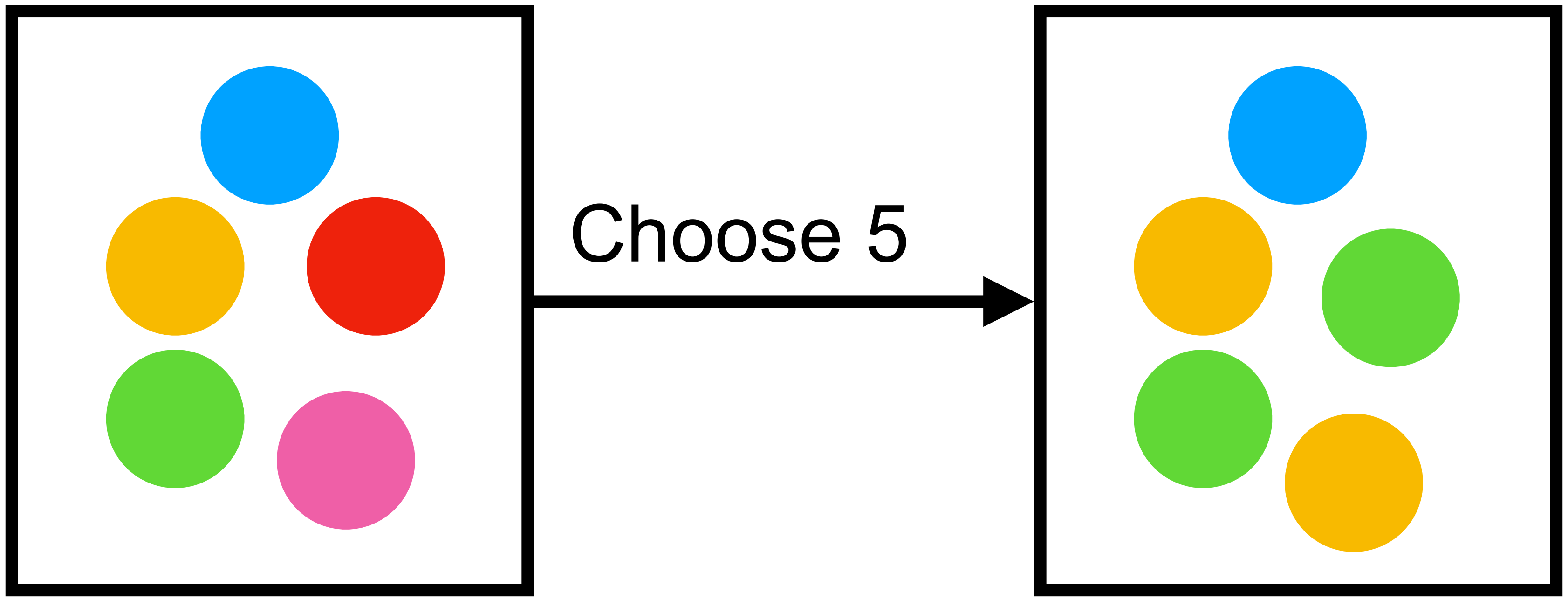
Lecture 20: Markov Chain Monte Carlo

Bootstrapping

- Lets say you have a fixed dataset $(\vec{x})$
  - You cannot generate more
  - You compute something very complicated on it
    - For example $\vec{y} = \mathrm{NN}(\vec{x})$
  - You want to know the uncertainty on $\vec{y}$ given by $\sigma_{\vec{y}}$
    - However your function $\frac{d\mathrm{NN}(\vec{x})}{dx} \notin \text{exists}$

Bootstrapping: Strategy



You will
Get Duplicates

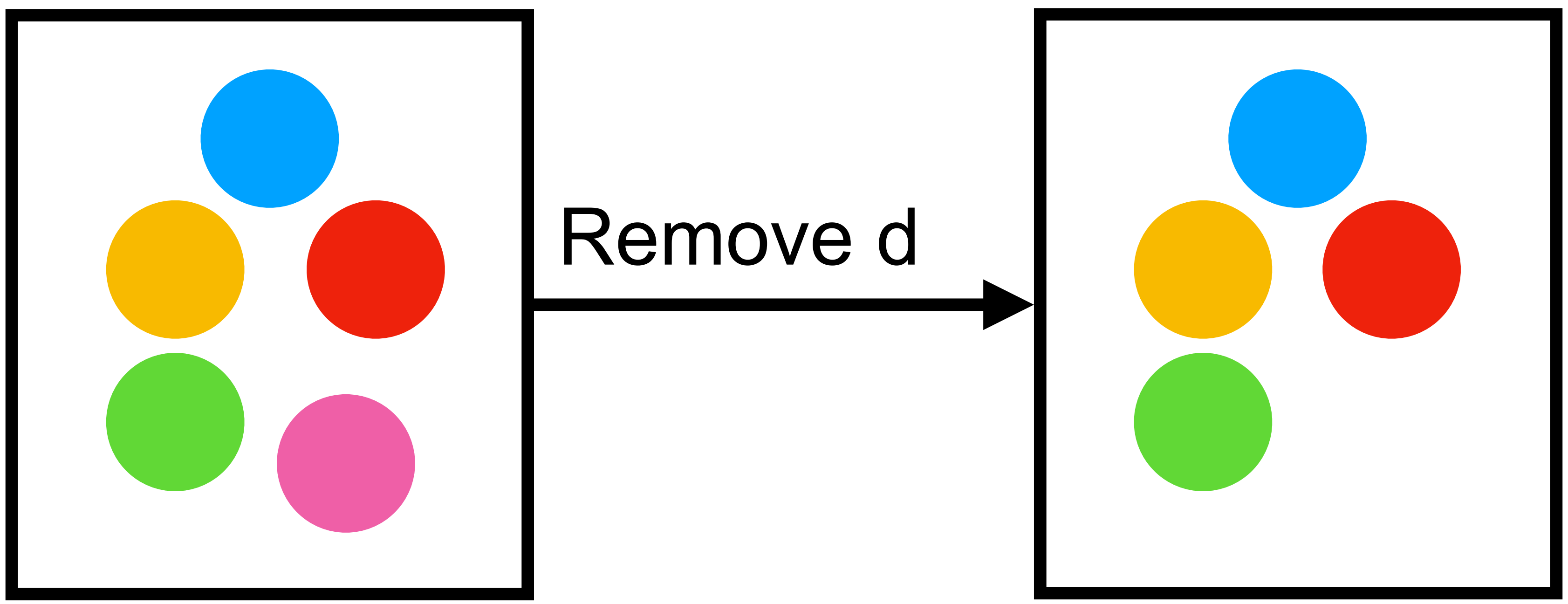
However if
things
Are truly
poission its ok

- Randomly sample the pool of events with the same size
  - Now use this sample to compute all our observables
- Variance over our random samples will be the uncertianty

$$\sigma_{\mathrm{boot}} = \frac{1}{N_{\mathrm{samples}} - 1} \boxed{\sum_{i}^{N_{\mathrm{samples}}} \left(\mathcal{O} - \bar{\mathcal{O}}\right)^2}$$

We can do this
with any
observable

Delete-D Jackknife



- Like what we did with Bootstrapping
  - However, doesn't duplicate events

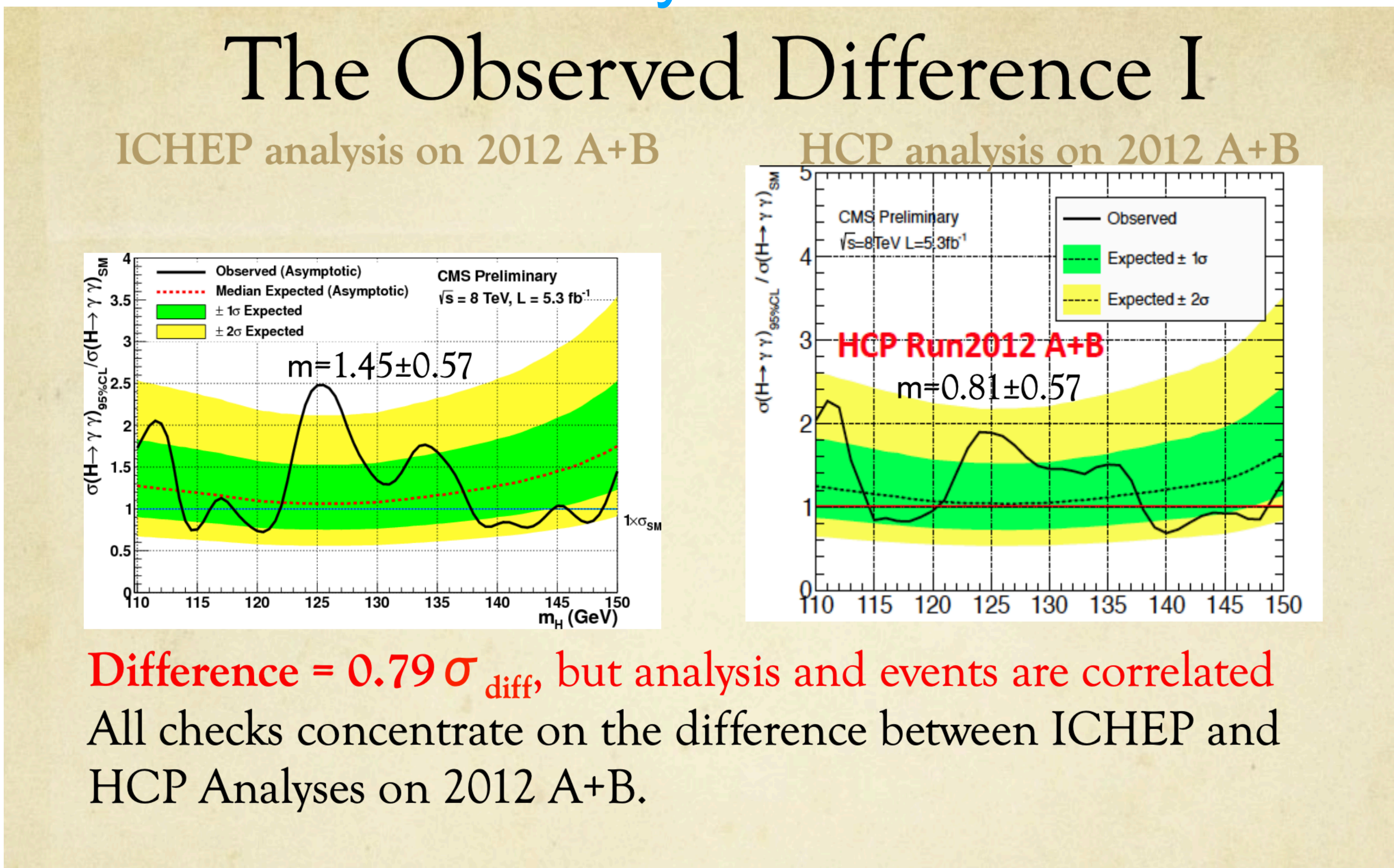
d=removed samples

$$\sigma_{\text{Jackknife}} = \frac{N_s - d}{\left({}_{N_s}C_d\right) d} \sum_{i}^{{}_{N_s}C_d} \left(\mathcal{O} - \bar{\mathcal{O}}\right)^2$$

