Intuition for MCMC Sampling

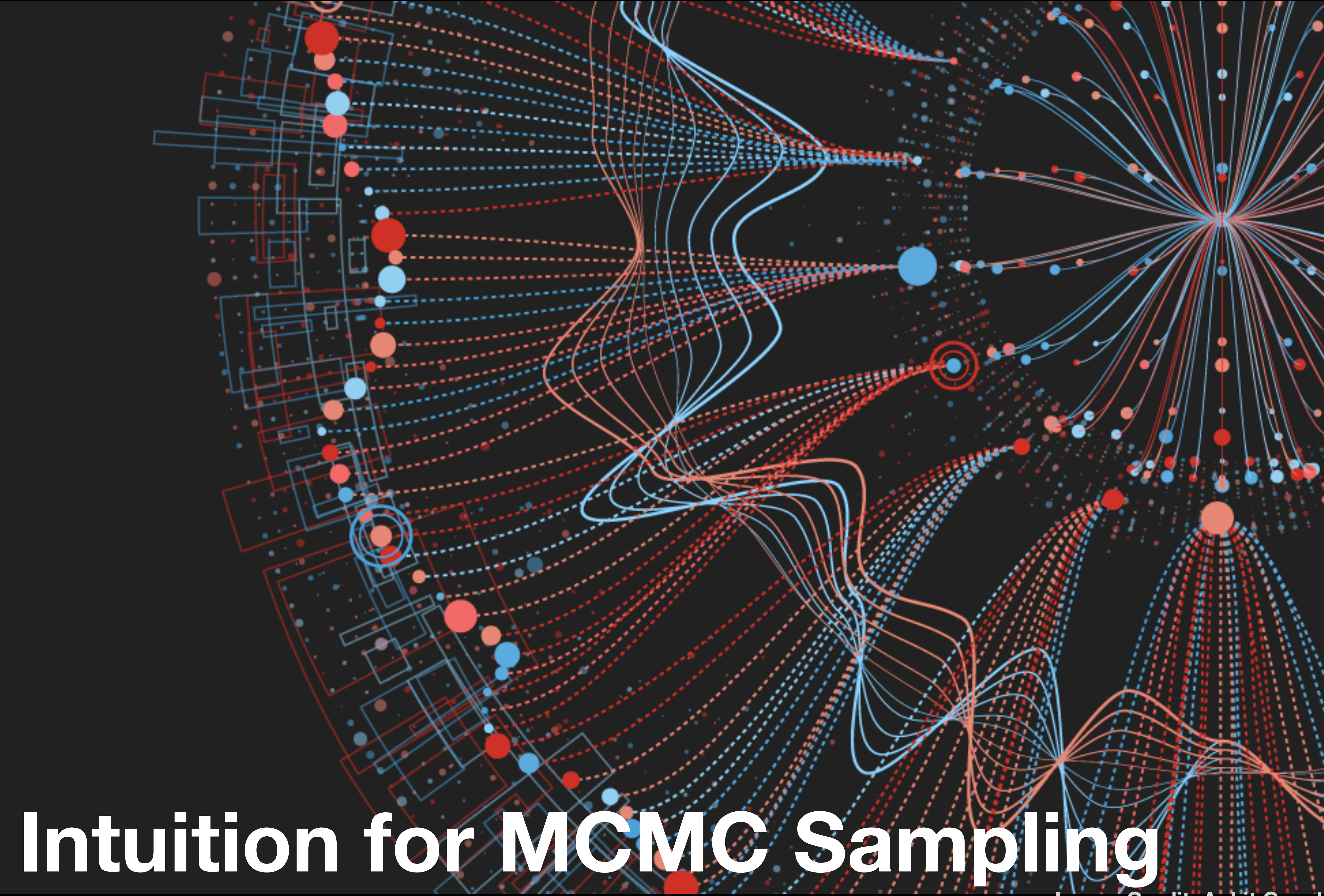
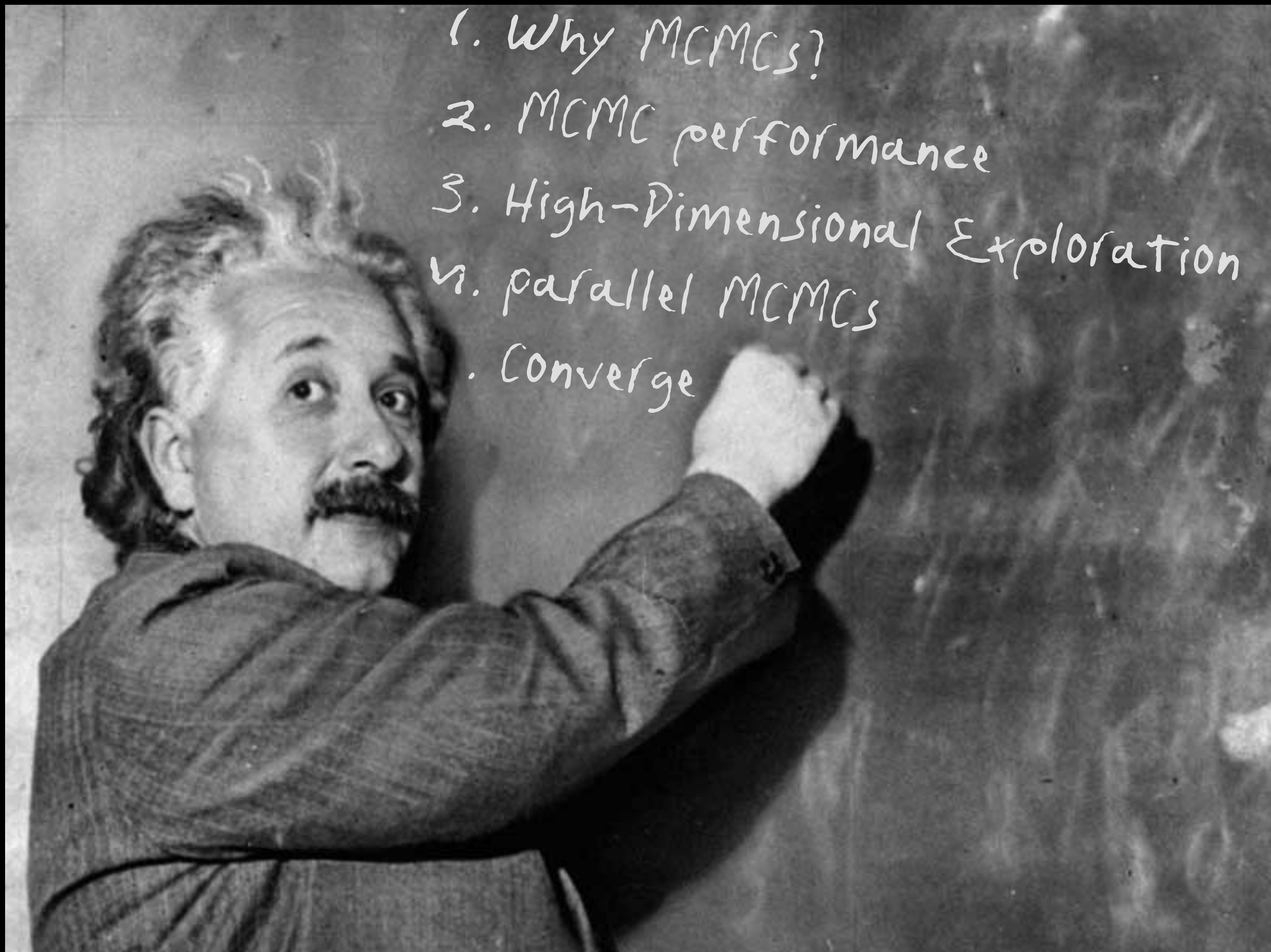


Image Credit: Ankit Goyal

Peter Behroozi

Outline


1. Why MCMCs?
2. MCMC performance
3. High-Dimensional Exploration
4. parallel MCMCs
. Converge

Why?

Observations

Why?

Observations

$$\mathcal{L}(x) = \exp(-\chi^2/2)$$

Models

MCMC

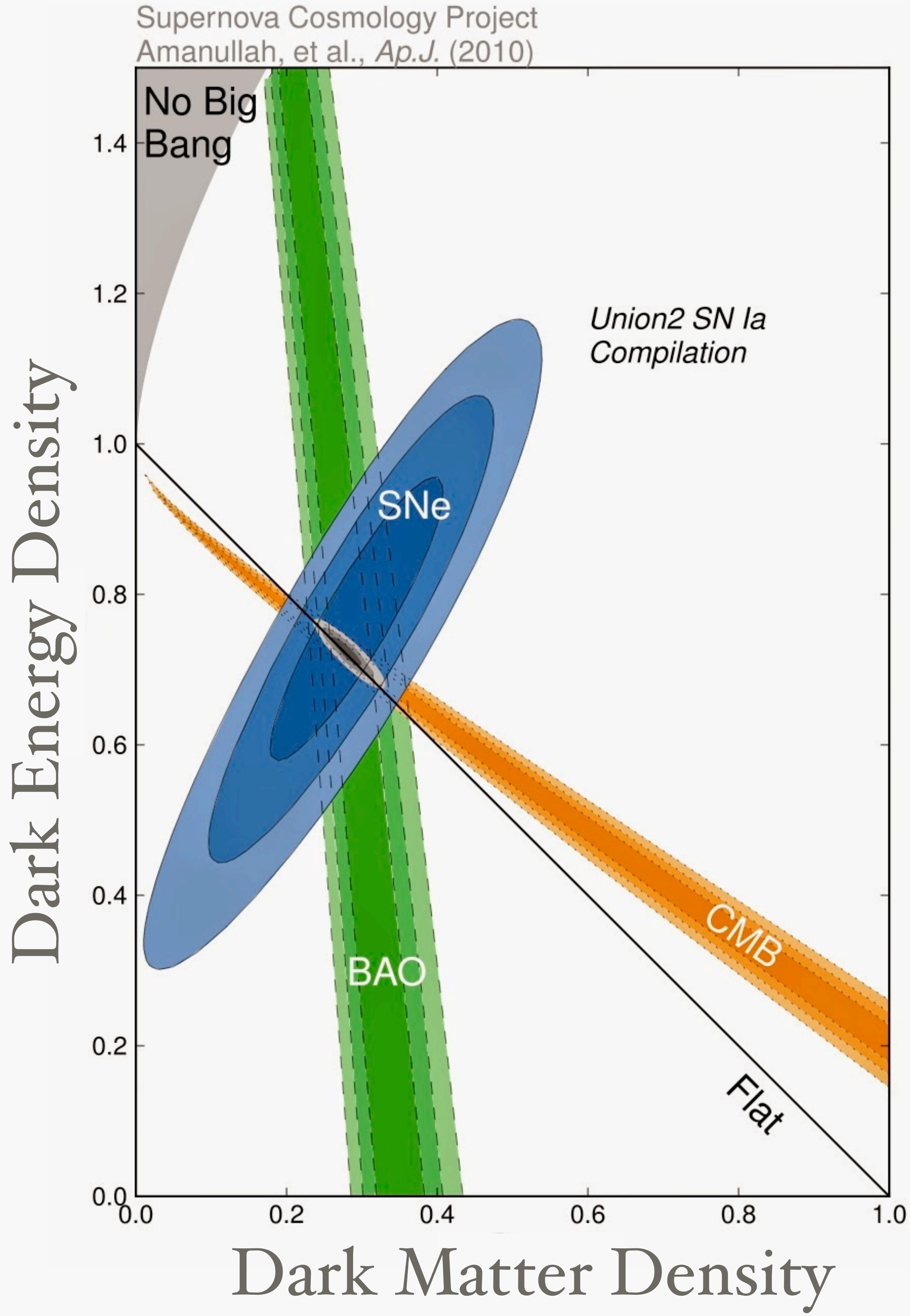
Why?

