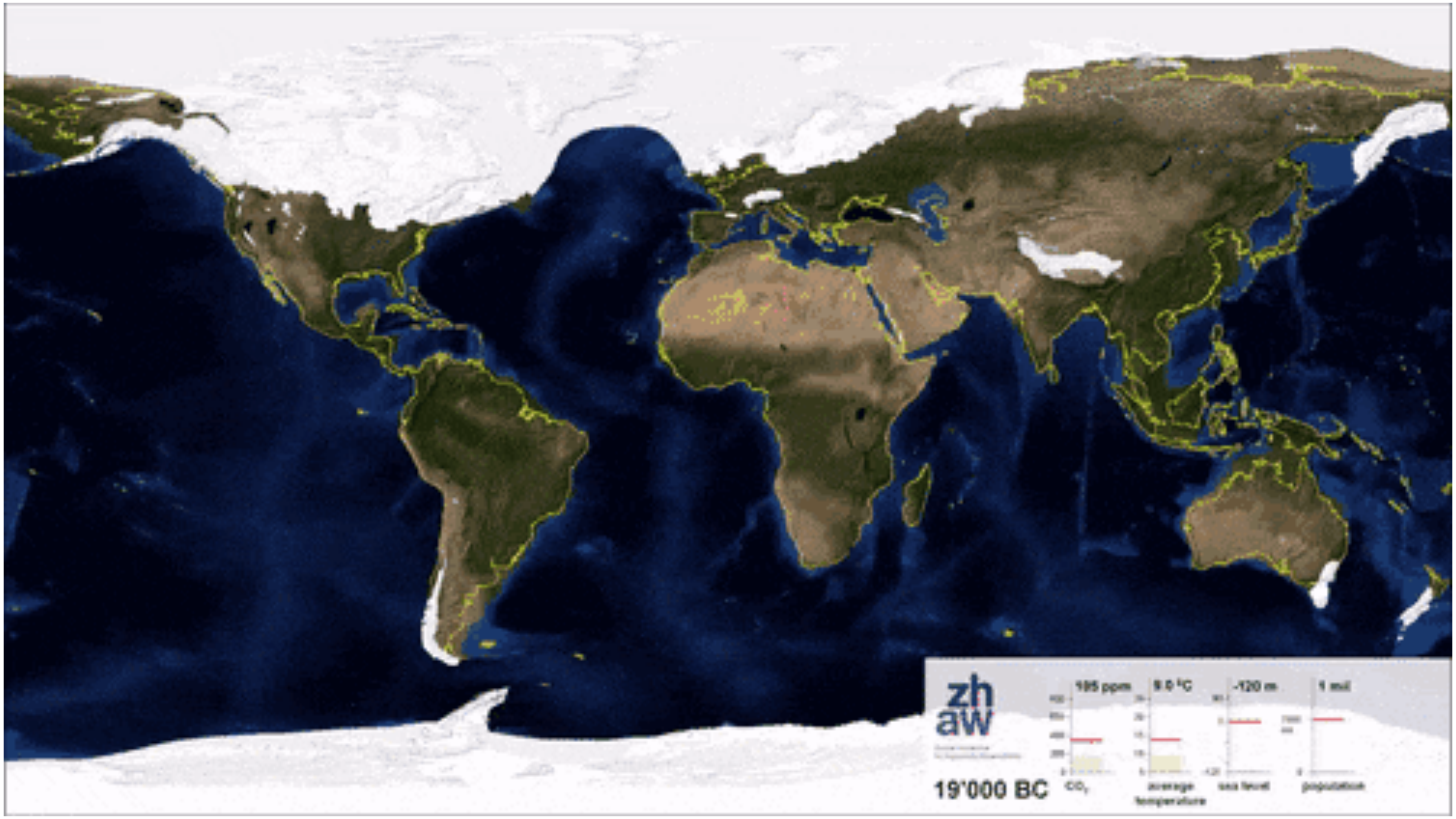
Lecture 22: Markov Chain Monte Carlo (update)

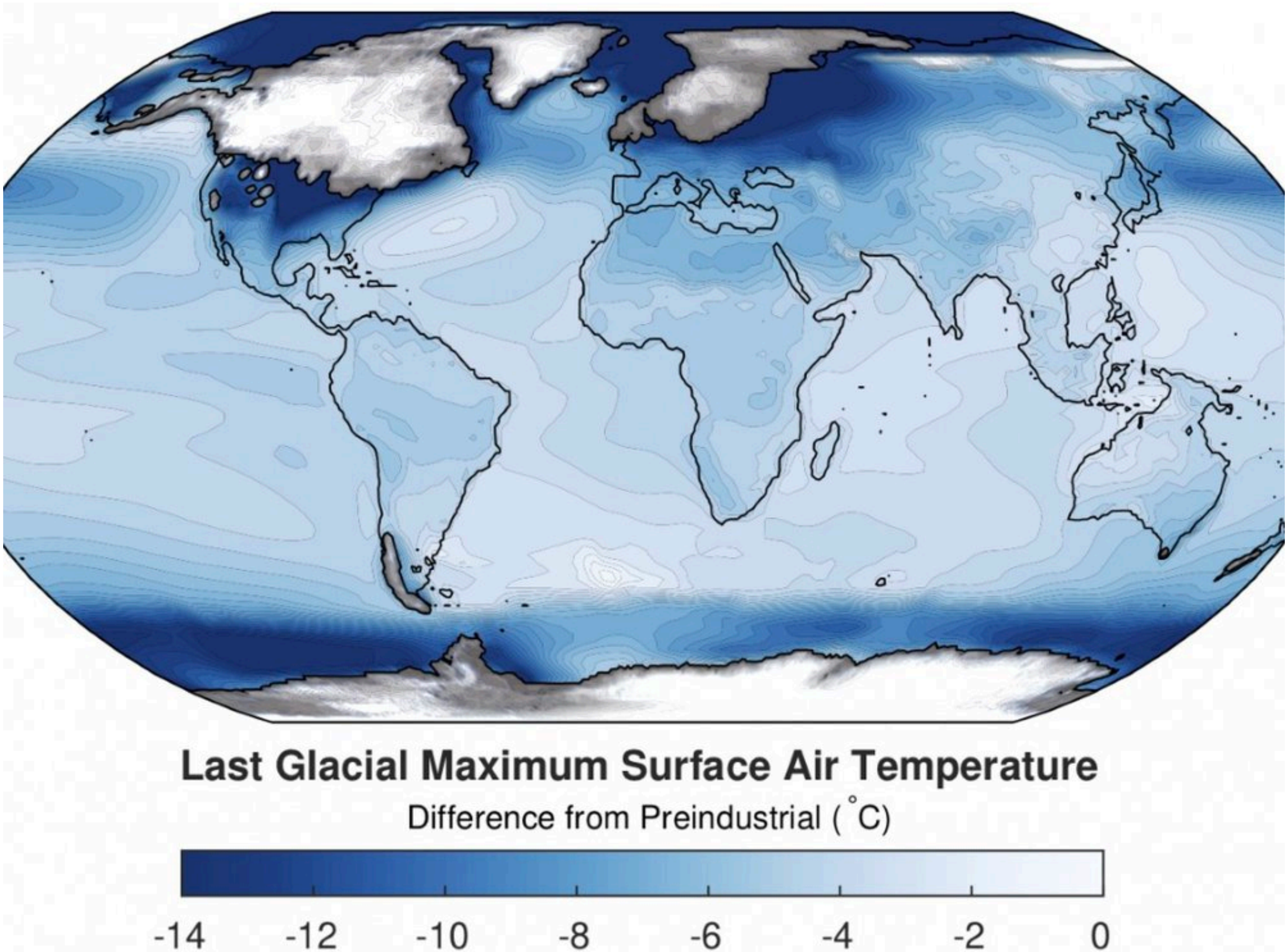
The Ice Age



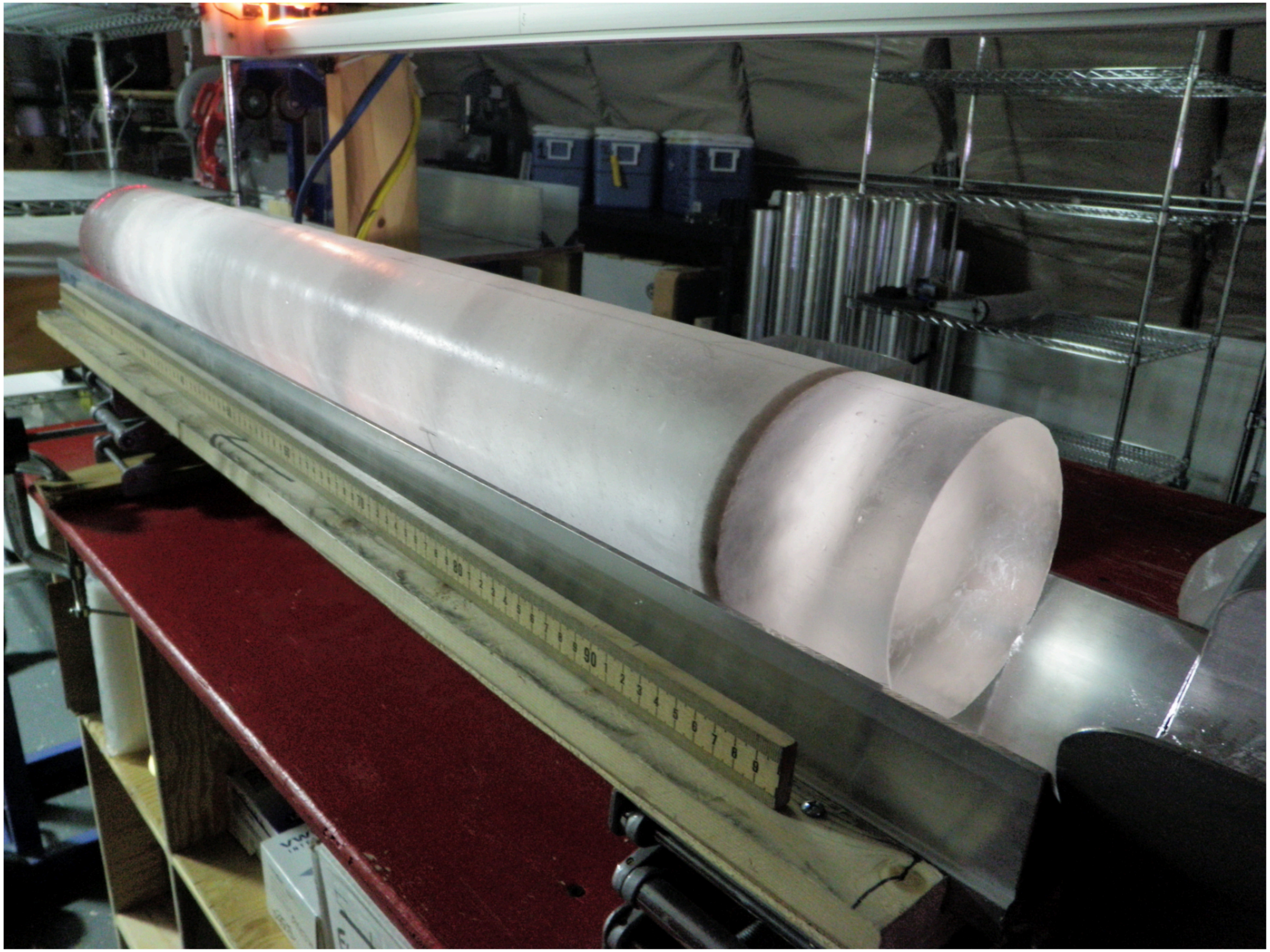
- Ice age had a profound impact on the earth