Total Unc From Jackknife

Fun Story

Higgs to diphoton result changed dramatically in 2012
On exactly the same data



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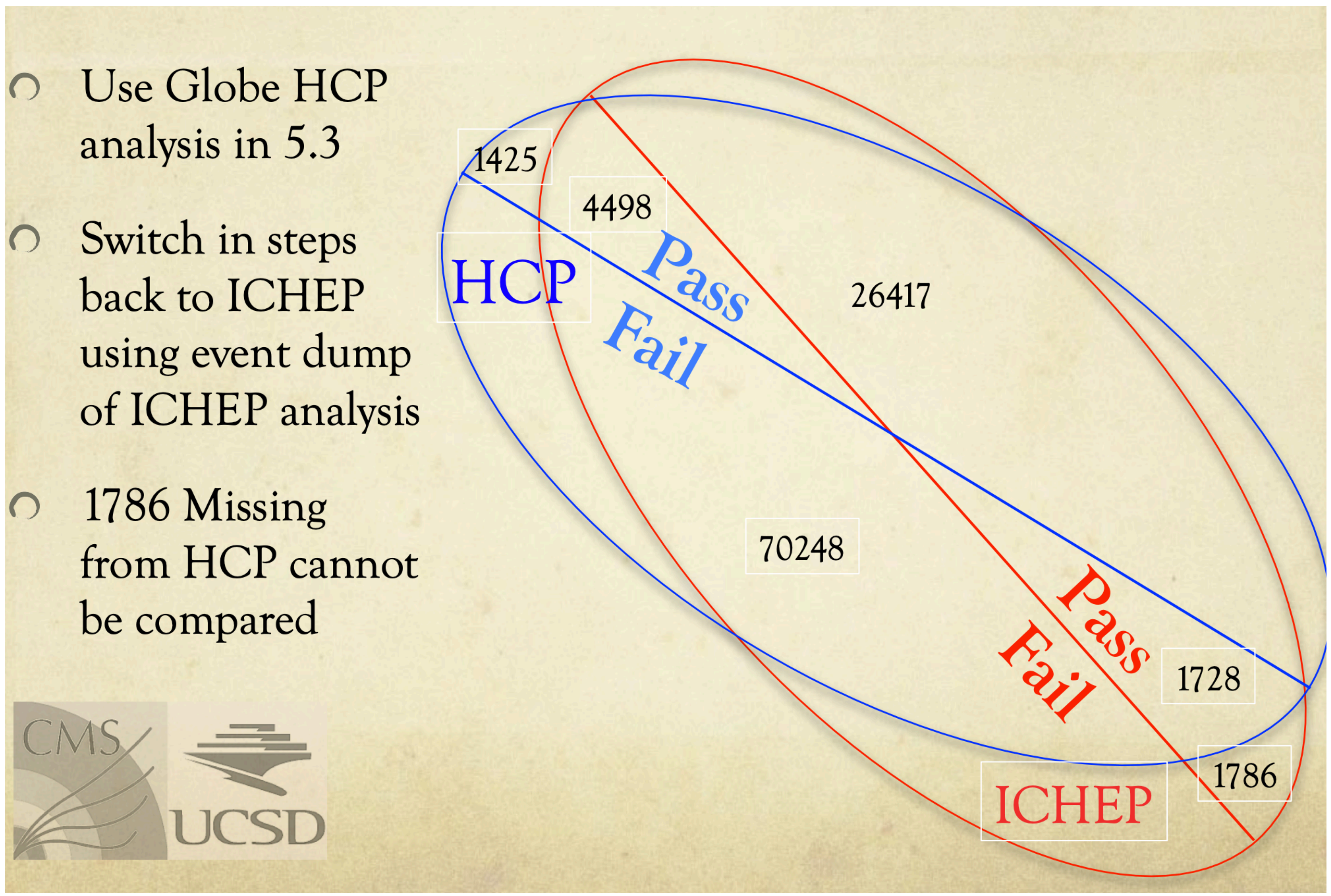
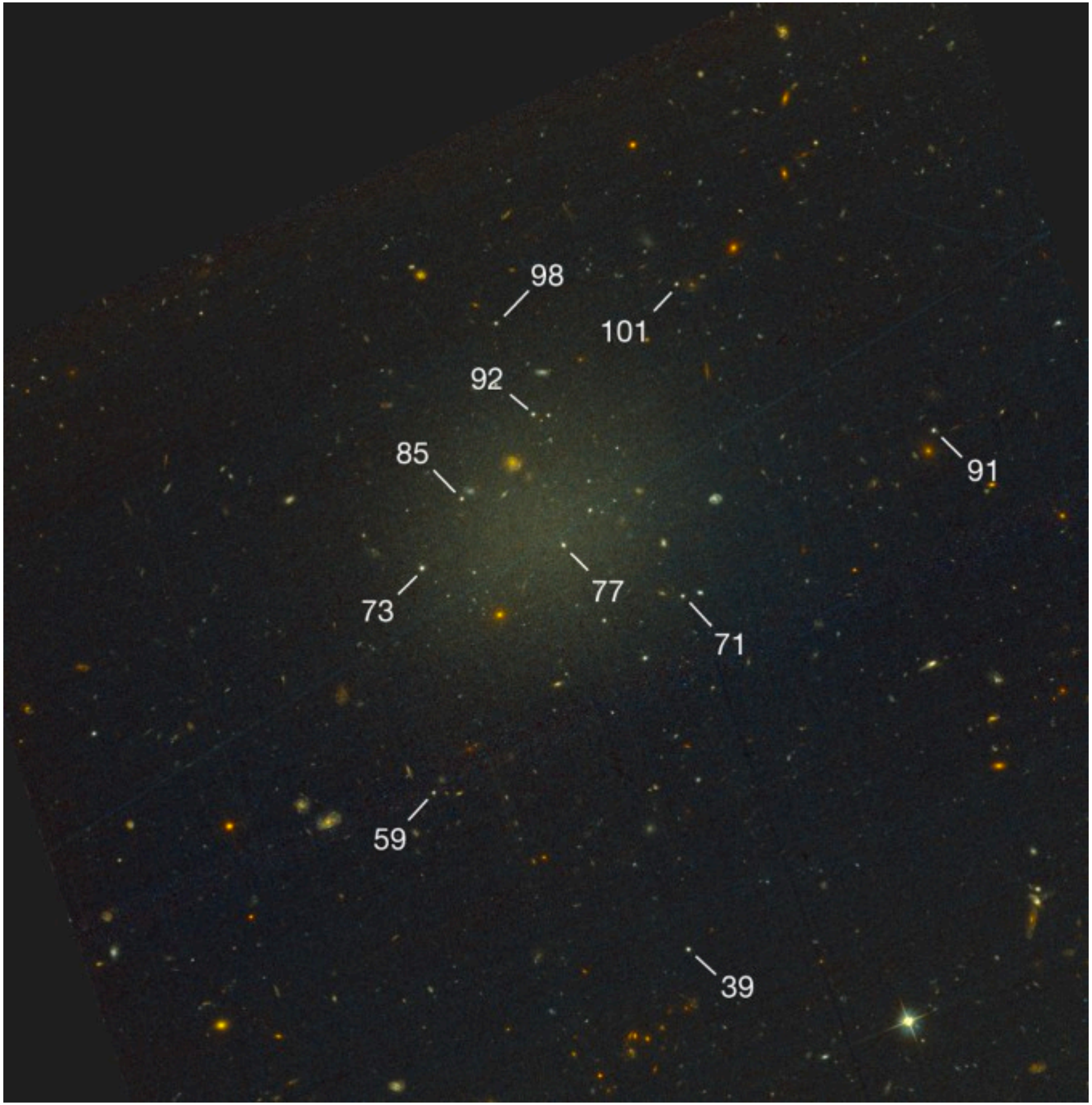
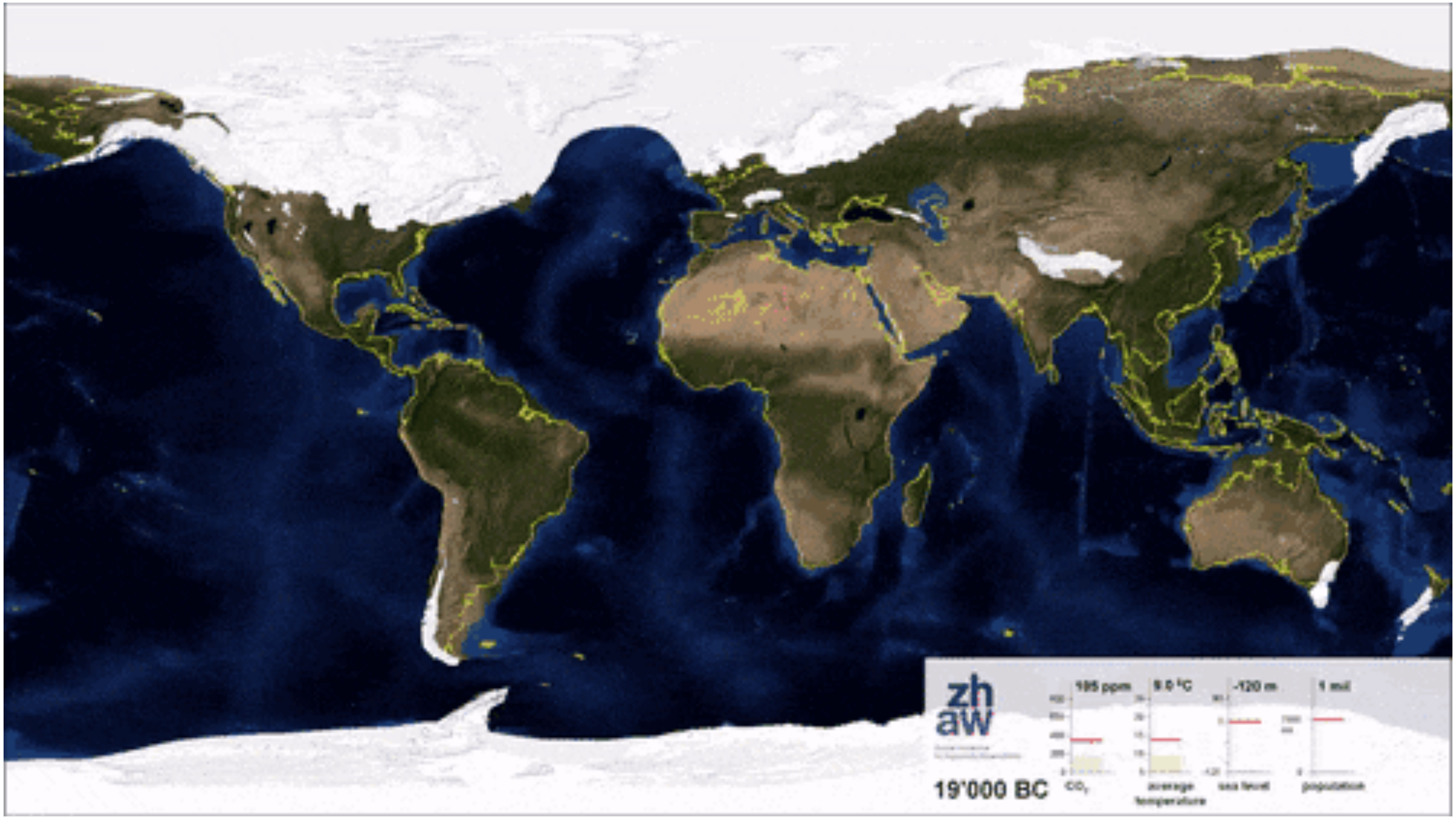


Delete-d Jackkinfe was the way we were able to analyze the unc.

MCMC

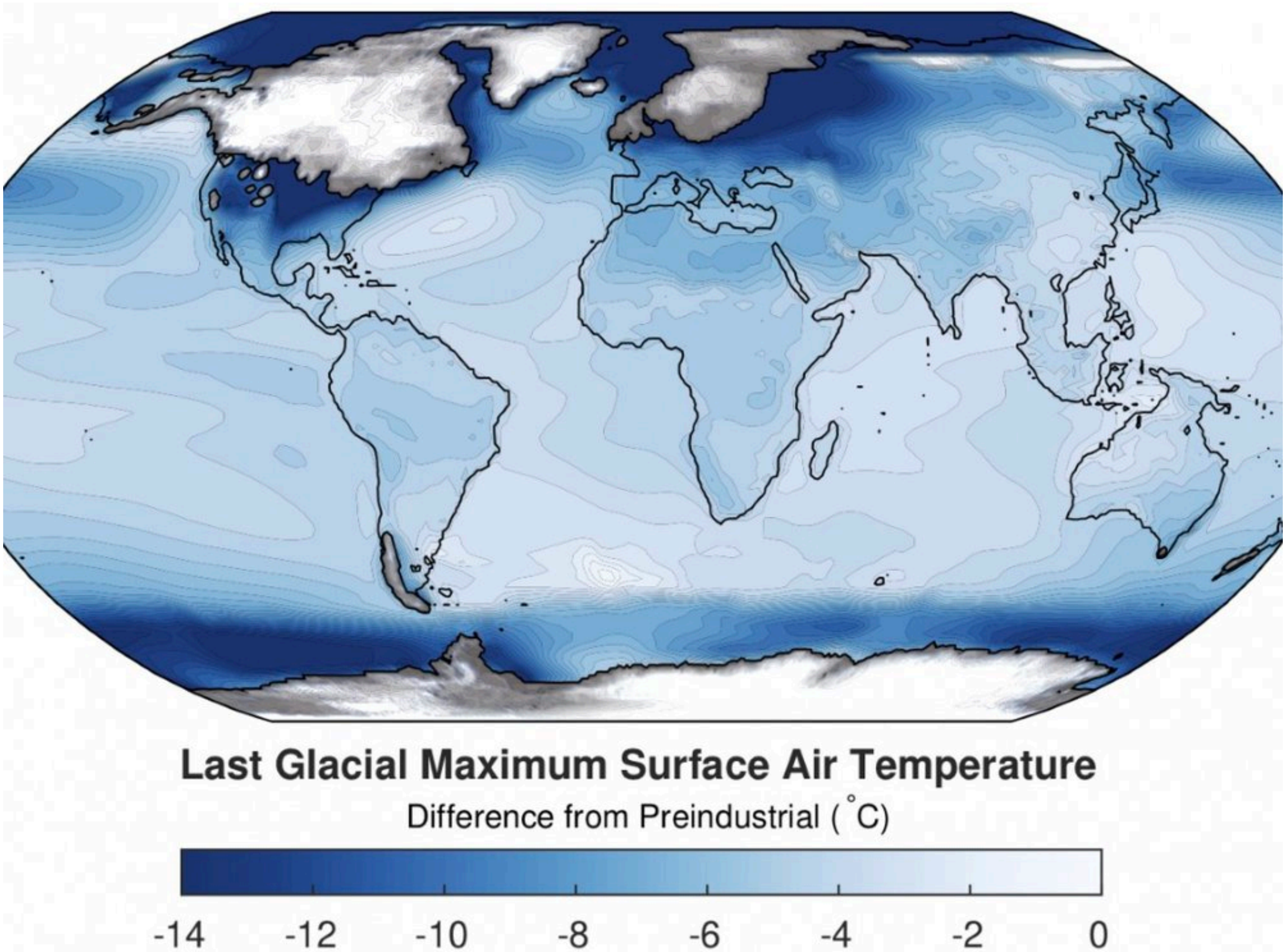


The Ice Age

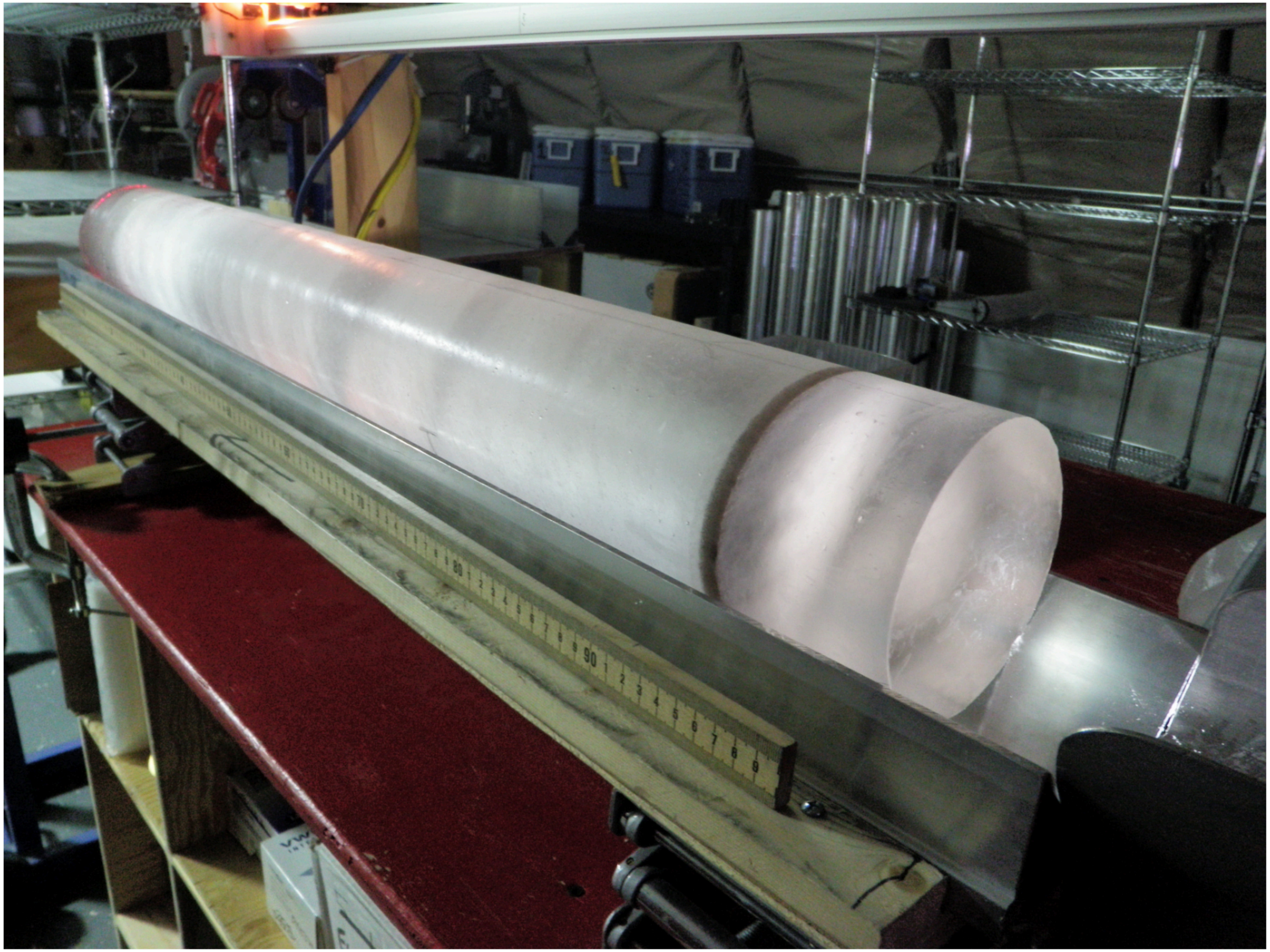


- Ice age had a profound impact on the earth
- Crazy to think humans were alive at this time

The Ice Age


Last Glacial Maximum Surface Air Temperature
Difference from Preindustrial (°C)
-14
-12
-10
-8
-6
-4
-2
0

Ice Core Temps

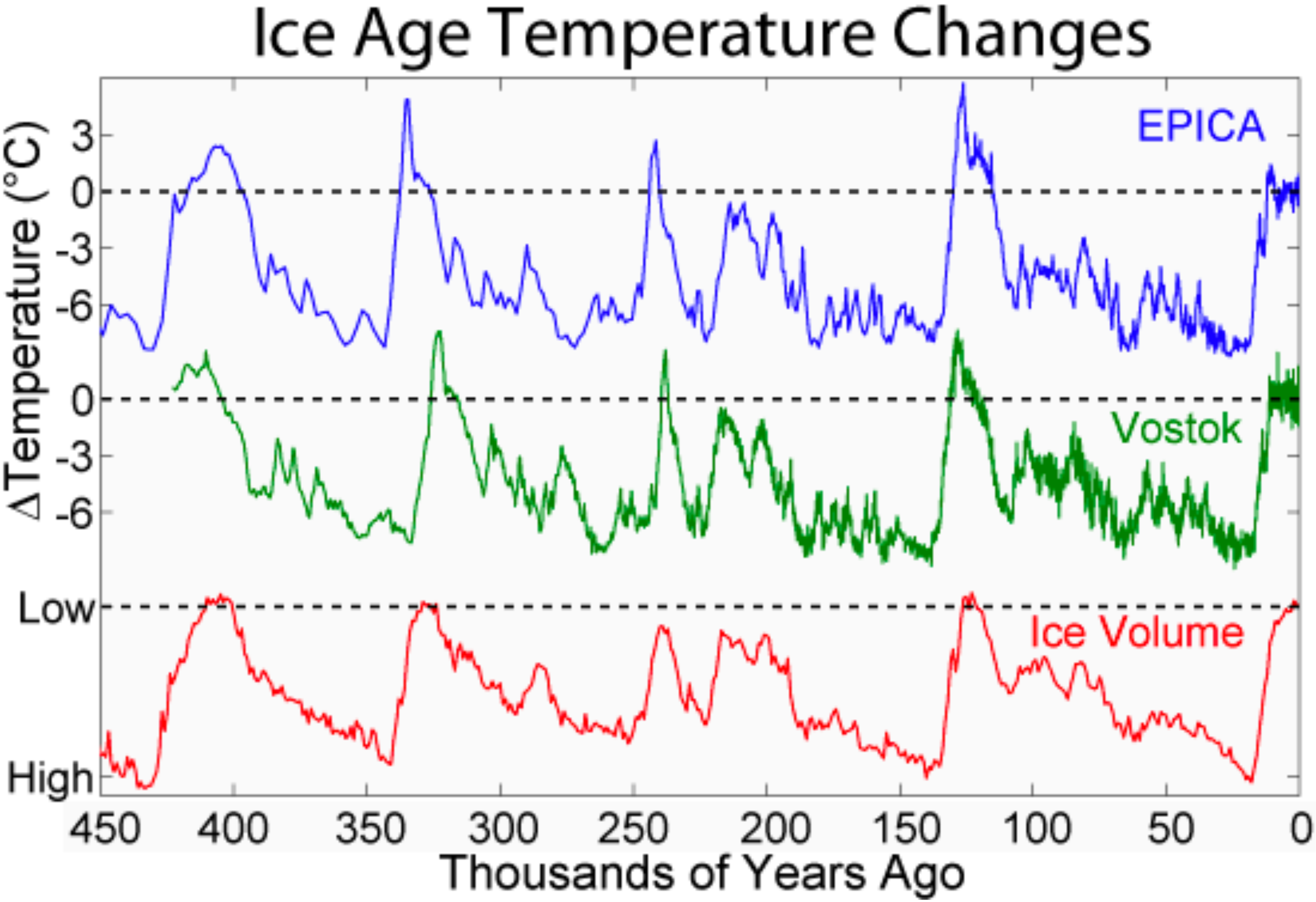


The dark band in this ice core from the West Antarctic Ice Sheet Divide (WAIS Divide) is a layer of volcanic ash that settled on the ice sheet approximately 21,000 years ago. — Credit: Heidi Roop, NSF