Observations

$$\mathcal{L}(x) = \exp(-\chi^2/2)$$

Models → **MCMC**

Range of Reasonable Physical Models


Supernova Cosmology Project
Amanullah, et al., Ap.J. (2010)
No Big Bang
Union2 SN Ia Compilation
SNe
BAO
CMB
Flat
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0.8
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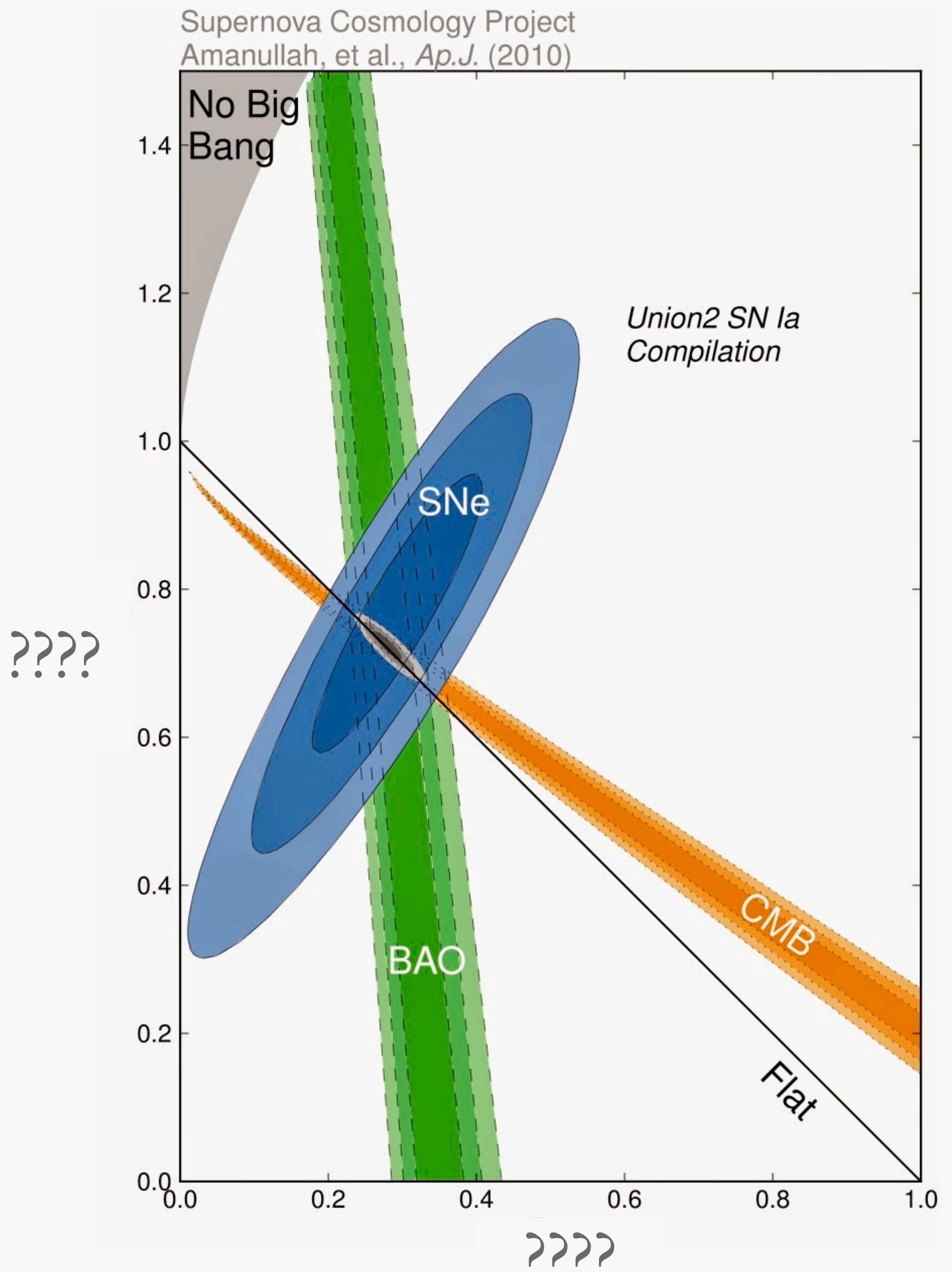
Dark Energy Density
Dark Matter Density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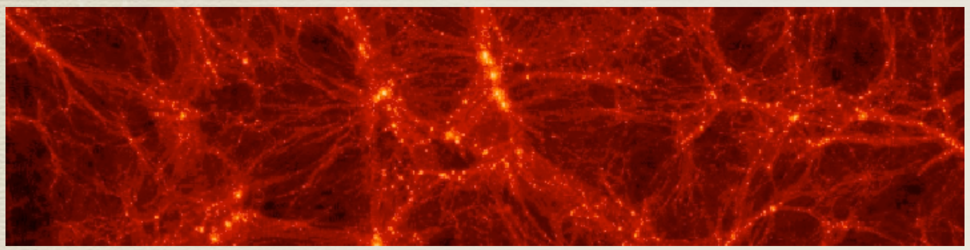
UniverseMachine



DM Simulation

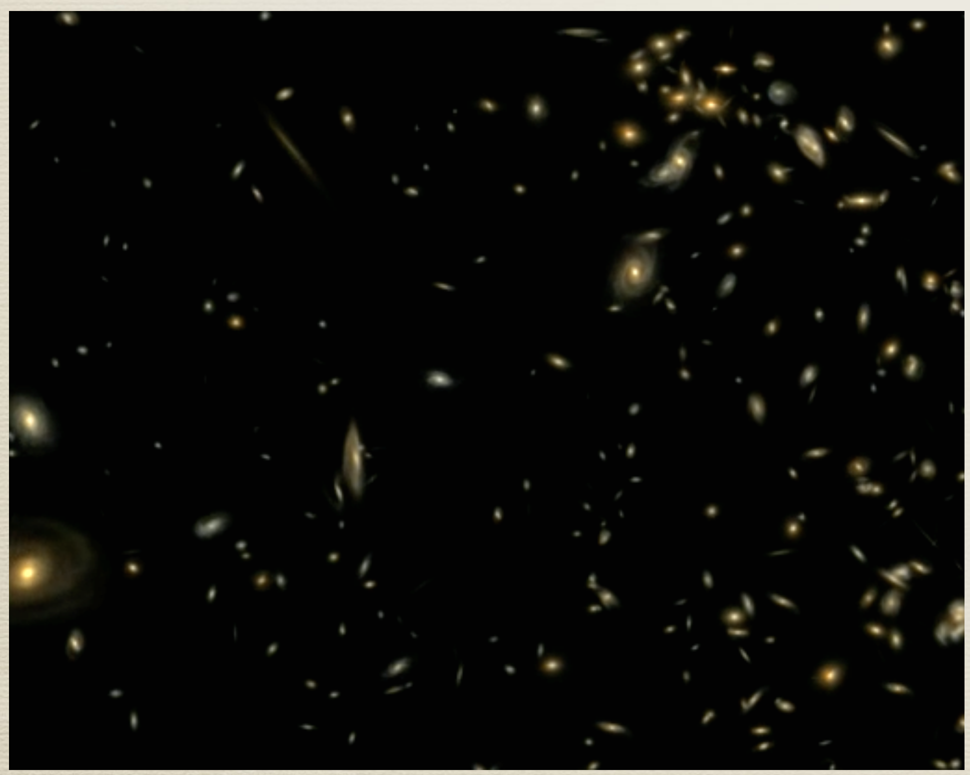
+

$$\mathrm{SFR} = f(M_h, \dot{M}_h, z)$$

=

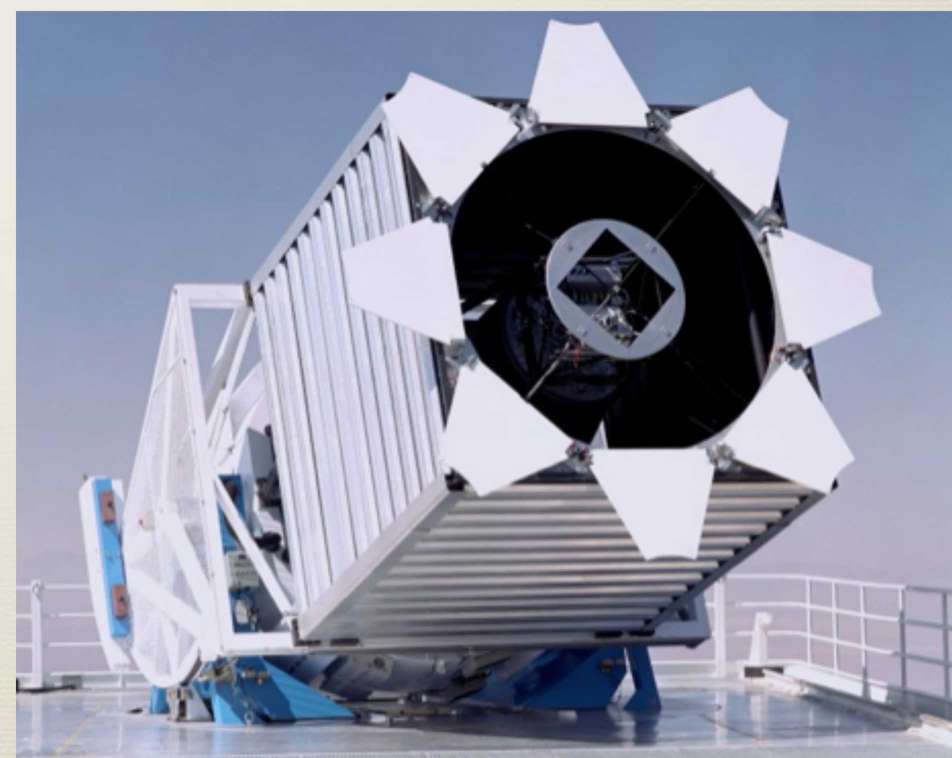
Minimal Galaxy Model

MCMC



Mock Universe

$\stackrel{?}{=}$



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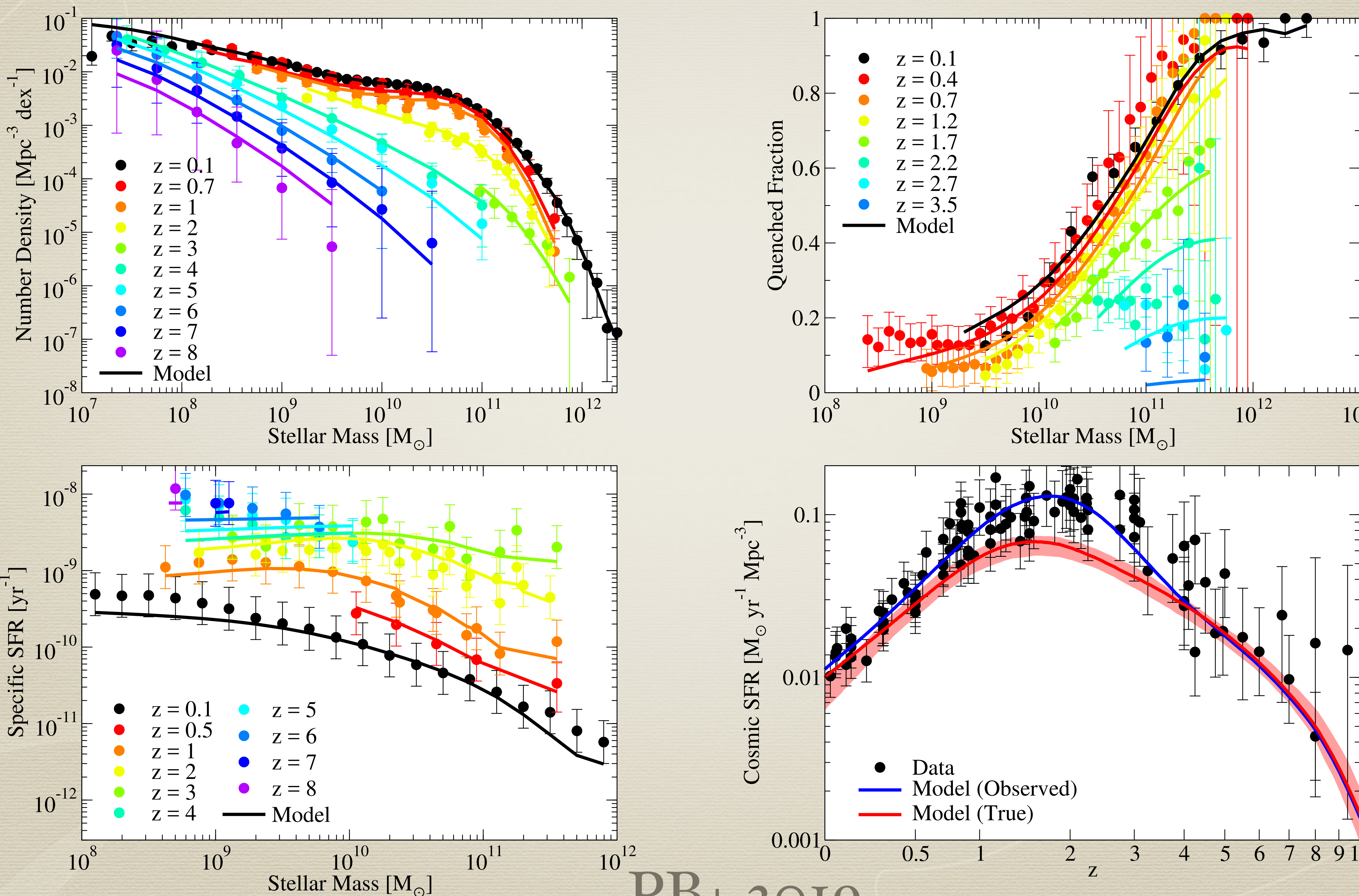
Observational Constraints



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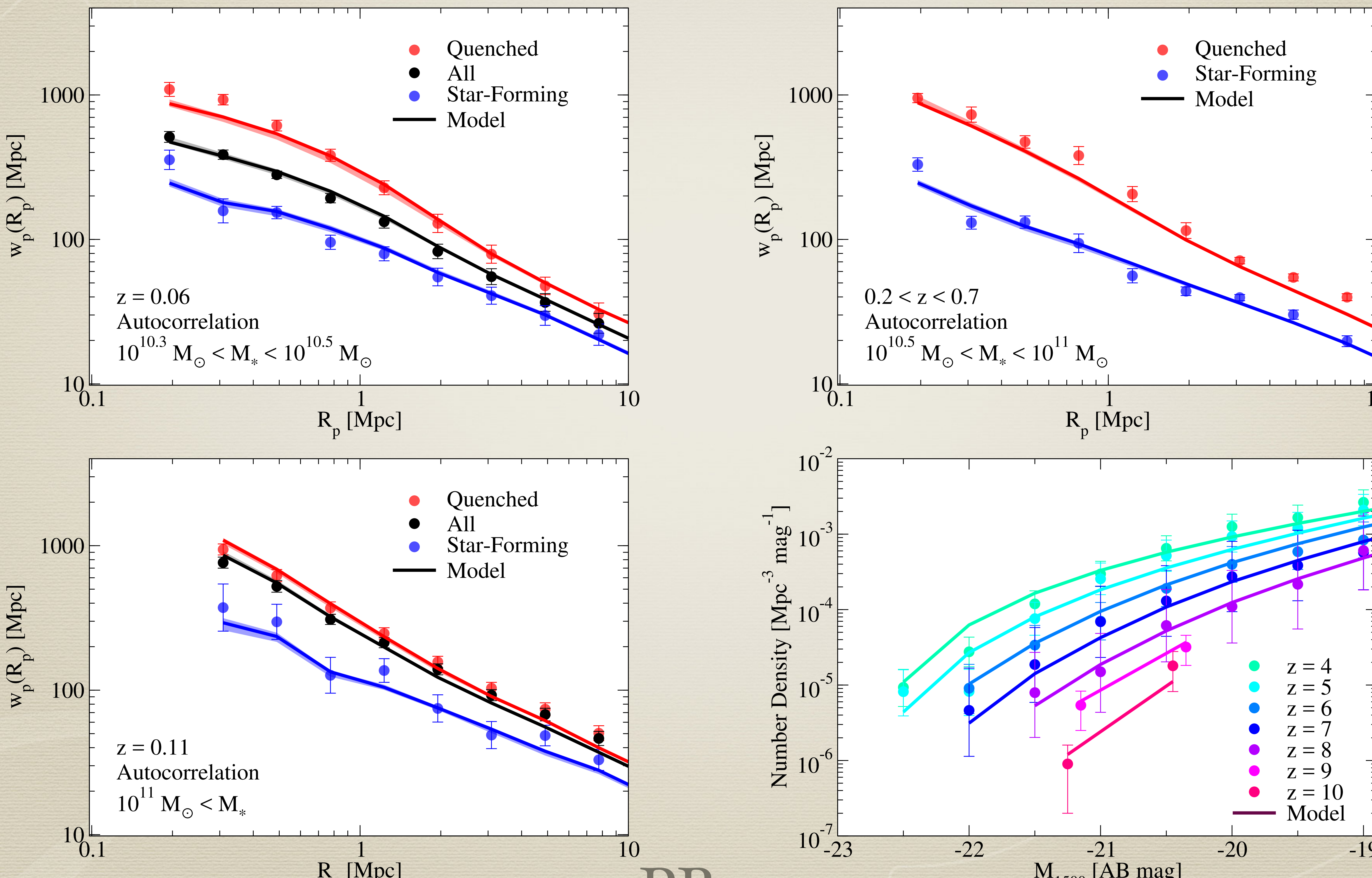

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Why?