- 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

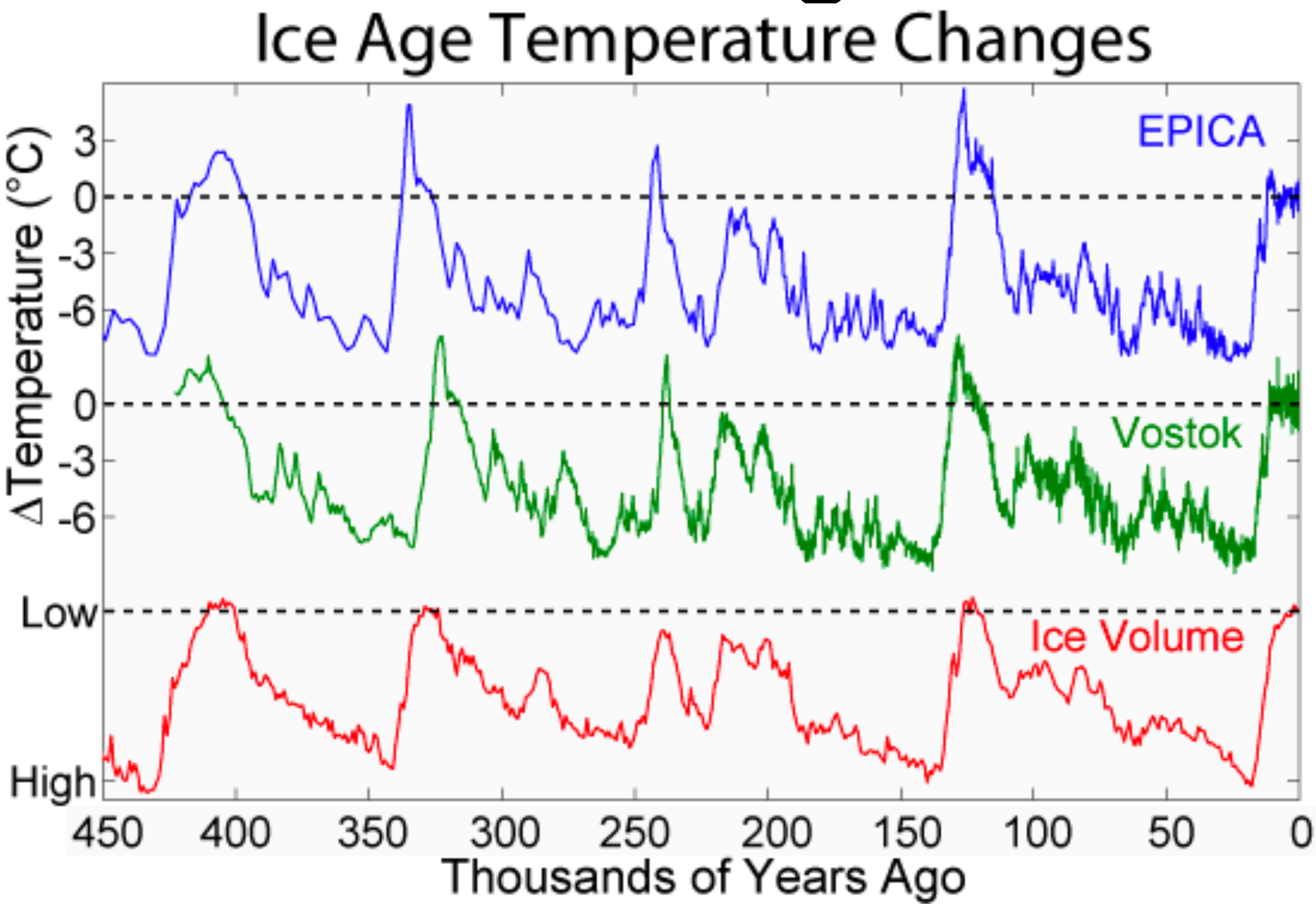


The dark band in this ice core from the West Antarctic Ice Sheet Divide (WAIS Divide) is a layer of volcanic ash that settled on the ice sheet approximately 21,000 years ago. — Credit: Heidi Roop, NSF

