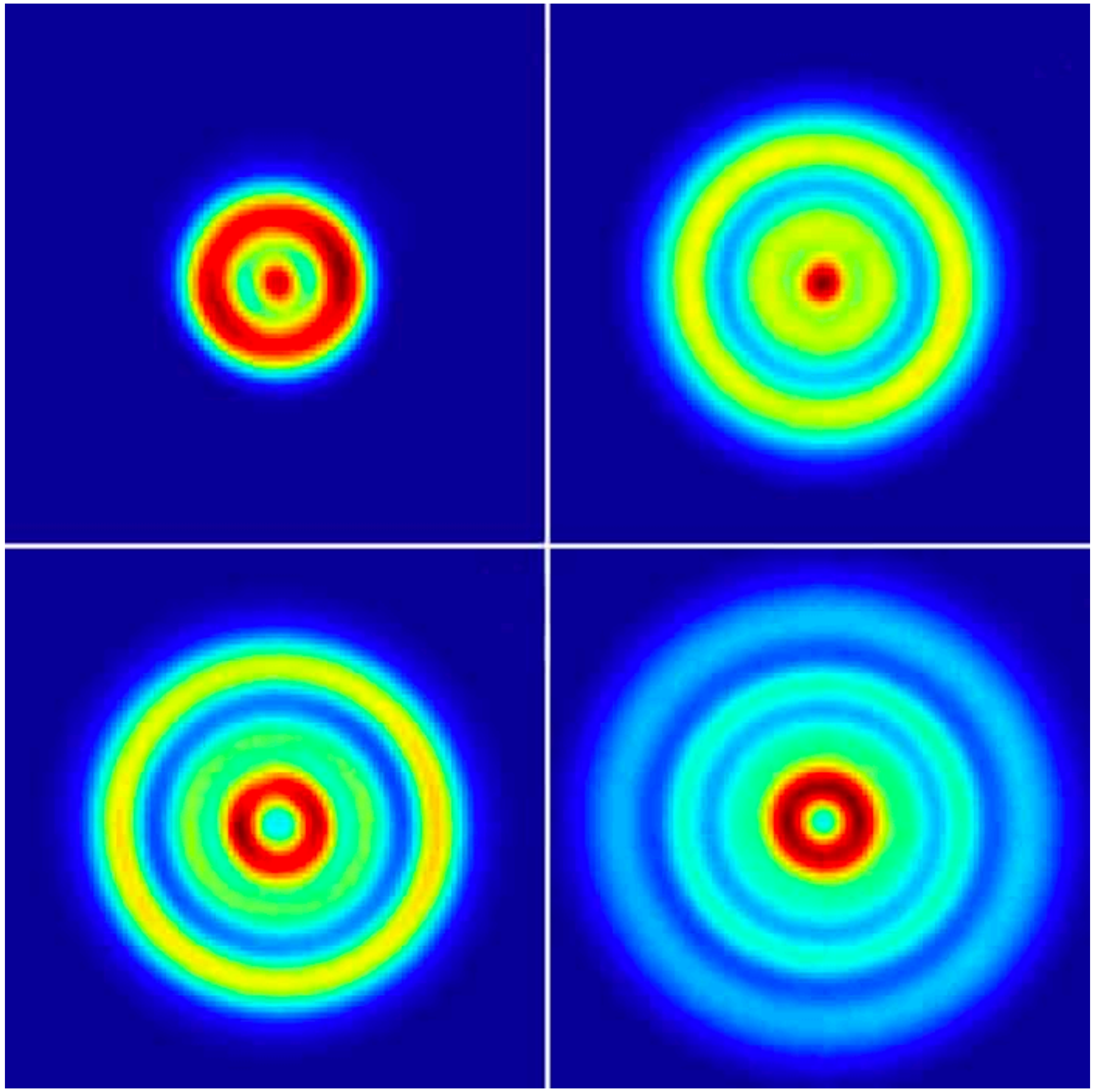
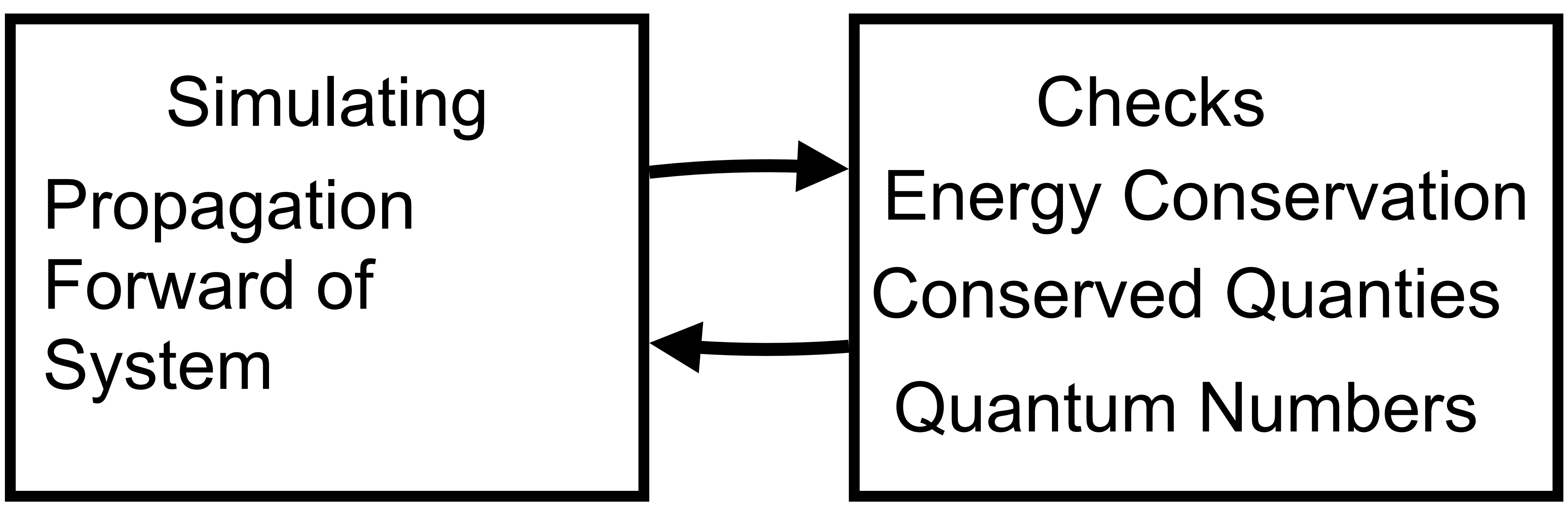


Lecture 22: Markov Chain Monte Carlo + More