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$$\mathcal{L}(x) = \exp(-\chi^2/2)$$

Models → **MCMC**

Range of Reasonable Physical Models

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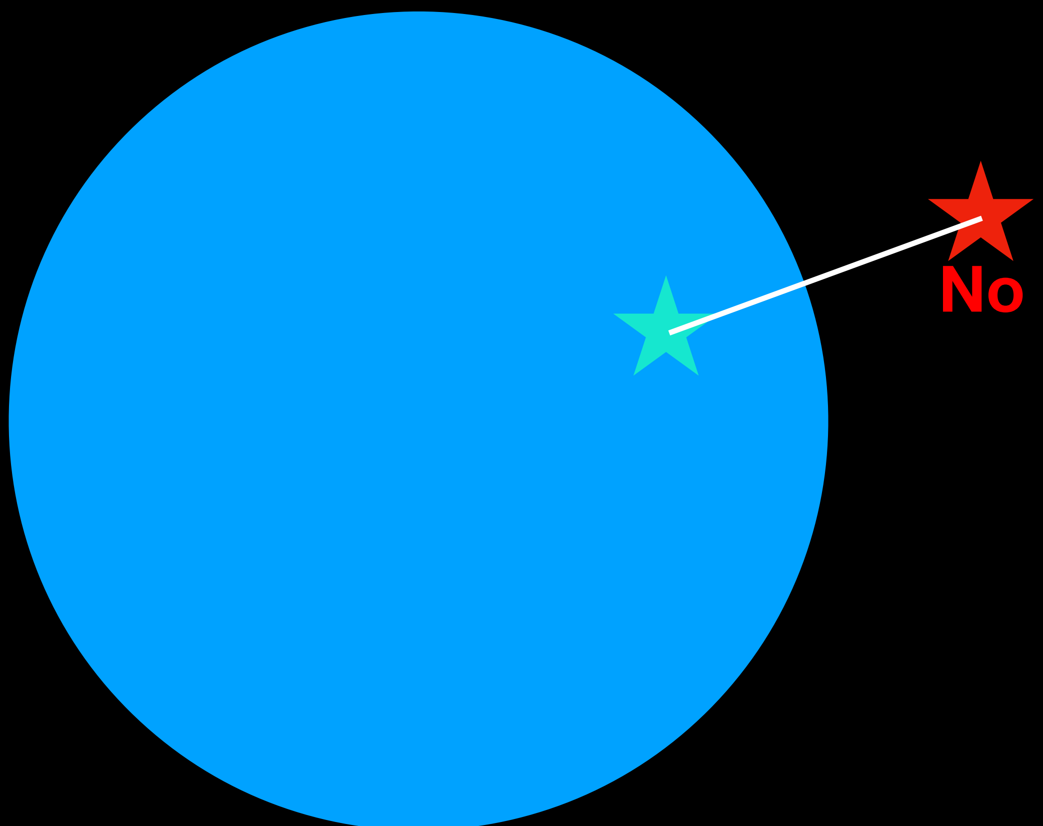
Models **MCMC**

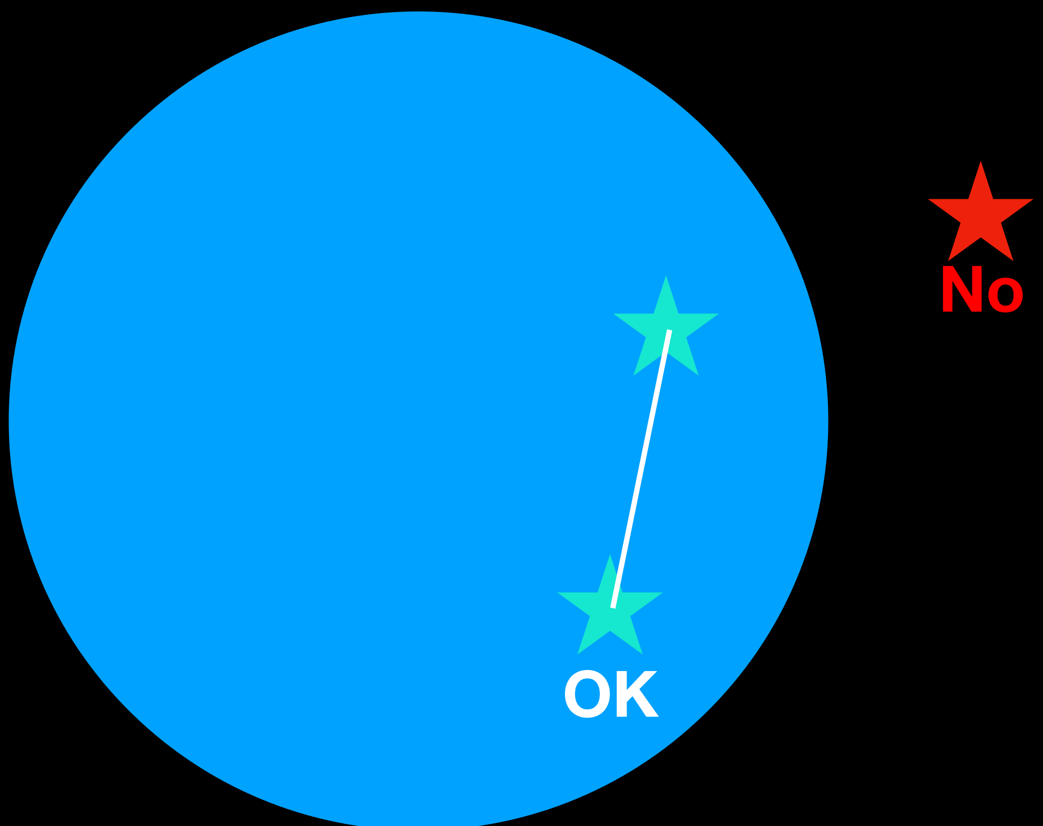
Career in Astronomy

MCMCs



Random walk w/ rejections

MCMCs



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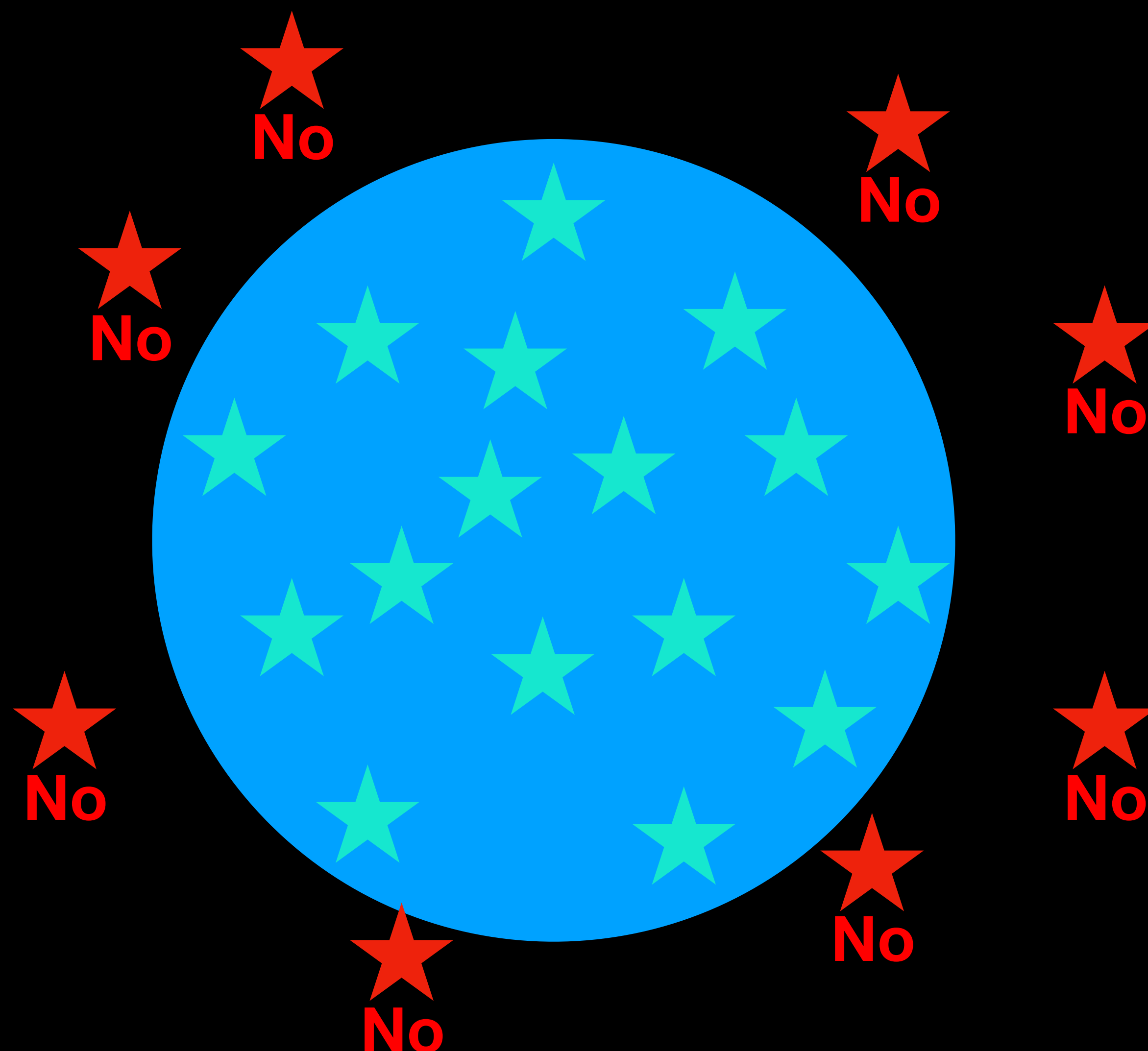
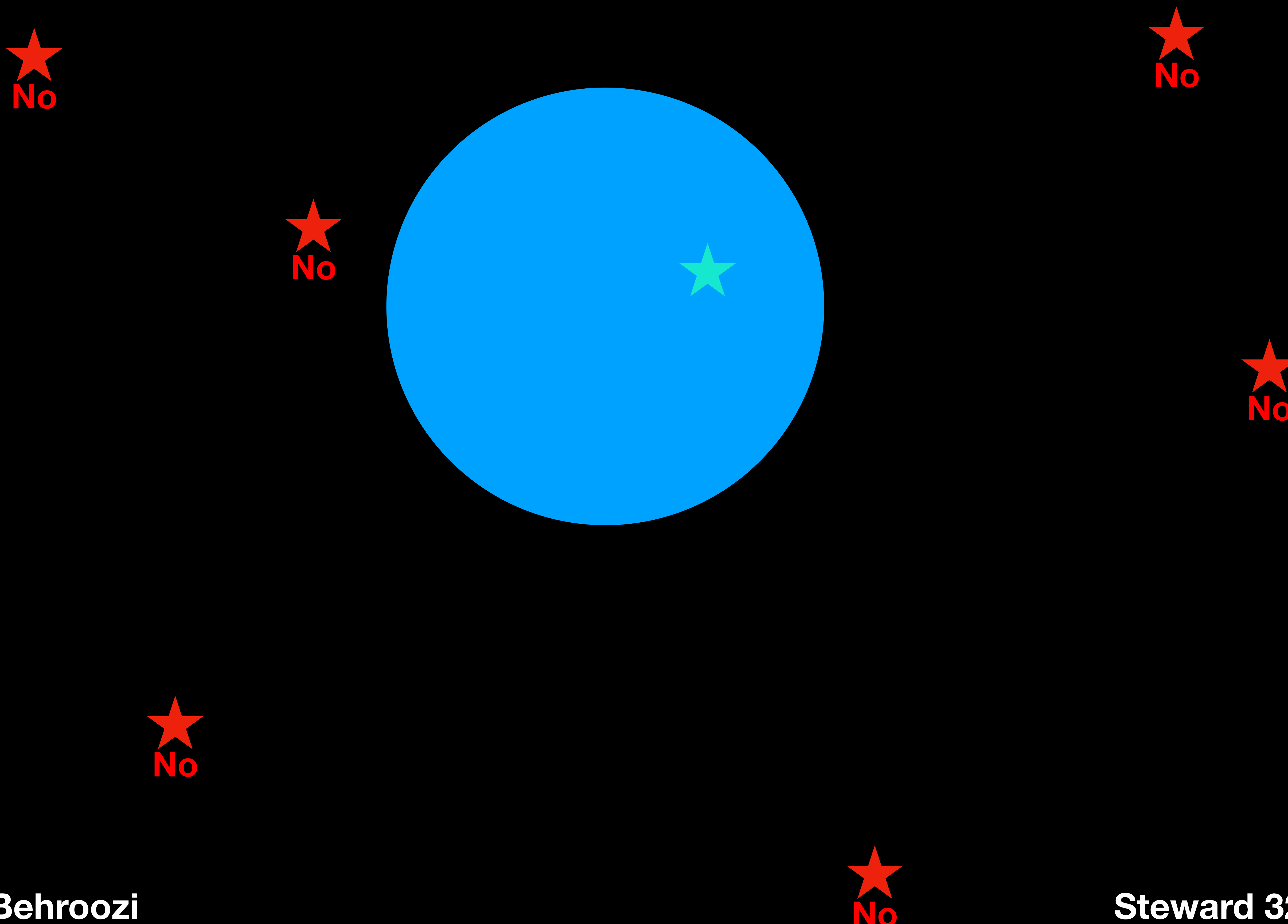
MCMCs



