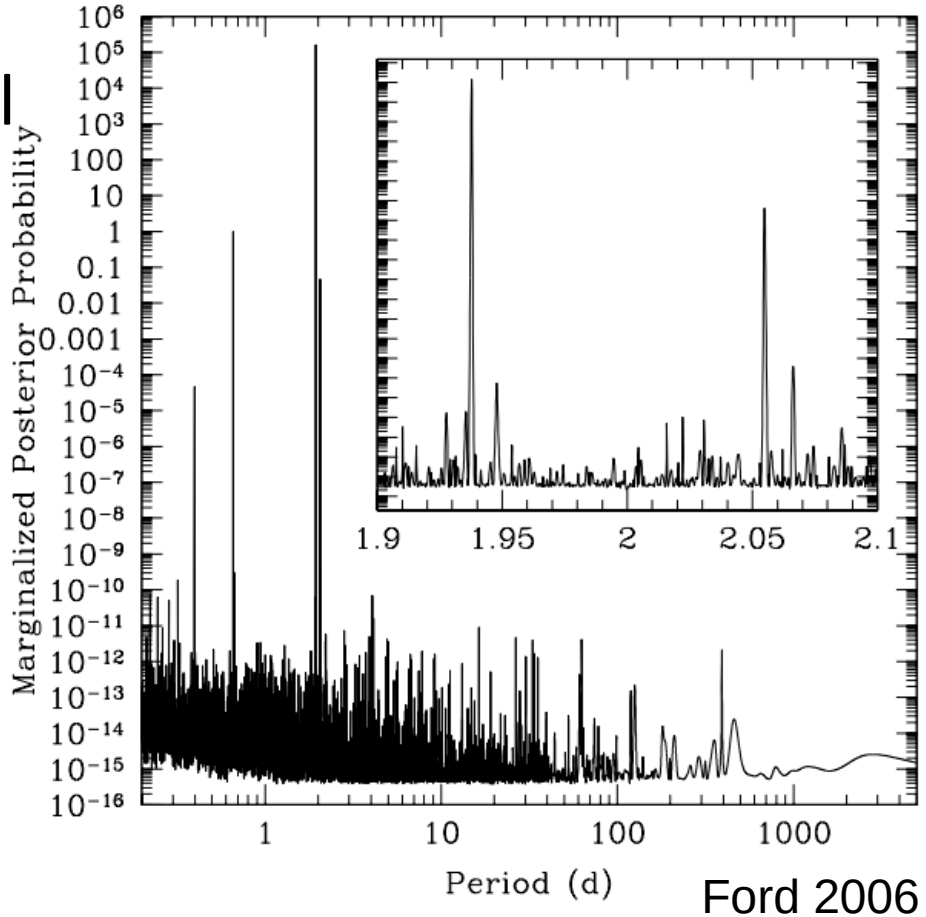
First, Identify Relevant Portion of Parameter Space

- Physical intuition
- Simplified statistical model
- Simplified physical model
- Analyze subset of data

Then, perform MCMC with good initial guesses

- Include samples from each viable mode

(See also Parallel Tempering)

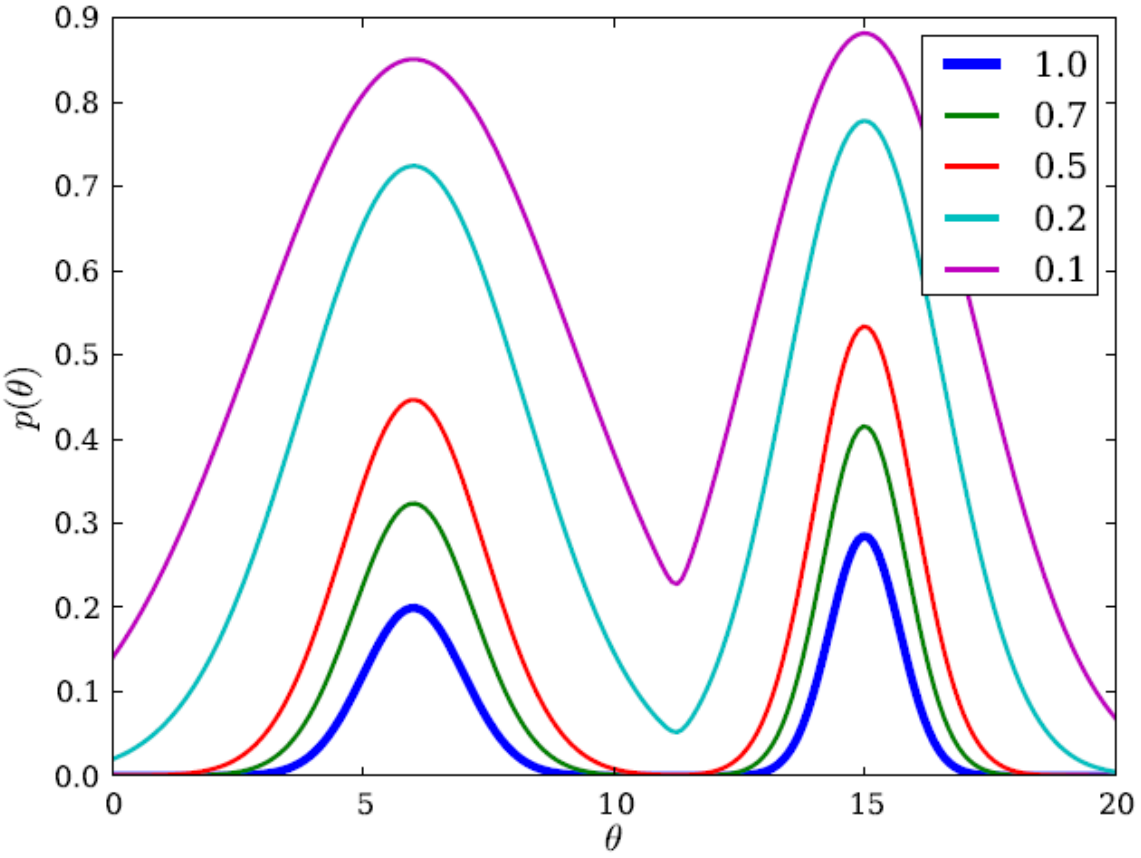


Ford 2006

Parallel Tempering MCMC

To enable large jumps, *anneal* or *temper* the posterior:

$$q_\beta(\theta) = [q(\theta)]^\beta, \qquad \beta \in [0, 1]$$



Loredo

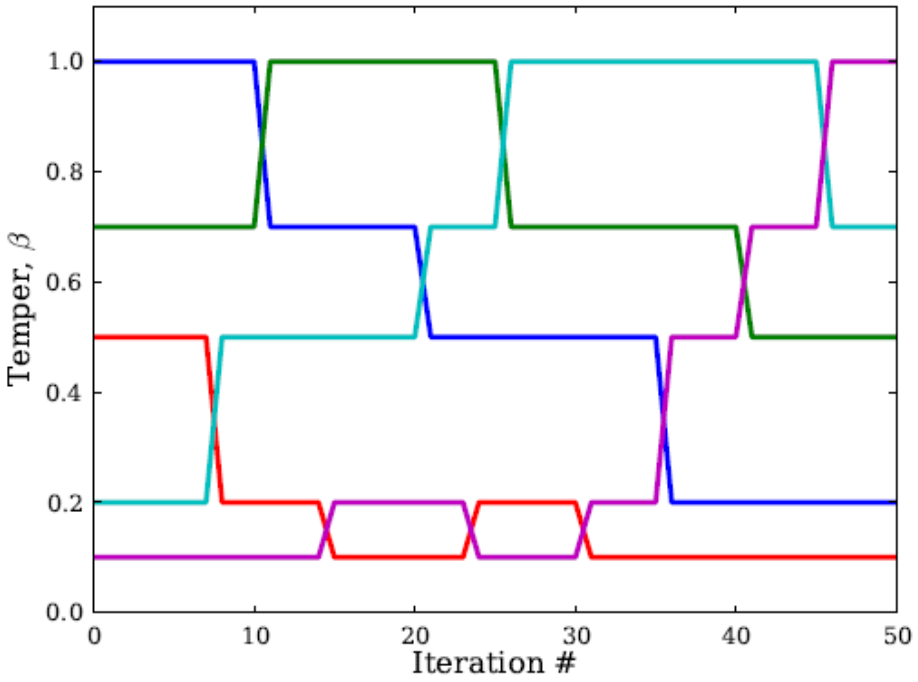
Consider a set of tempers ("inverse temperatures") $\{\beta_i\}$

Think of each $q_i = q_{\beta_i}$ as its own "model" with its own parameters, and construct a sampler for the joint distribution

$$p(\theta_1, \ldots, \theta_m) = \prod_i q_i(\theta_i)$$

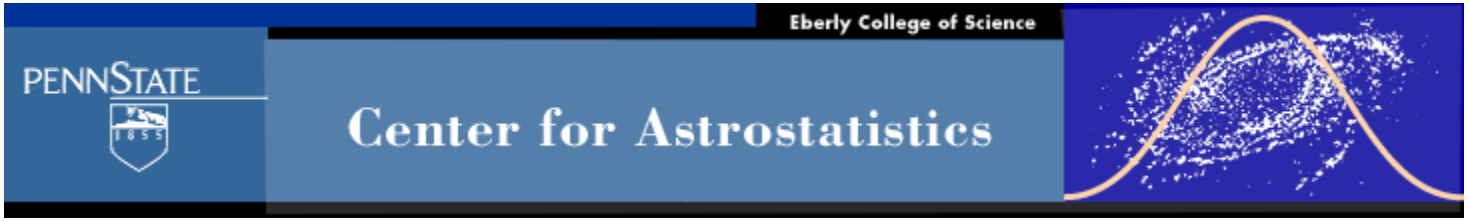
Alternate within-temper proposals and swap proposals between adjacent tempers

Swaps between tempered chains



Loredo

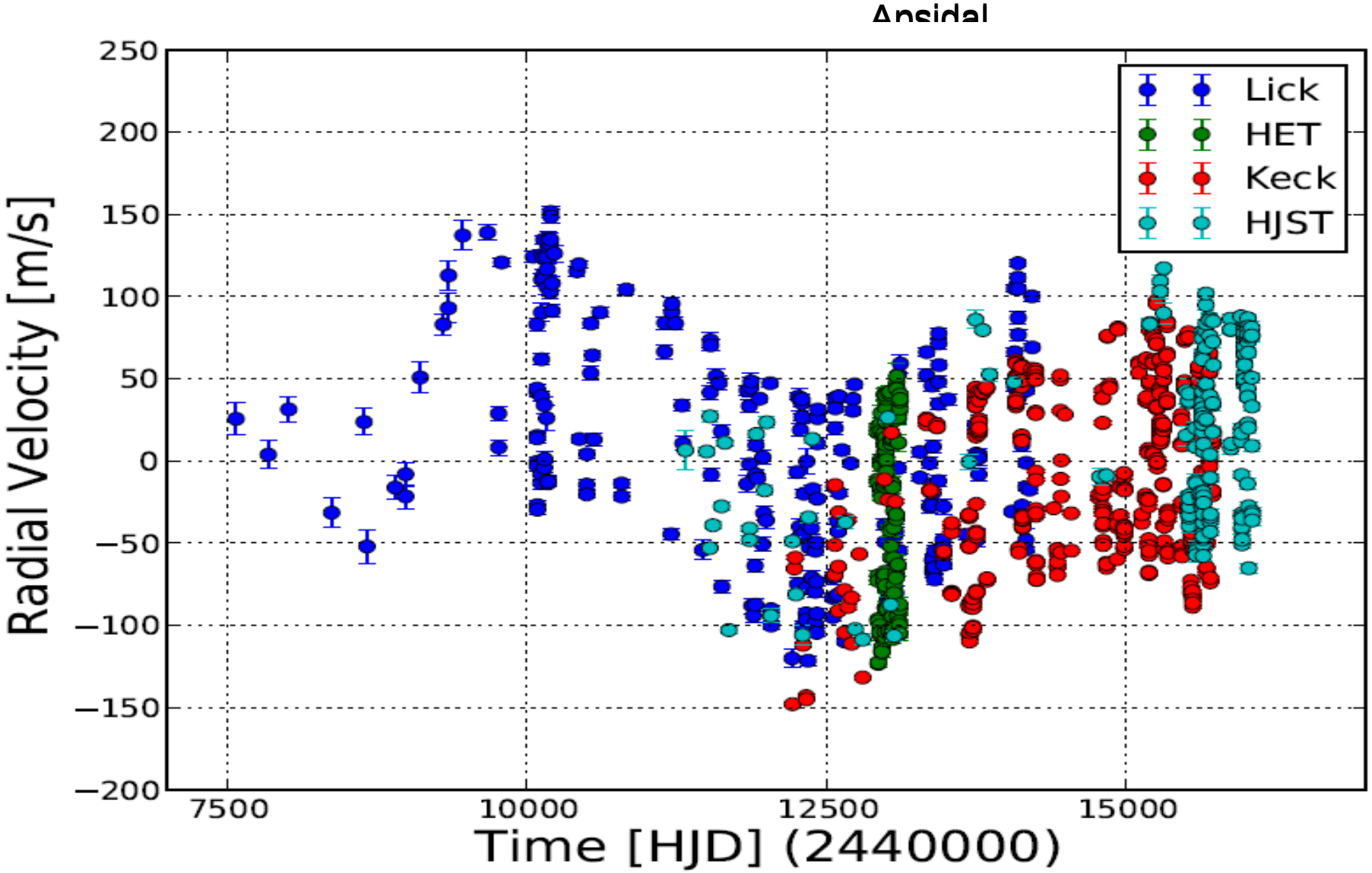
Pause for Questions



Example Application of DEMCMC

- Non-interacting systems & Doppler observations:
  - ~5x$N_{planets}$ physical model parameters
  - Model evaluation is very fast
  - Can require ~10^7 model evaluations
  - Parameter estimation is “solved” problem
  - Use dozens of physically-motivated proposals that deal with non-linear correlations
- Strongly Interacting planetary systems:
  - ~7x$N_{planets}$ physical model parameters
  - Can require ~10^{10} model evaluations
  - Model evaluation is slow, since requires n-body integration
  - Computationally demanding
  - Requires clever algorithms & parallel computation