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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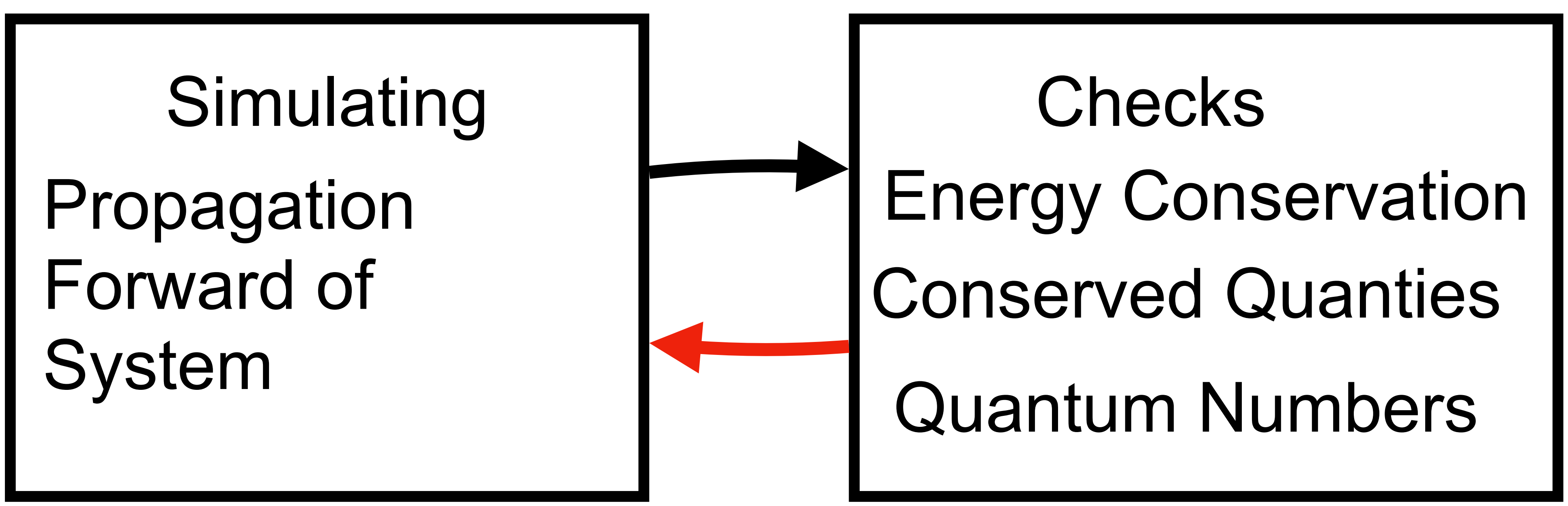
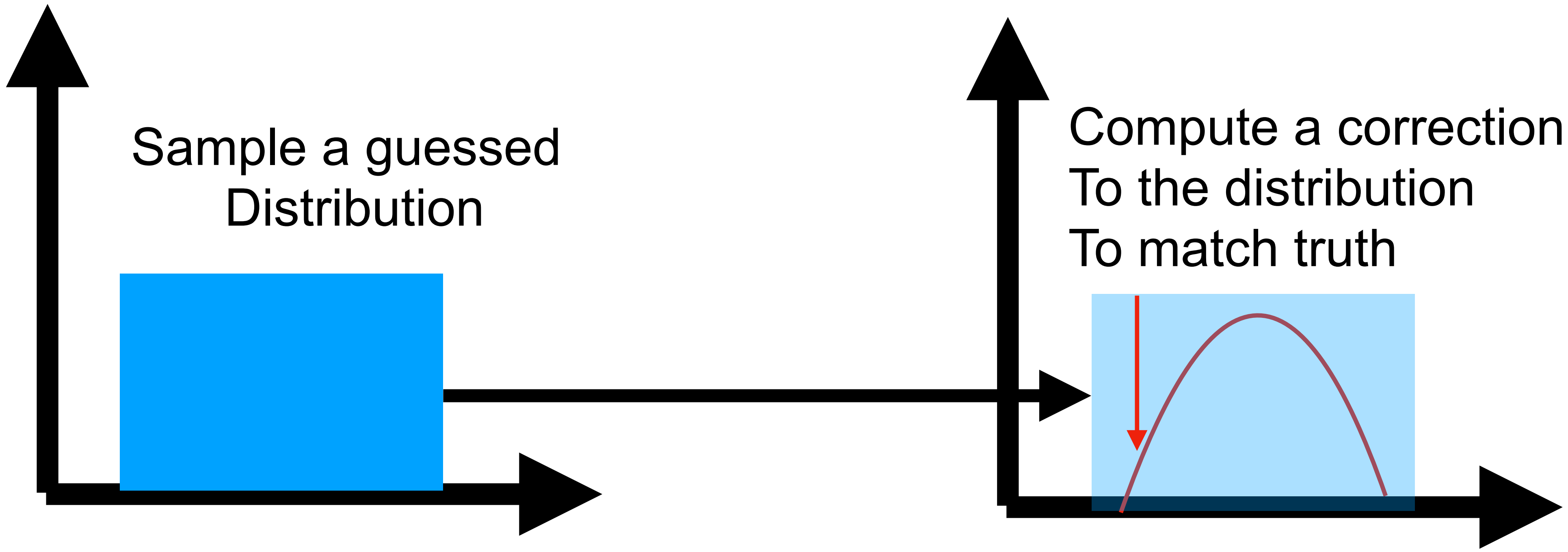