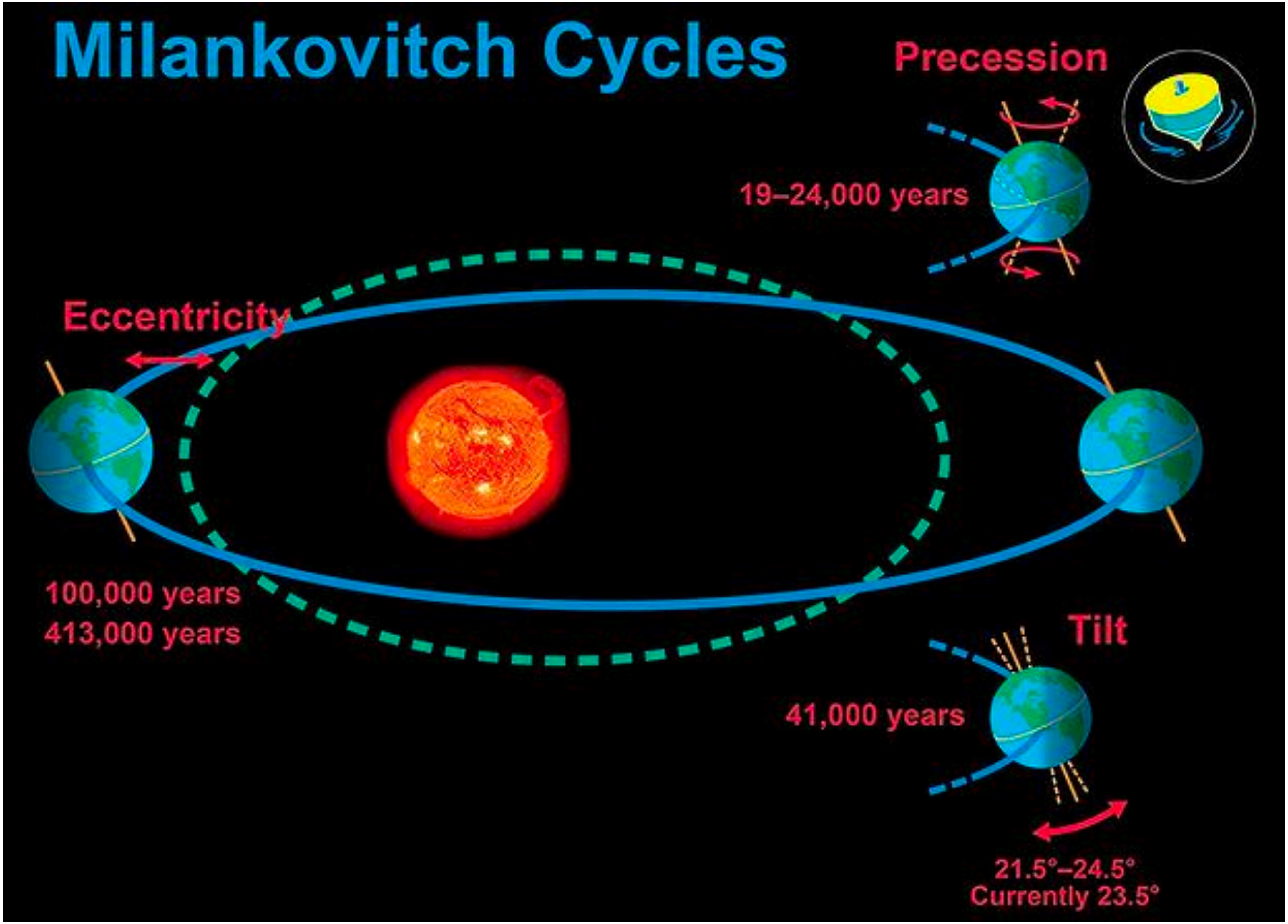
Ice Core

Ice Core recovery has been
A critical element In many
locations on earth

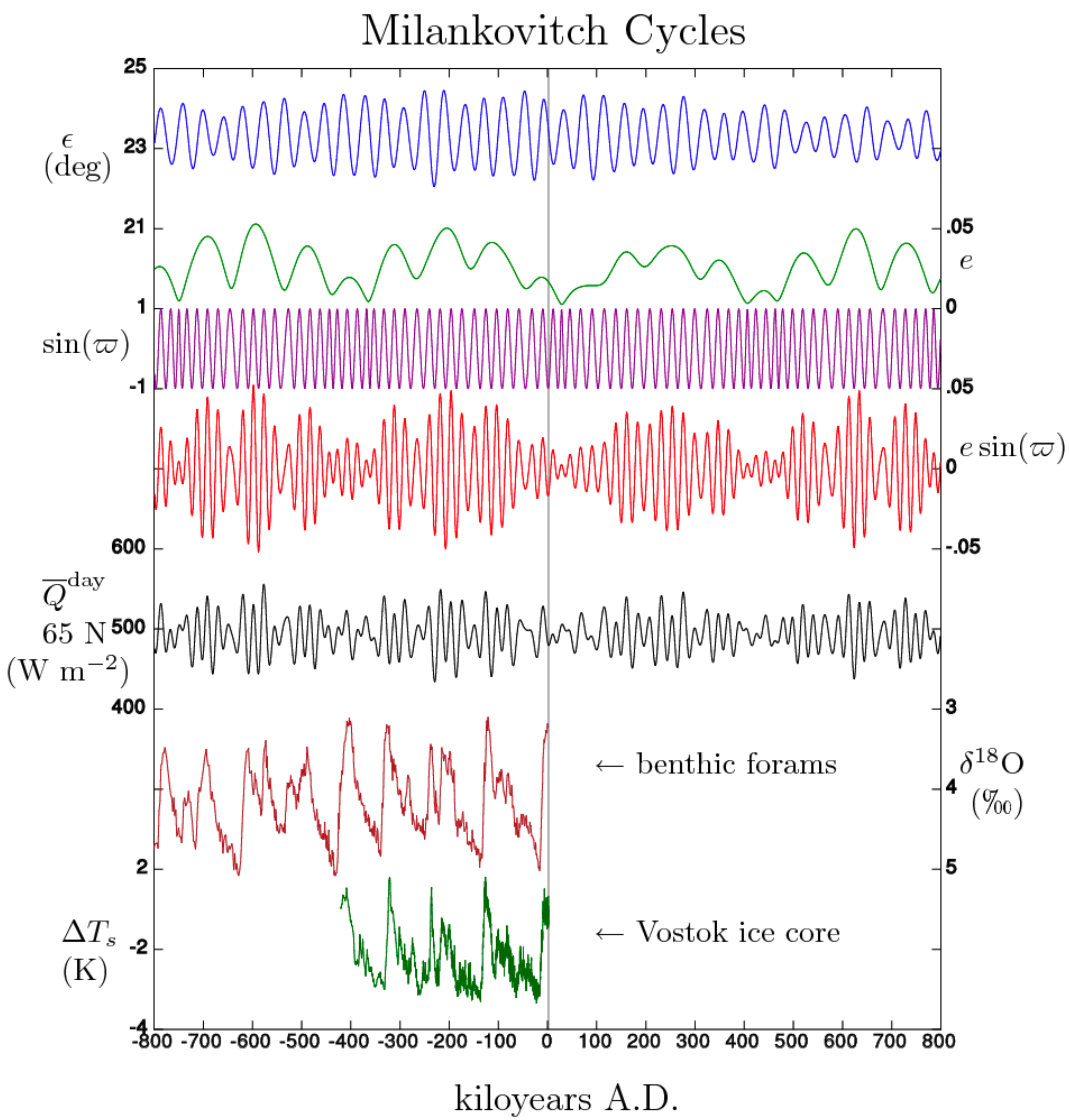
Ice Age over time



Milhanovitch Cycles

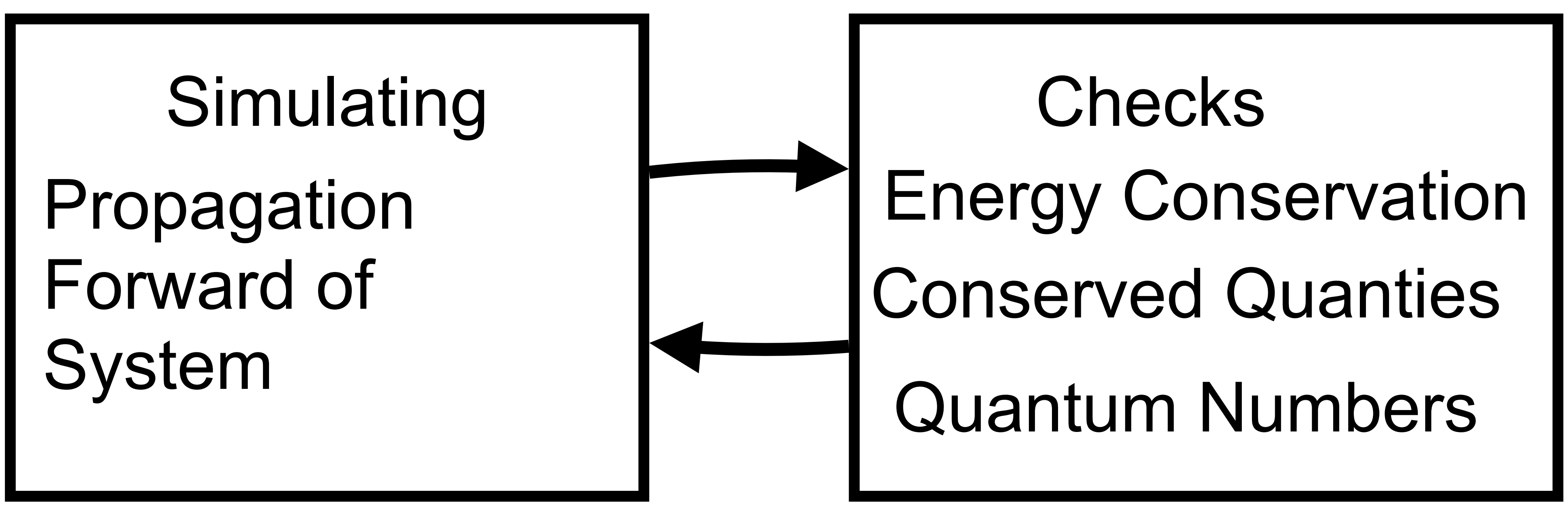


Scale of Eccentricity



Making MC Better

- In this simulation part of this class
    - We have learned that simulations are not accurate
    - There are a few things we can do to make it better
        - Key is to have a notion of when we are going wrong



Correcting

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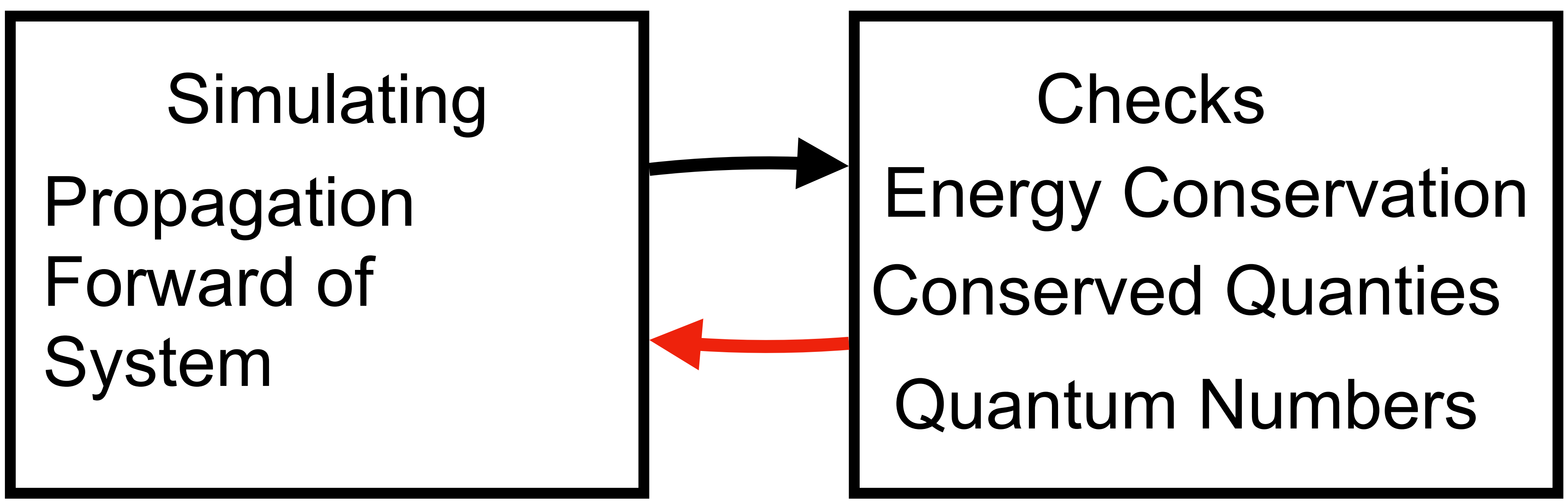
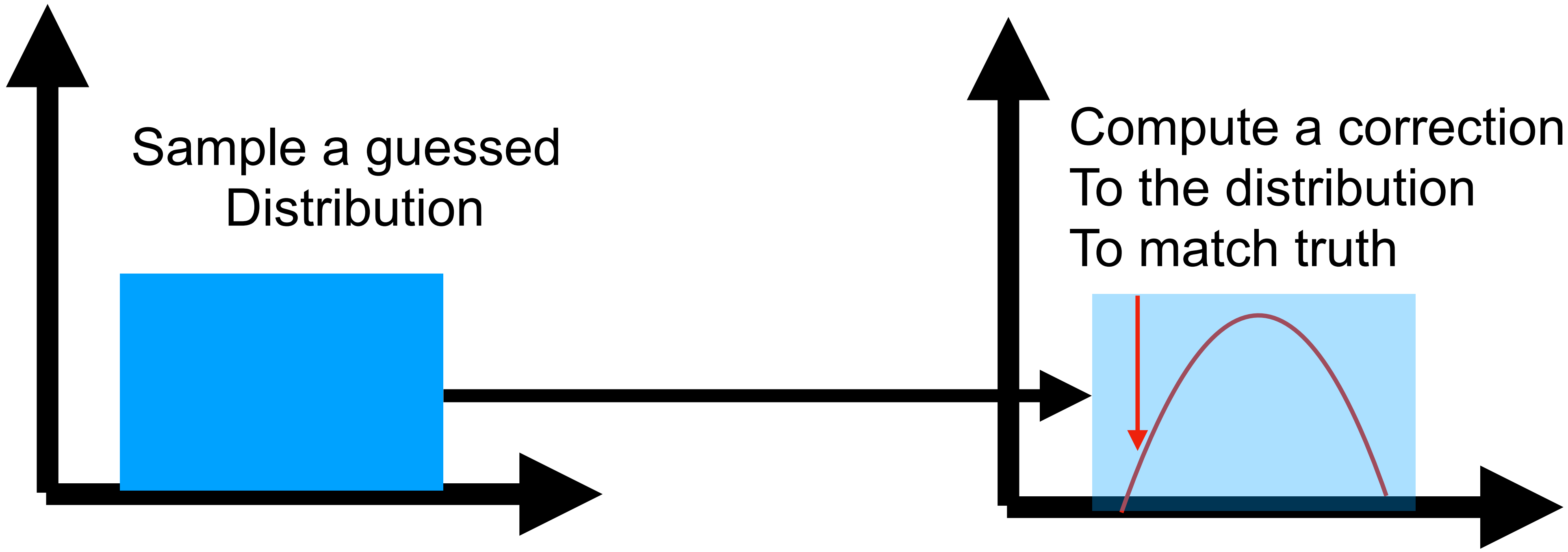
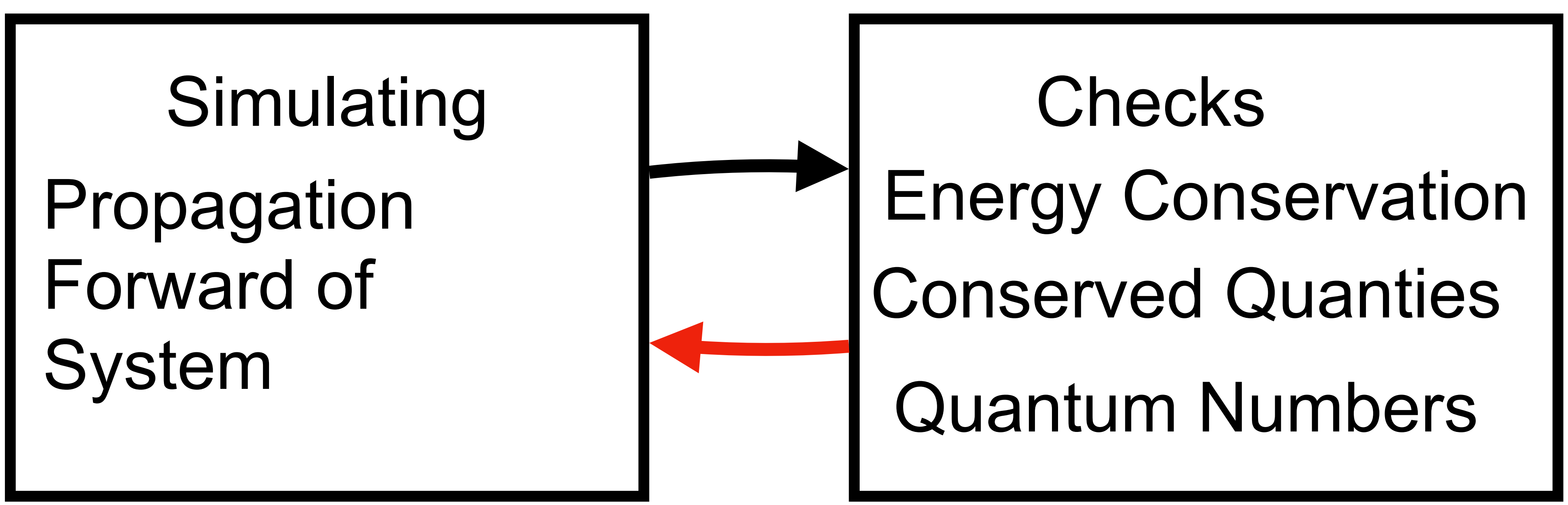
    - Key is to have a notion of when we are going wrong