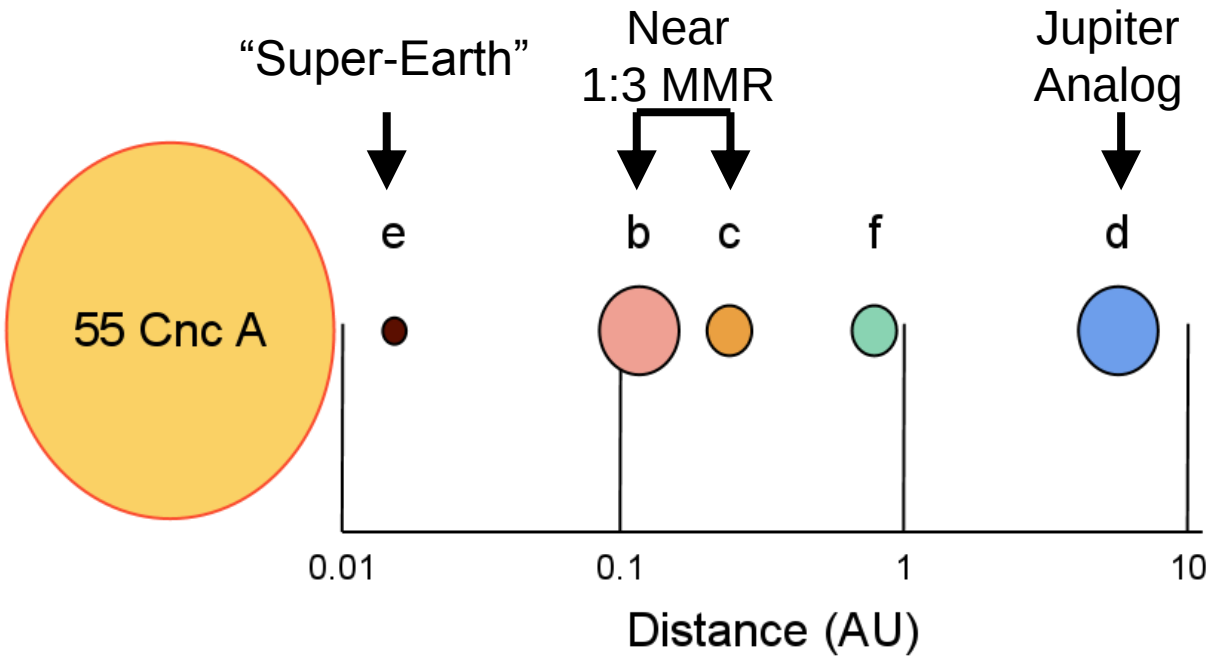
55 Cnc: An RV Classic



Butler+ 1996; Marcy+ 2002; McArthur+ 2004; Endl et al 2012; Nelson et al. 2014

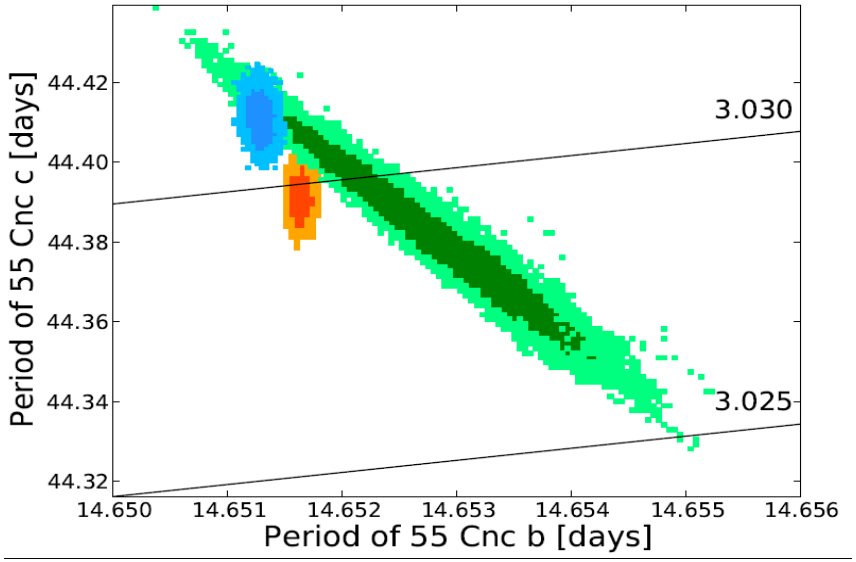
55 Cnc: Astroinformatics in Action

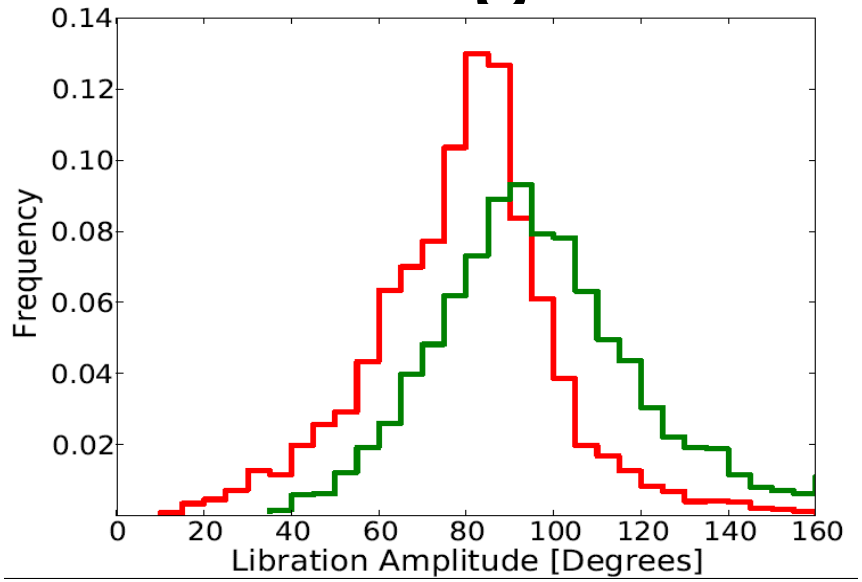
- 1,086 RVs from 4 observatories, spanning over 23 years
- Self-consistent Bayesian Analysis w/ full N-body treatment
- 40 dimensional parameter space
- ~3 weeks of computation w/ GPU (before stability tests)
- N-body integrations using Swarm-NG GPU (Dindar+ 2012)