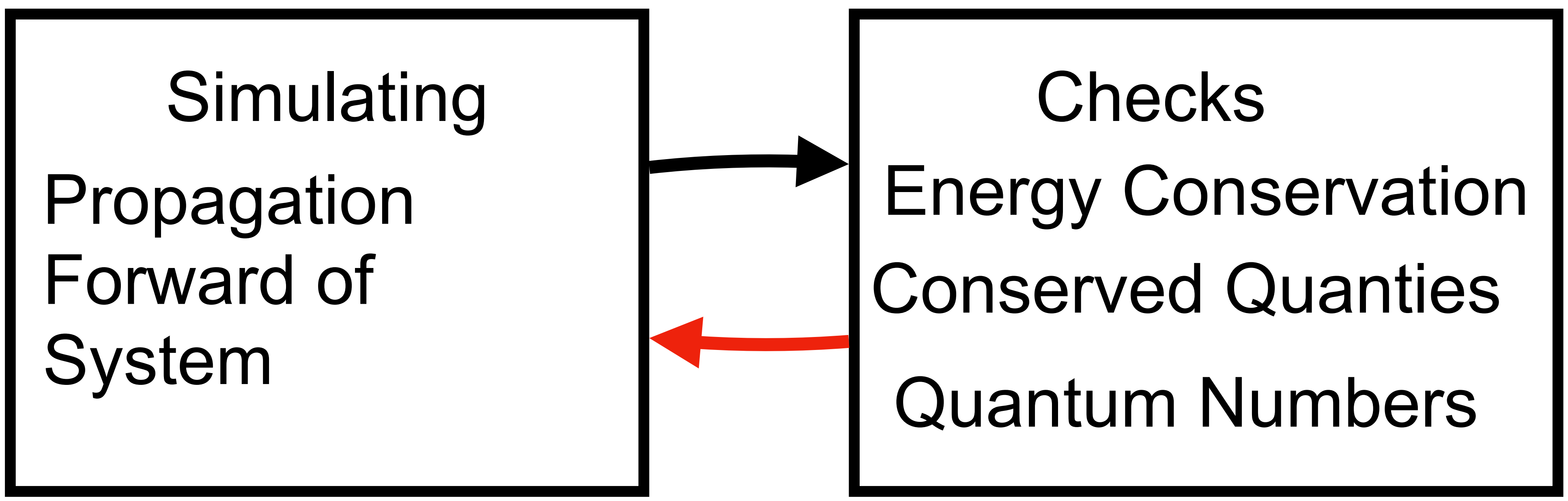
    - There are a few things we can do to make it better
        - Key is to have a notion of when we are going wrong