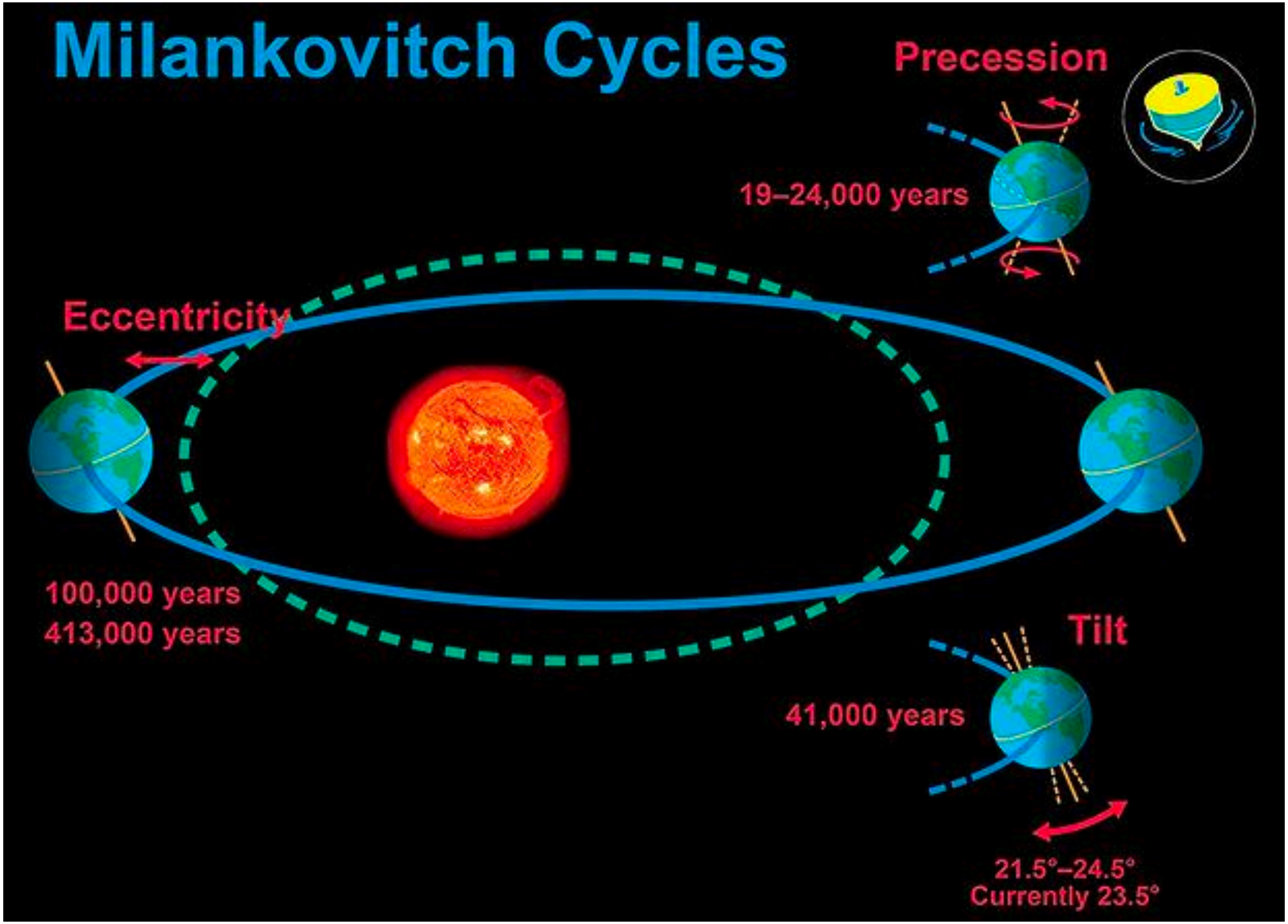
Ice Core

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

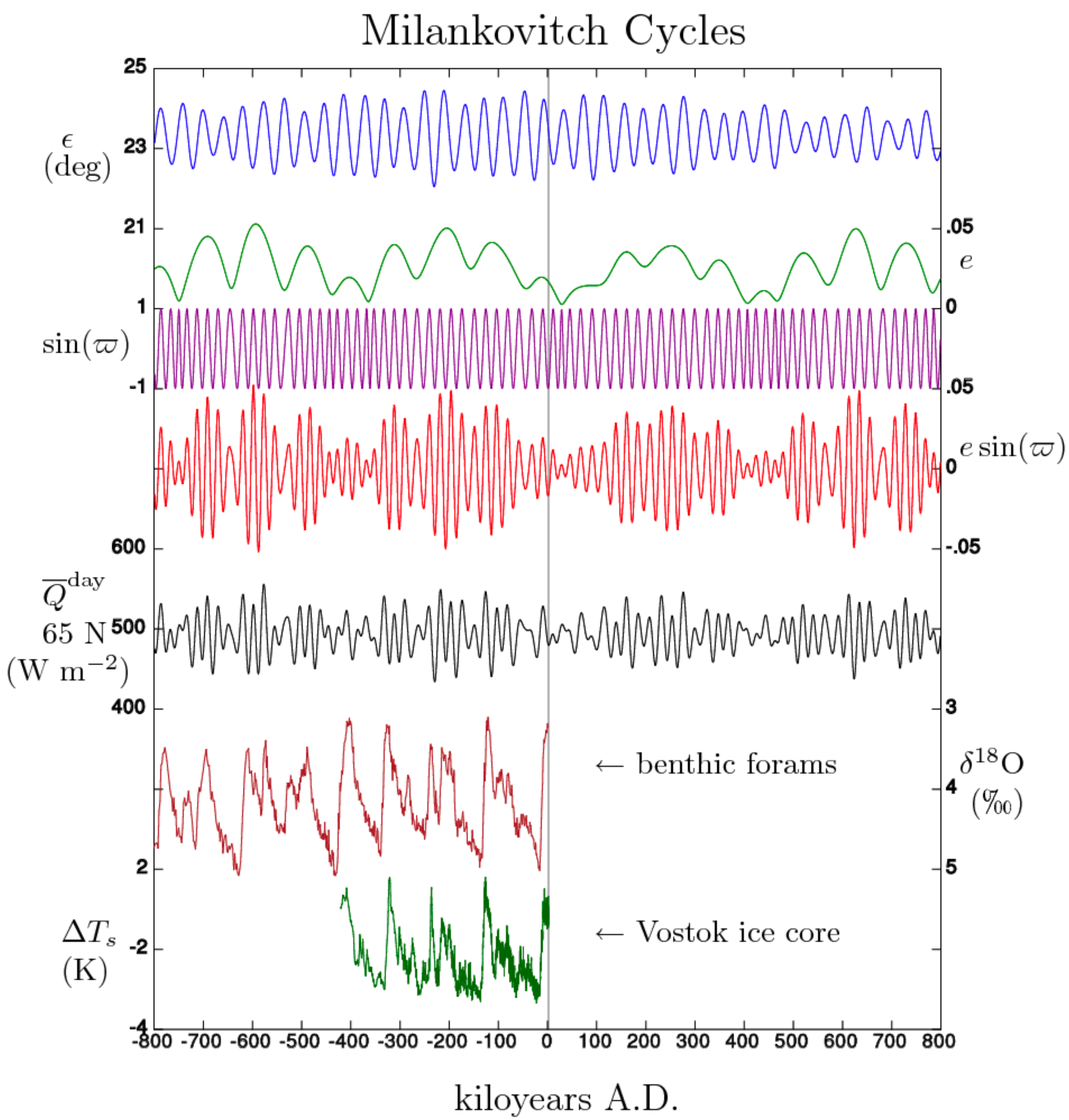
Ice Age over time



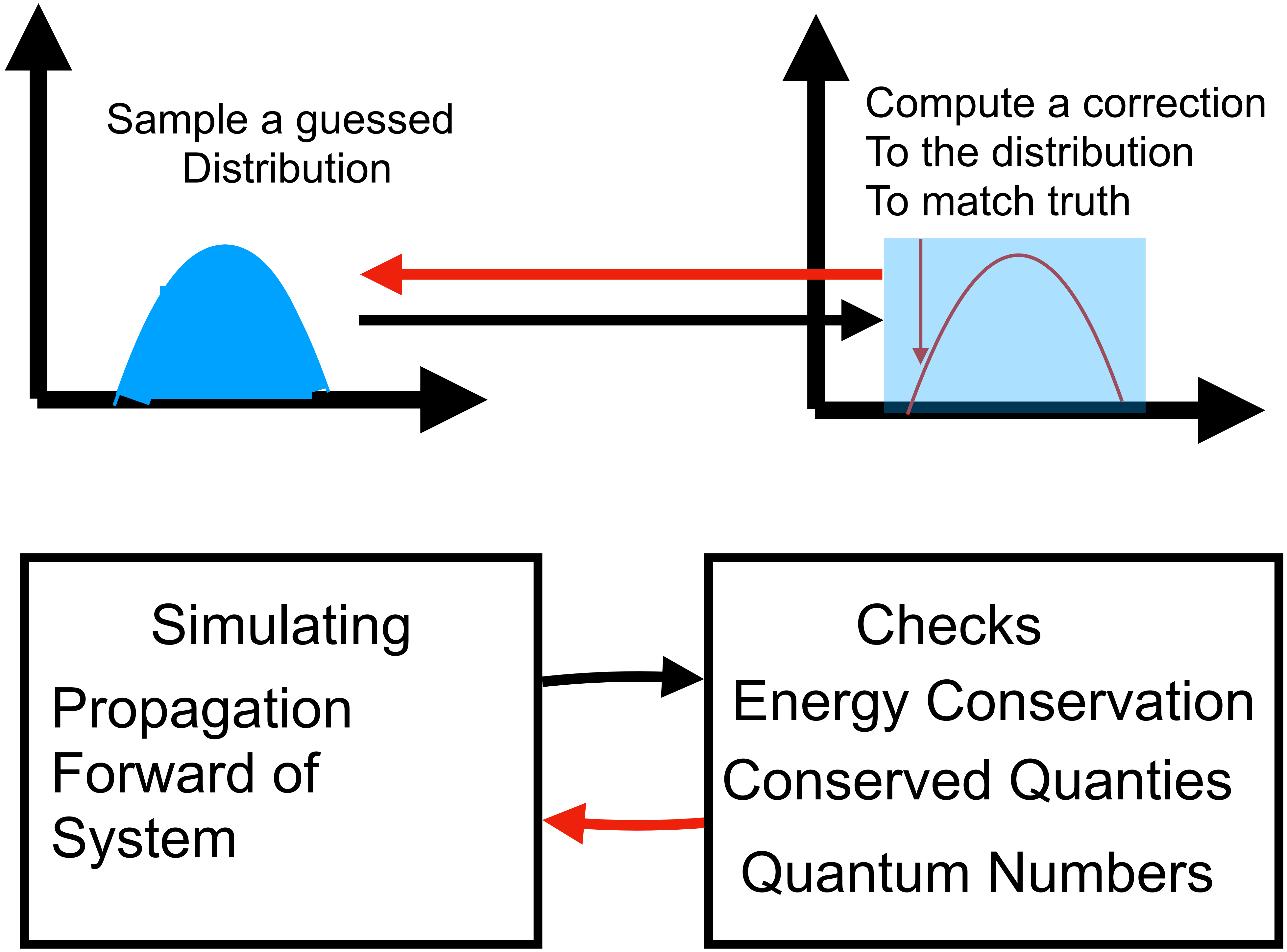
Milhanovitch Cycles



Scale of Eccentricity



Markov Chain MC



Correct Our Simulation Through a Probabilistic Rescaling

Metropolis-Hastings

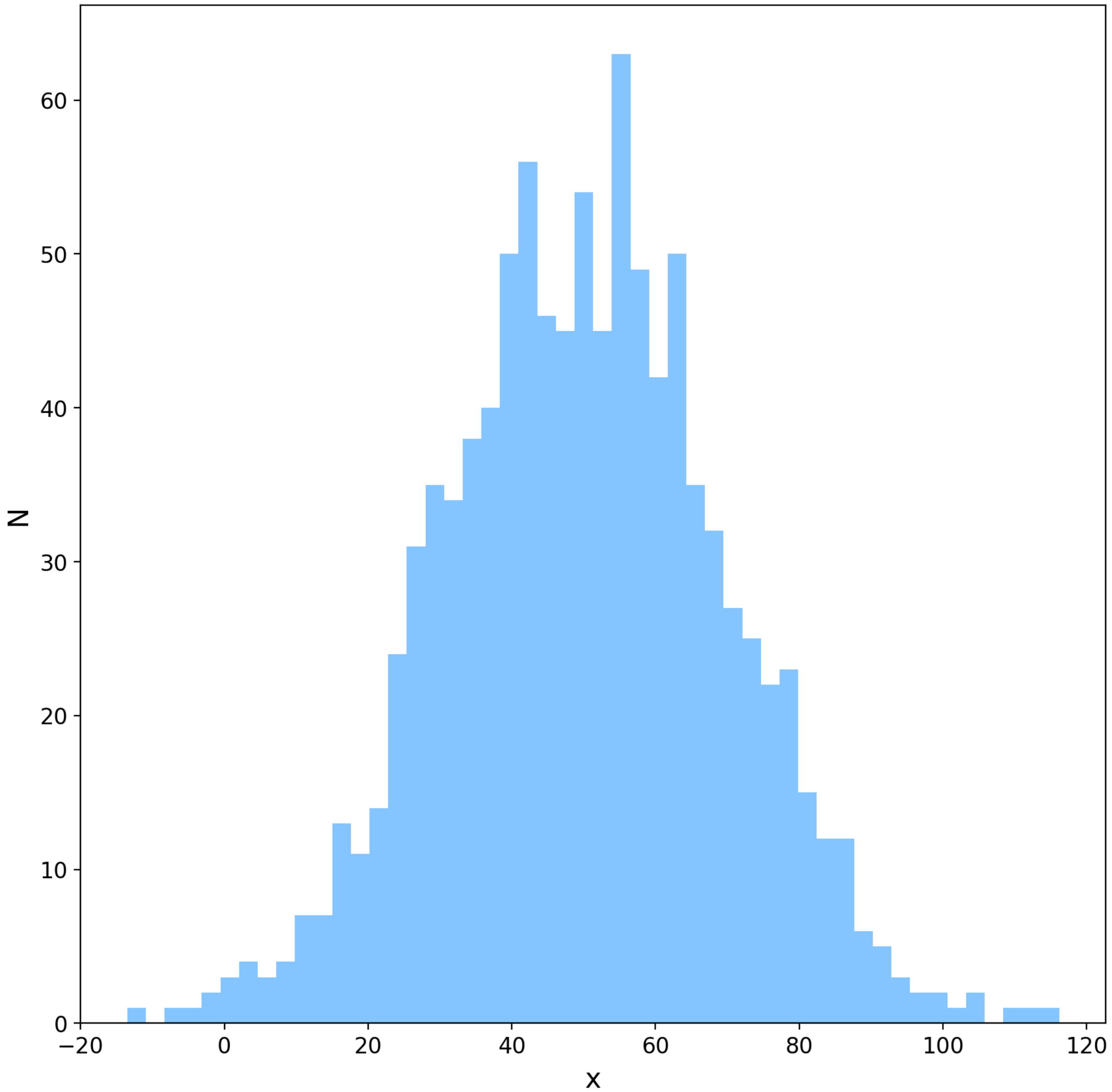
- Step 0: Randomly sample a parameter $\boldsymbol{x_1}$
- Step 1: Sample a new parameter $\mathbf{x_2}$
    - Use a chosen “Proposal Function” for sampling
    - Compute the probability of stepping $\mathbf{x_2}$ to stepping $\mathbf{x_1}$
- Step 2: Sample a flat distribution from 0 to 1 ($\mathbf{s_2}$)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

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

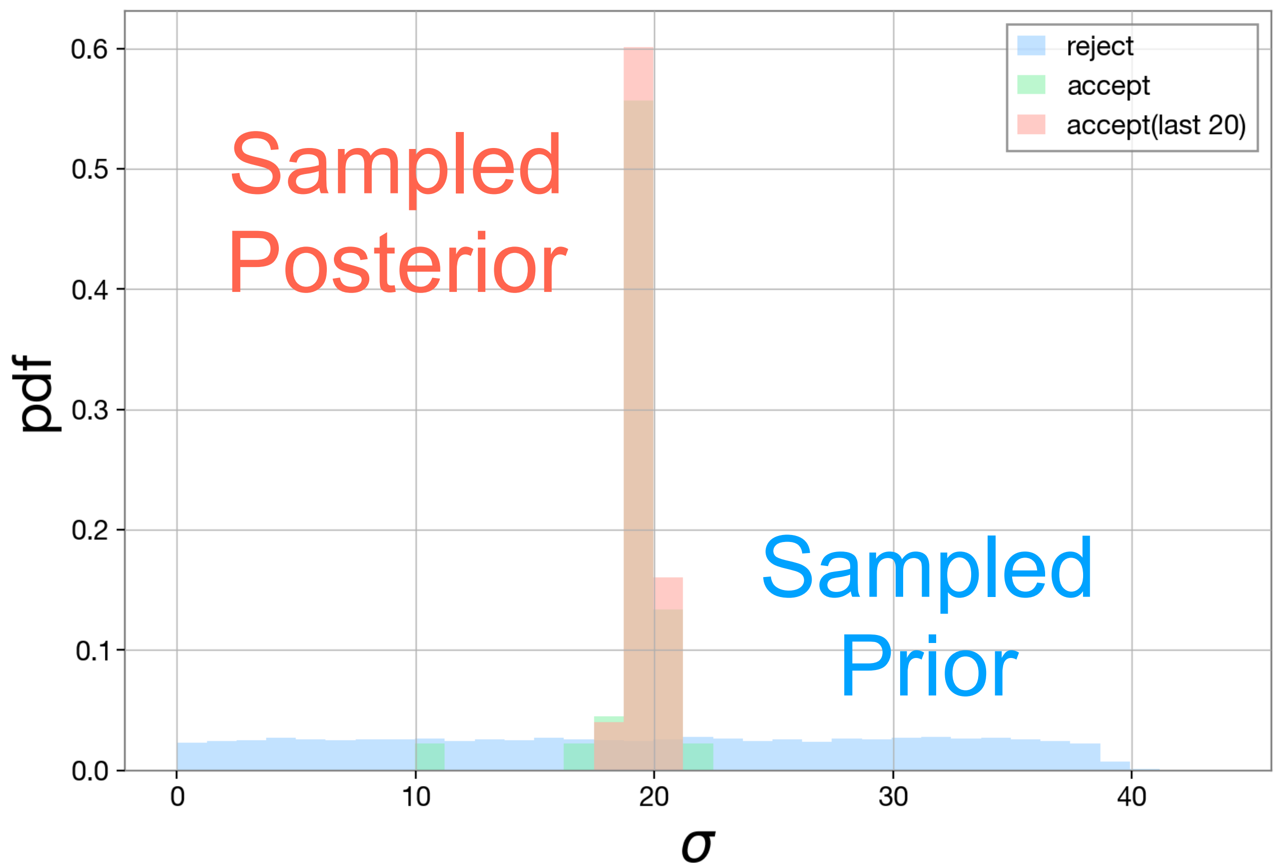


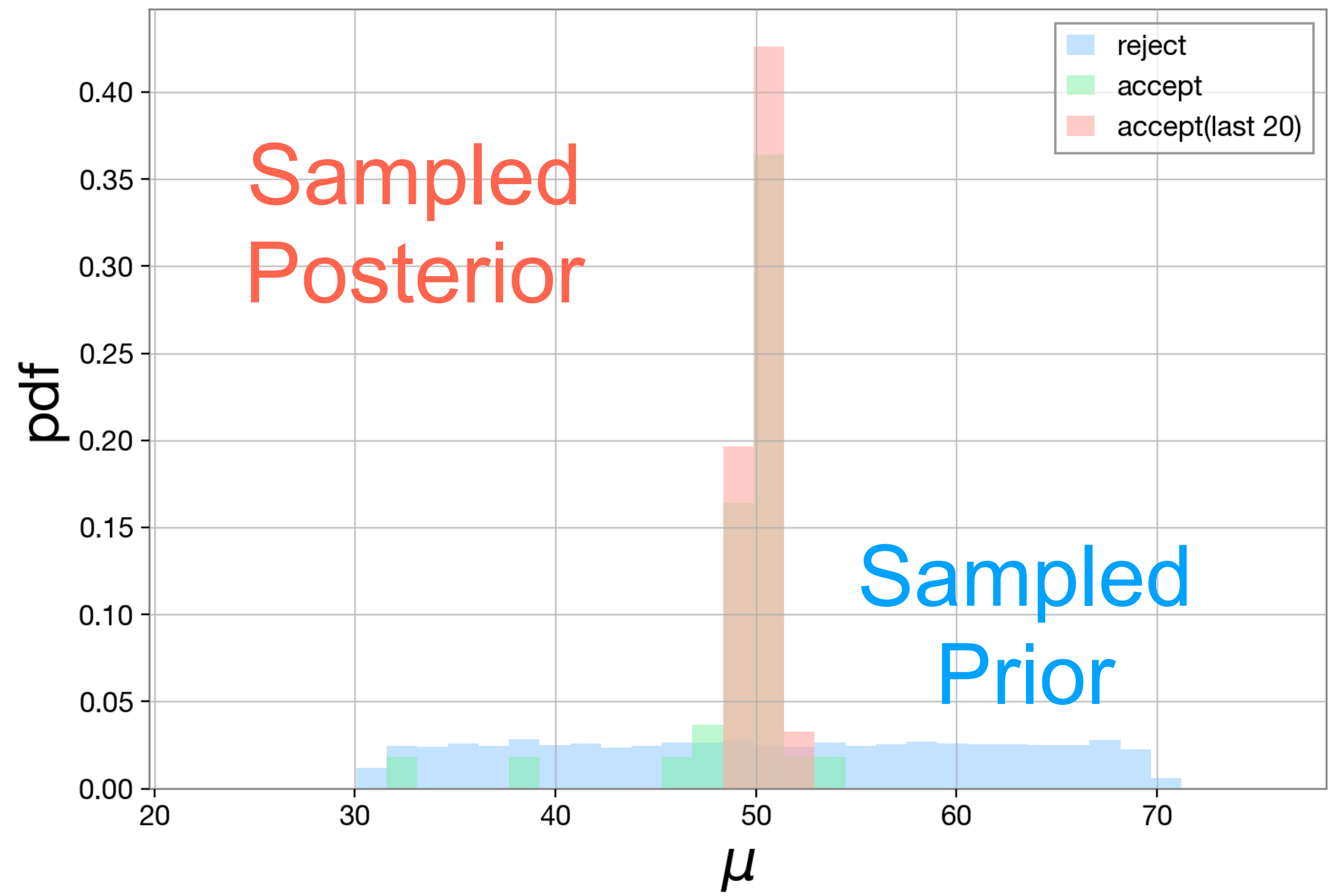
Log(Probability)