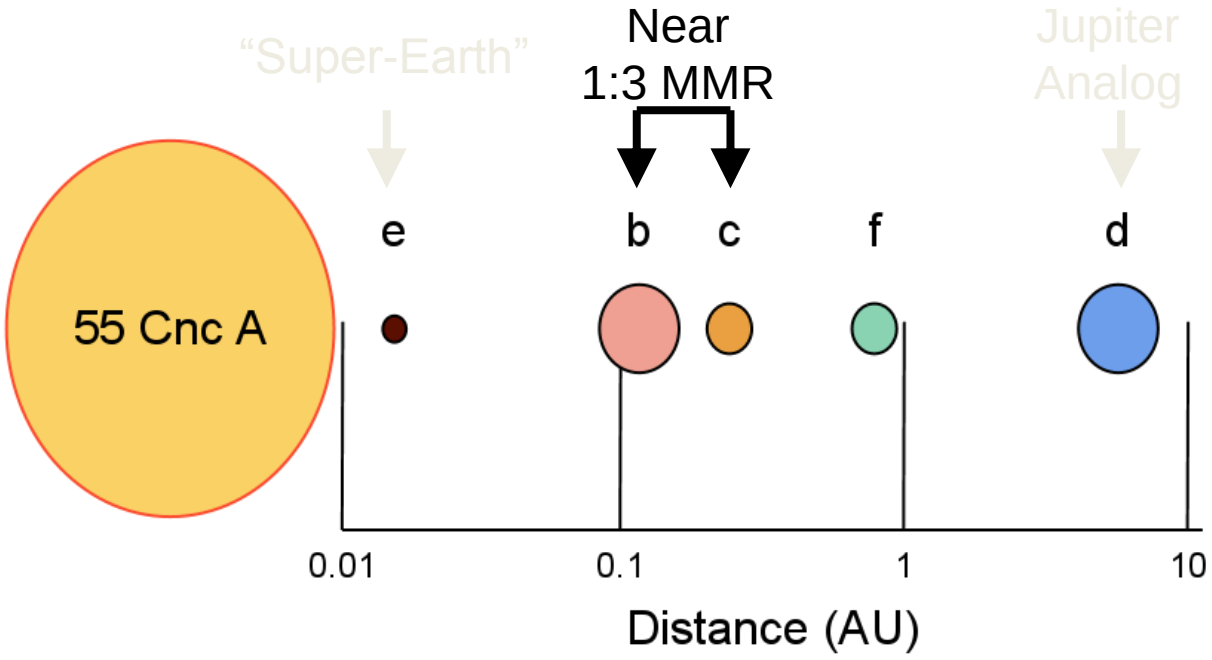


B. Nelson et al. 2014

55 Cnc: Evidence for Disk Migration

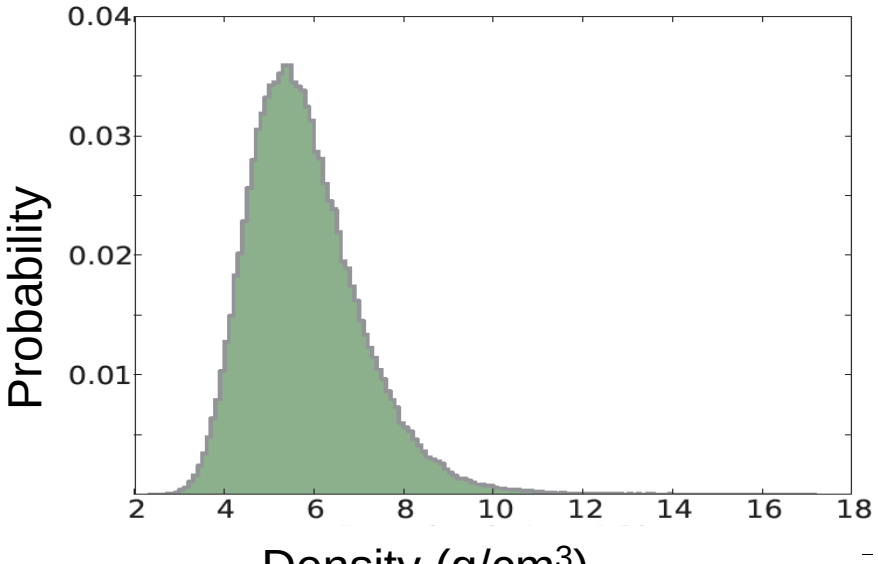


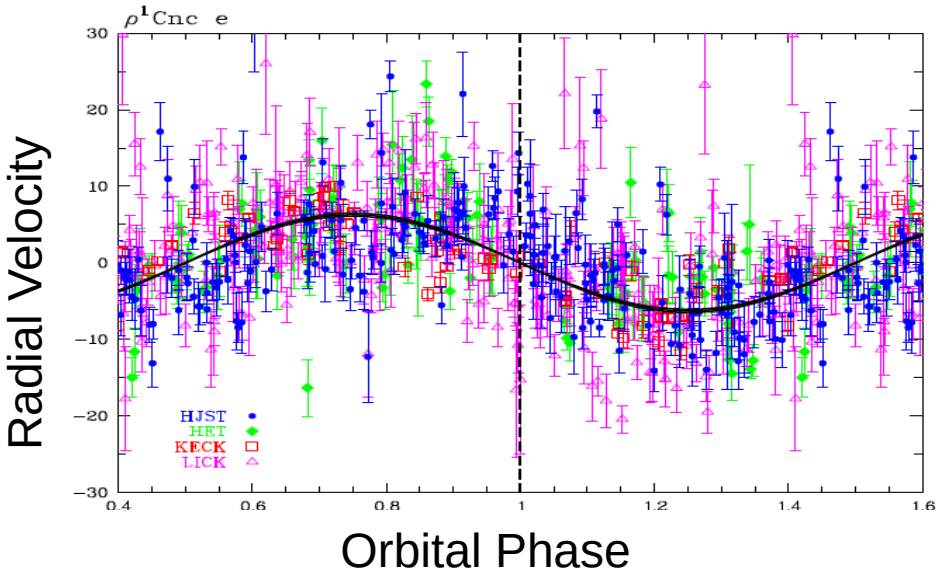




B. Nelson et al. 2014

55 Cnc: Density of a Super-Earth



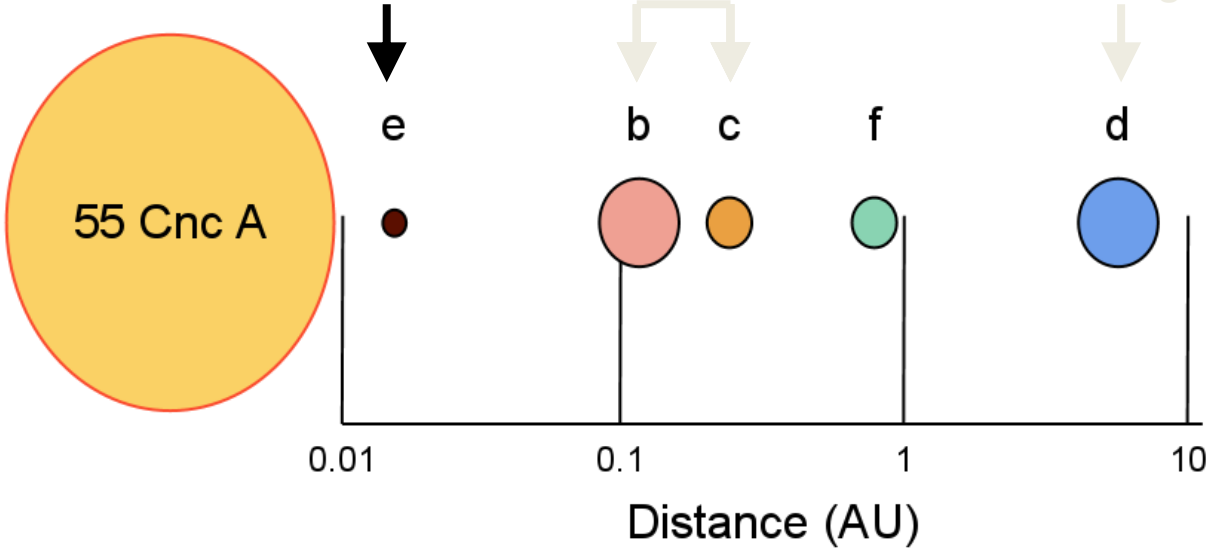


"Super-Earth"