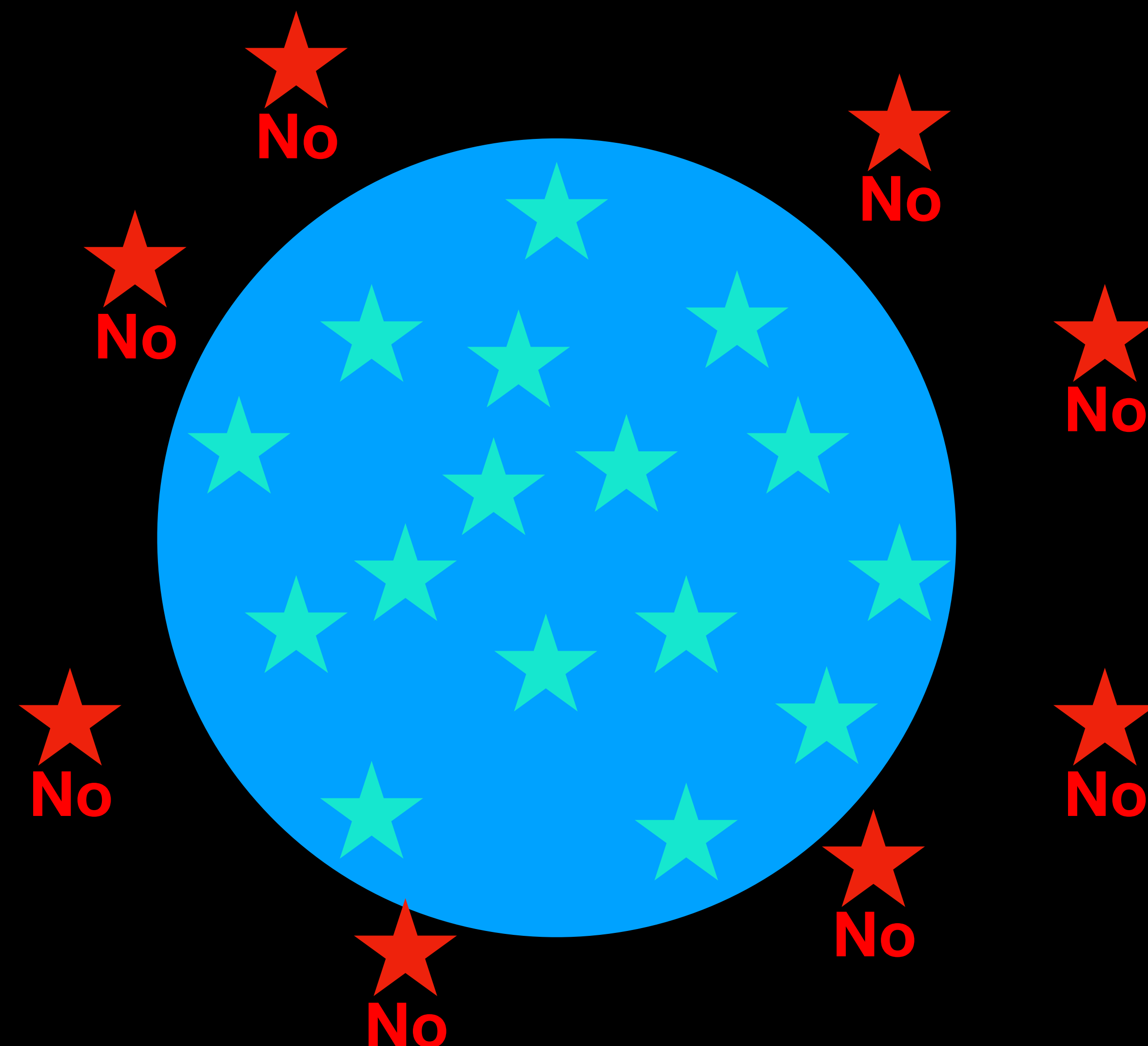
Random walk w/ rejections

MCMC Performance

MCMC Performance

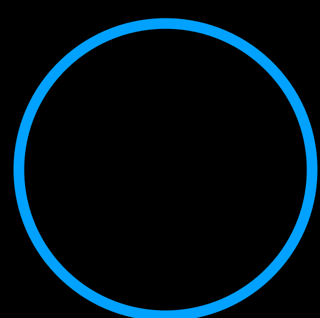


MCMC Performance



Rapidly degrades when step size is not ~ distribution size.

Which distribution will be hardest to explore with a uniform random walk?

1. 

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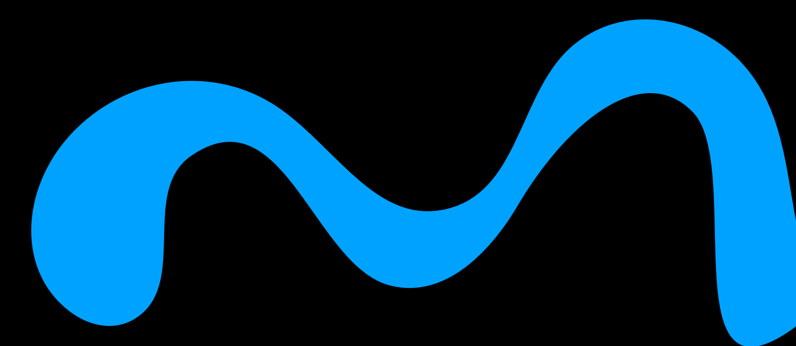
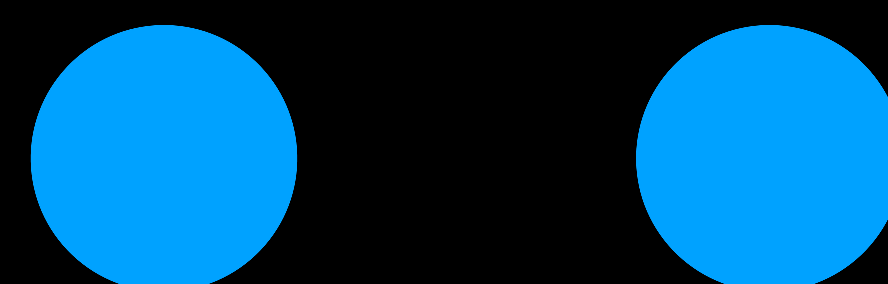
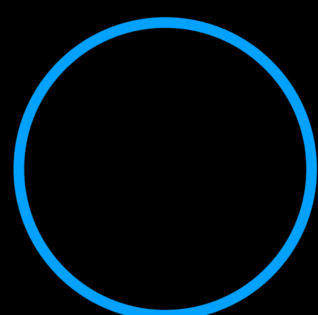
3. 

4. 

Which distribution will be second hardest to explore with a uniform random walk?

1. 

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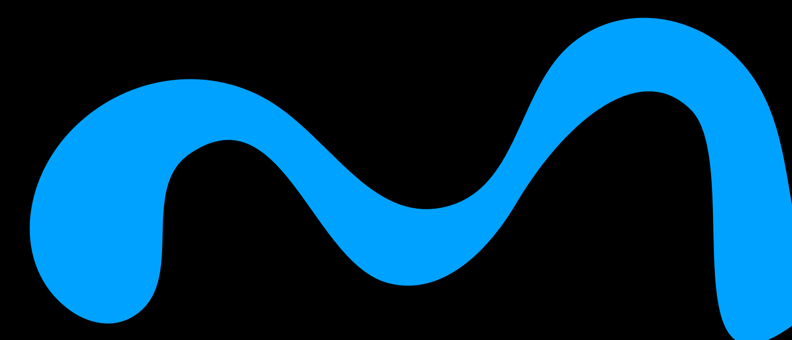
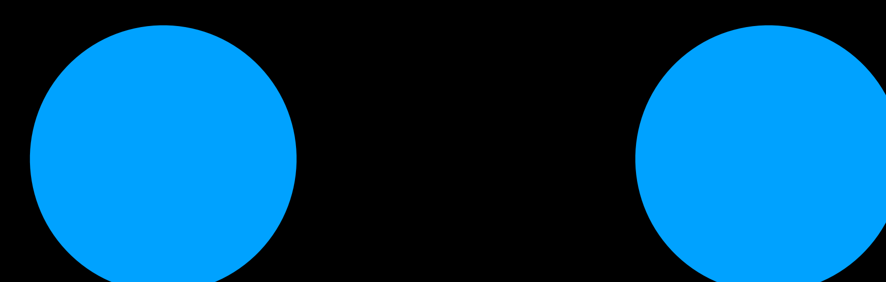
3. 

4. 

Takeaway point:

MCMC algorithms that adapt to the target distribution are vastly more efficient.

Takeaway point:

emcee (stretch-step)
Adaptive Metropolis
NUTS (Hamiltonian)

Hamiltonian Sampling Demo

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$$U(\vec{x}) = \frac{1}{2}\chi^2(\vec{x}) \qquad\qquad T(\vec{v}) = \frac{1}{2}v^2$$

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$$\mathcal{H}(\vec{x}, \vec{v}) = U(\vec{x}) + T(\vec{v})$$

$$\mathcal{L}(\vec{x}, \vec{v}) = \exp(-\mathcal{H}(\vec{x}, \vec{v}))$$

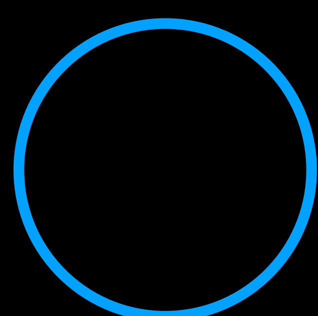
Hamiltonian Sampling Demo

$$U(\vec{x}) = \frac{1}{2}\chi^2(\vec{x}) \qquad T(\vec{v}) = \frac{1}{2}v^2$$

$$\mathcal{H}(\vec{x},\vec{v}) = U(\vec{x}) + T(\vec{v})$$
$$\mathcal{L}(\vec{x},\vec{v}) = \exp(-\mathcal{H}(\vec{x},\vec{v}))$$

$$\frac{\partial\vec{x}}{\partial t} = \nabla T = \vec{v} \qquad \frac{\partial\vec{v}}{\partial t} = -\nabla U = -\frac{1}{2}\nabla\chi^2$$

Which distribution will be second hardest to explore with a uniform random walk?

1. 

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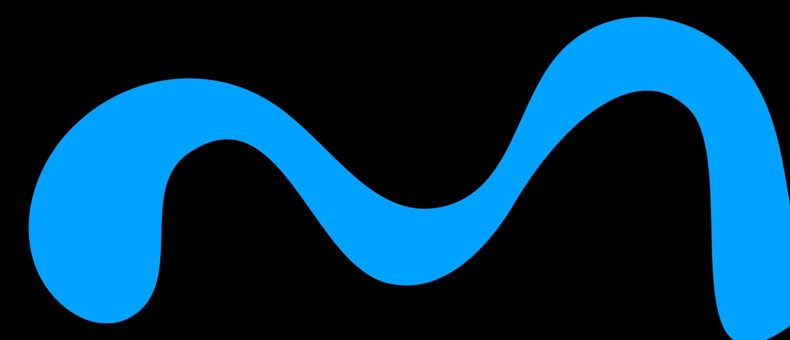
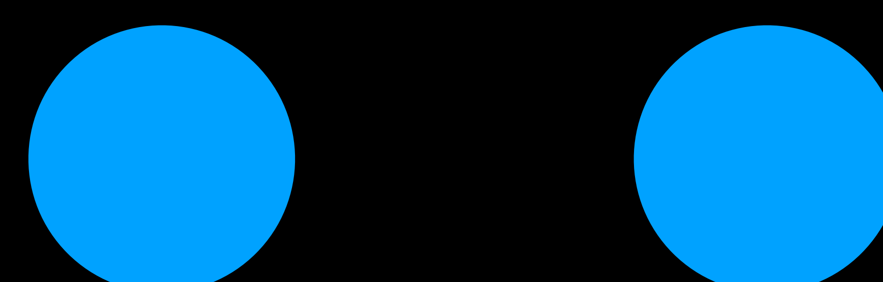
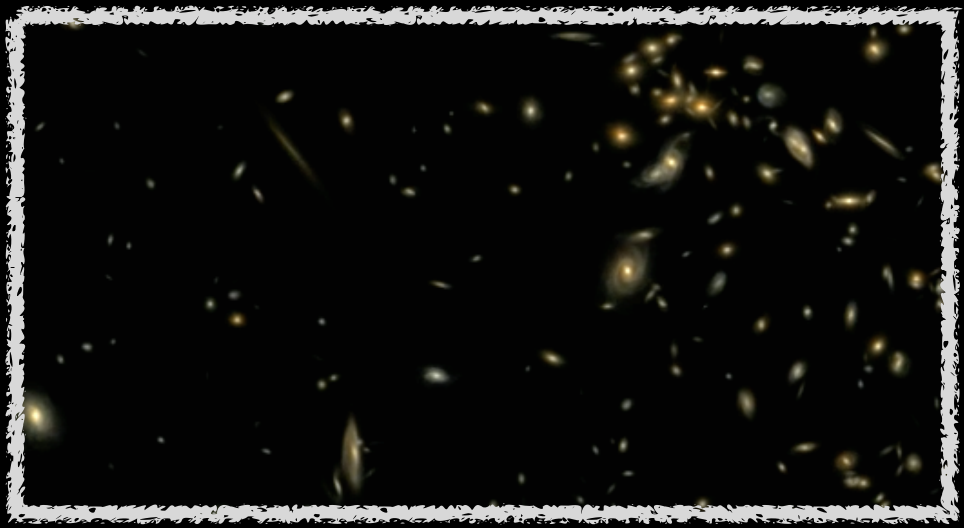
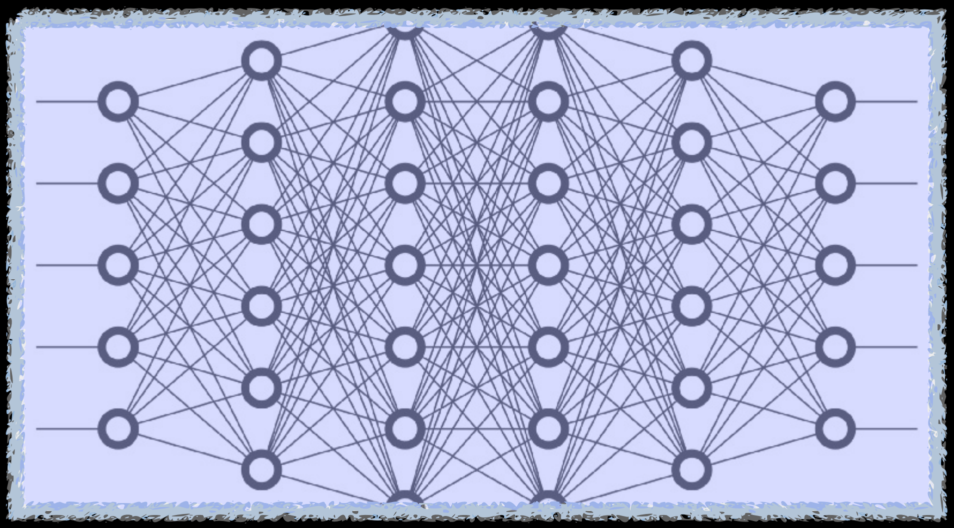
3. 