Correct Our Simulation Through a Probabilistic Rescaling

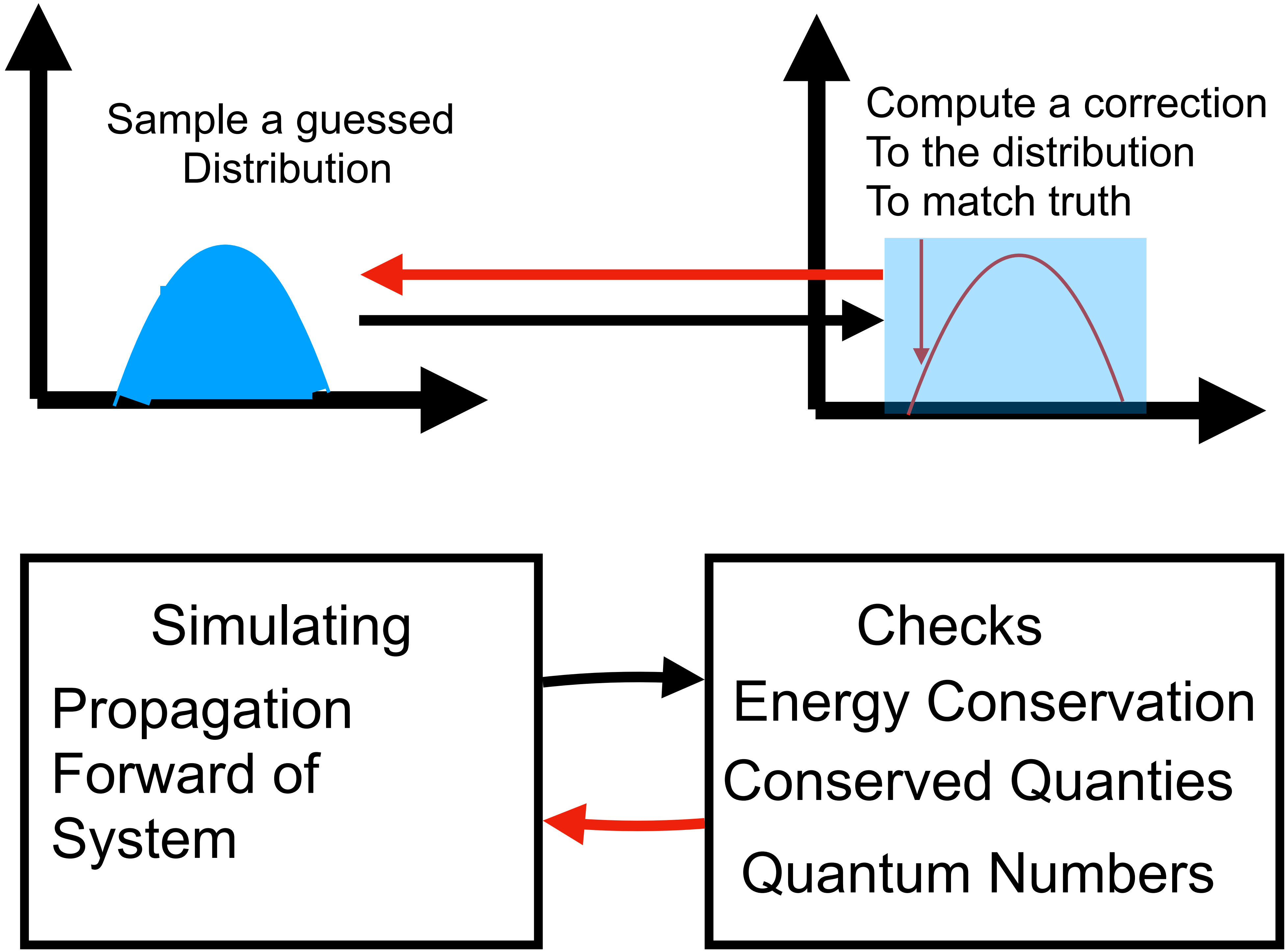
Markov Chain MC





Correct Our Simulation Through a Probabilistic Rescaling

Markov Chain MC



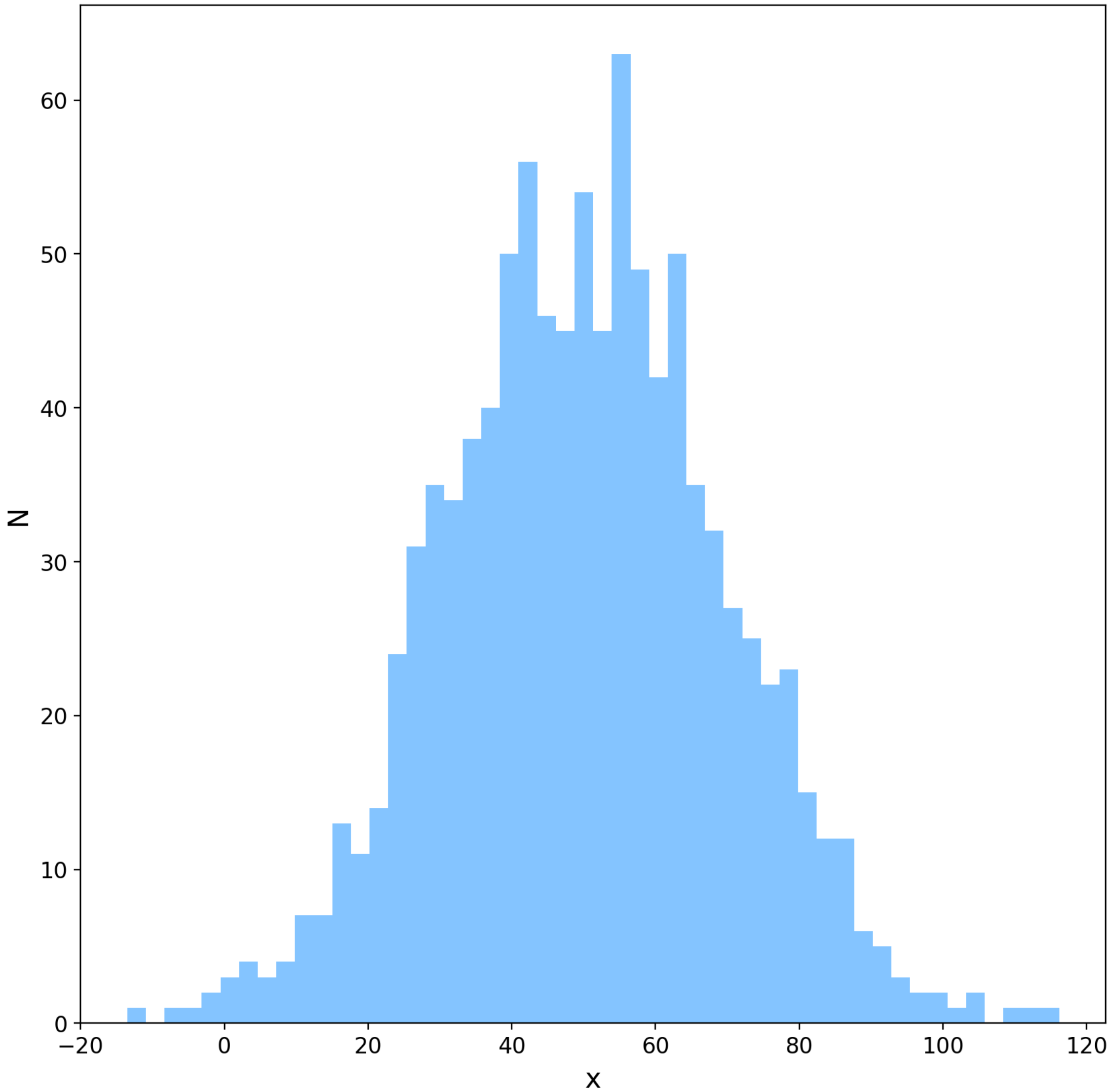
Correct Our Simulation Through a Probabilistic Rescaling

Fitting a Guassian

- Strategy to randomly sample mean(μ) and sigma σ

  - Accept the values for μ, σ if probability is higher

  - Keep accepting/rejecting until we hit equilibrium



Log(Probability)

$$\log(\mathcal{L}) = \sum_i \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(\mu - x_i)^2}{\sigma^2}}\right)$$

$$= \sum_i \left(\frac{x_i - \mu}{\sigma}\right)^2 - \frac{1}{2}\log\left(2\pi\sigma^2\right)$$

Accepted μ, σ yield the best fits

Visualizing in Bayes

Posterior probability of the model in light of the data

Likelihood function of the data given the model

Prior probability of the model

$$\boxed{P(\text{model}|\text{data})} = \frac{\boxed{P(\text{data}|\text{model})}\boxed{P(\text{model})}}{P(\text{data})}$$

Sampled Distribution
Aka Proposal

Equilibrated Best Fit

Probability Driving
Decision

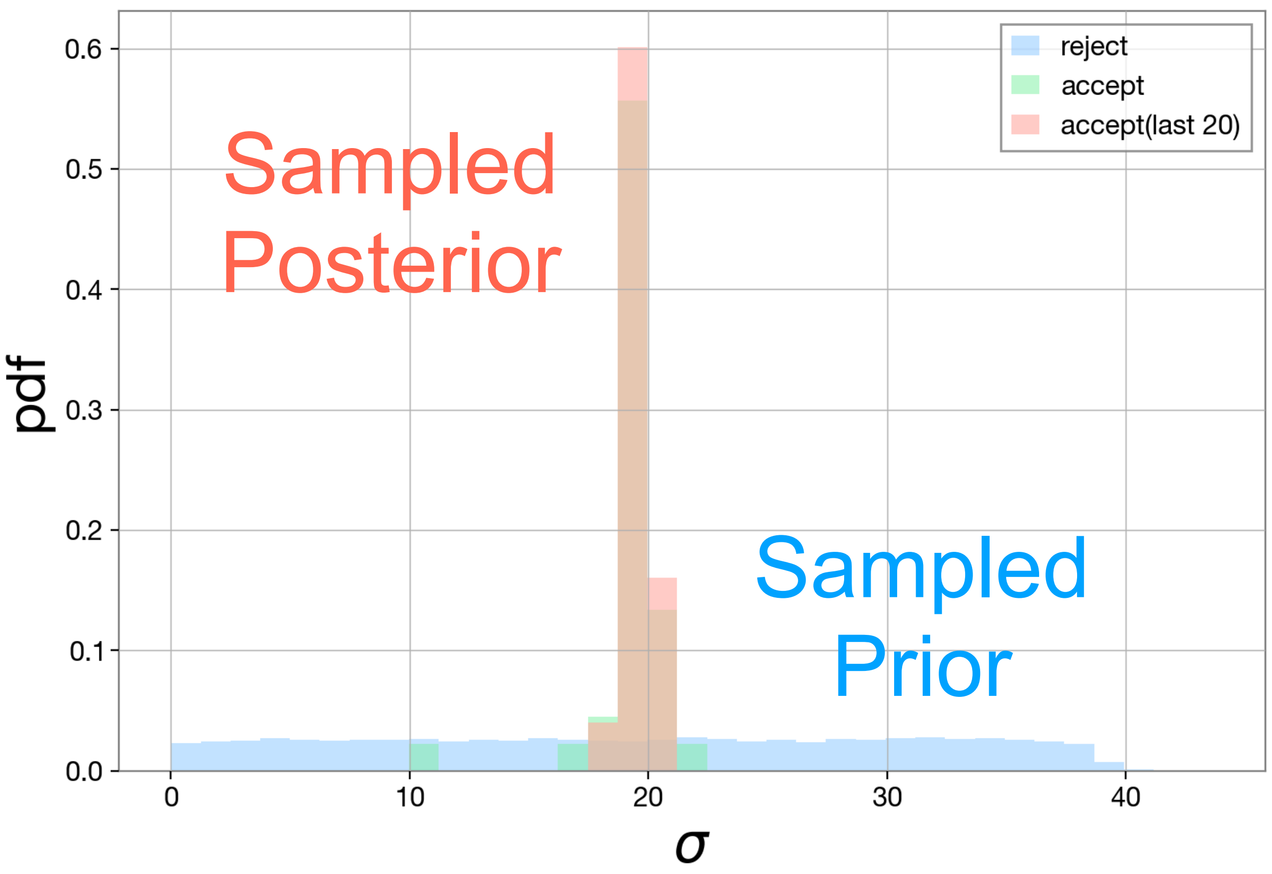
Evidence [can typically be absorbed into the normalization of the posterior]