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

Accepted μ, σ yield the best fits

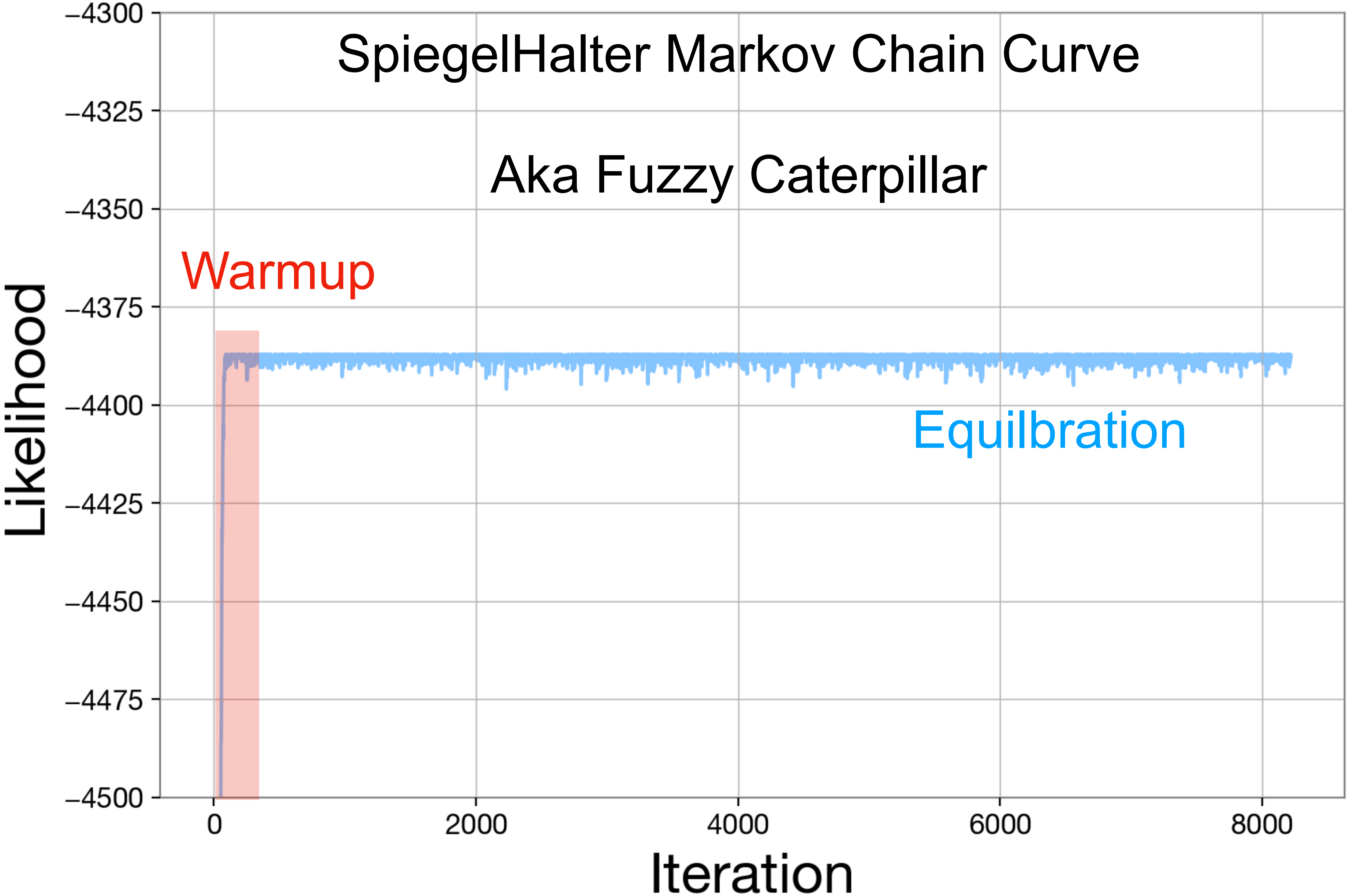
Best Fit Paramters





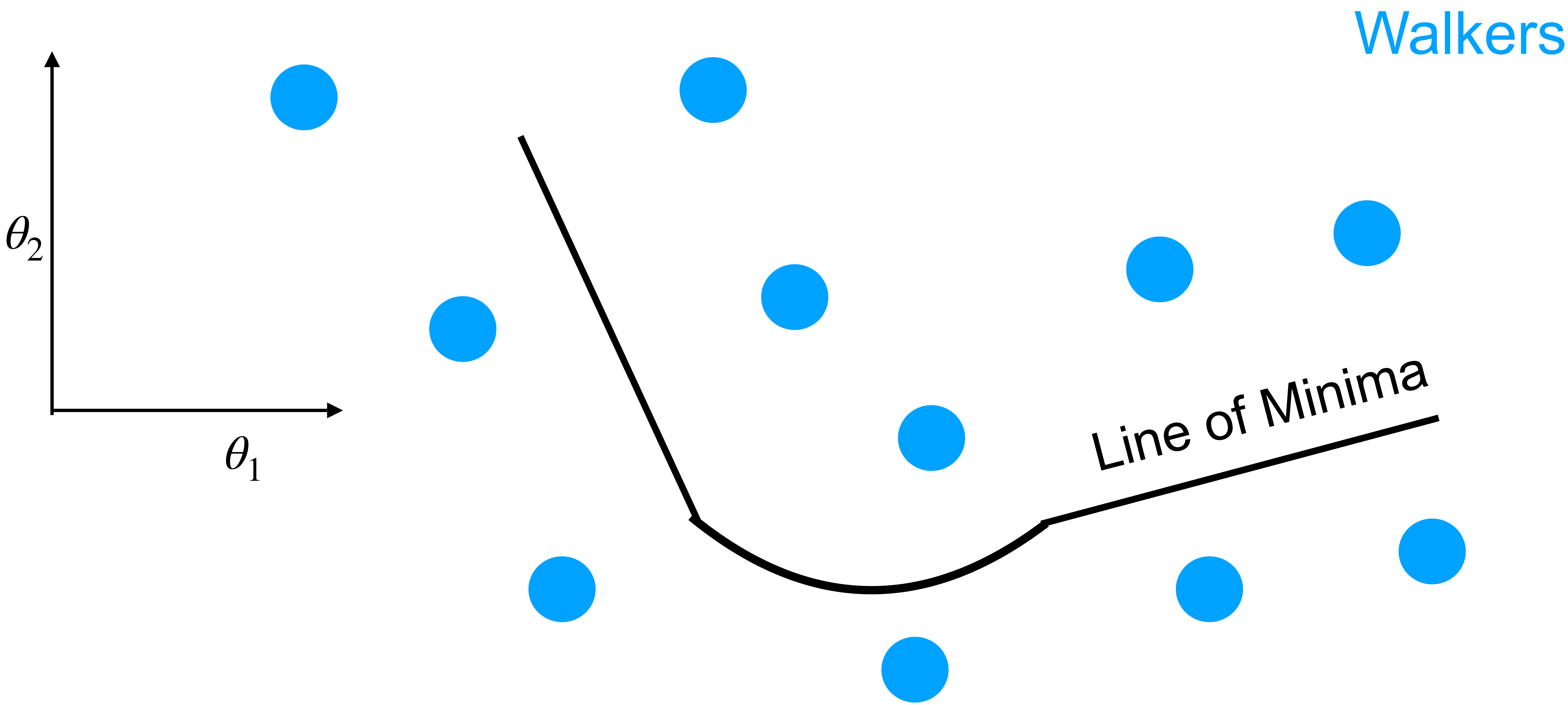
- This is where I start to hint that there are limitations here
- What we are doing is running a check
  - We are not taking a derivative (No gradients or Hessians)

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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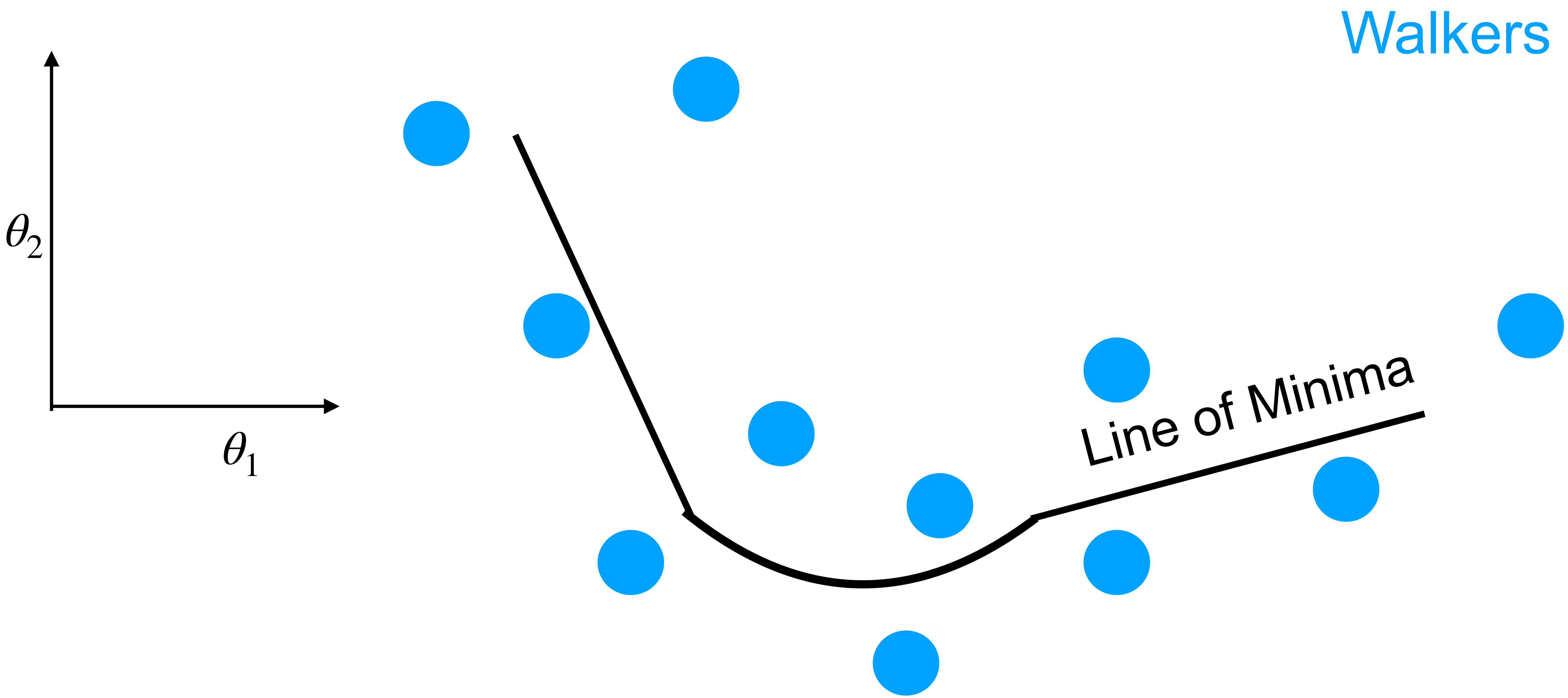