4. 

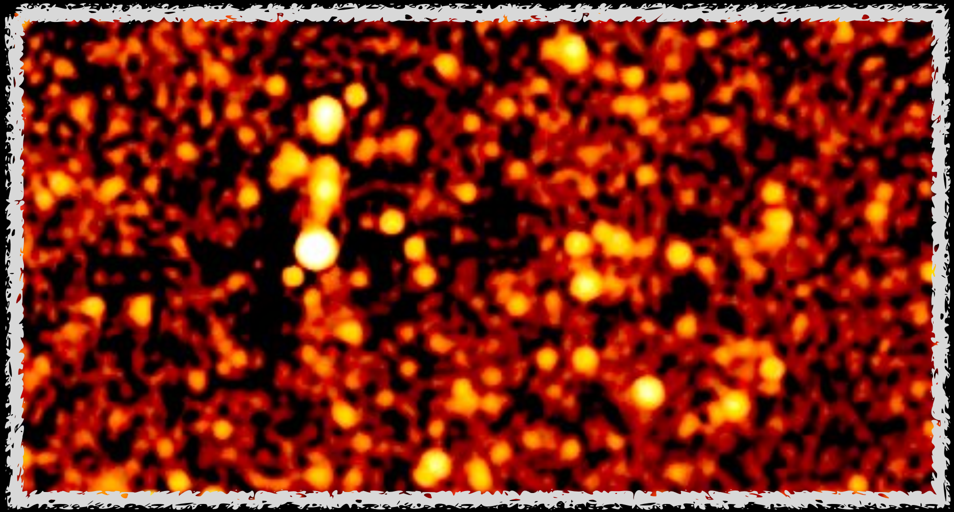
High-Dimensional Problems



Empirical Galaxy Modeling
40-70 dimensions



Deep Neural Networks
50-10,000 dimensions

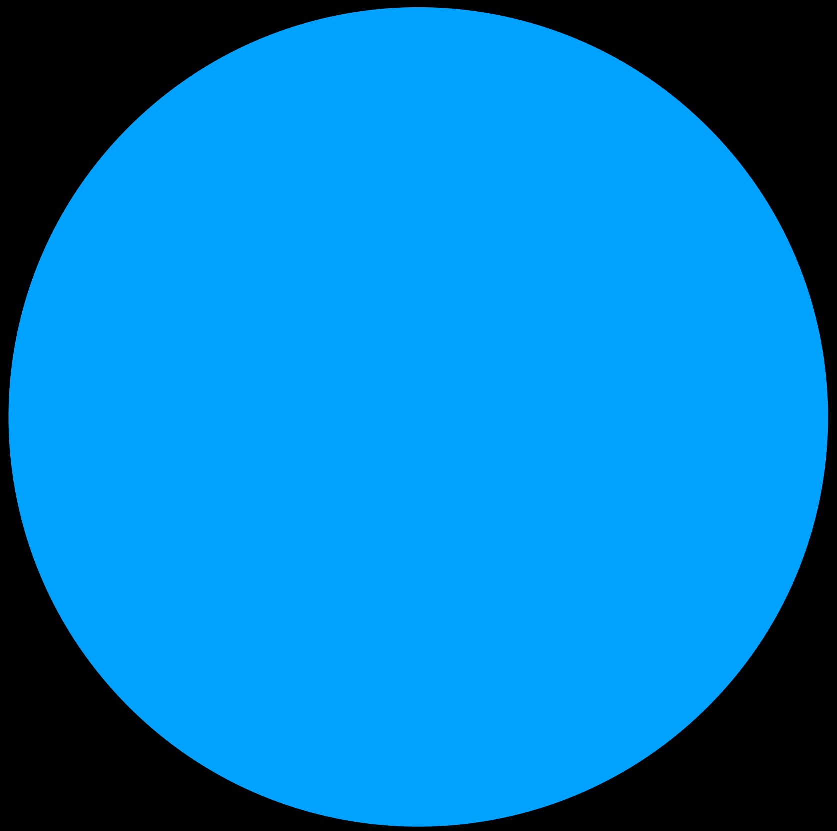


Confused Source Recovery
100 - 10^9 dimensions

Constrained Realizations
> 10^9 dimensions

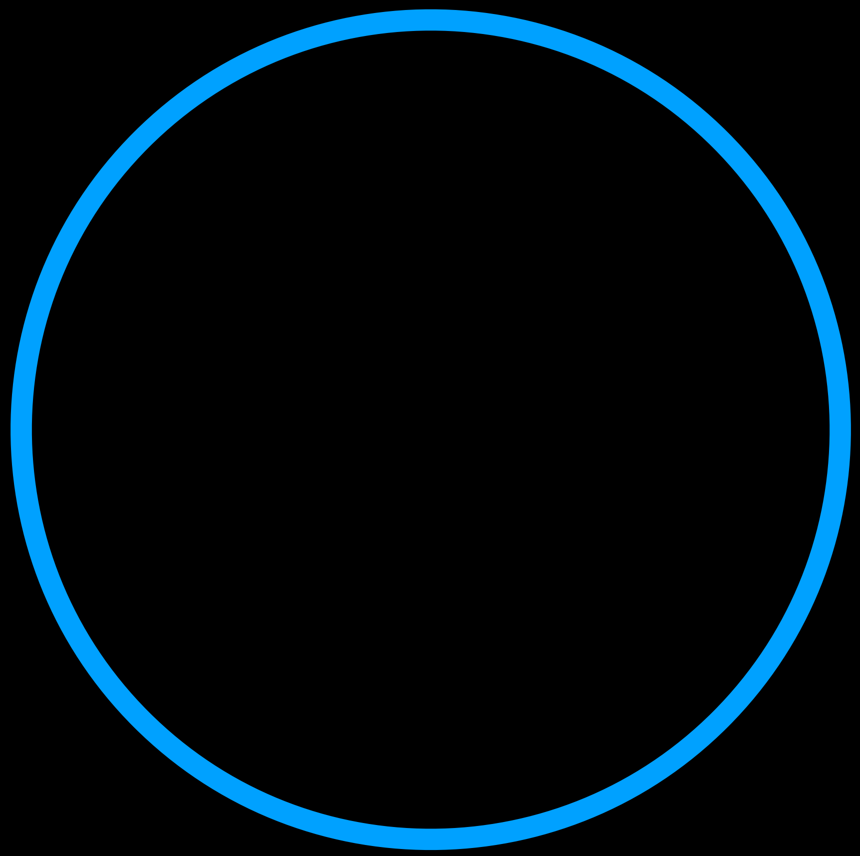
Image Credits: SDSS, Radu Raicea, Jim Condon, CLUES

High-Dimensional Problems



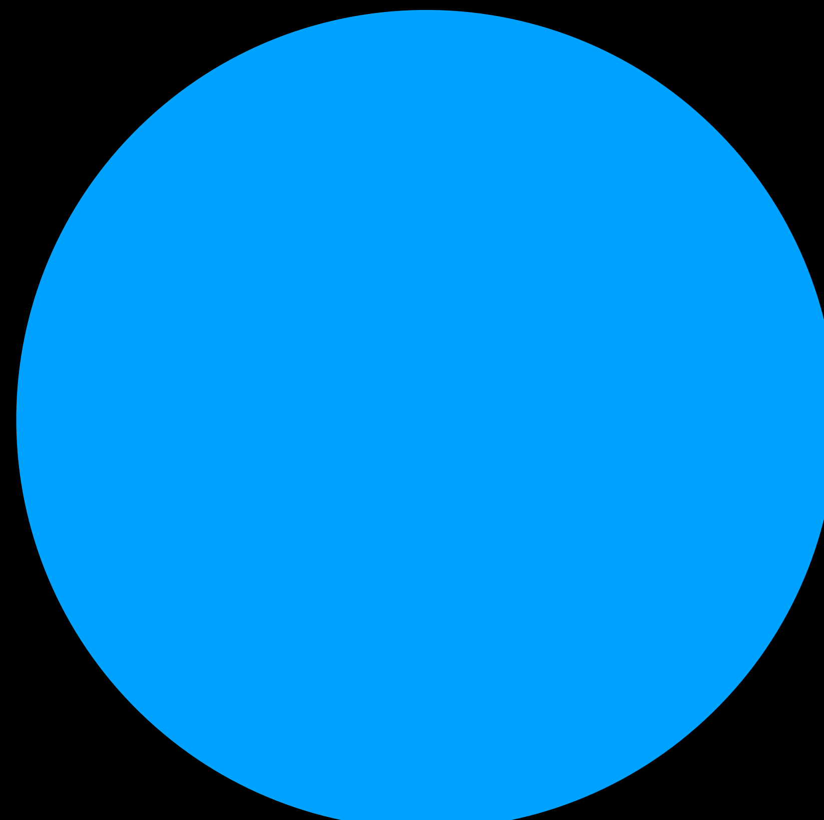
In 3D: 5% change in radius = 15% change in volume.

High-Dimensional Problems



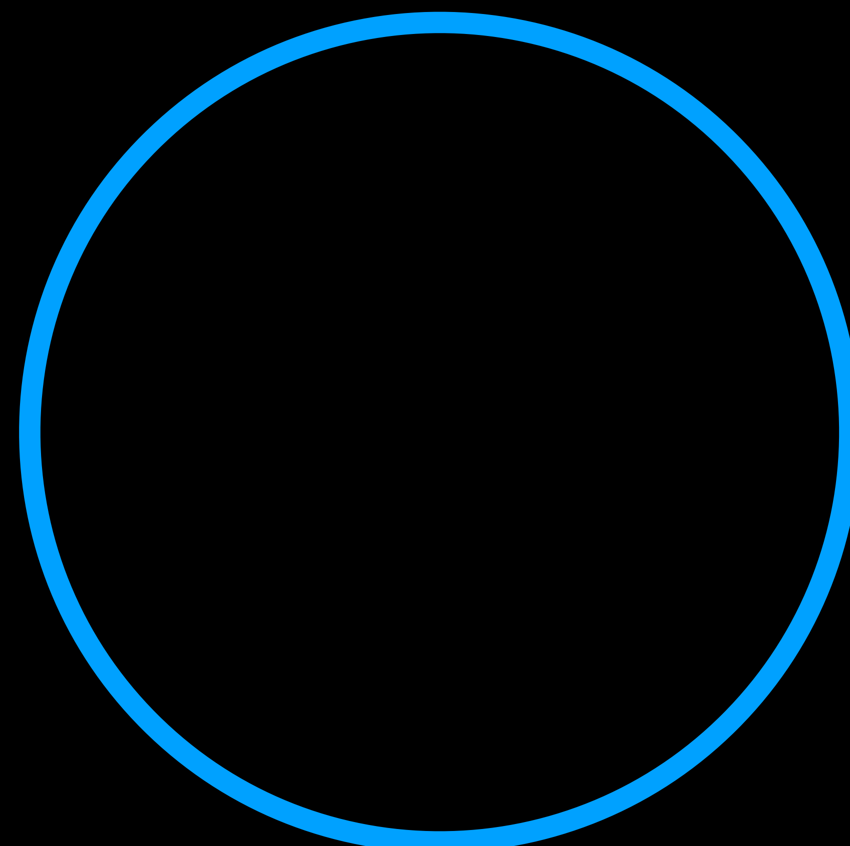
In 20D: 5% change in radius = 165% change in volume.

High-Dimensional Problems



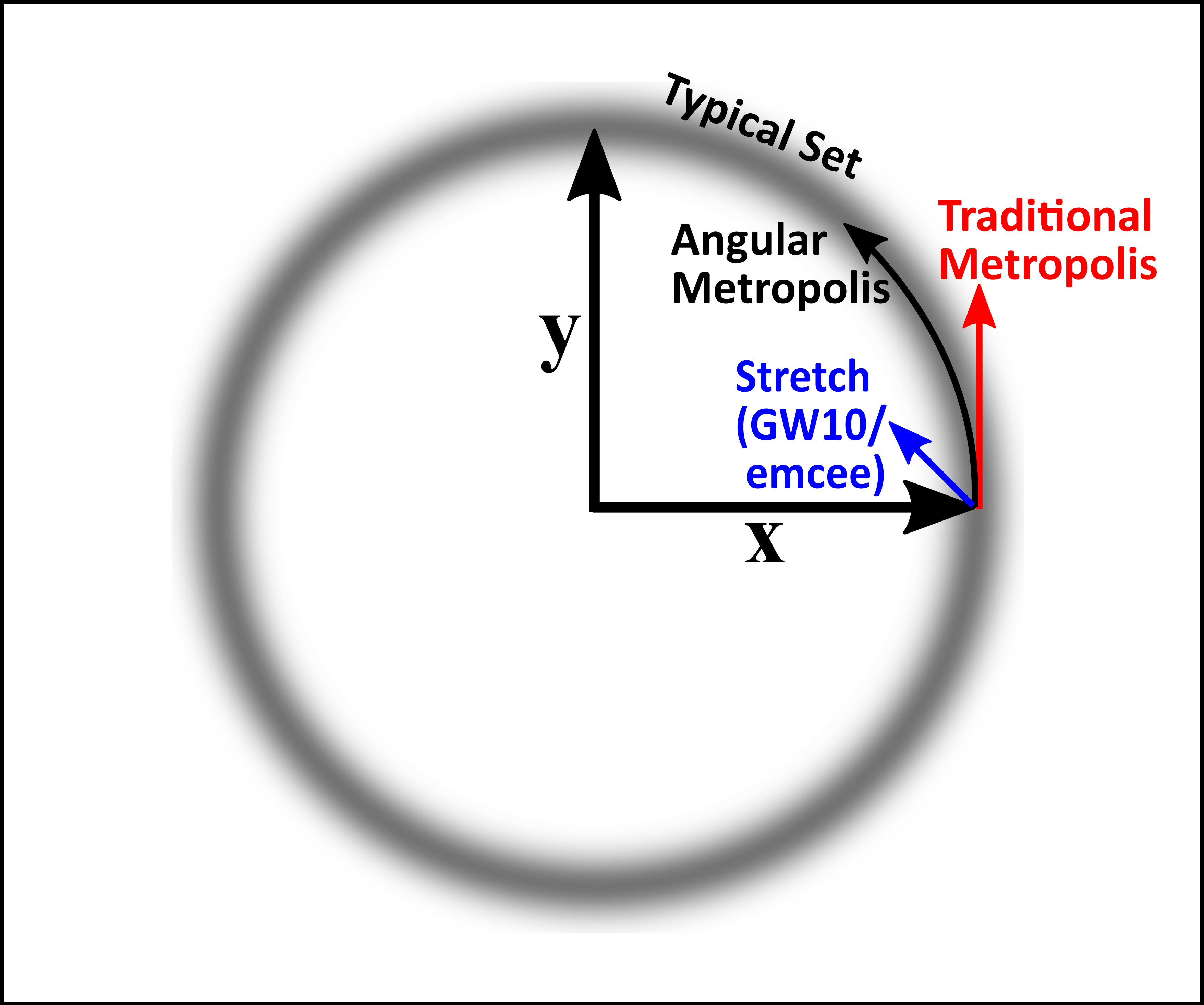
In 3D: covariance matrix has 6 parameters.