Correct Our Simulation Through a Probabilistic Rescaling

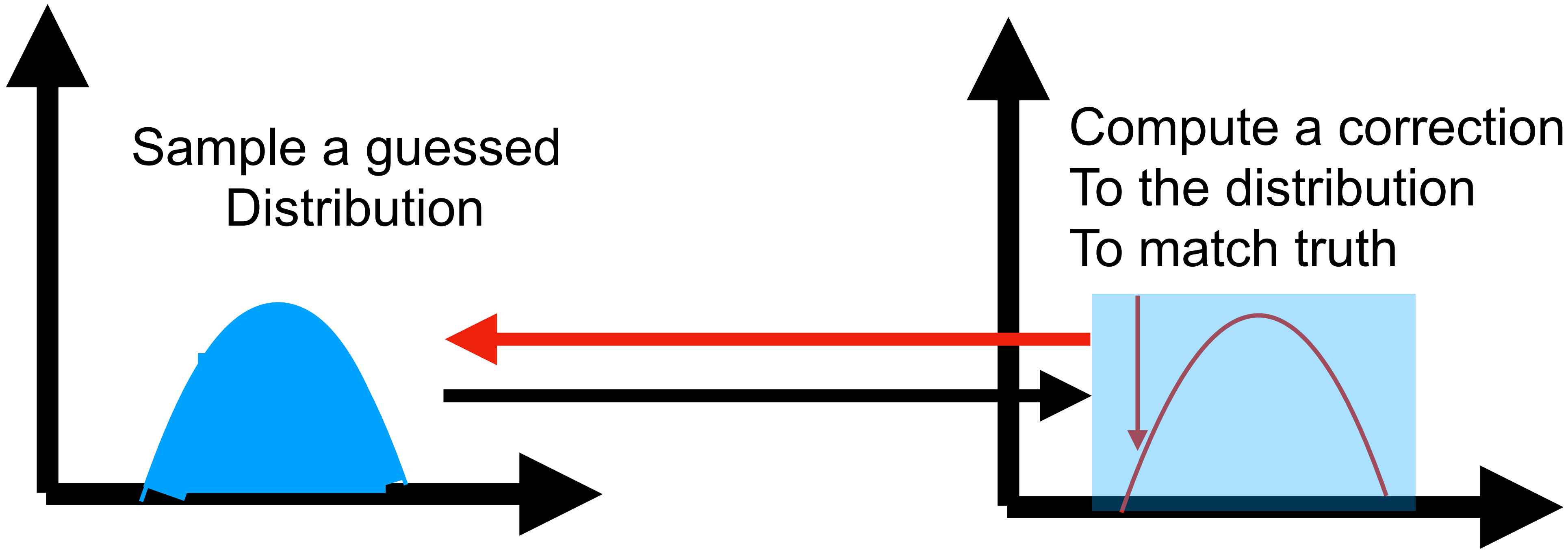
Markov Chain MC