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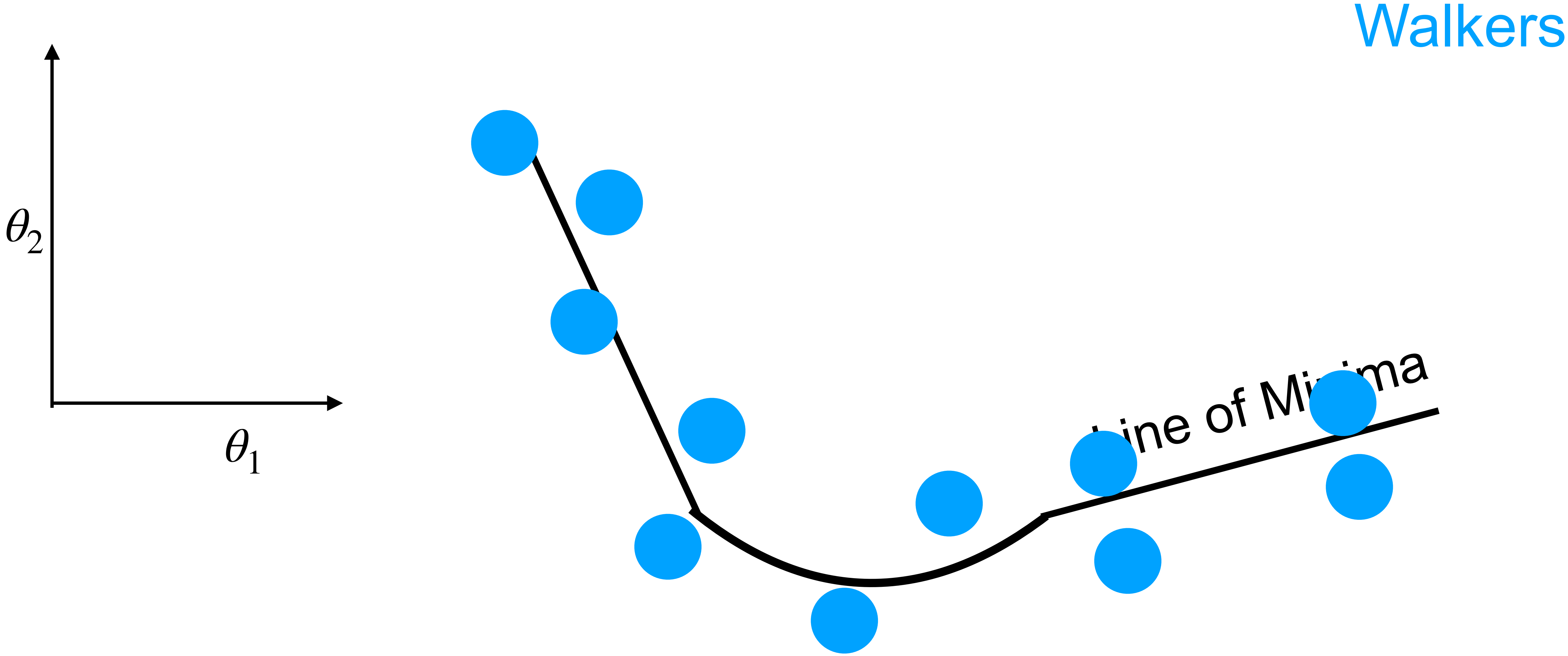
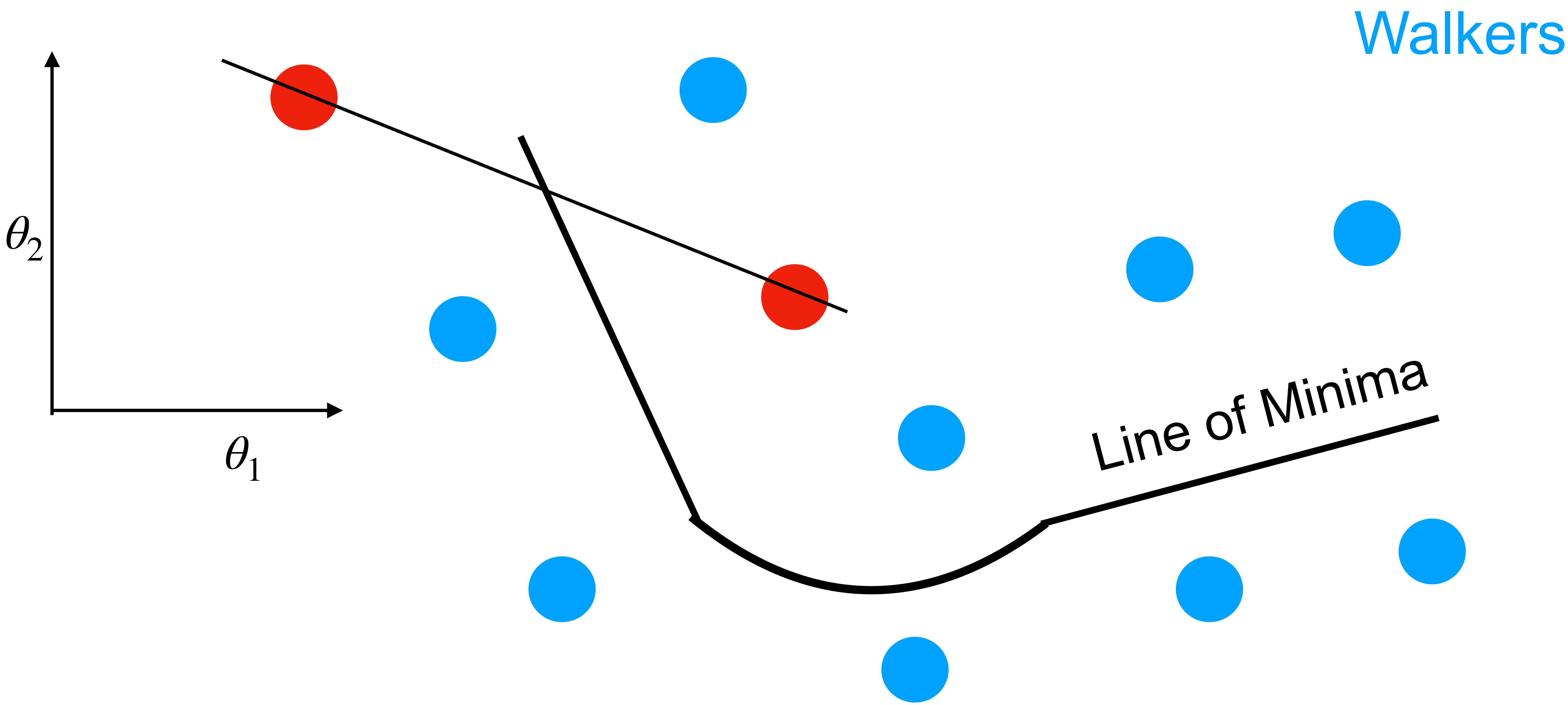


Updating w/Random Points

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



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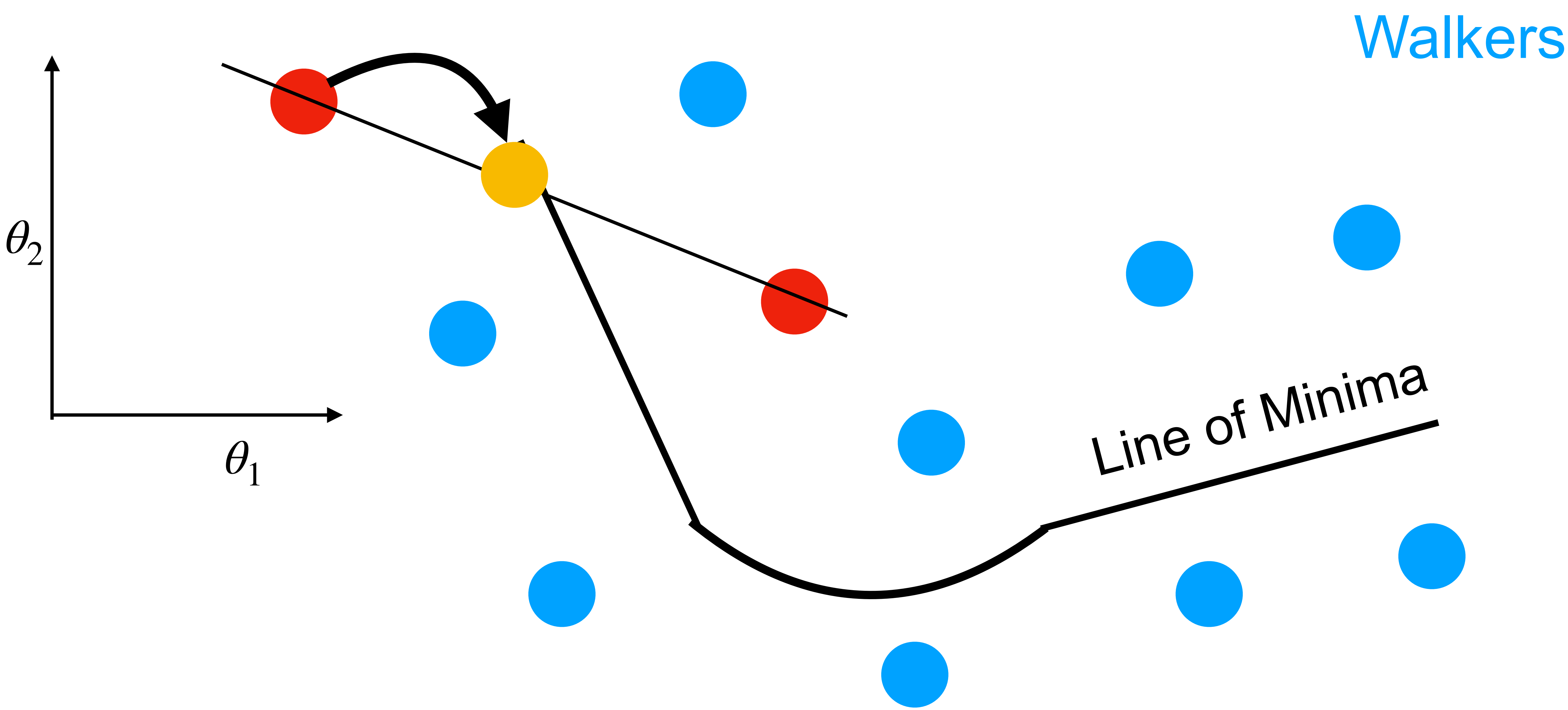