Near 1:3 MMR

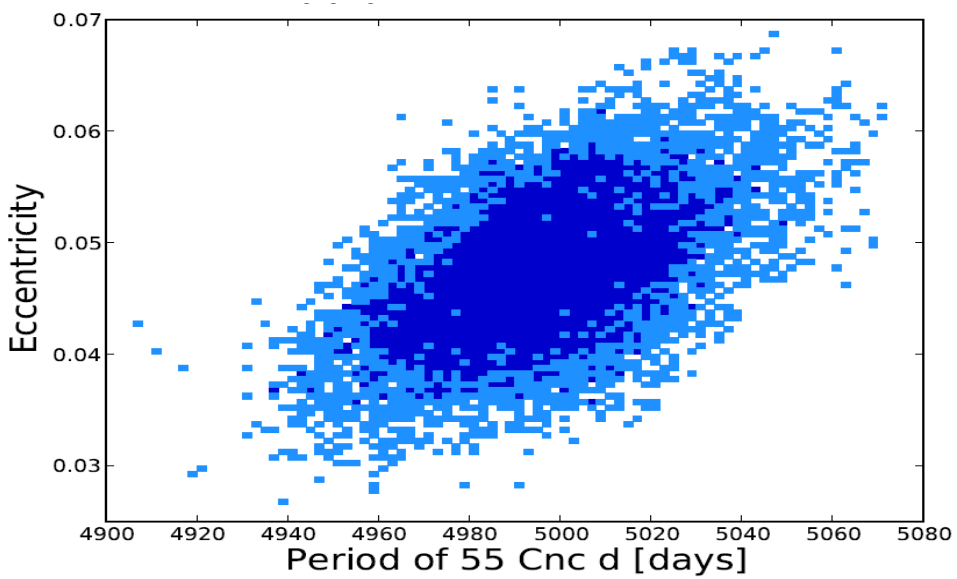
Jupiter Analog

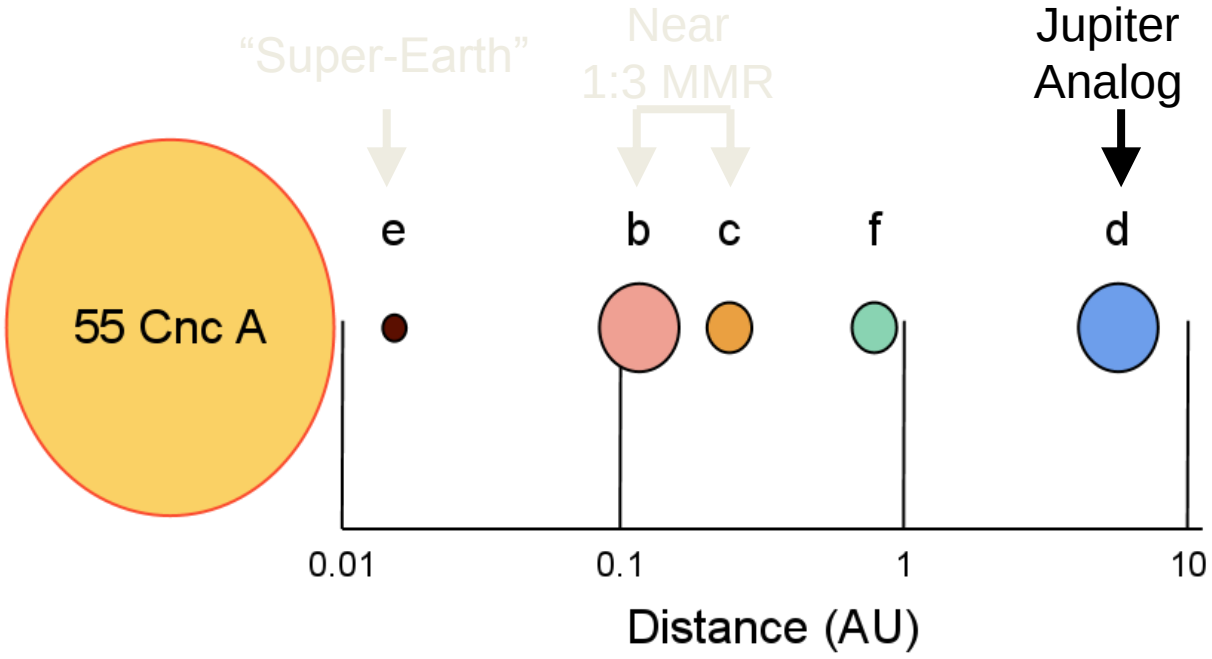
Endl et al. 2012



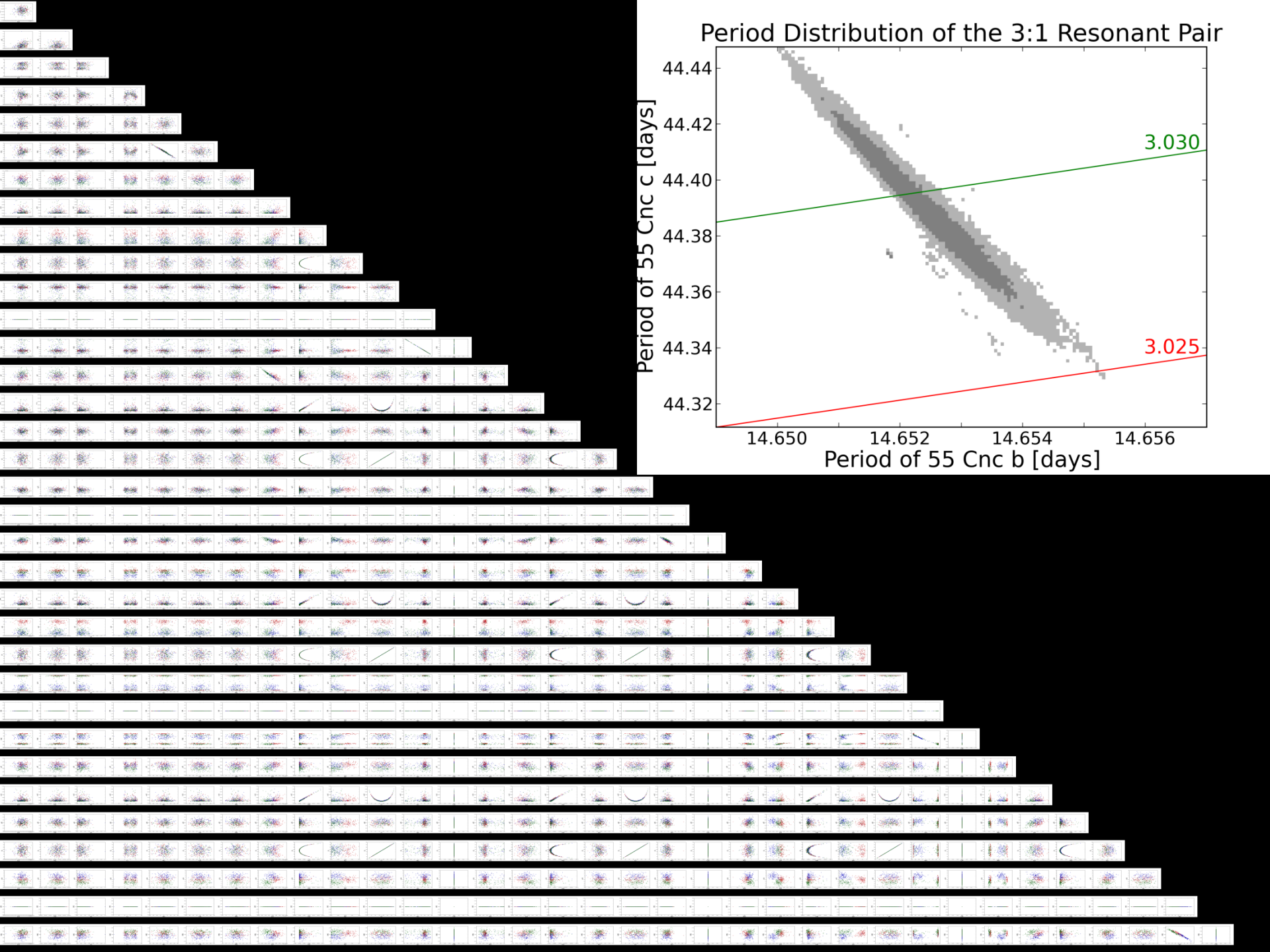
B. Nelson et al. 2014

55 Cnc: A True Jupiter Analog





B. Nelson et al. 2014

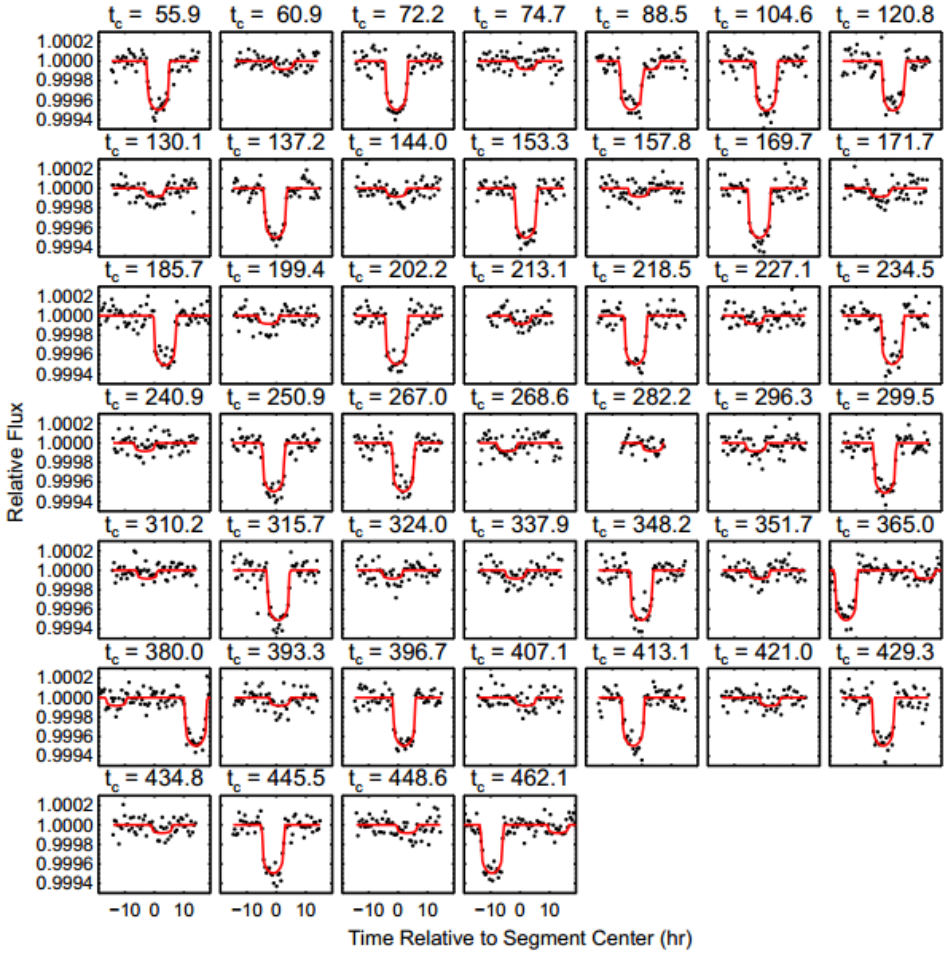

Period Distribution of the 3:1 Resonant Pair