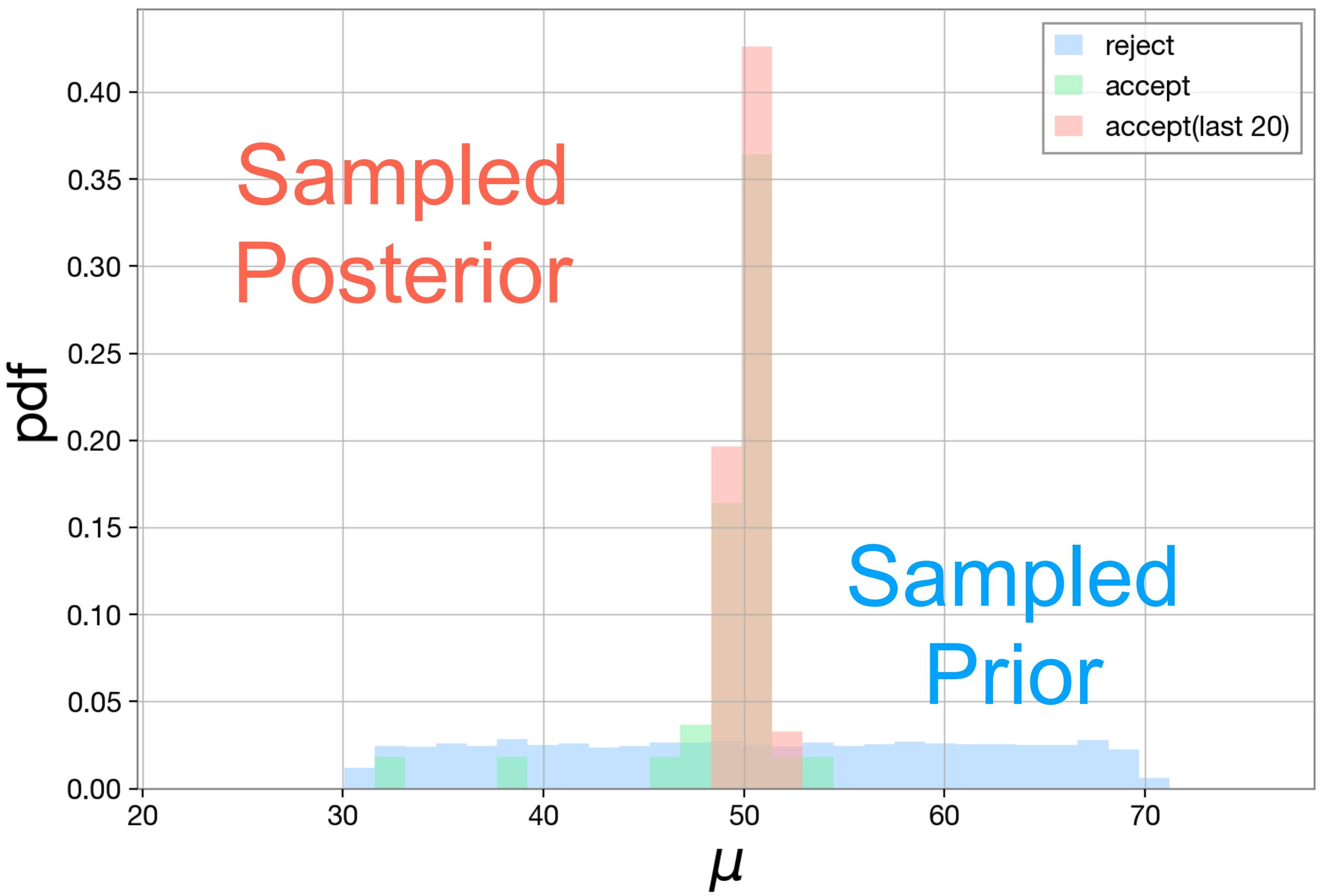
The Likelihood reweights the Prior to the Posterior

Metropolis-Hastings

- Step 0: Randomly sample a parameter $\boldsymbol{x_1}$
- Step 1: Sample a new parameter $\mathbf{x_2}$
  - Use a chosen "Proposal Function" for sampling
  - Compute the probability of stepping $\mathbf{x_2}$ to stepping $\mathbf{x_1}$
- Step 2: Sample a flat distribution from 0 to 1 ($\mathbf{s_2}$)
  - Accept $\mathbf{x_2}$ if $s_2 < \dfrac{p(x_2)}{p(x_1)}$
- Step 3 : Go back to step 1

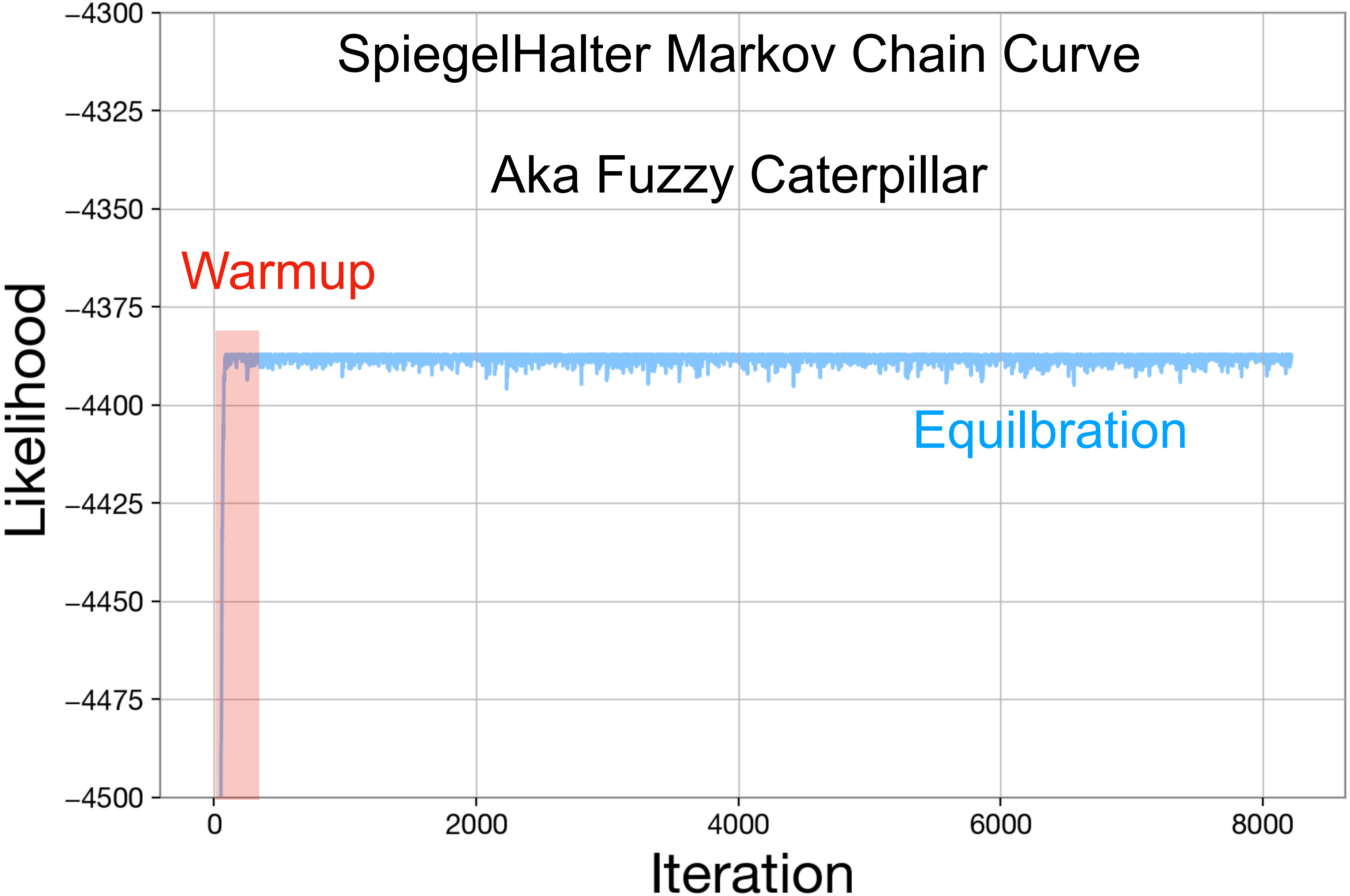
Best Fit Paramters





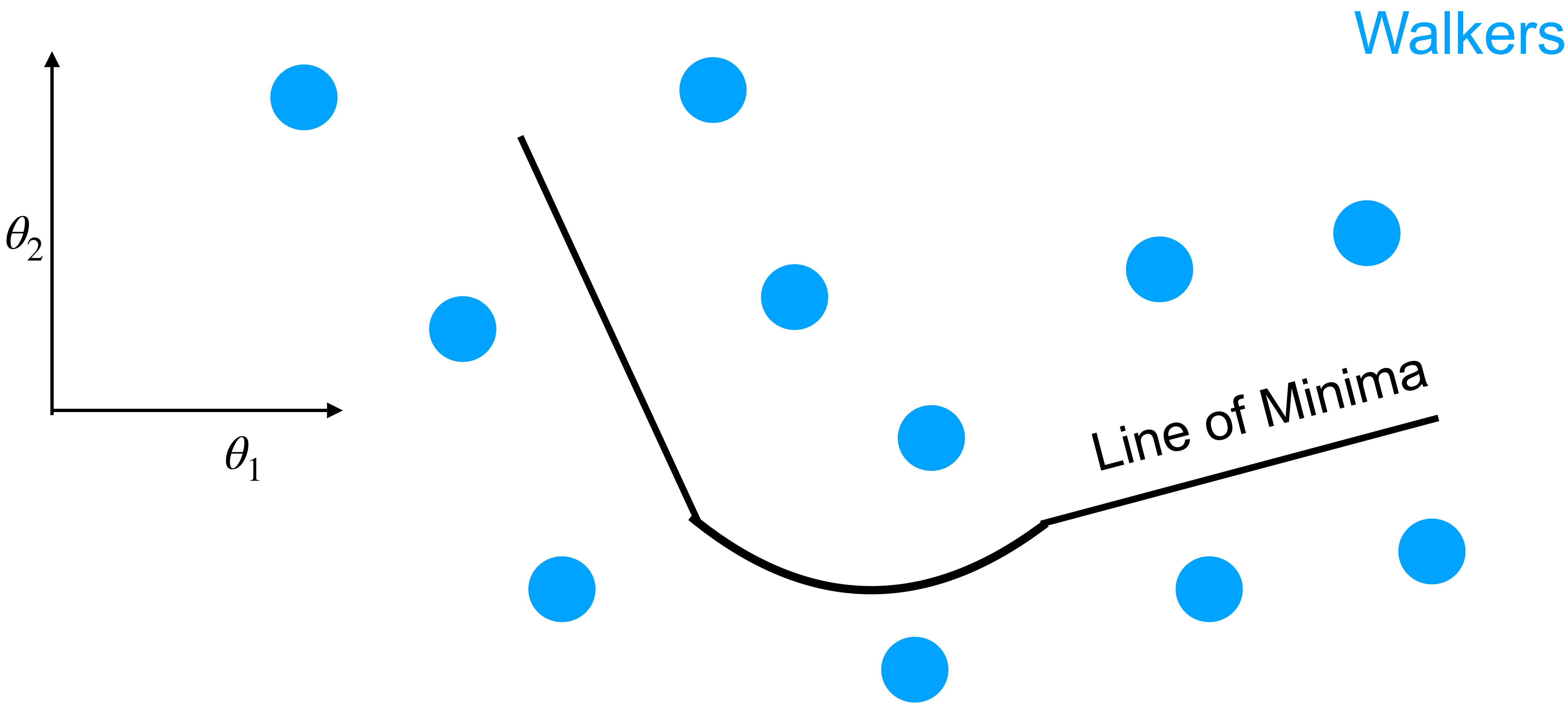
- This is where I start to hint that there are limitations here
- What we are doing is running a check
  - We are not taking a derivative (No gradients or Hessians)

Best Fit Paramters



Speeding up MCMC

- We can consider having many walkers probe our space
  - Many walkers at the same time speed up convergence



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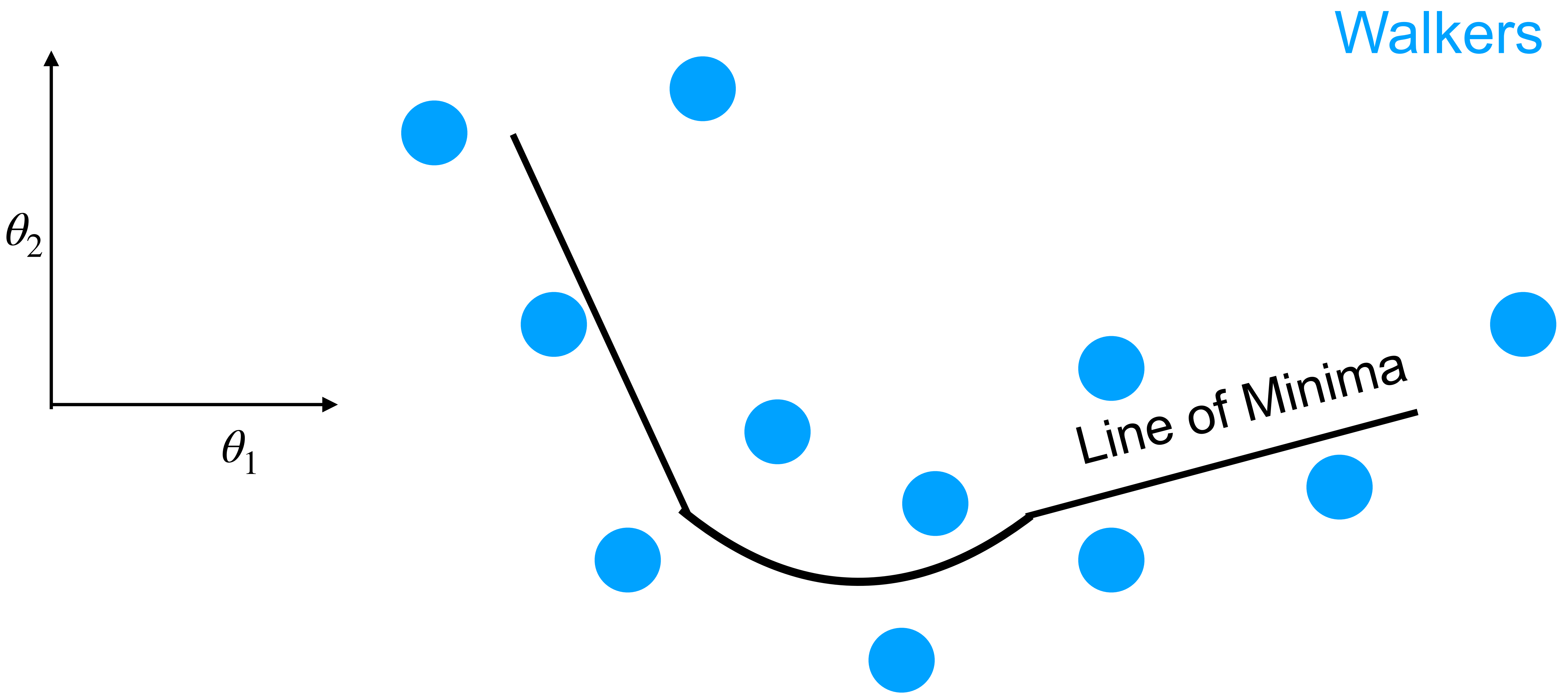