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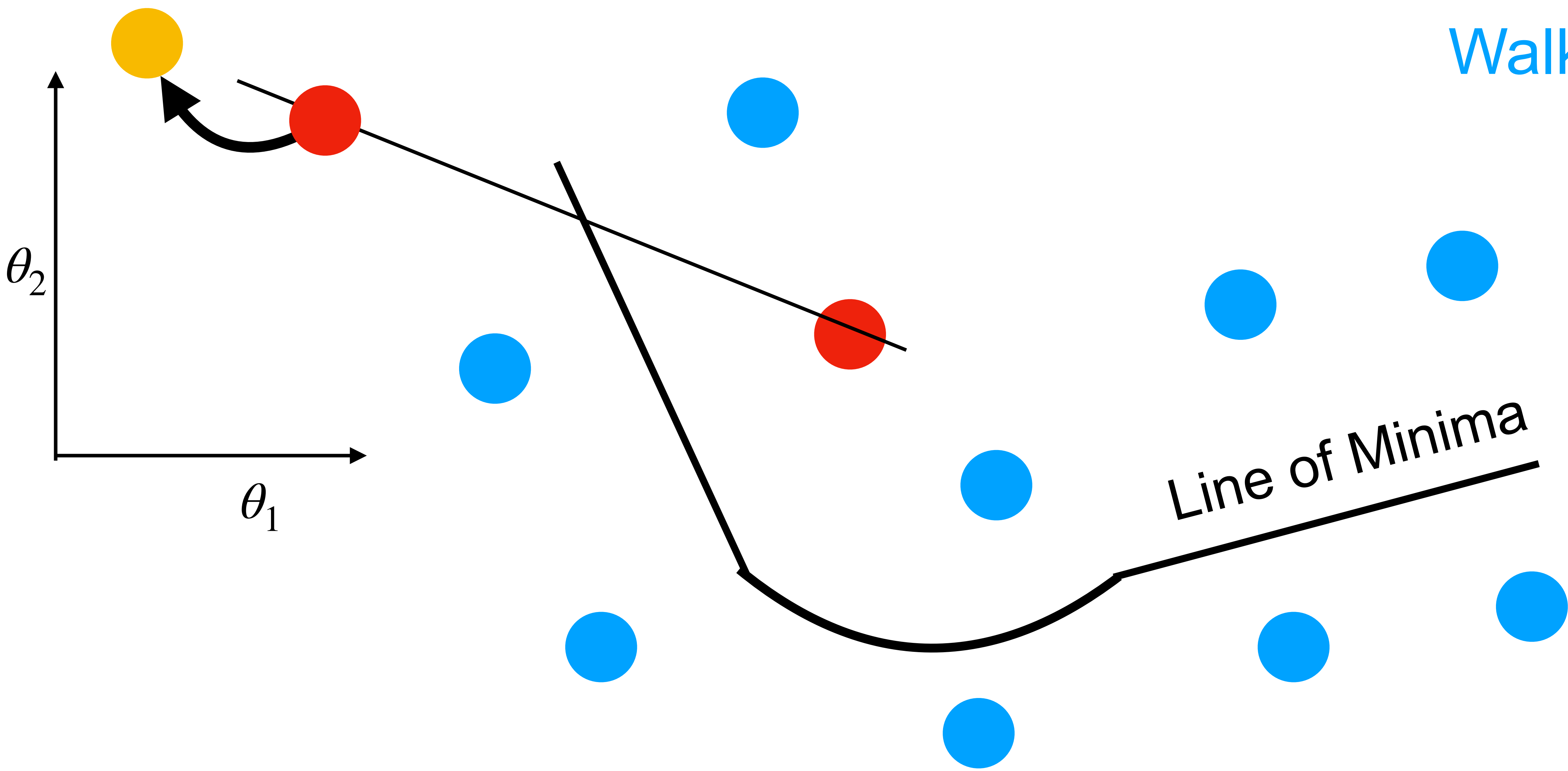

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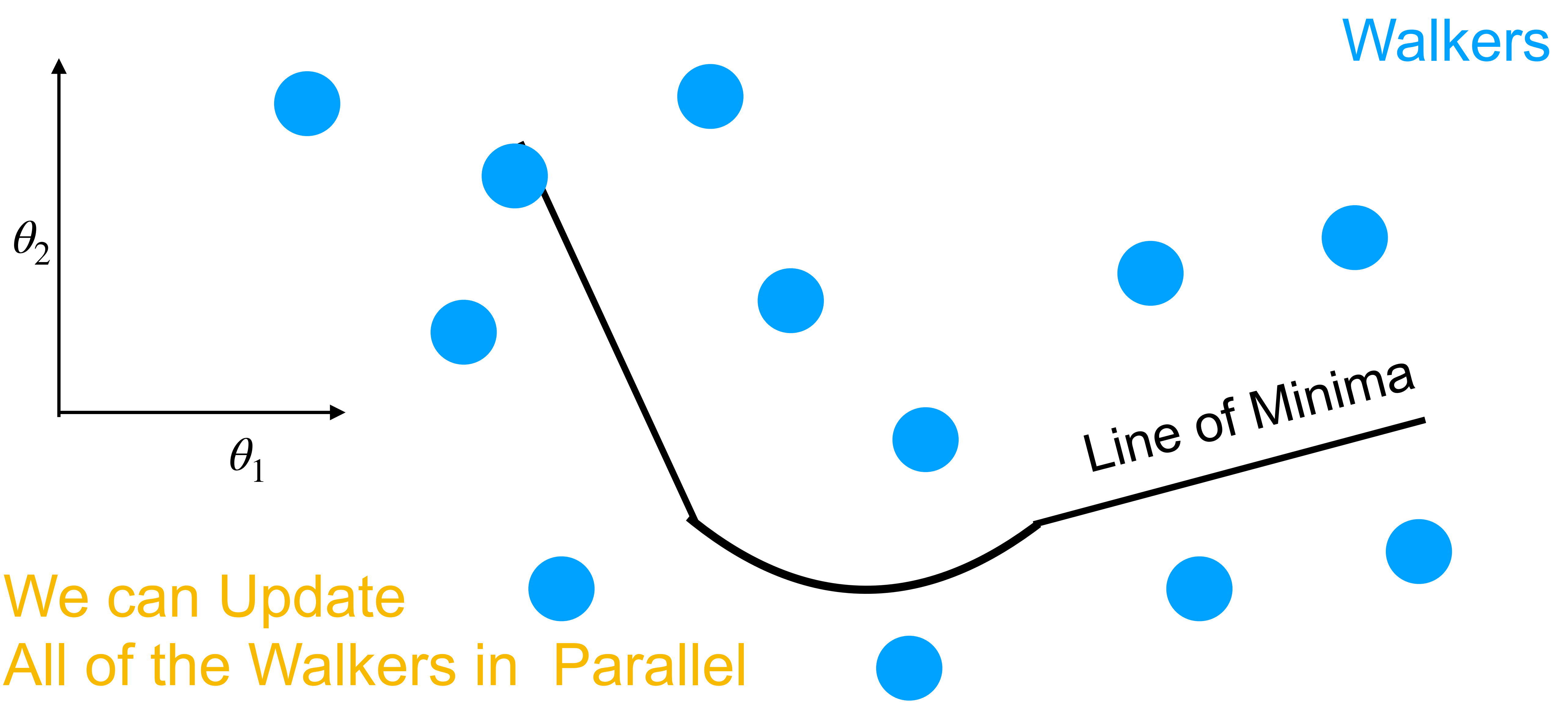
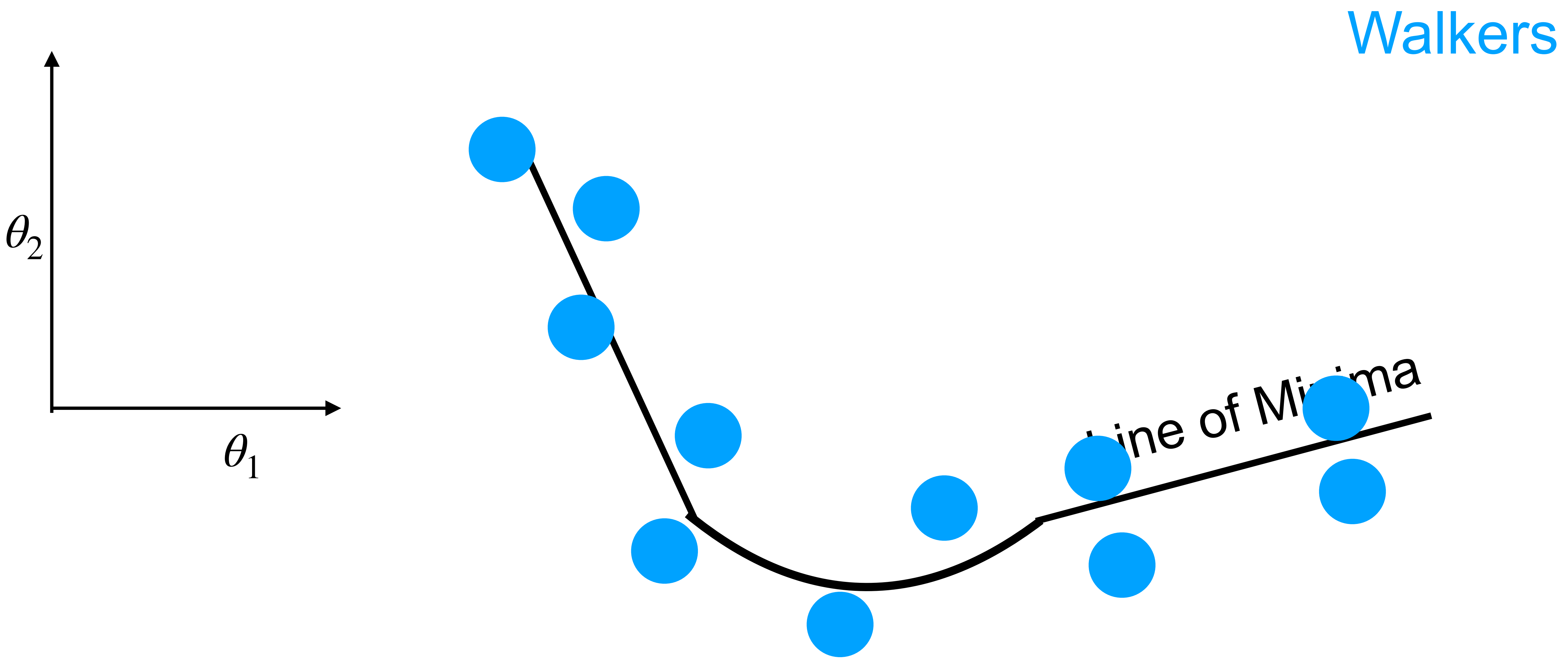


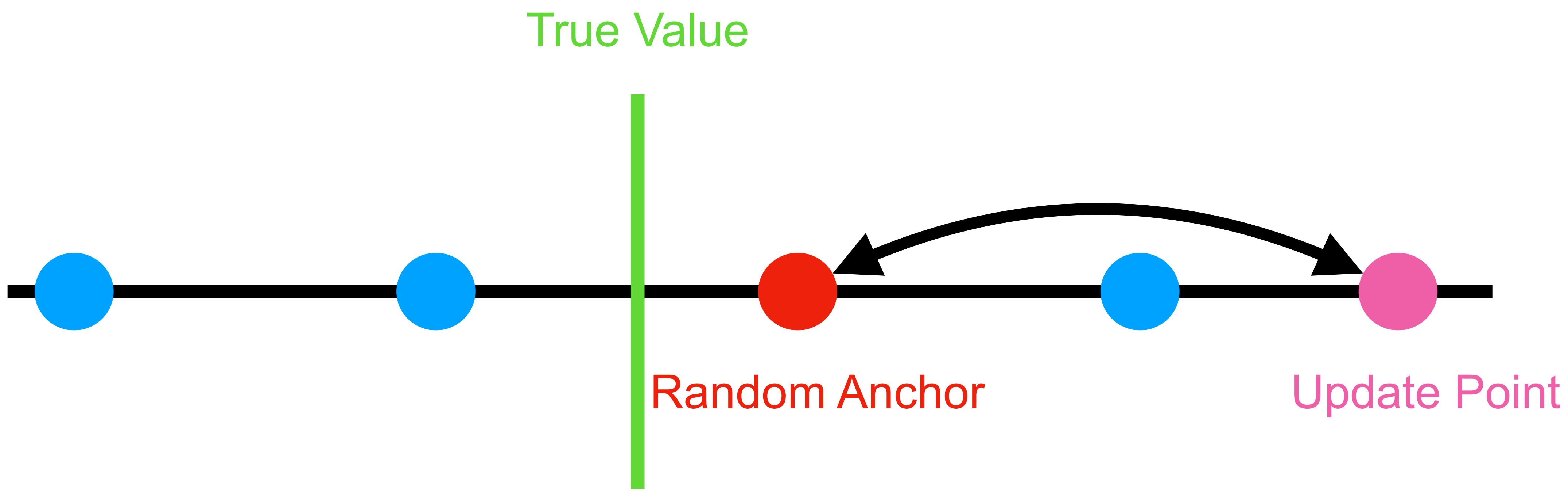
We can Update
All of the Walkers in Parallel