Period of 55 Cnc c [days]
44.44
44.42
44.40
44.38
44.36
44.34
44.32
3.030
3.025
14.650
14.652
14.654
14.656
Period of 55 Cnc b [days]

Example Application of DEMCMC

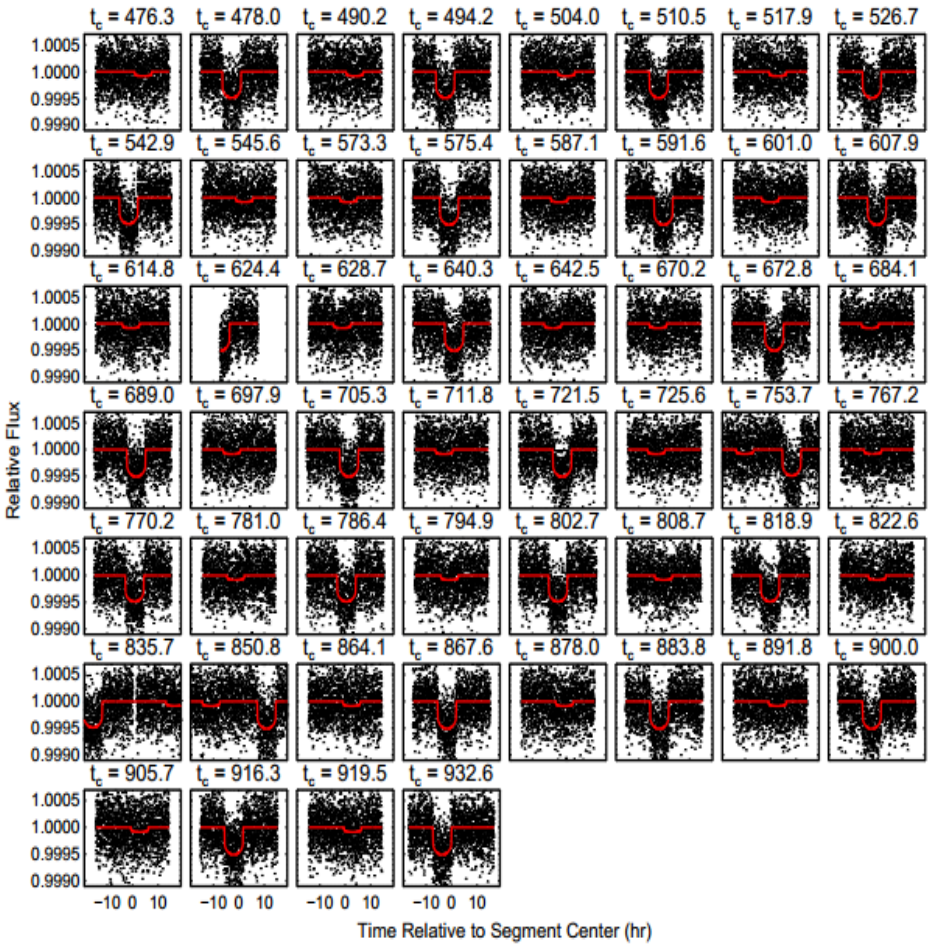
Measuring planet masses & orbits from Kepler light curves of stars with multiple transiting planets