High-Dimensional Problems

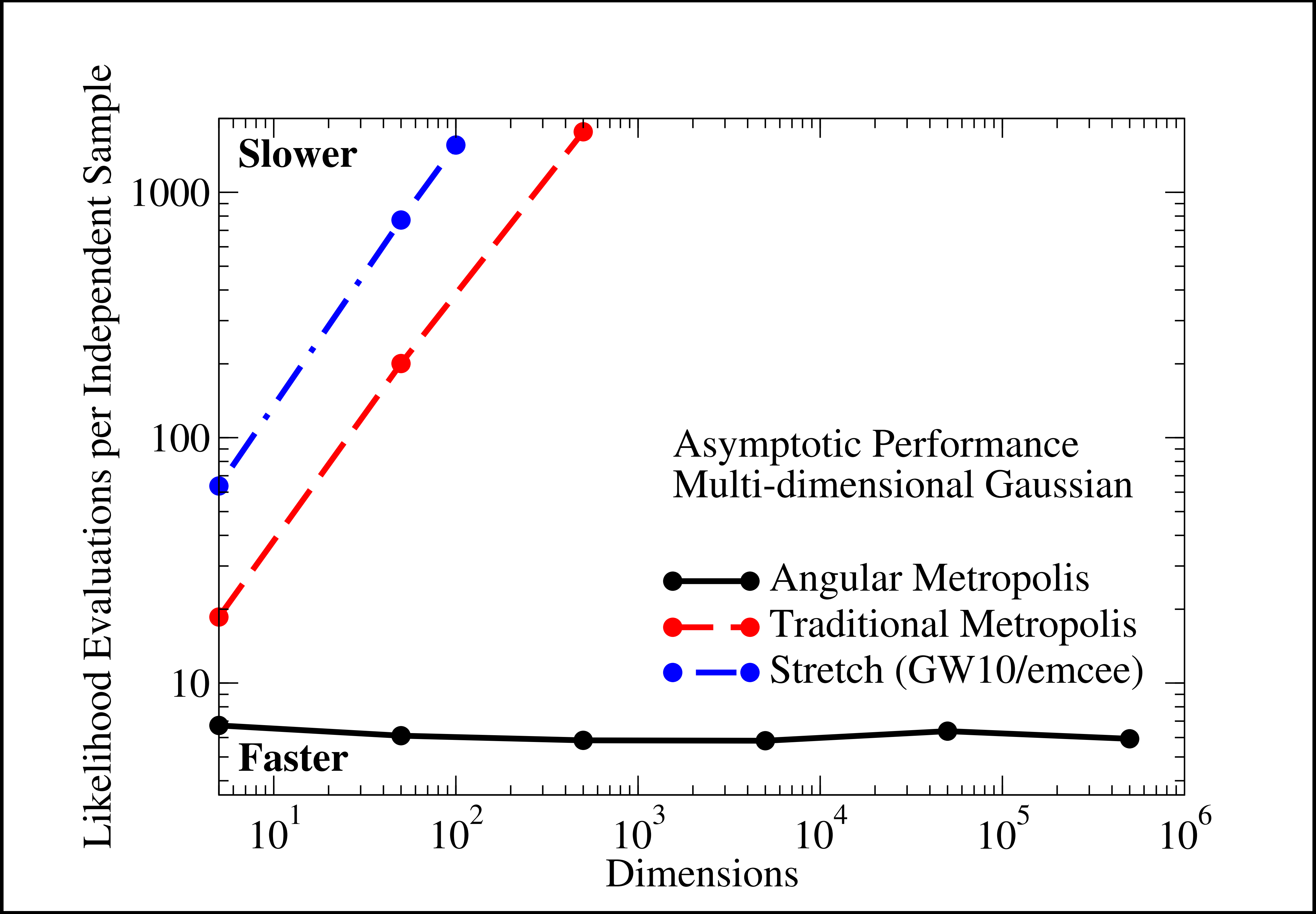


In 20D: covariance matrix has 210 parameters (D*(D+1)/2).

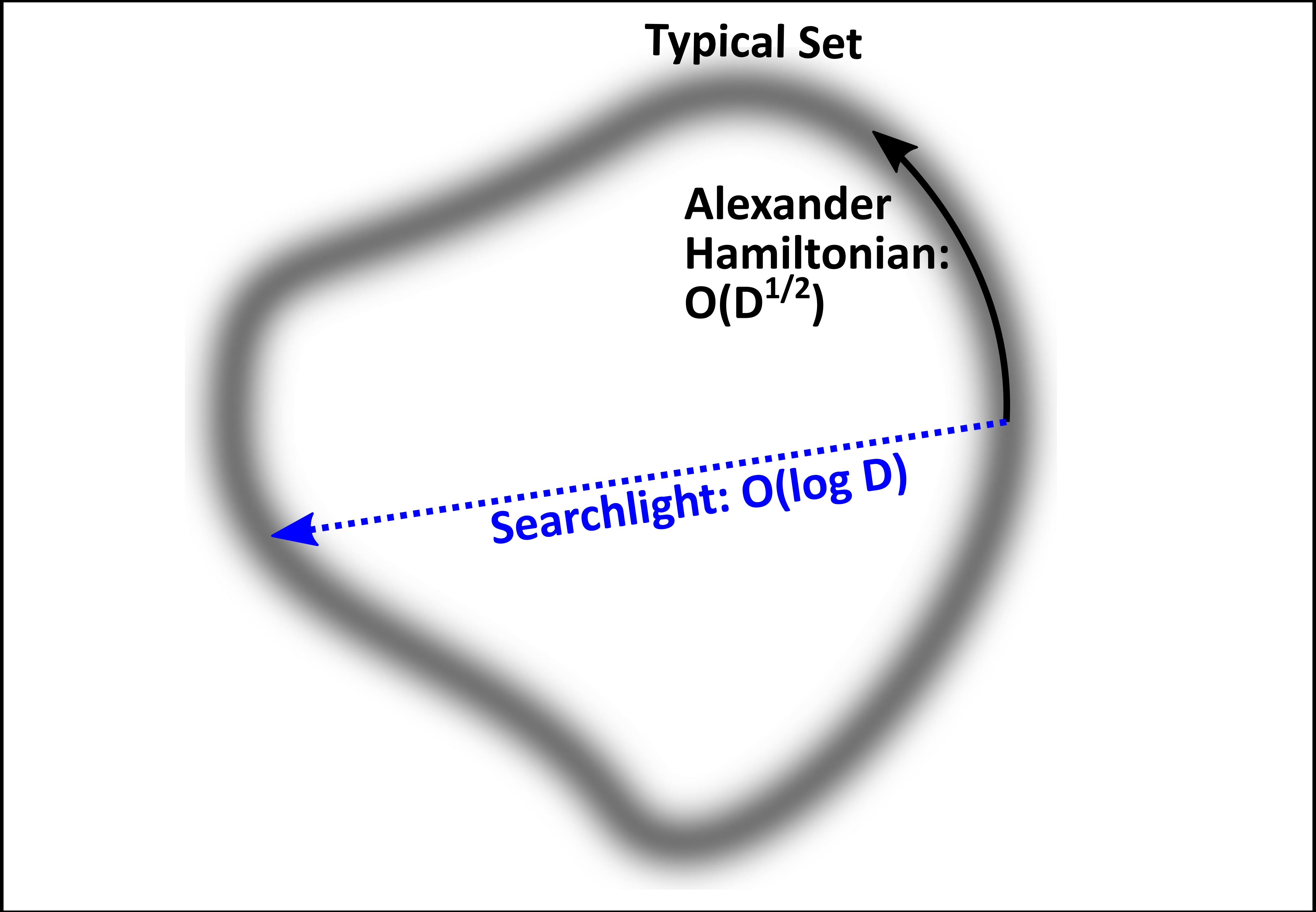
(Future) Solutions



(Future) Solutions



(Future) Solutions



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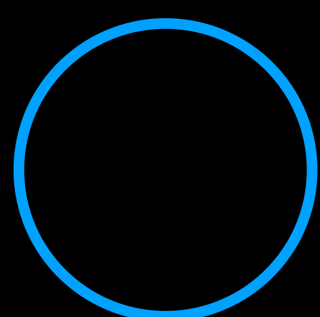
1. 

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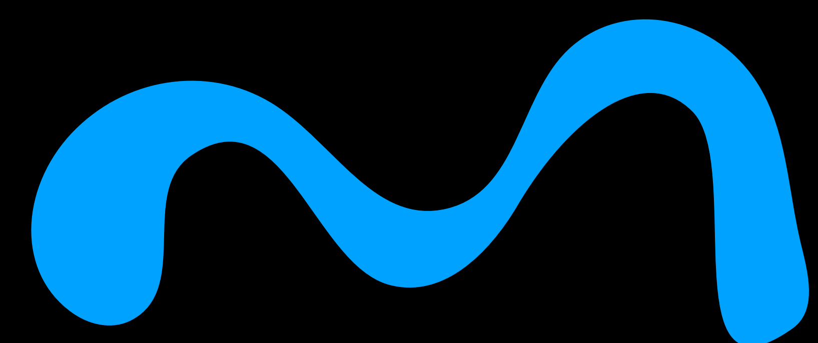
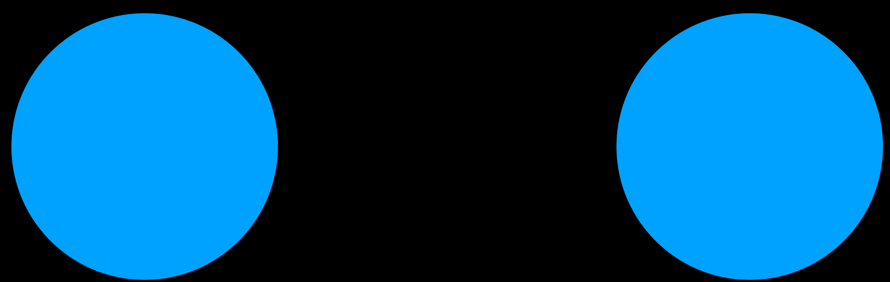
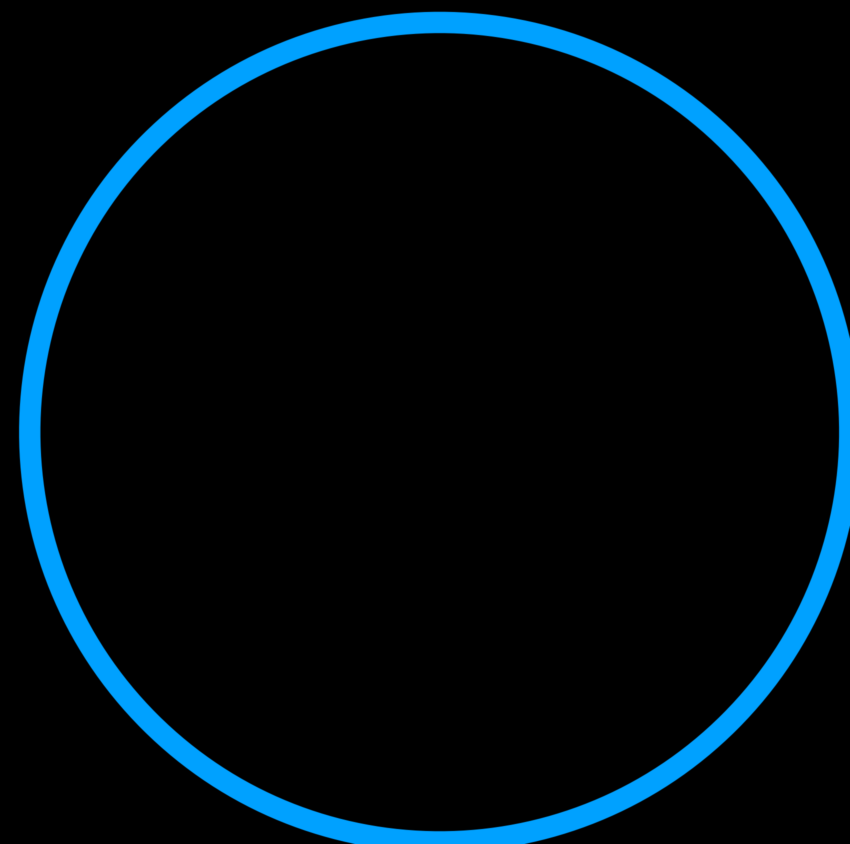
3. 