Speeding up MCMC

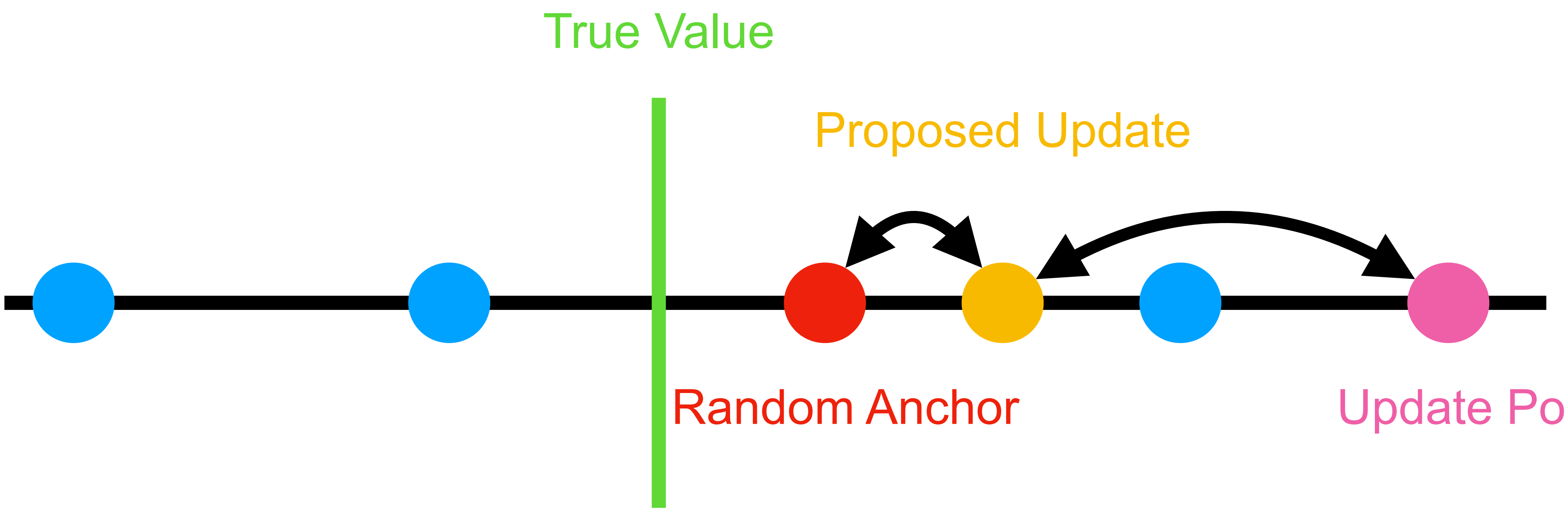
- We randomly choose a pair of points
  - Move one of the points along the line between them



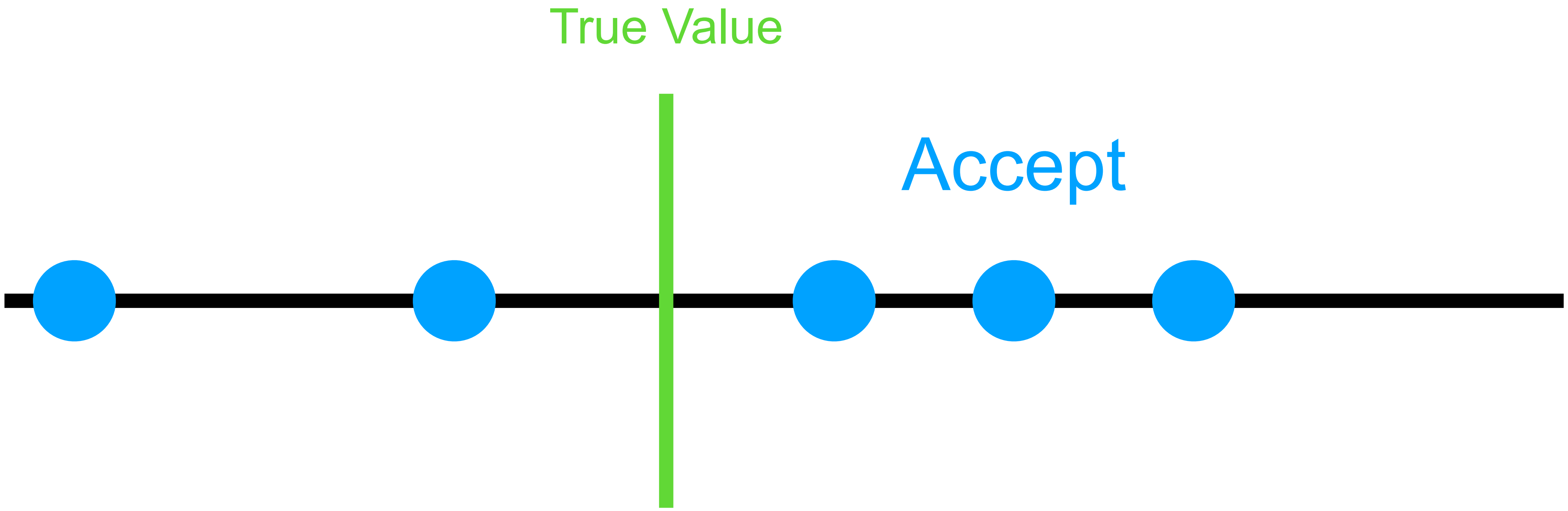
Example Fit



Example Fit



Example Fit



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

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

Equilibrated Best Fit

Sampled Distribution
Aka Proposal

Probability Driving
Decision

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

The Likelihood reweights the Prior to the Posterior

Quantum Monte Carlo

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

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

Guess a Form for the wavefunction

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

We can define probability from wavefunction

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

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

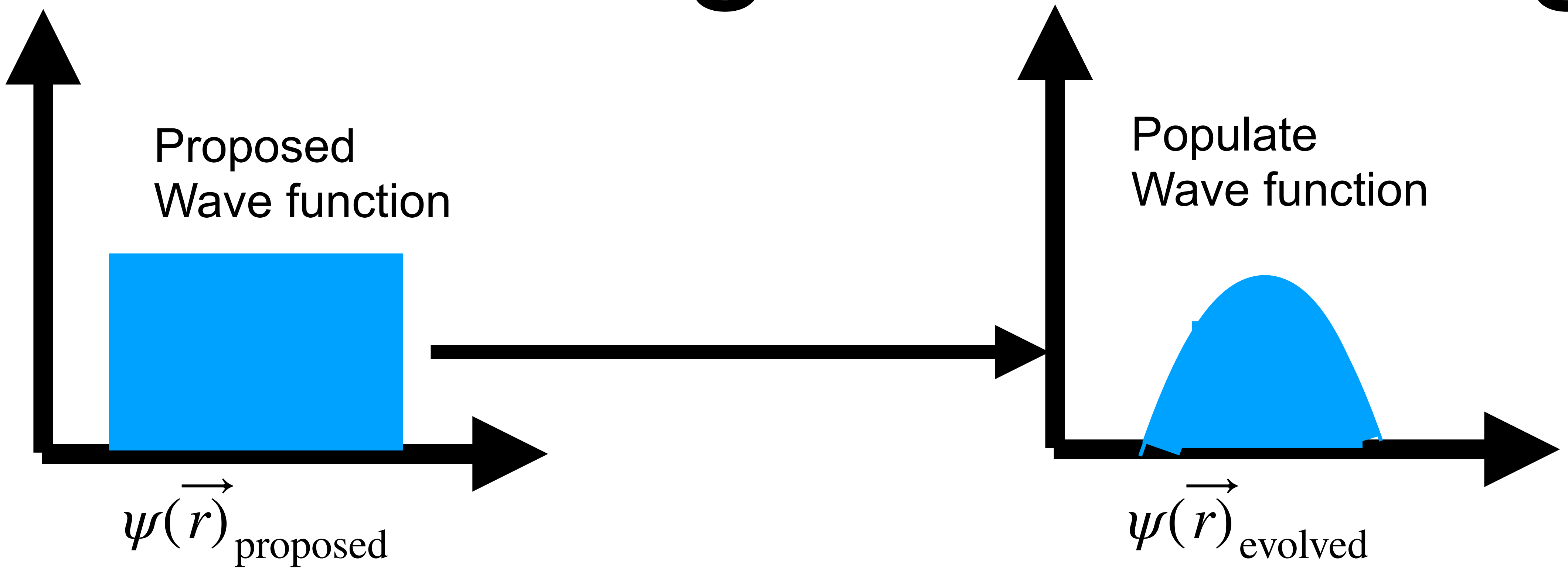
$$\sum_j p_j(\vec{r}\,|\,\vec{\theta}) = \frac{\psi_j^*(\vec{r}\,|\,\vec{\theta})\psi_j(\vec{r}\,|\,\vec{\theta})}{\langle\psi\,|\,\psi\rangle}$$

We can define probability from wavefunction

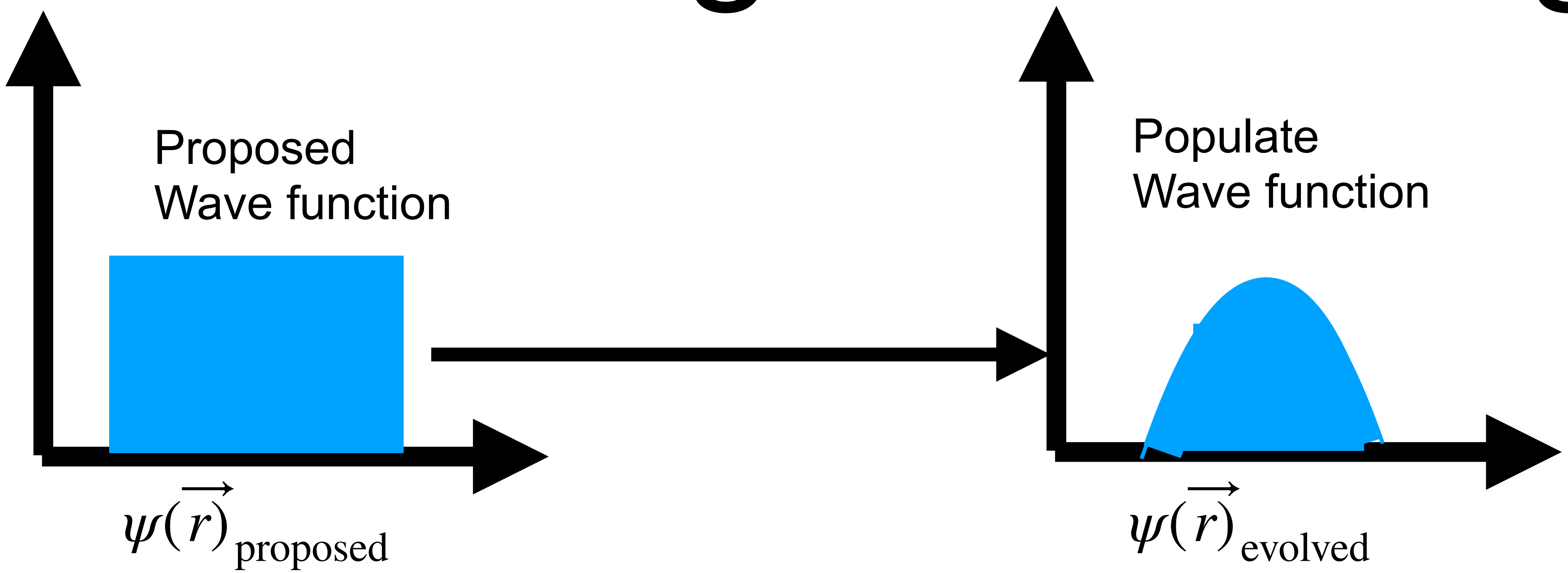
$$\sum_j w_{i+1}^j = \frac{p_j(\overrightarrow{r_{i+1}}\,|\,\vec{\theta})}{p_j(\overrightarrow{r_i}\,|\,\vec{\theta})}$$