- Physical Model:
  - Orbits: Either non-interacting or full n-body model
  - Light curves: Limb darkening, stellar activity
- Likelihood:
  - Assume each flux measurements has uncorrelated, Gaussian uncertainties, or
  - Could account for correlated noise

Characterizing Kepler's Systems with Interacting Planets: Kepler-36 b & c



30 min exposure time

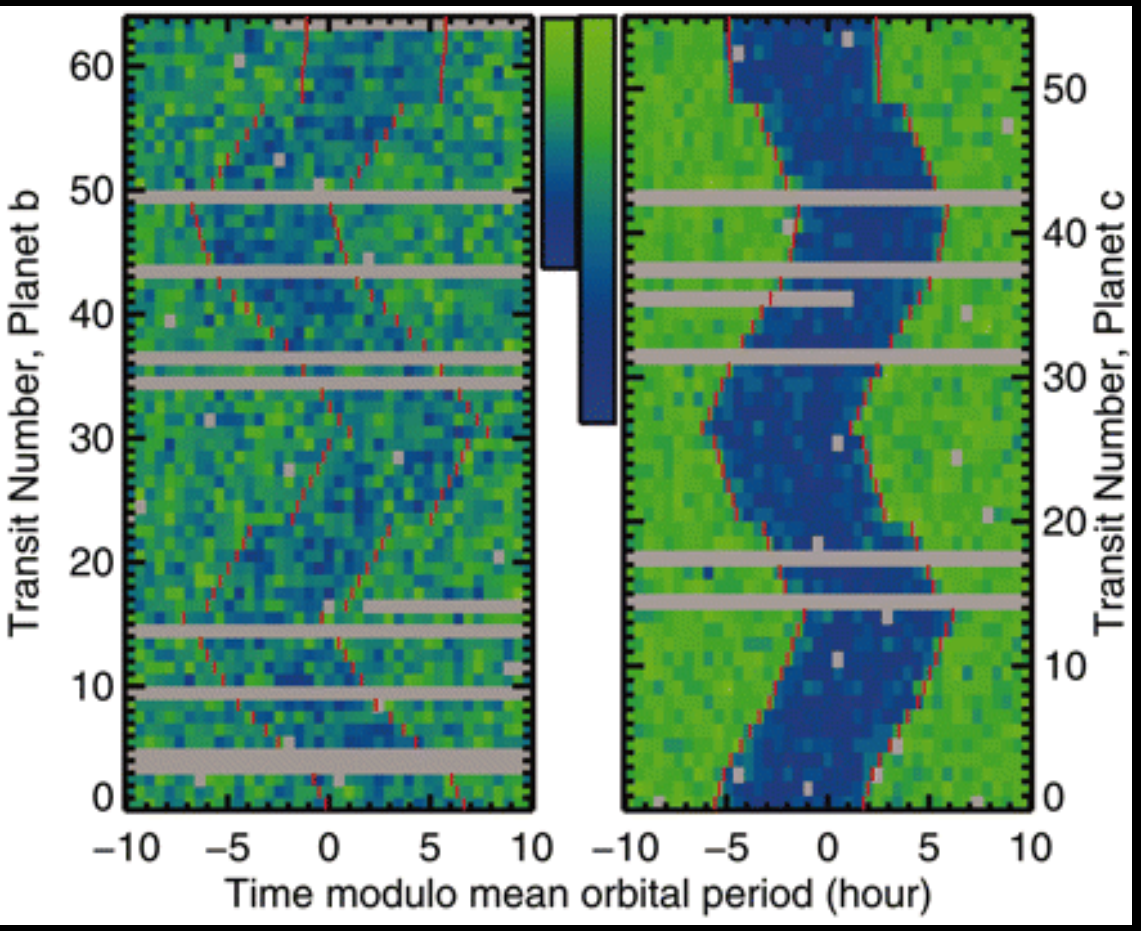


1 min exposure time

Carter et al. 2012

Characterizing Planet Masses for Rapidly Interacting Systems

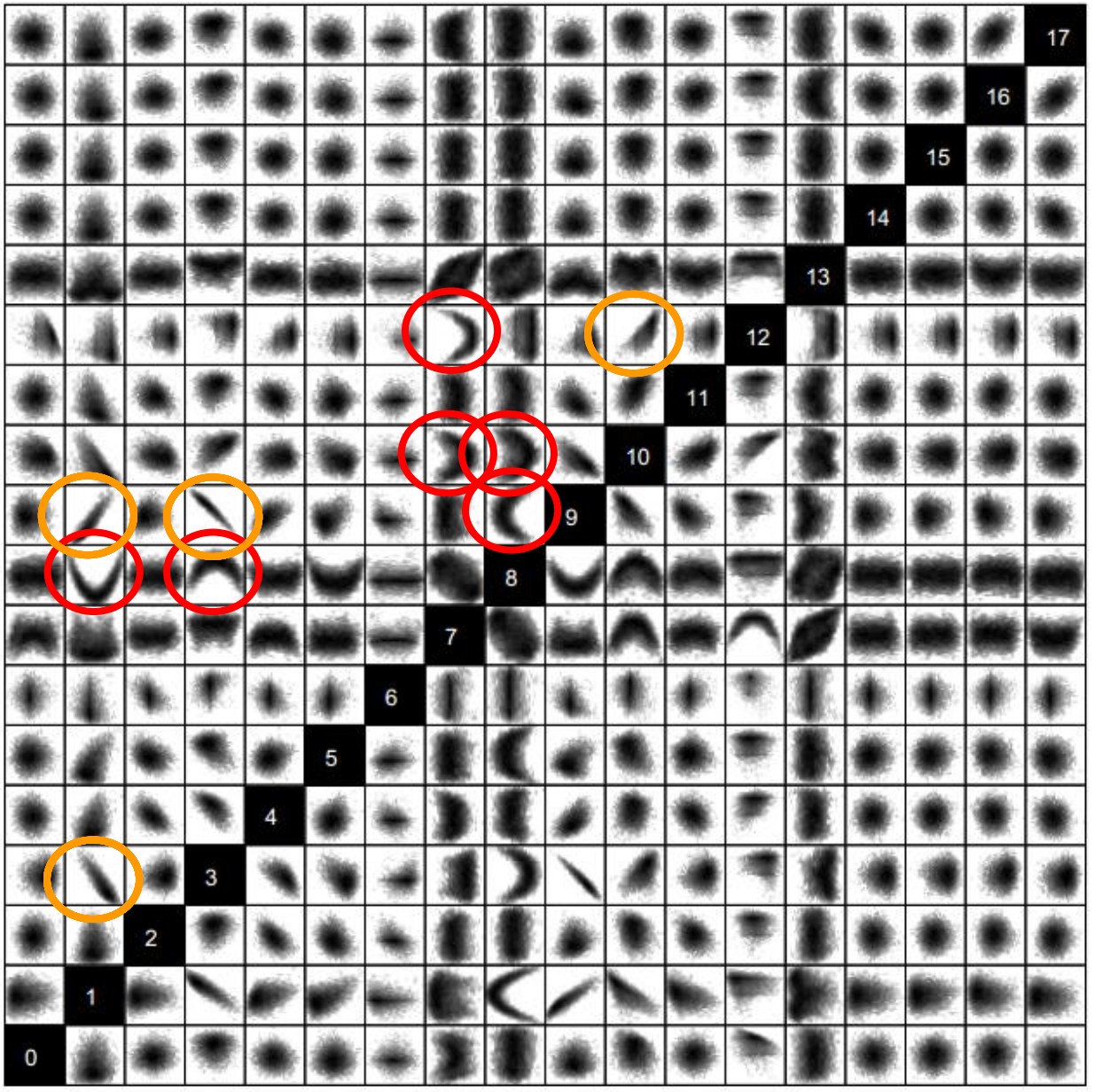
Kepler-36b&c: Chaotic due to 29:34 and 6:7 MMRs!