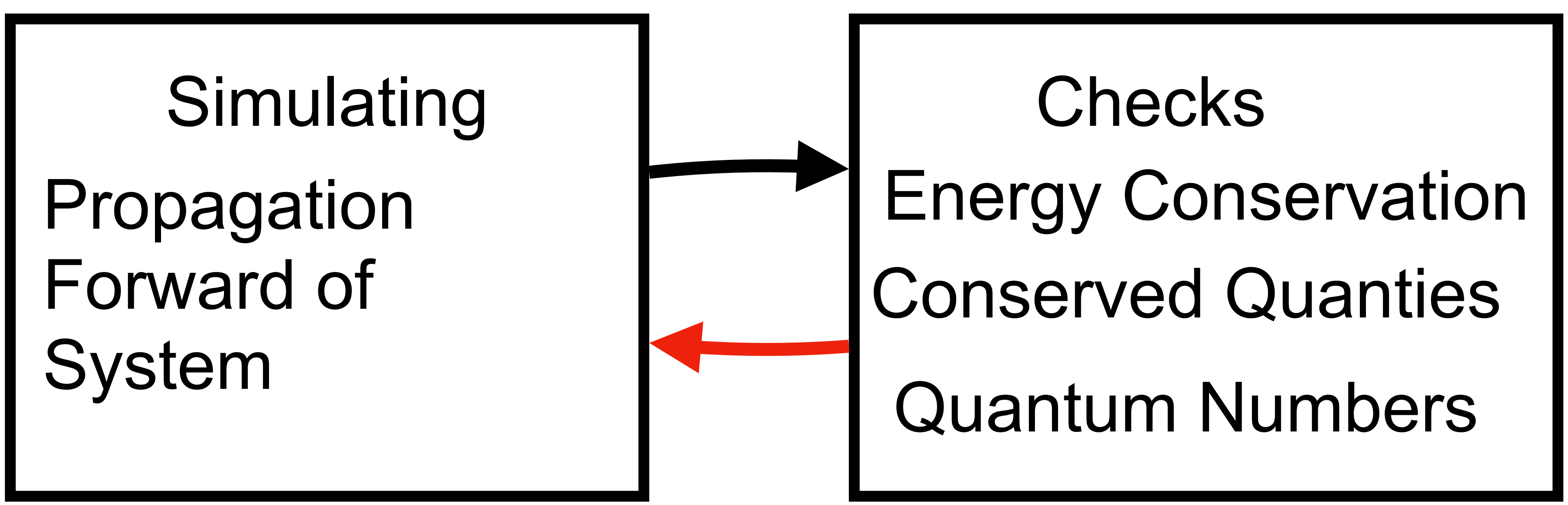




Correct Our Simulation Through a Probabilistic Rescaling

Markov Chain MC





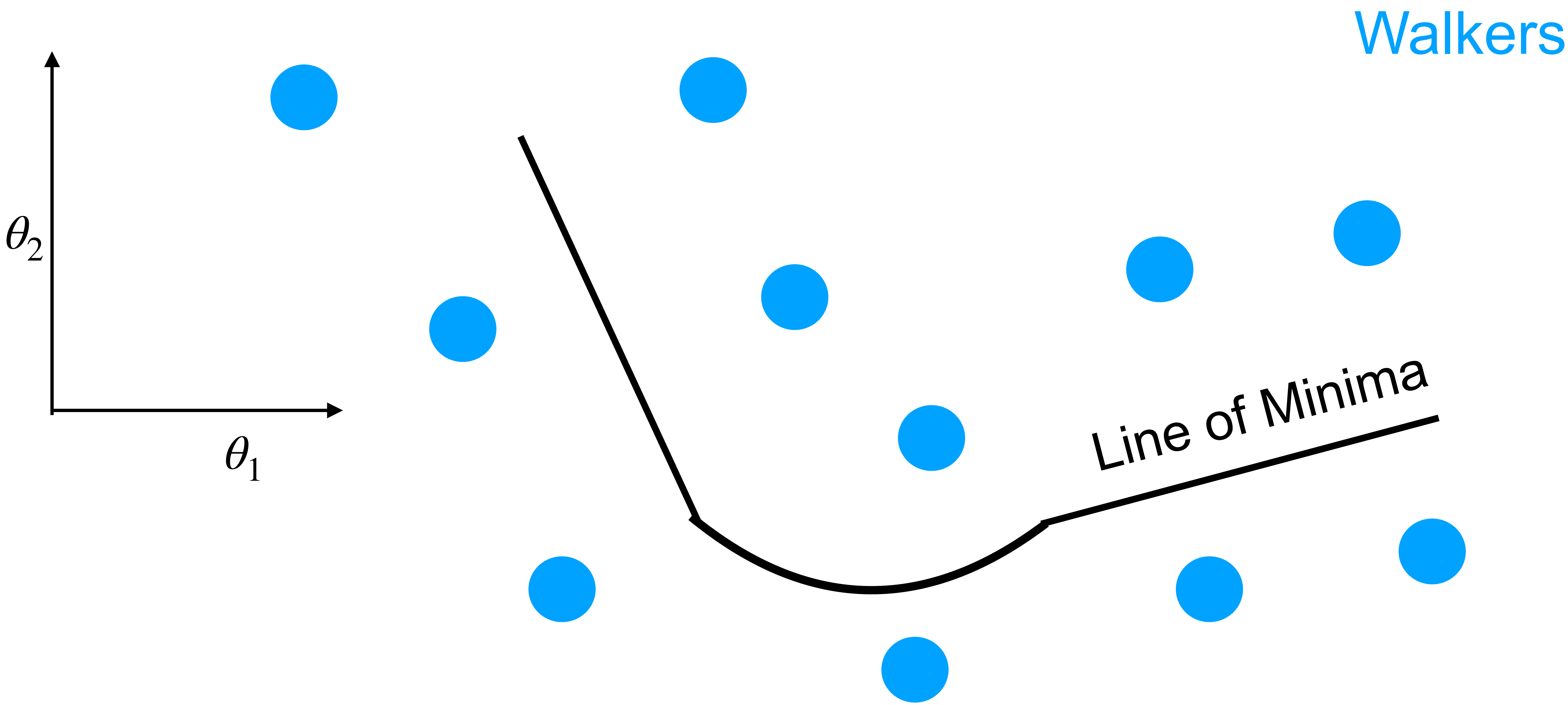