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

Solving Schroedinger



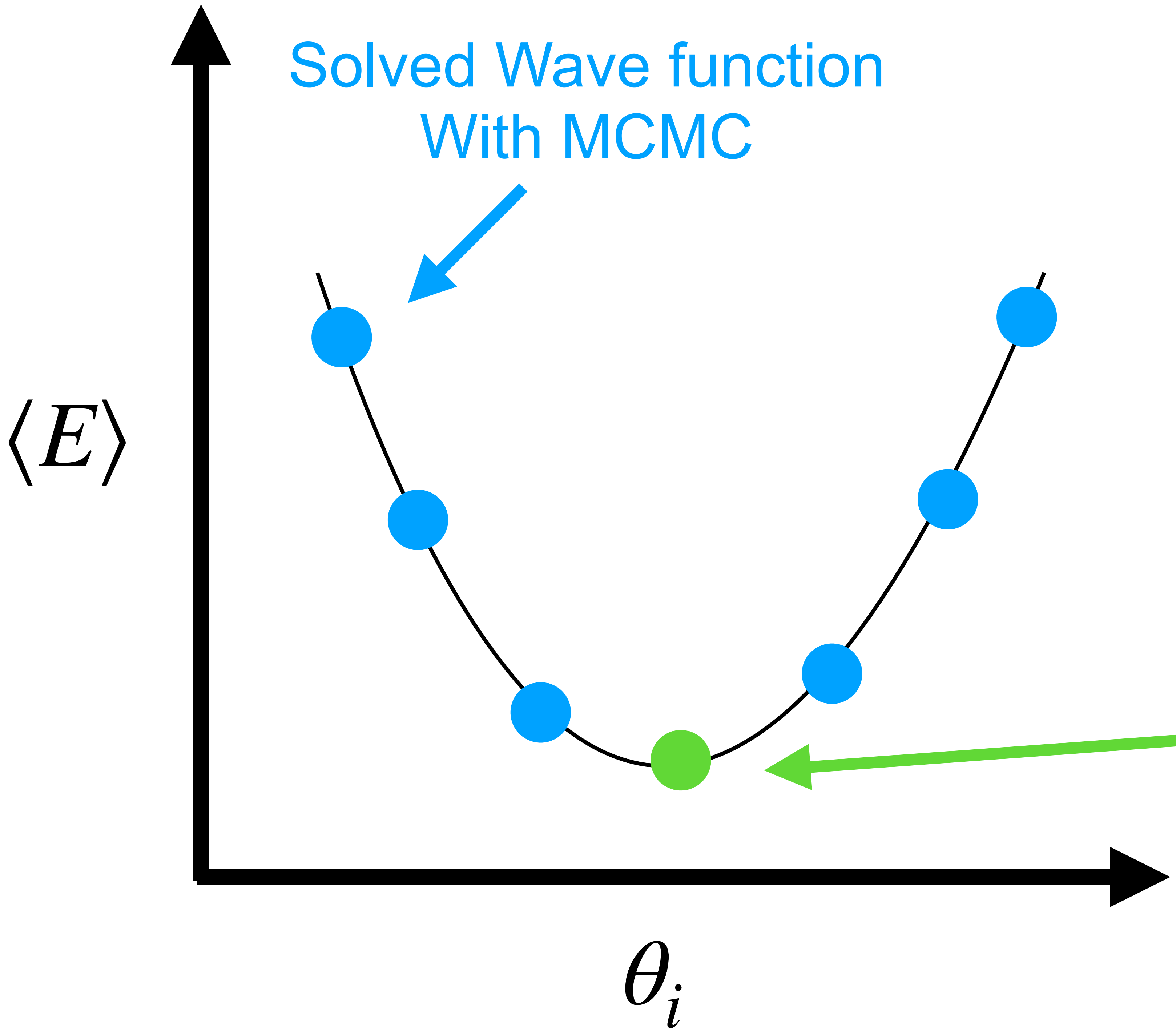
Solving Schroedinger



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

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

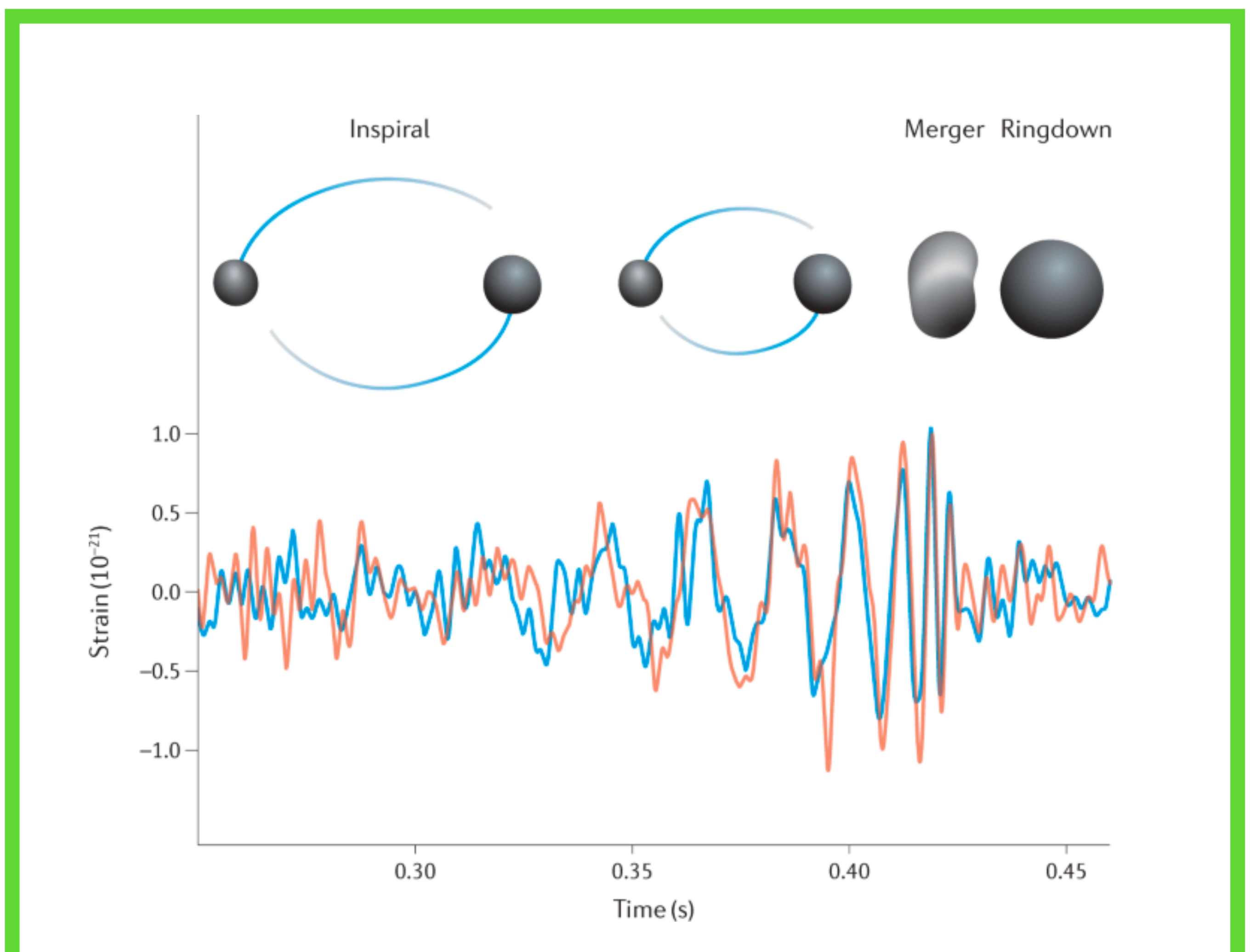
Solving Schroedinger

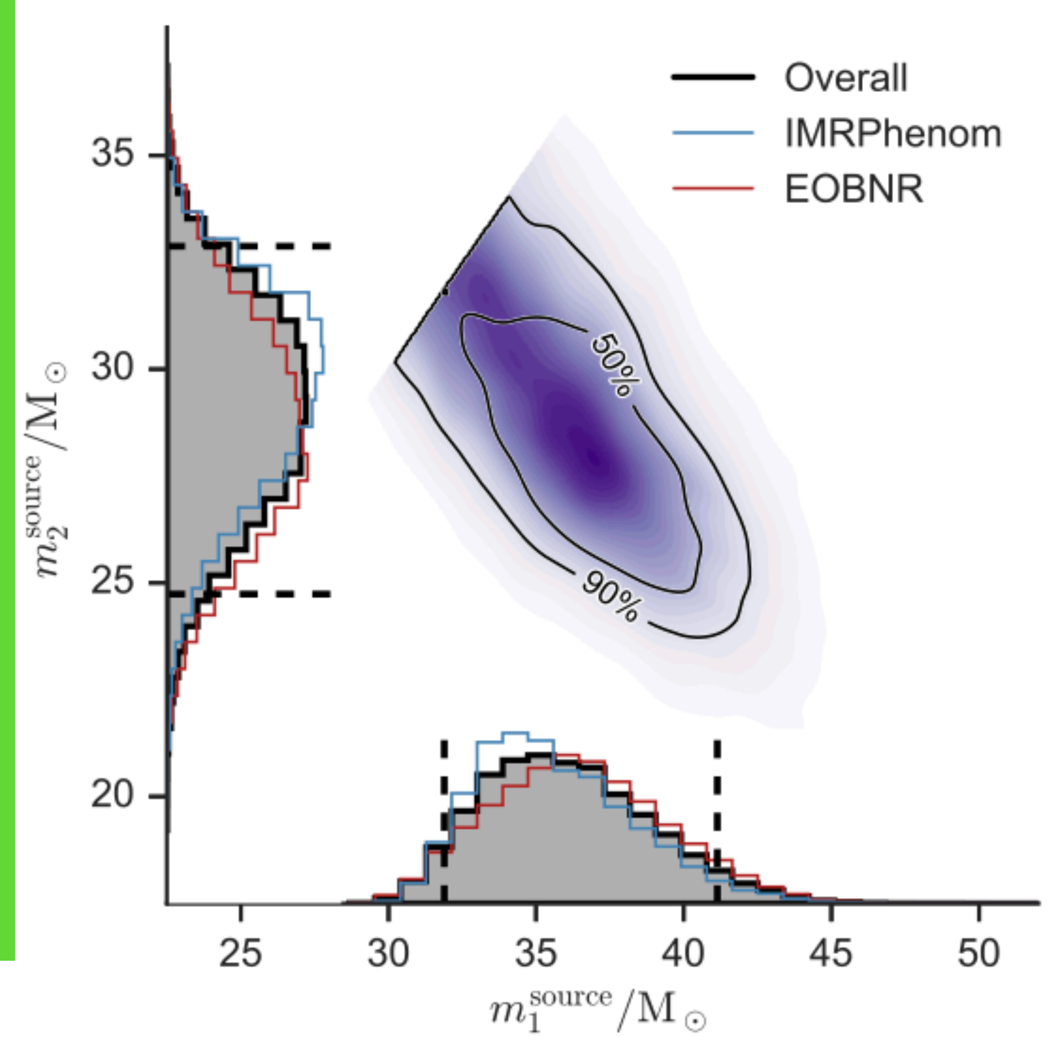


Our goal is to minimize the Energy given a wave functional form

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

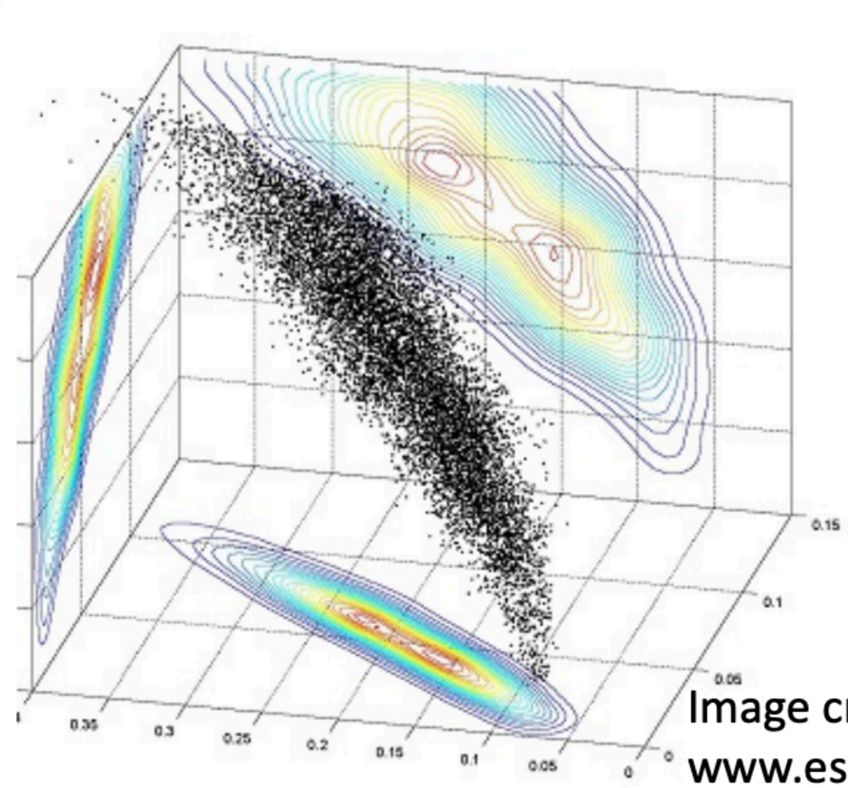


Image credit: www.essenceps.com

- 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