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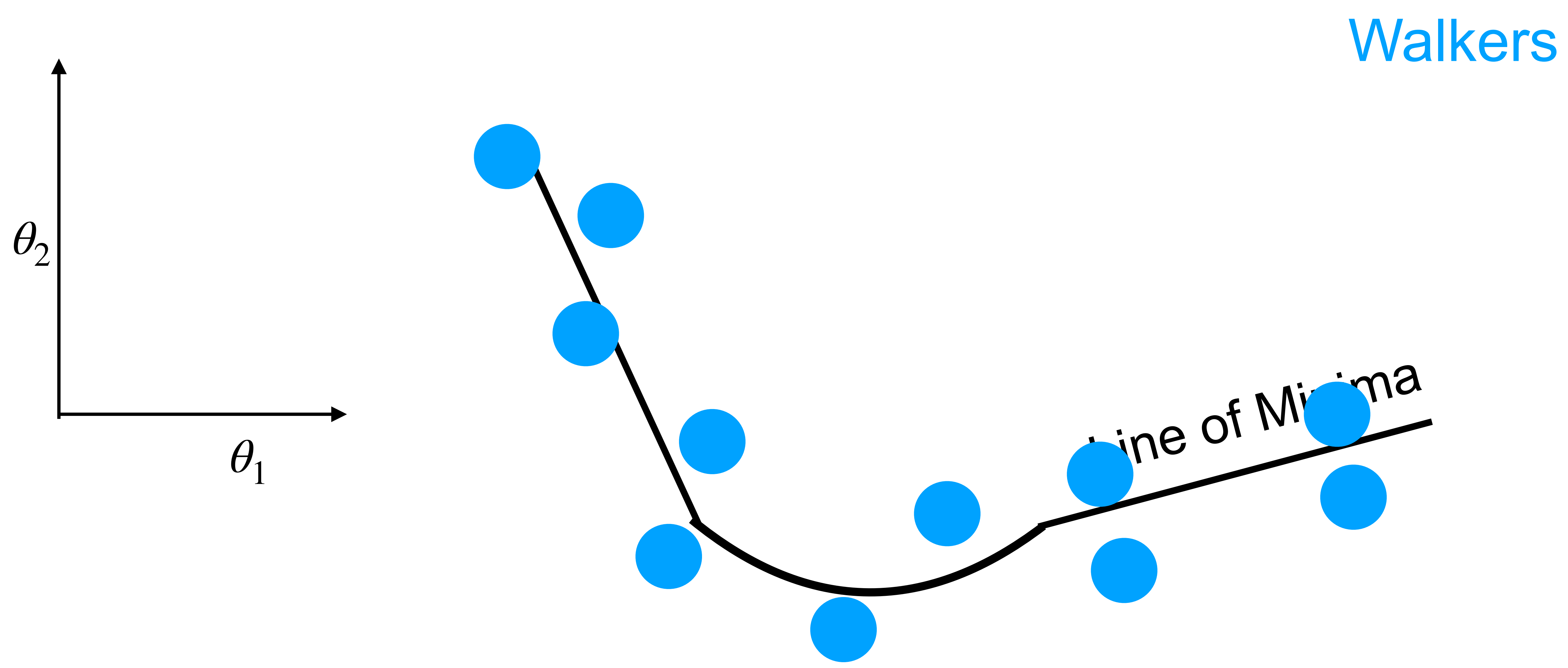
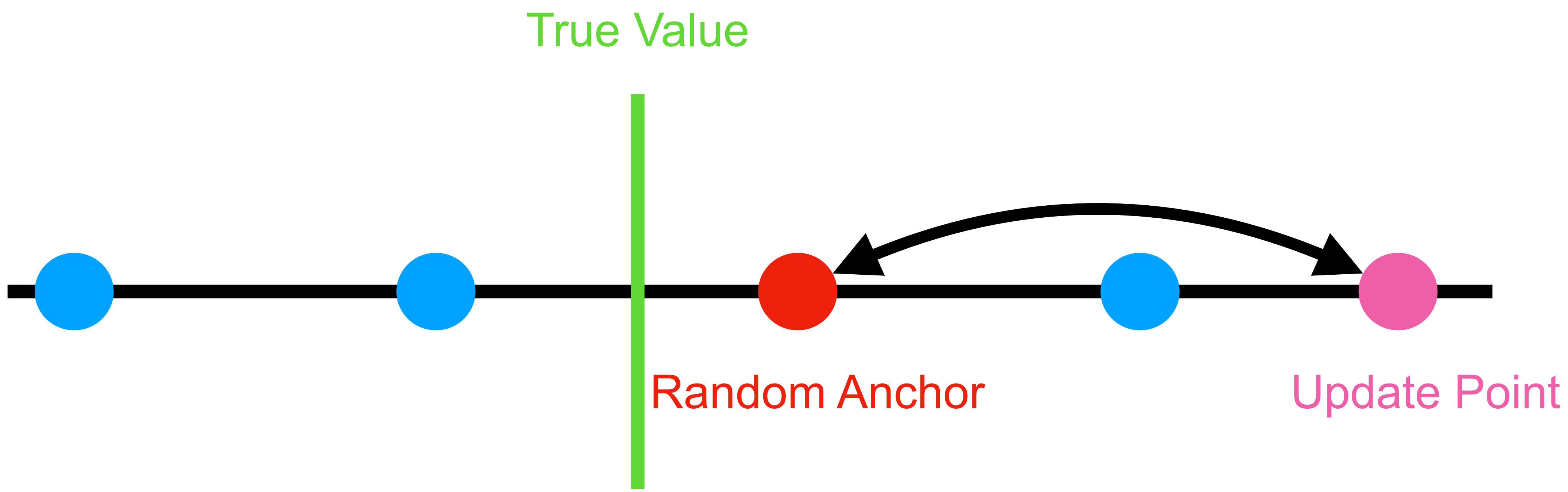


Example Fit



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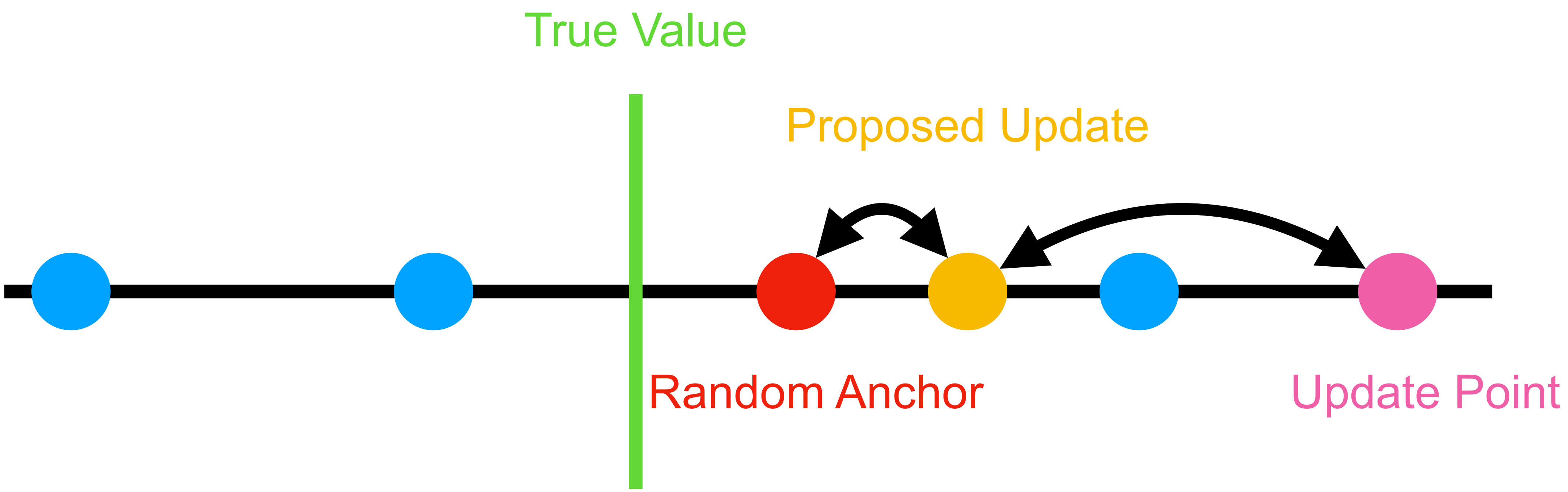

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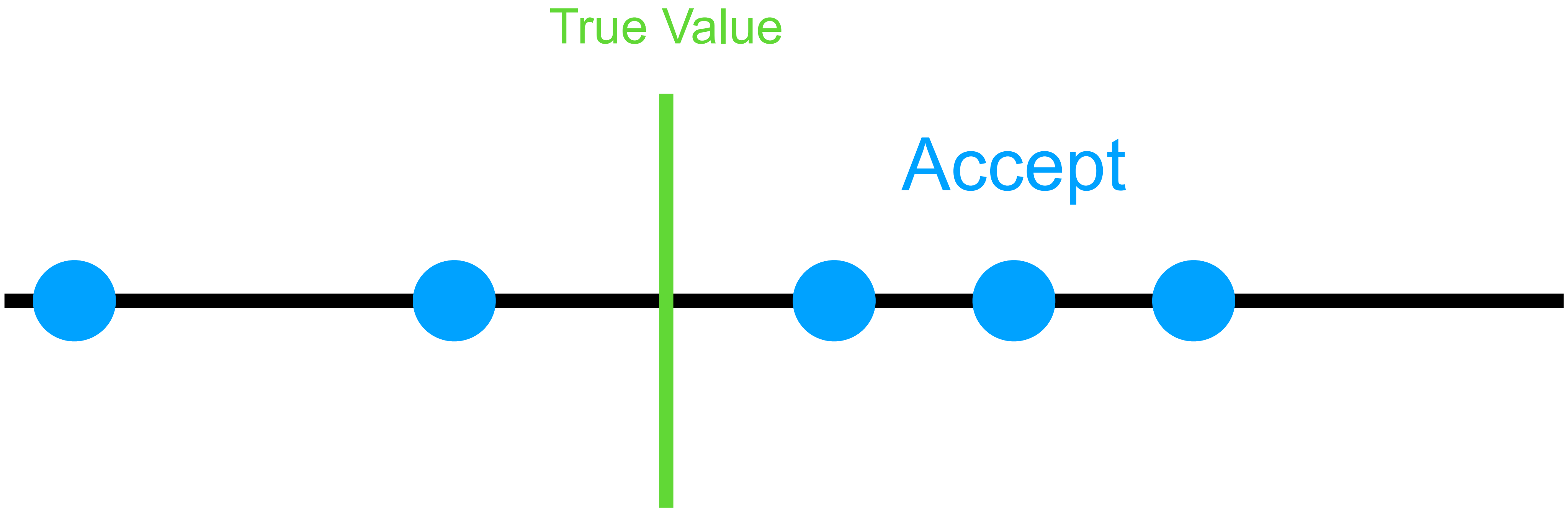
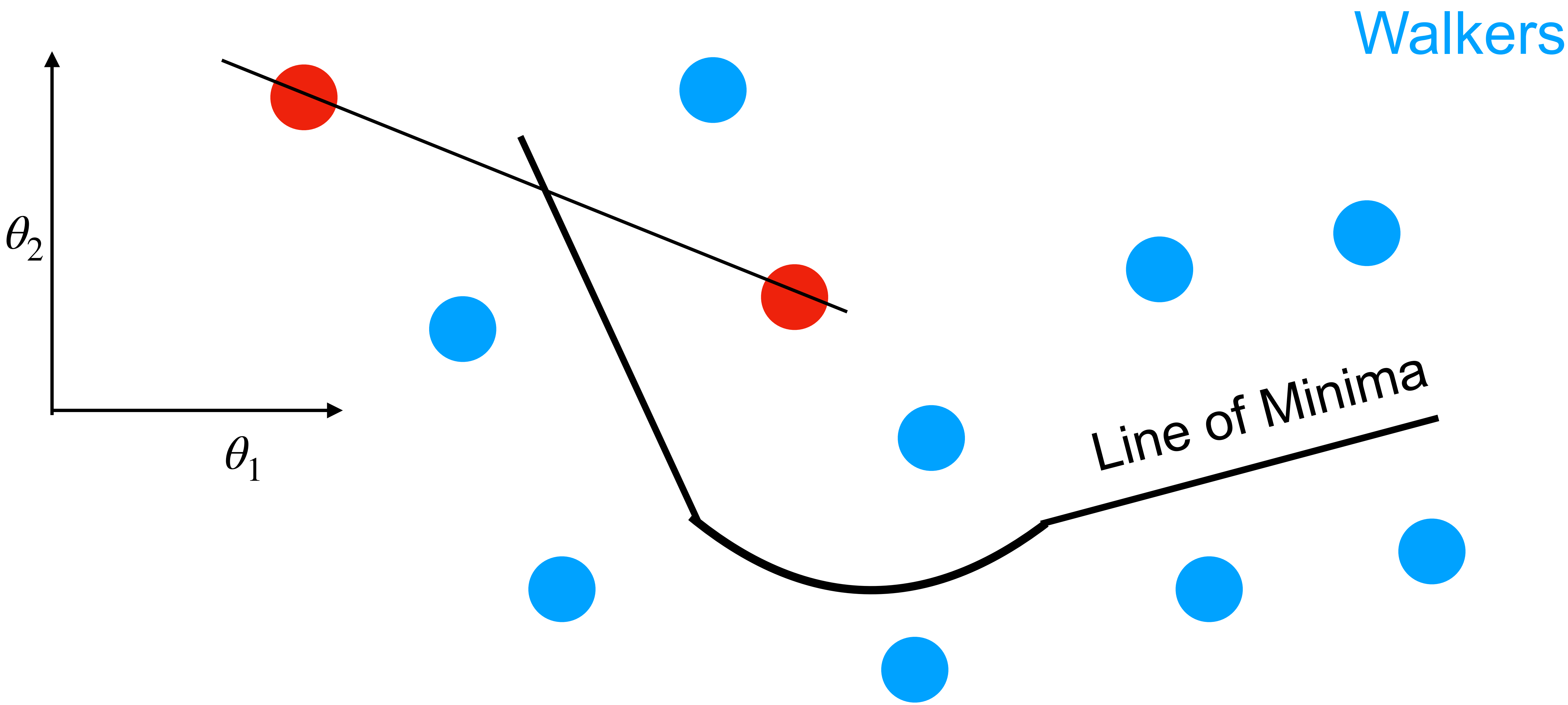


Updating w/Random Points

- We randomly choose a pair of points
  - Move one of the points along the line between them



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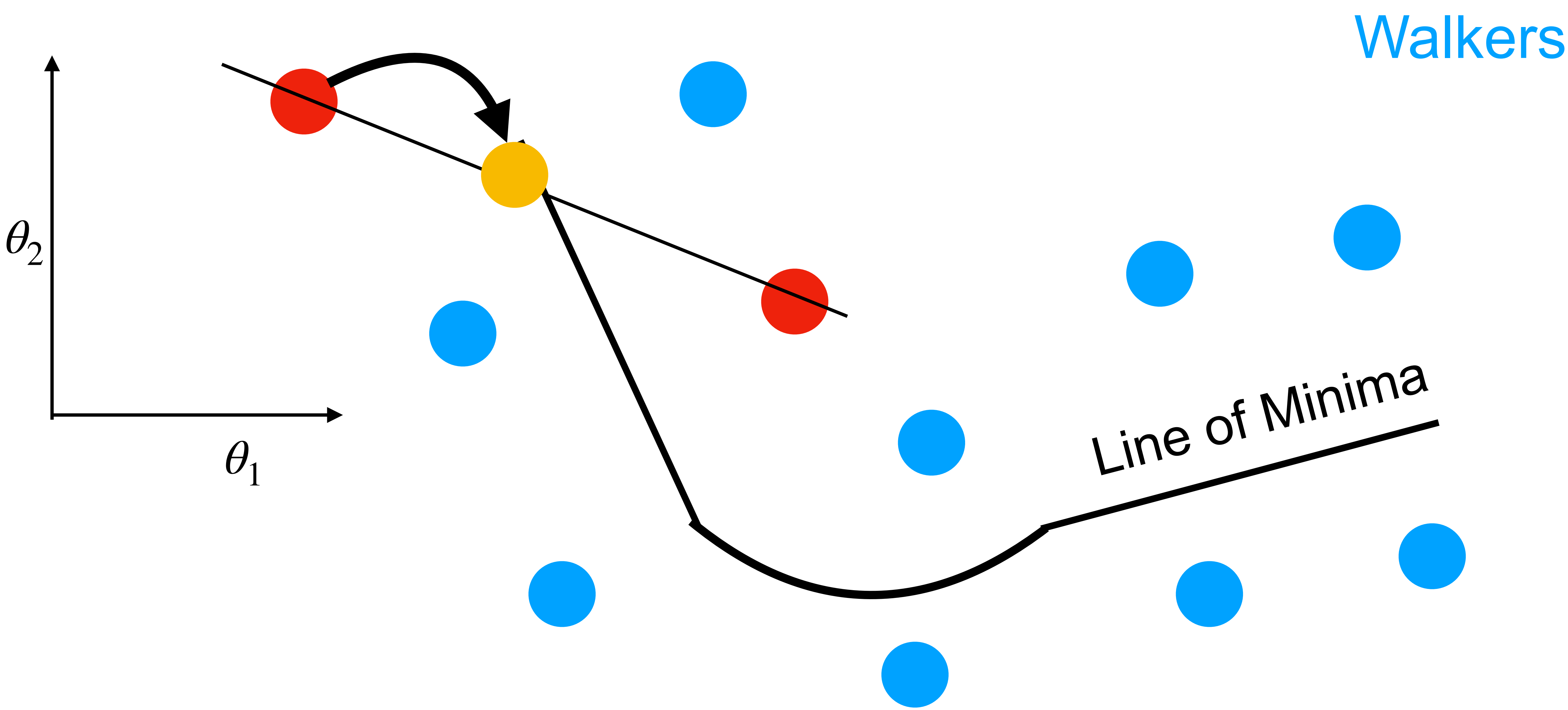