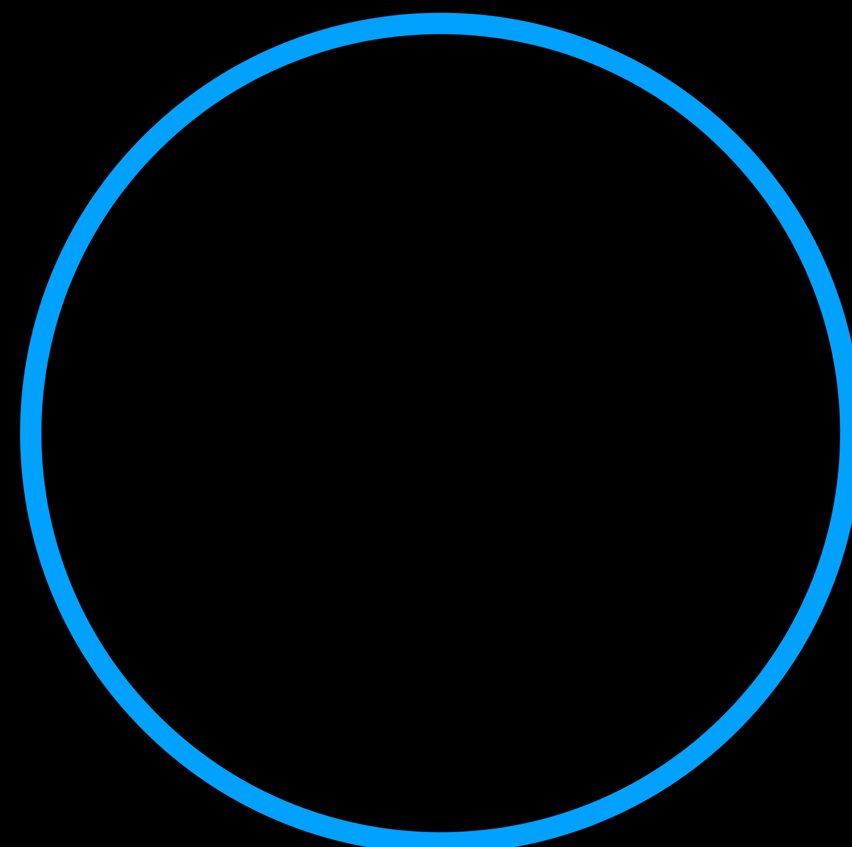
4. 

High-Dimensional Problems



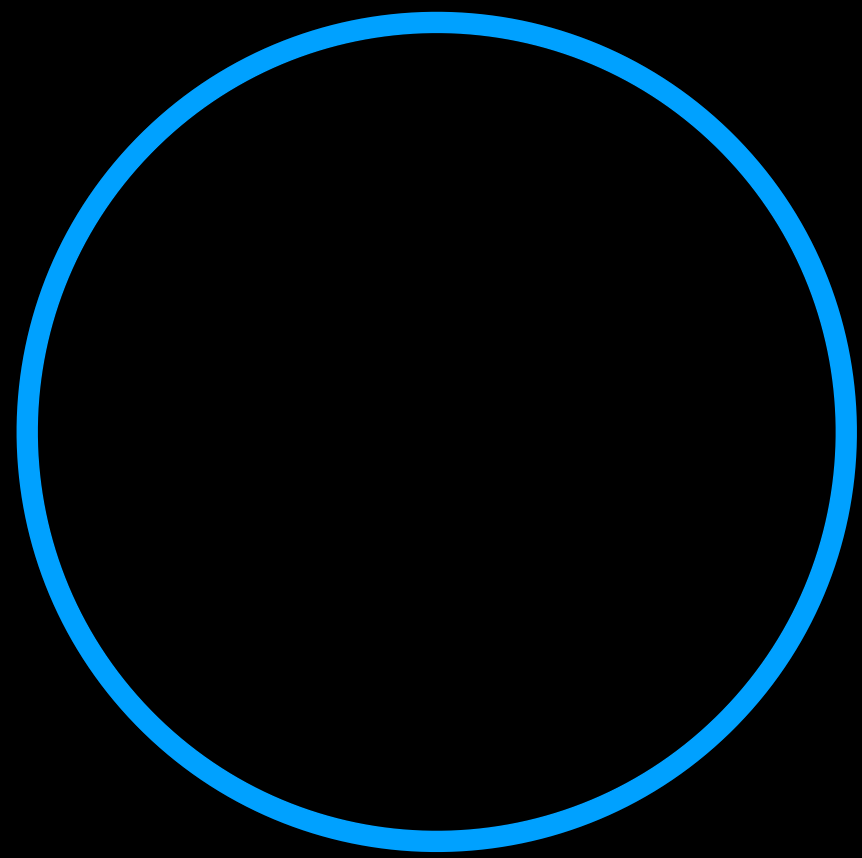
Use another algorithm (e.g. from scipy.optimize) to find minimum first.

High-Dimensional Problems



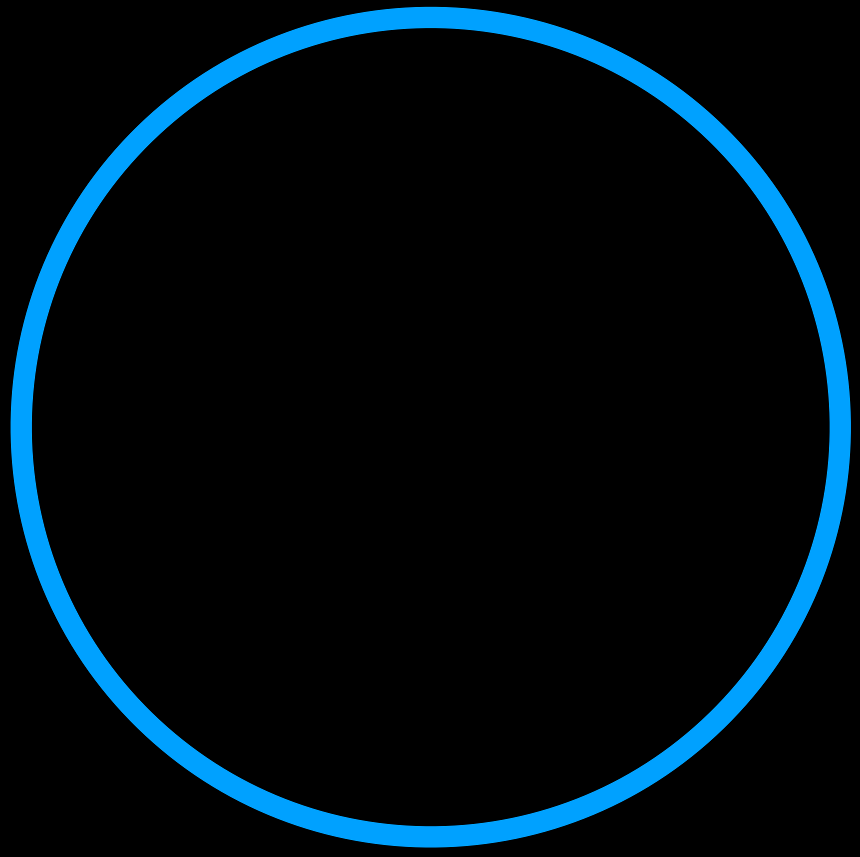
Estimate covariance matrix around minimum using the Fisher Information Matrix.

High-Dimensional Problems



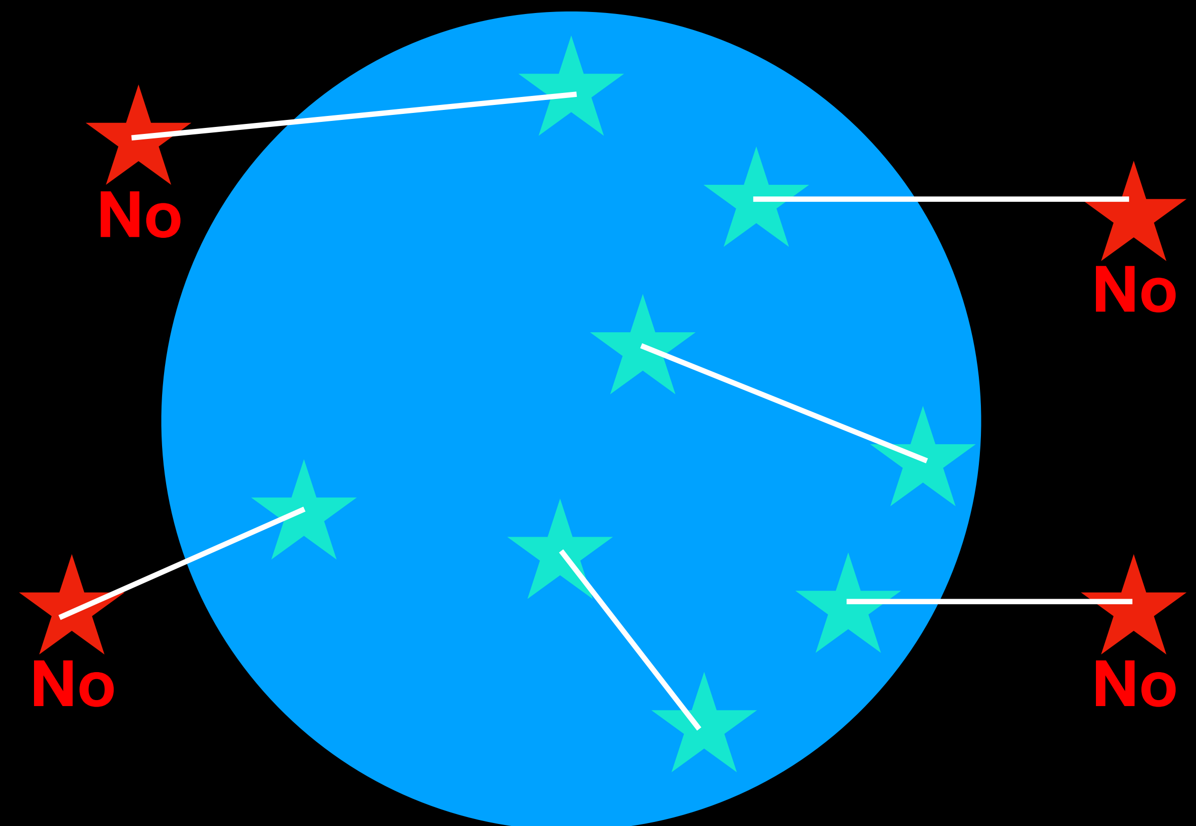
Use a Gaussian distribution with the estimated covariance matrix as starting points.

High-Dimensional Problems



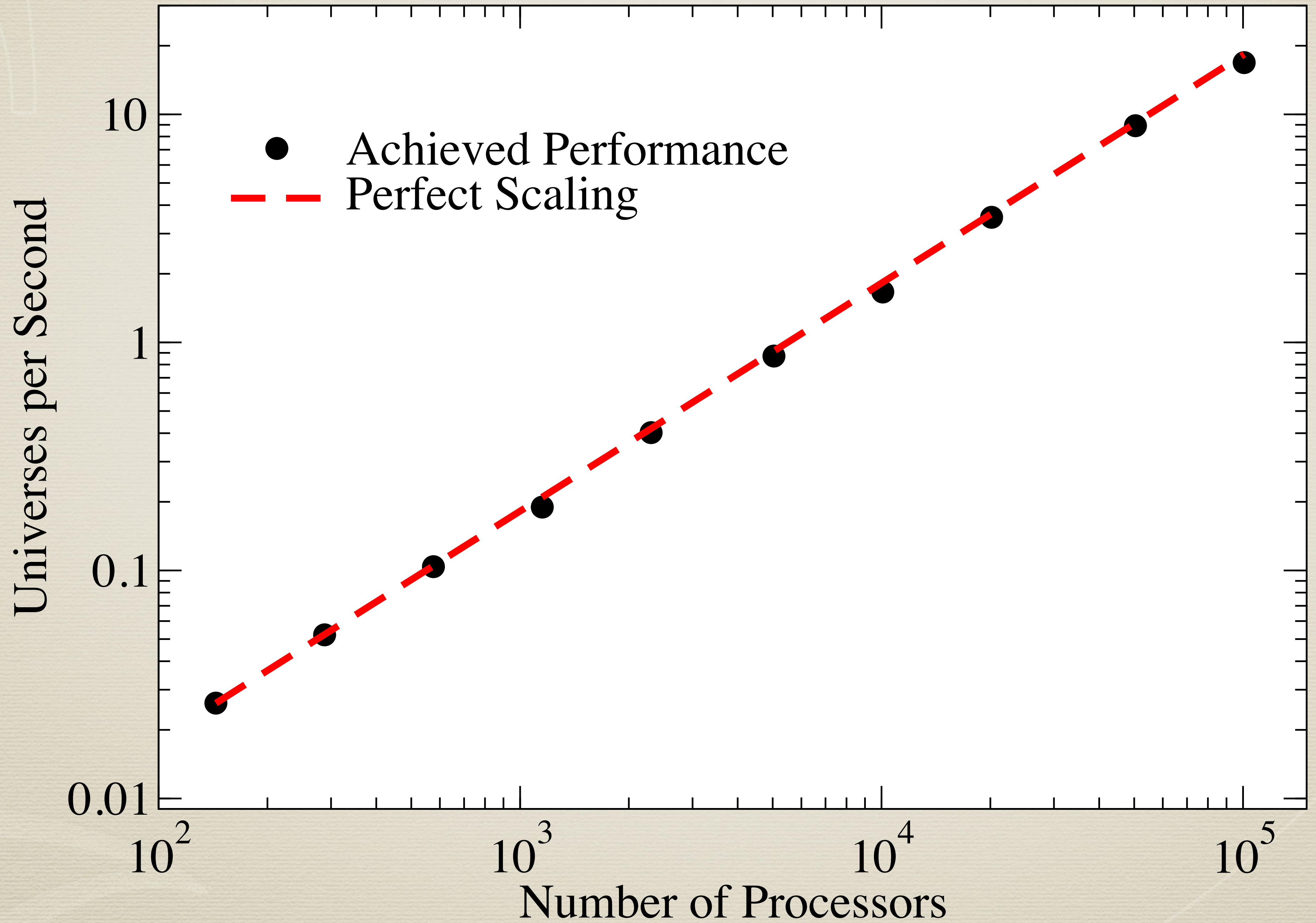
Use parallel sampling.