Correct Our Simulation Through a Probabilistic Rescaling

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

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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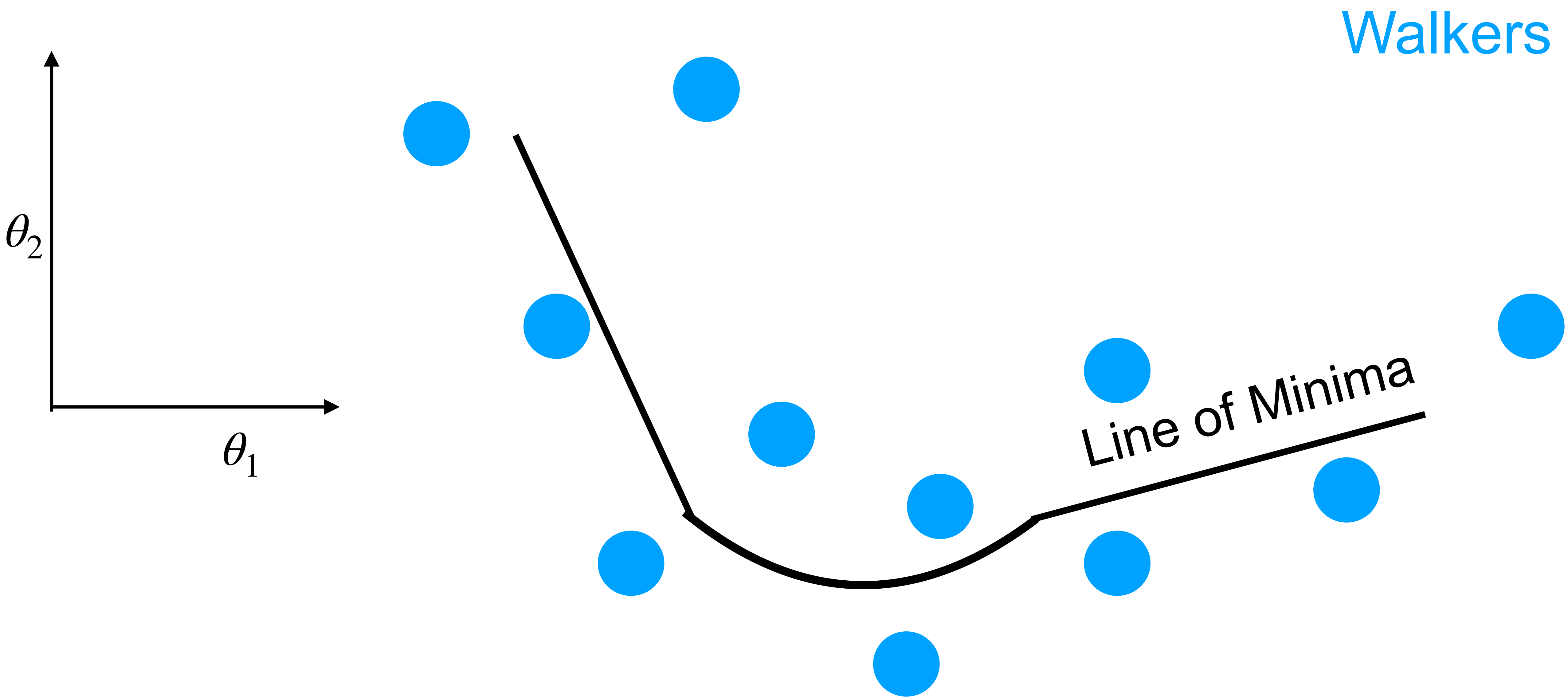

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