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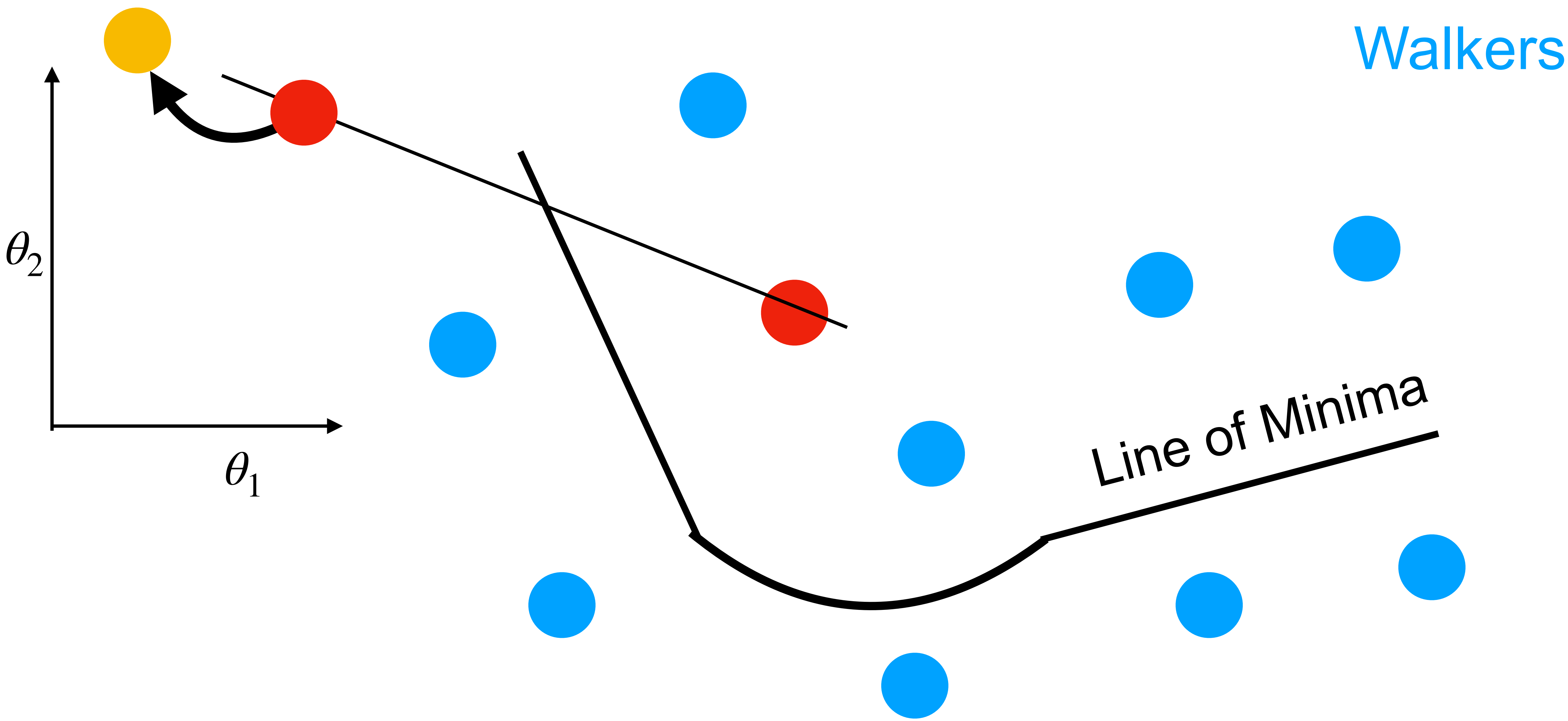

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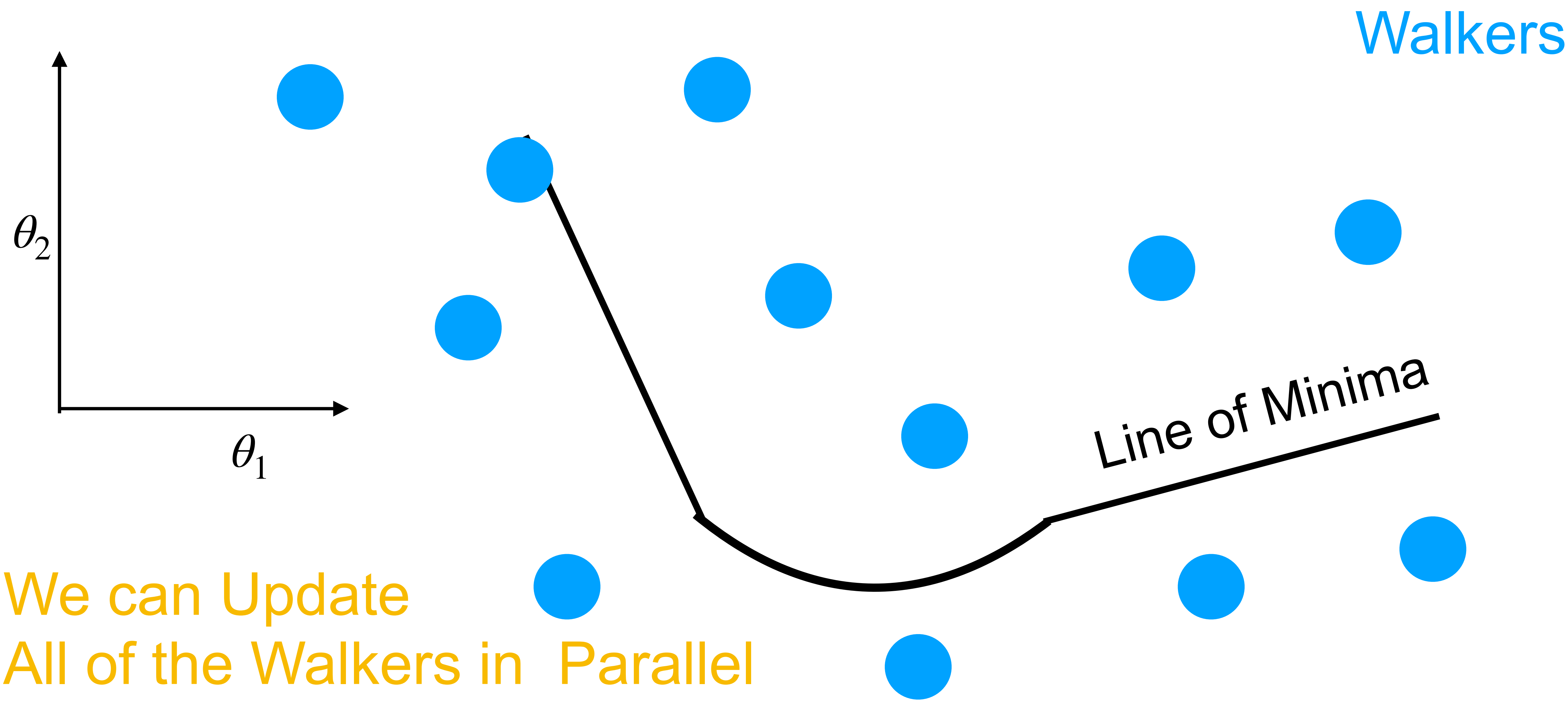

We can Update
All of the Walkers in Parallel

Speeding up MCMC

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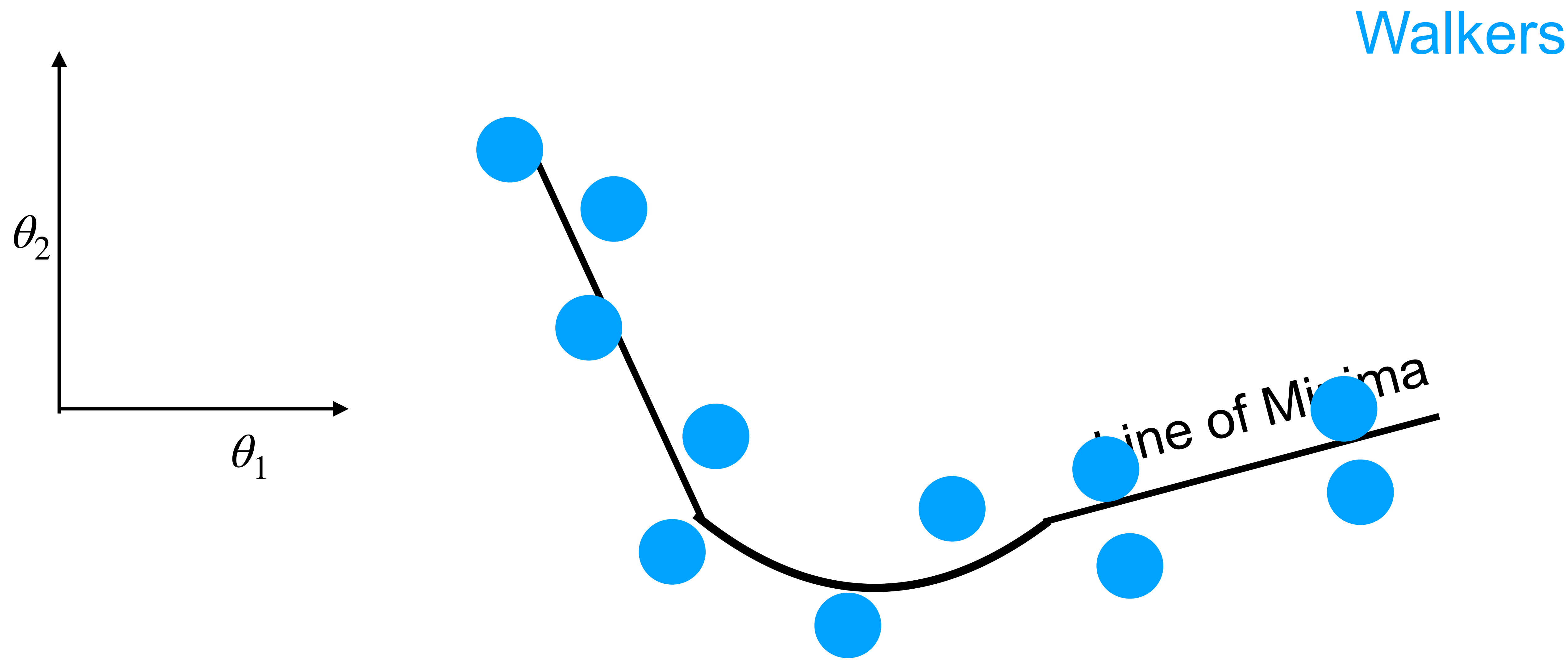

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Equilibrated Best Fit

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Aka Proposal

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Quantum Monte Carlo

- Can use the same MCMC to populate a wave function
  - We can then scan paramaters to solve Shroedinger's Eq

$$\boxed{\psi(\vec{r}\,|\,\vec{\theta}) = Ae^{-r/\theta_0}}$$

Guess a Form for the wavefunction

$$\boxed{p(\vec{r}\,|\,\vec{\theta}) = \frac{\psi^*(\vec{r}\,|\,\vec{\theta})\psi(\vec{r}\,|\,\vec{\theta})}{\langle\psi\,|\,\psi\rangle}}$$

We can define probability from wavefunction

$$\boxed{w_{i+1} = \frac{p(\overrightarrow{r_{i+1}}\,|\,\vec{\theta})}{p(\overrightarrow{r_i}\,|\,\vec{\theta})} = \frac{\psi^*(\vec{r}_{i+1})\psi(\vec{r}_{i+1})}{\psi^*(\vec{r}_i)\psi(\vec{r}_i)}}$$

Our proposal Doesn't need integral Aka $\langle\psi\,|\,\psi\rangle$

Multiple Walkers Populate

- The key is to MCMC evolve the wave function many times
  - We can use the aggregate Particles solve QM stuff

$$\sum_j \psi_j(\vec{r}\,|\,\vec{\theta}) = Ae^{-r/\theta_0}$$

Guess a Form for the wavefunction

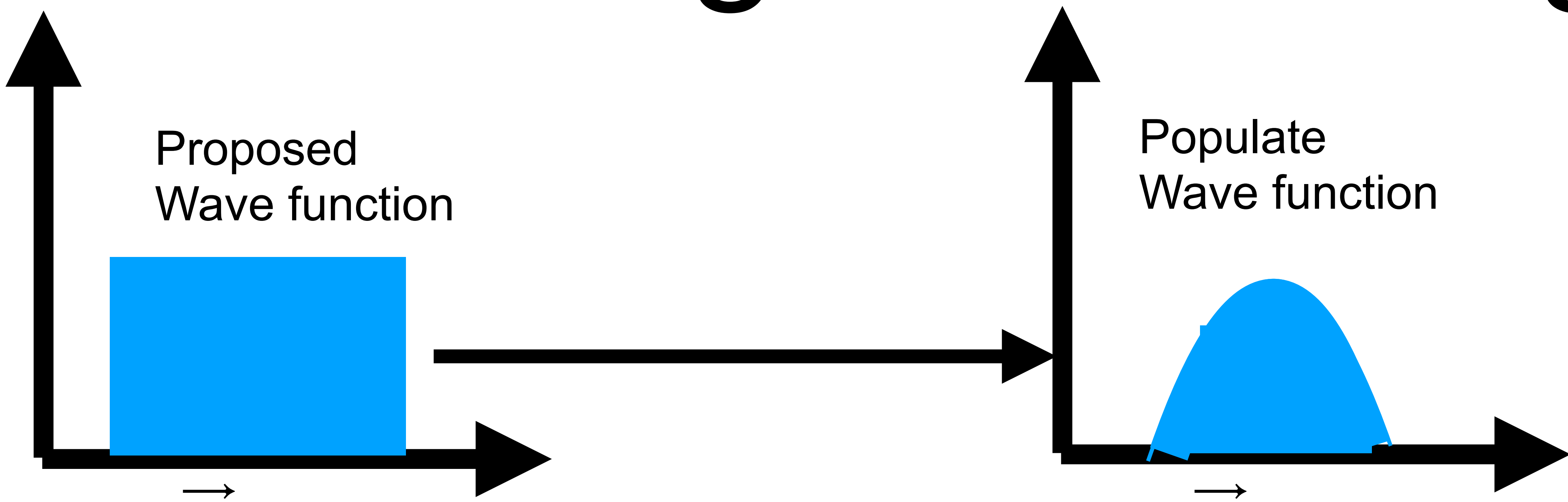
$$\sum_j p_j(\vec{r}\,|\,\vec{\theta}) = \frac{\psi_j^*(\vec{r}\,|\,\vec{\theta})\psi_j(\vec{r}\,|\,\vec{\theta})}{\langle\psi\,|\,\psi\rangle}$$

We can define probability from wavefunction

$$\sum_j w_{i+1}^j = \frac{p_j(\overrightarrow{r_{i+1}}\,|\,\vec{\theta})}{p_j(\overrightarrow{r_i}\,|\,\vec{\theta})}$$