Parallel Sampling



Multiple walkers generating multiple MCMC chains.

Universe Machine



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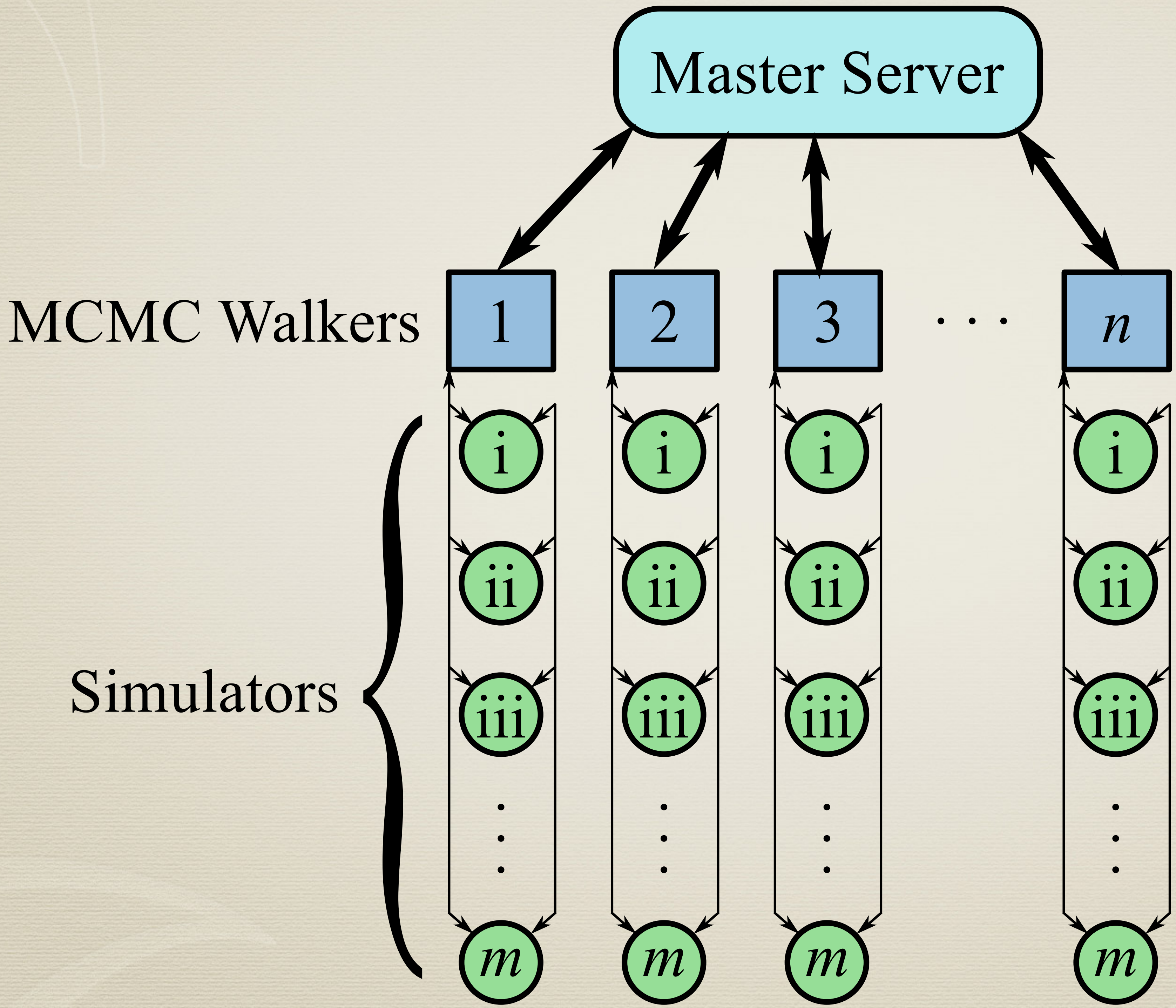

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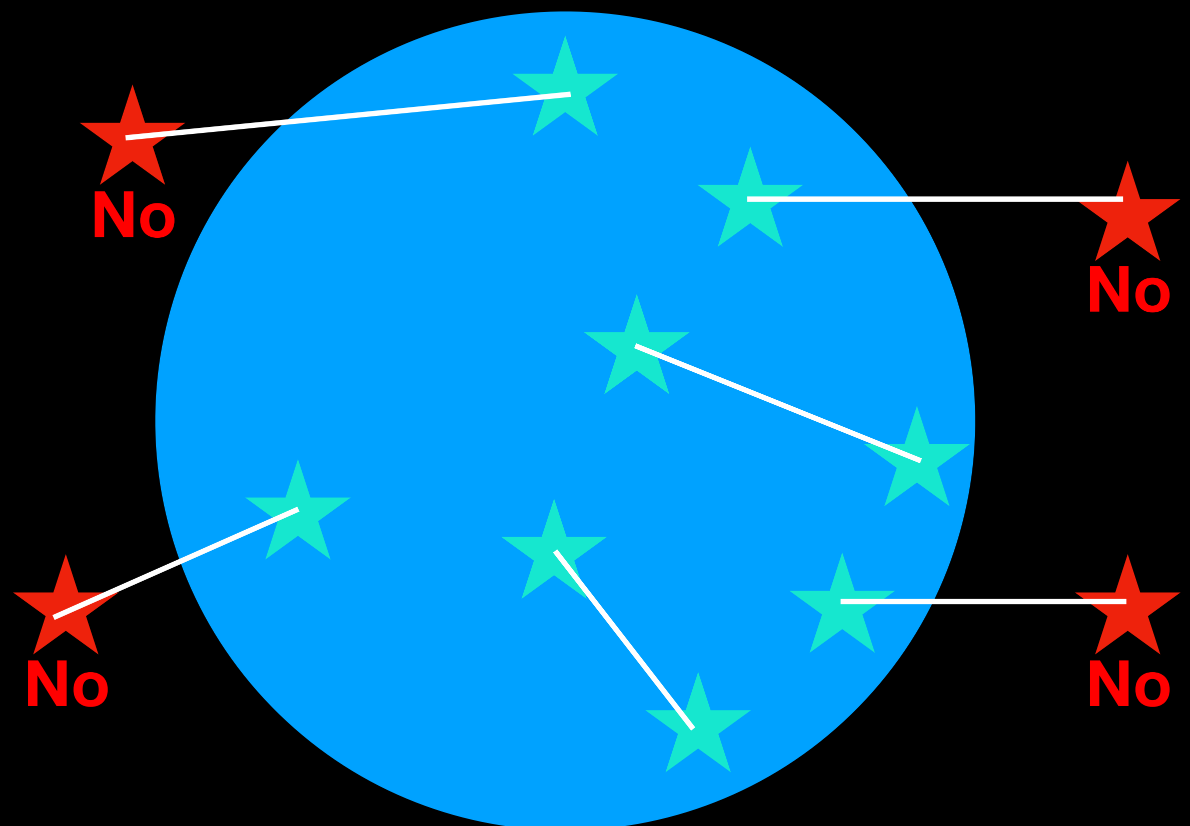
Convergence



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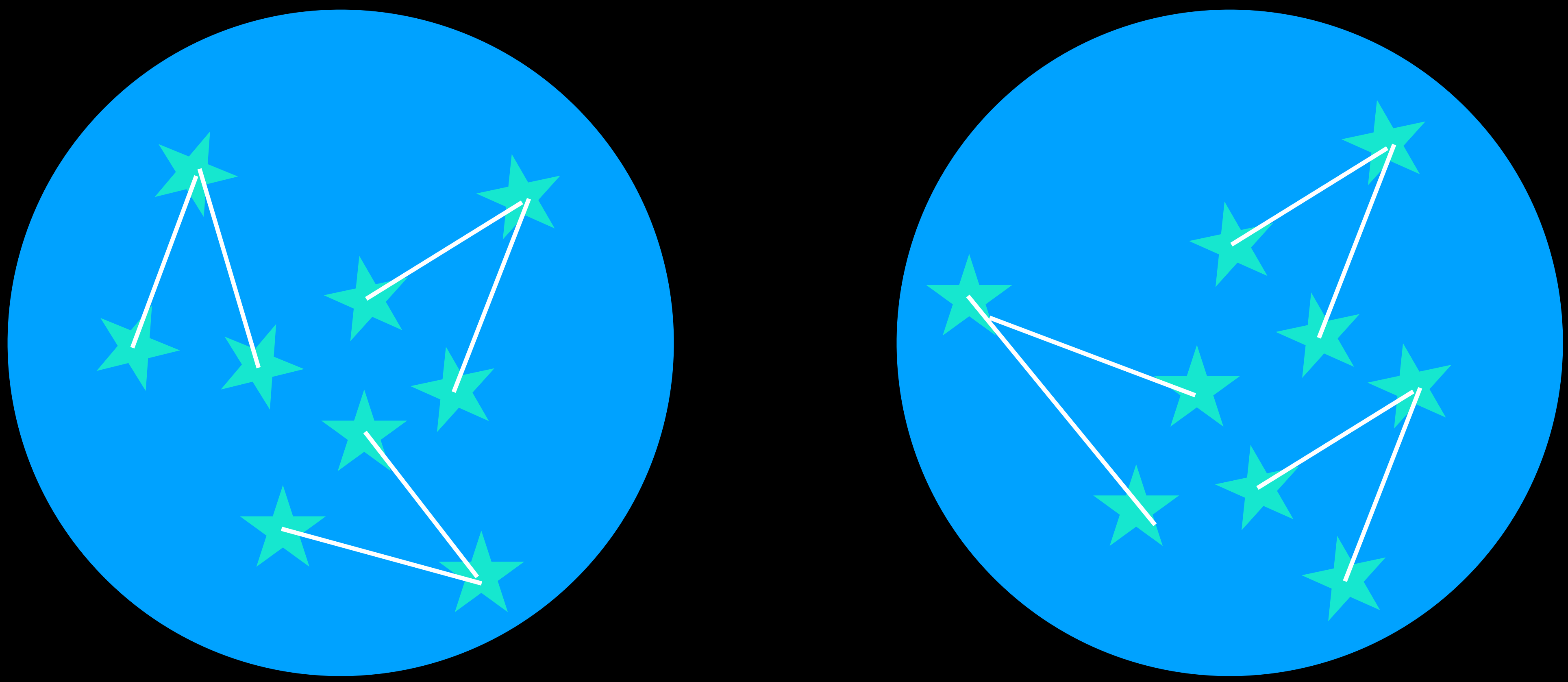

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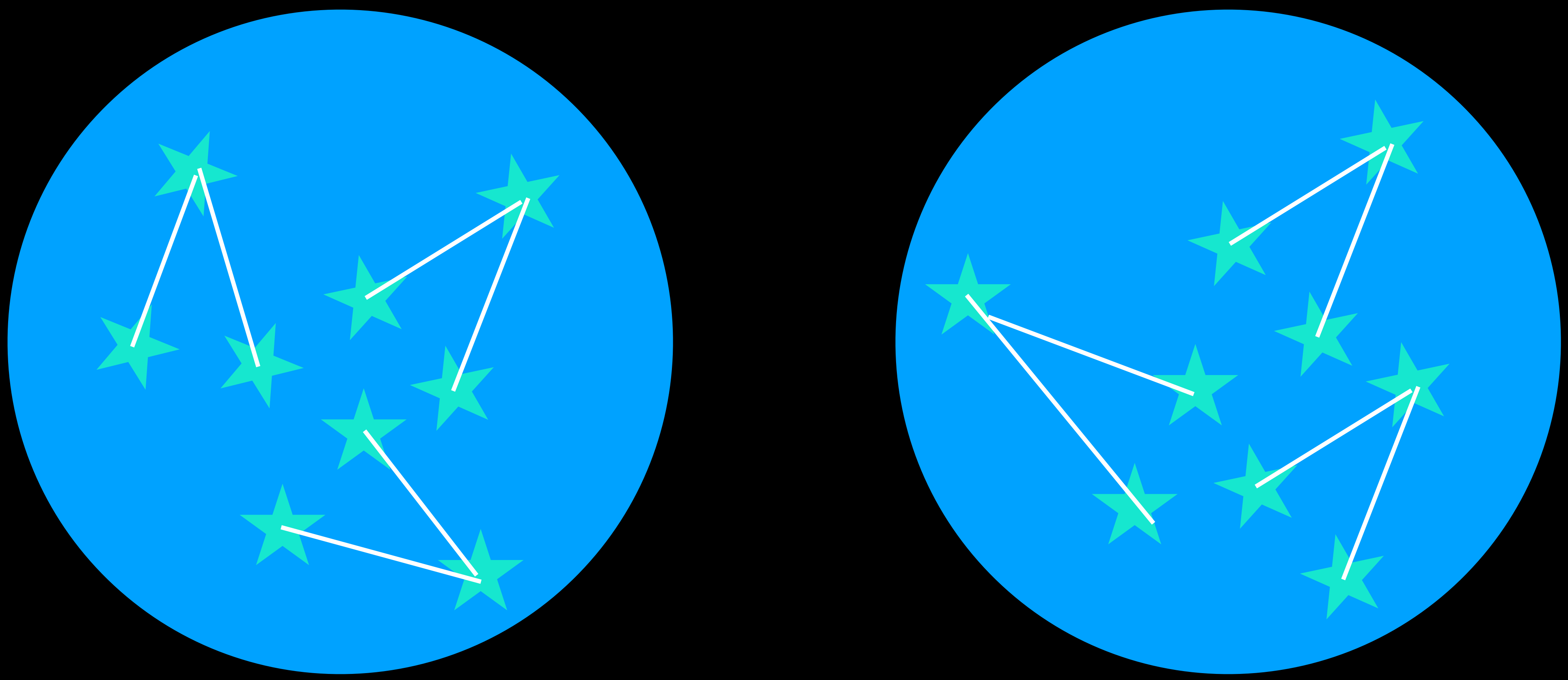

Gelman-Rubin ~ $\frac{\text{Total SD}}{\text{Within-chain SD}}$

Summary

MCMCs help convert obs. to physics.

Use adaptive algorithms

Good algorithms exist in <5D;
not so much (currently) for >10D

Testing for convergence is generally hard, but easier if you parallel sample.

come talk to me if you have MCMC questions

(behroozi@email.arizona.edu)

Peter Behroozi

Steward 326