Carter et al. 2012; Deck et al. 2012

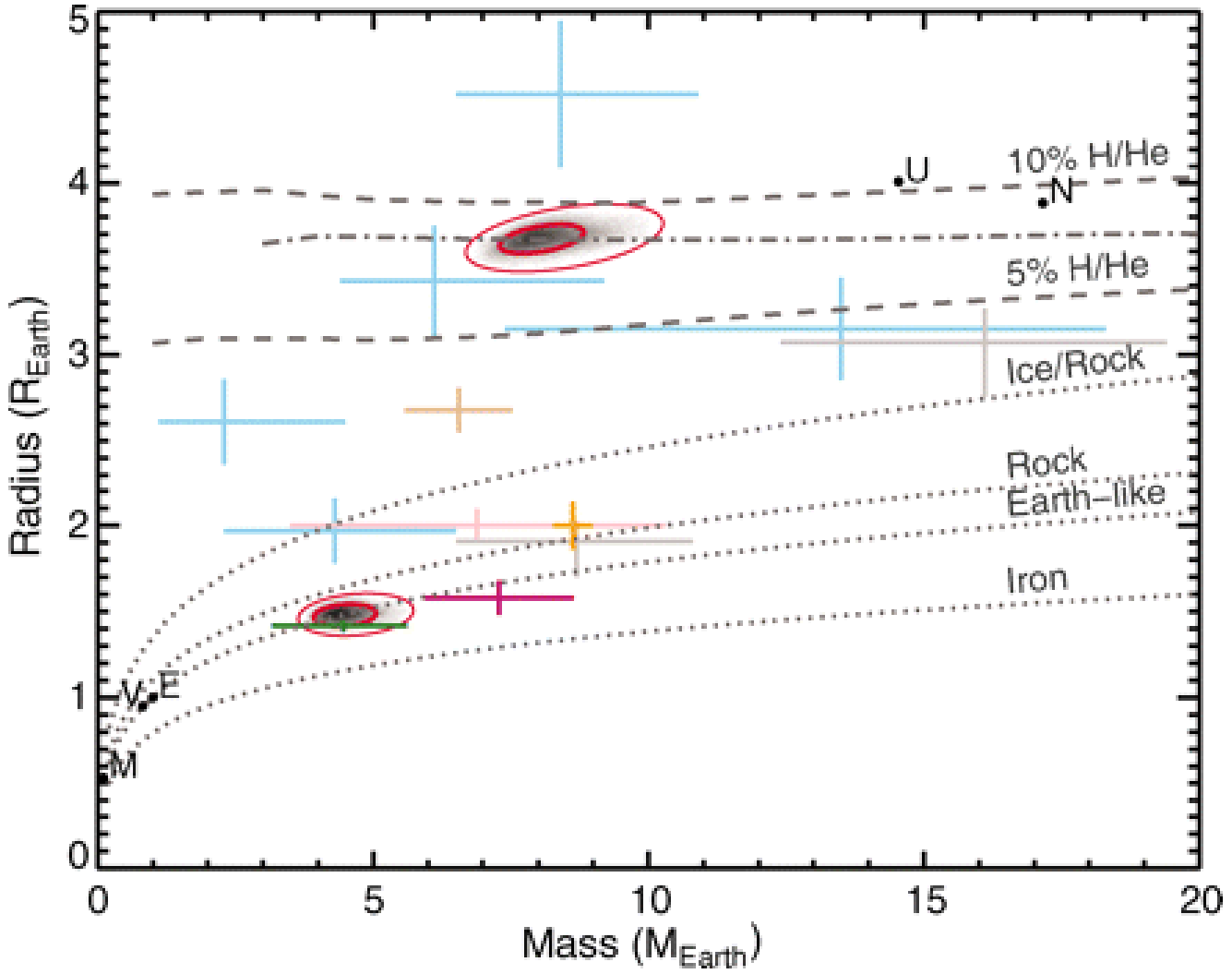
Two-Parameter Marginal Posterior Distributions

- Complex observational constraints
- Impractical to understand correlations a priori
- DEMCMC unphased by correlations
- ~10,000 CPU hours using
  128 cores (MPI) for
  ~1¼ years of observations



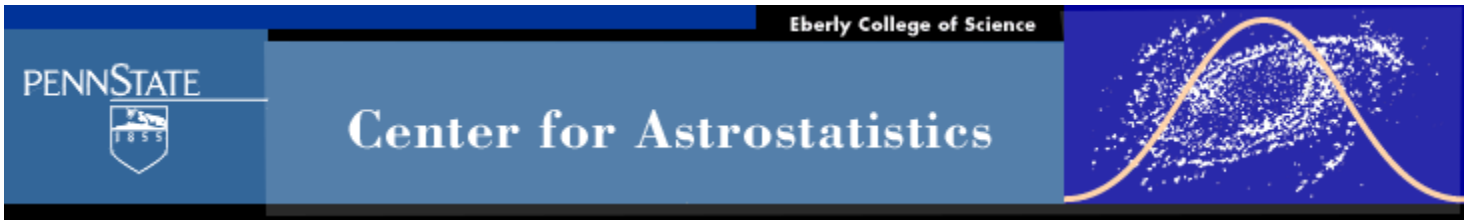
Carter et al. 2012

High-precision masses key for studying planet mass-radius relationship



Carter et al. 2012

Questions


PENNSTATE
1855
Eberly College of Science
Center for Astrostatistics