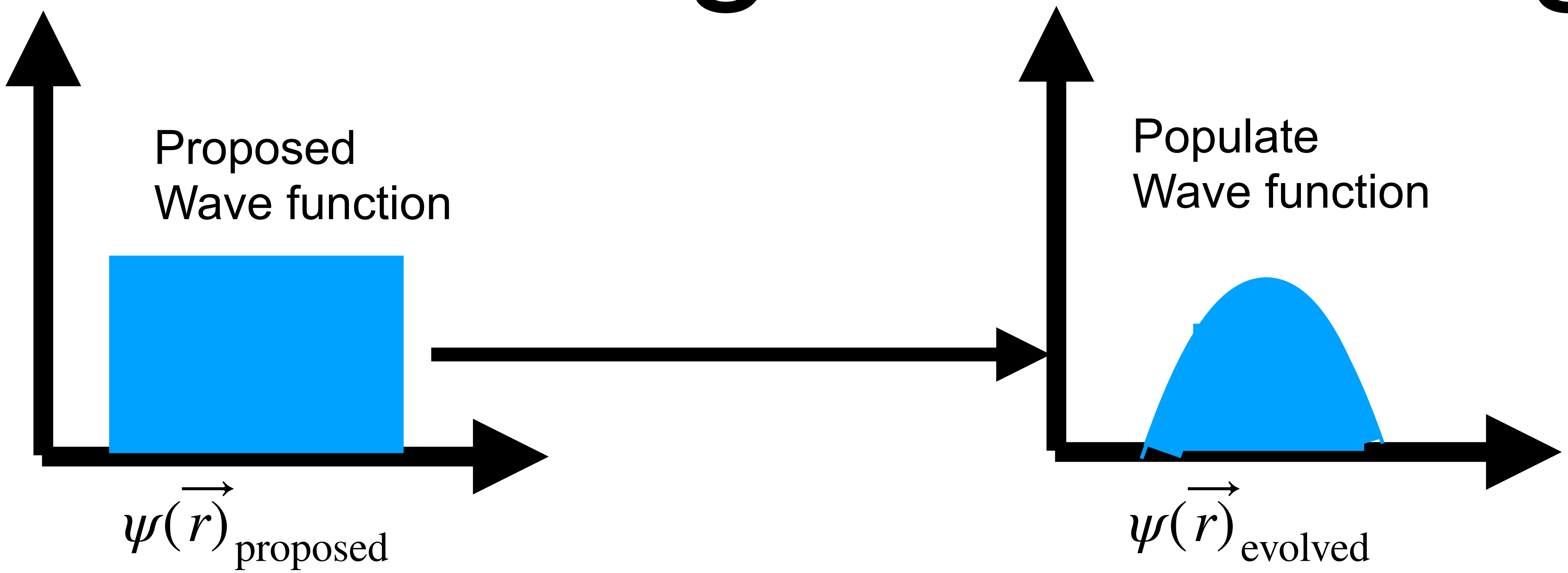
Our proposal Doesn't need $\langle\psi\,|\,\psi\rangle$

Solving Schroedinger



$\psi(\overrightarrow{r})_{\text{proposed}}$ $\psi(\overrightarrow{r})_{\text{evolved}}$

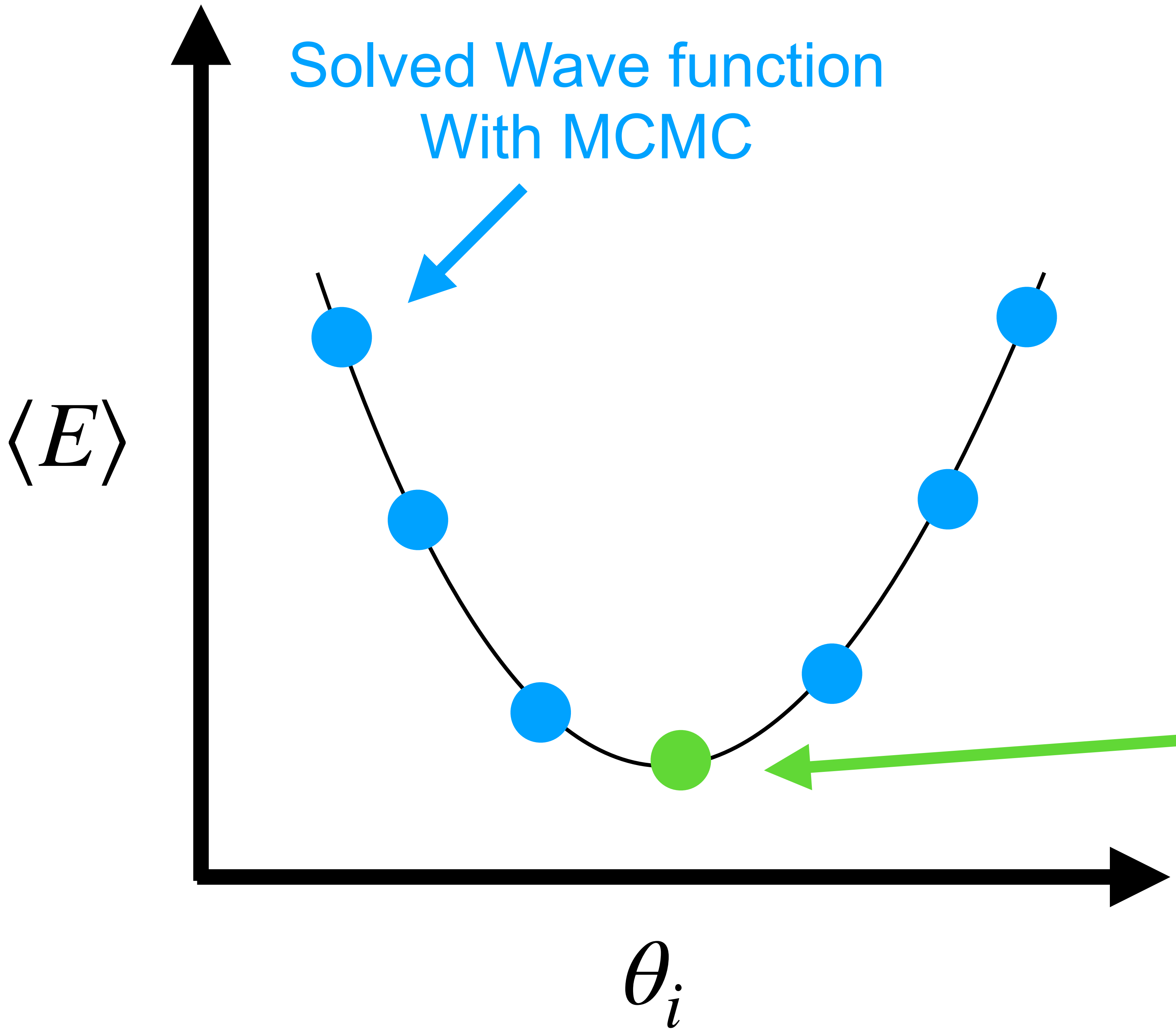
Solving Schroedinger



- Once we have the evolved wave funciton
  - We can compute expectations
  - No need to integrate (Really this is MC integration)

$$\boxed{\langle E\rangle = \sum_j p_j(\vec{r}\,|\,\vec{\theta})E_j(\vec{r}\,|\,\vec{\theta}) = \sum_j \psi_j^*(\vec{r}\,|\,\vec{\theta})\psi_j(\vec{r}\,|\,\vec{\theta})E_j(\vec{r}\,|\,\vec{\theta})}$$

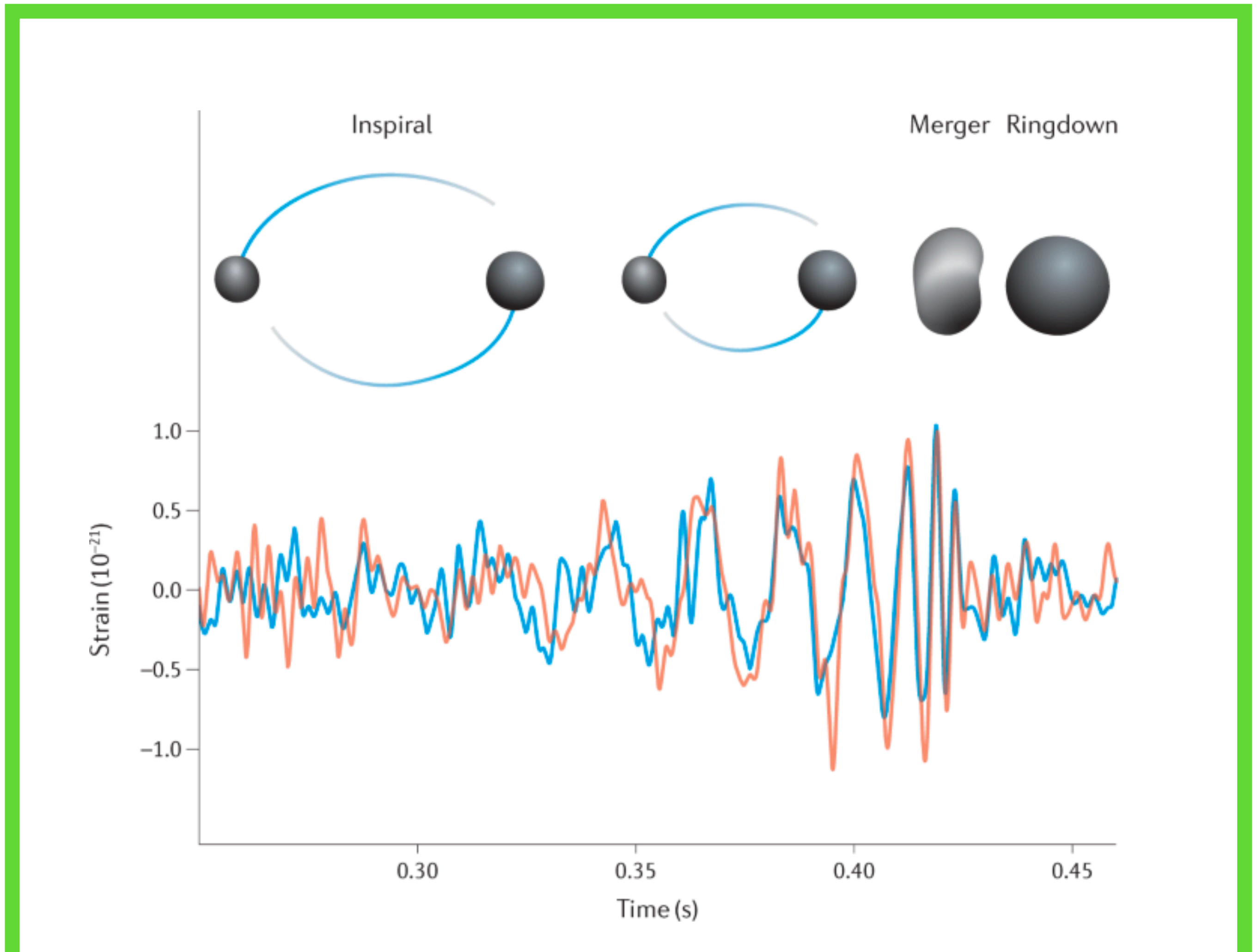
Solving Schroedinger



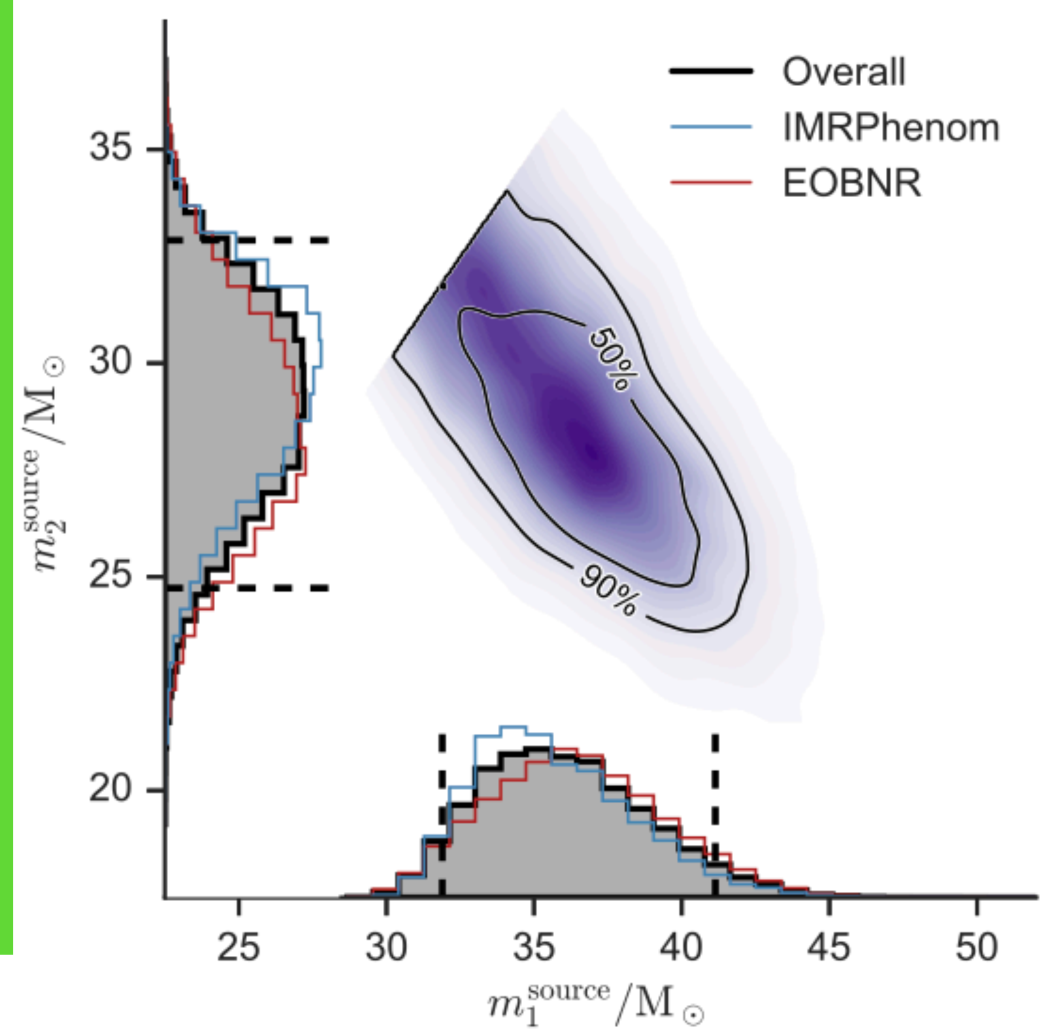
Our goal is to minimize the Energy given a wave functional form

Full Blow MCMC

- Ultimately the big gain from this are complex fits
  - Cases where normal gradient descent breaks down
  - What better case than to go back to LIGO



Full Waveform not differentiable (cannot fit it)



Observations

- There is some elegance to the MCMC approach
  - Builds directly to Bayesian fitting
  - MC allows us to explore parameters and correlations

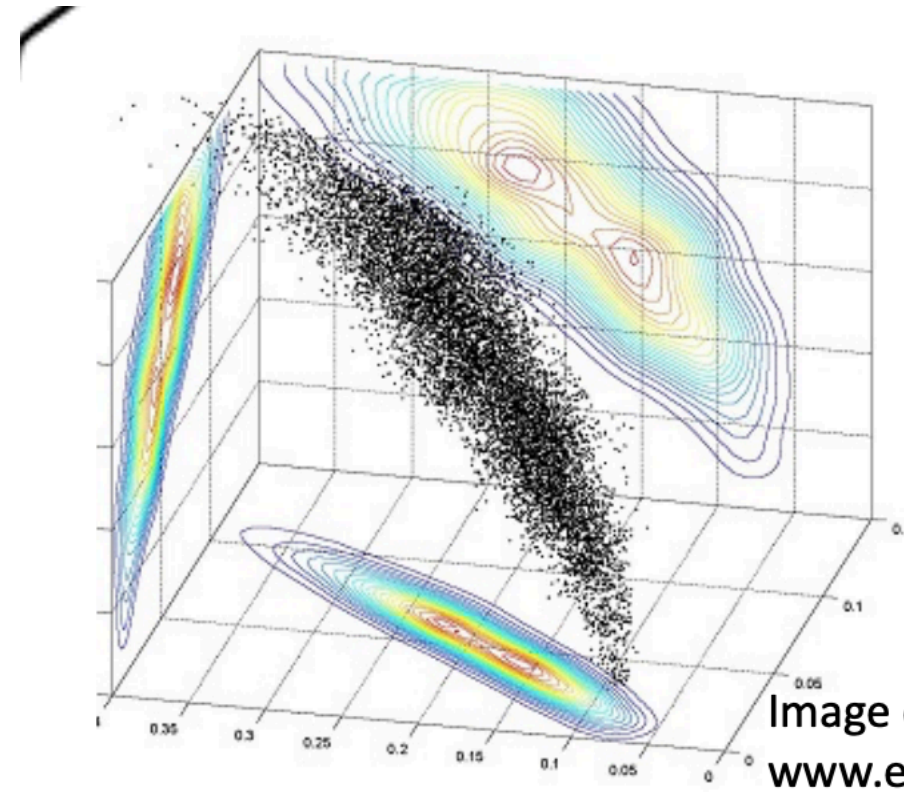


Image credit: www.essenceps.com

- However, it is really slow
  - Migration towards differentiable loss is becoming popular
  - Training an NN to replace part of sampling helps with this
  - Project 3 starts to illustrate modern approach to this all