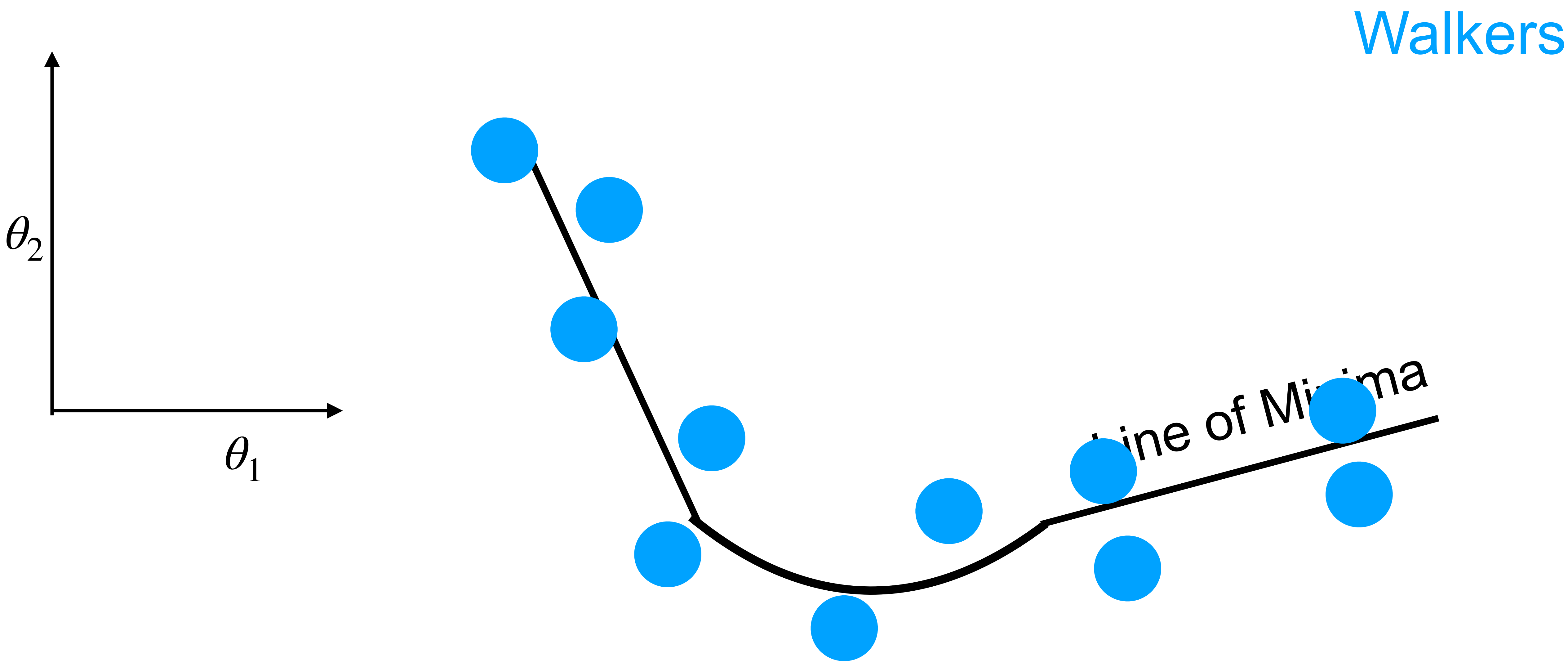
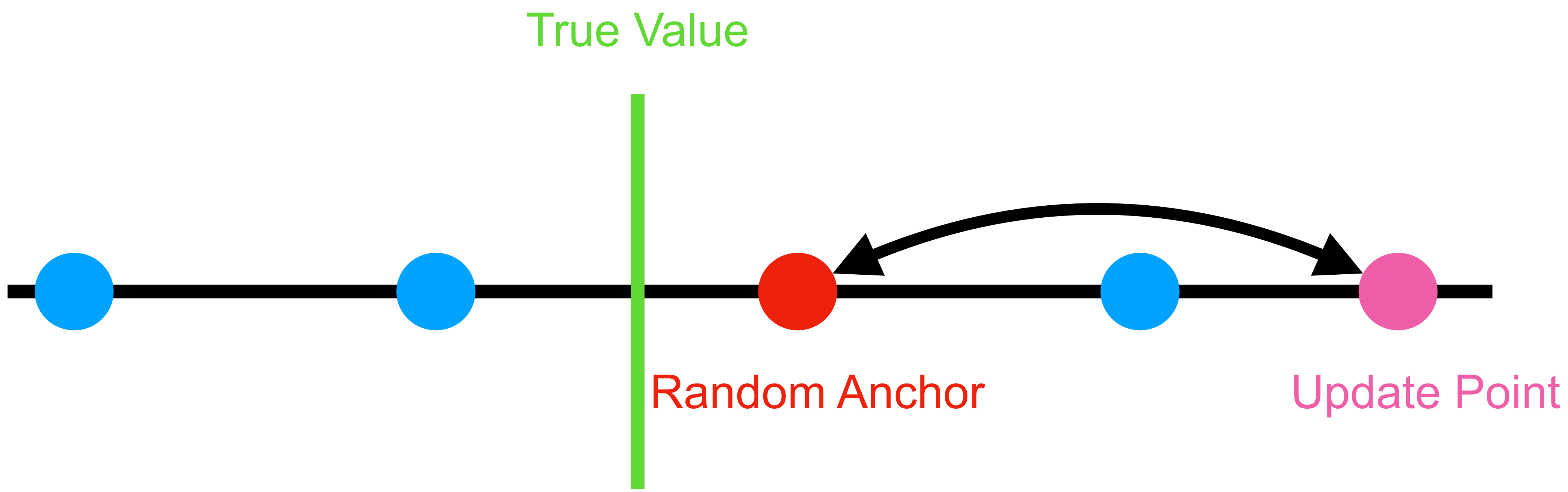


Example Fit



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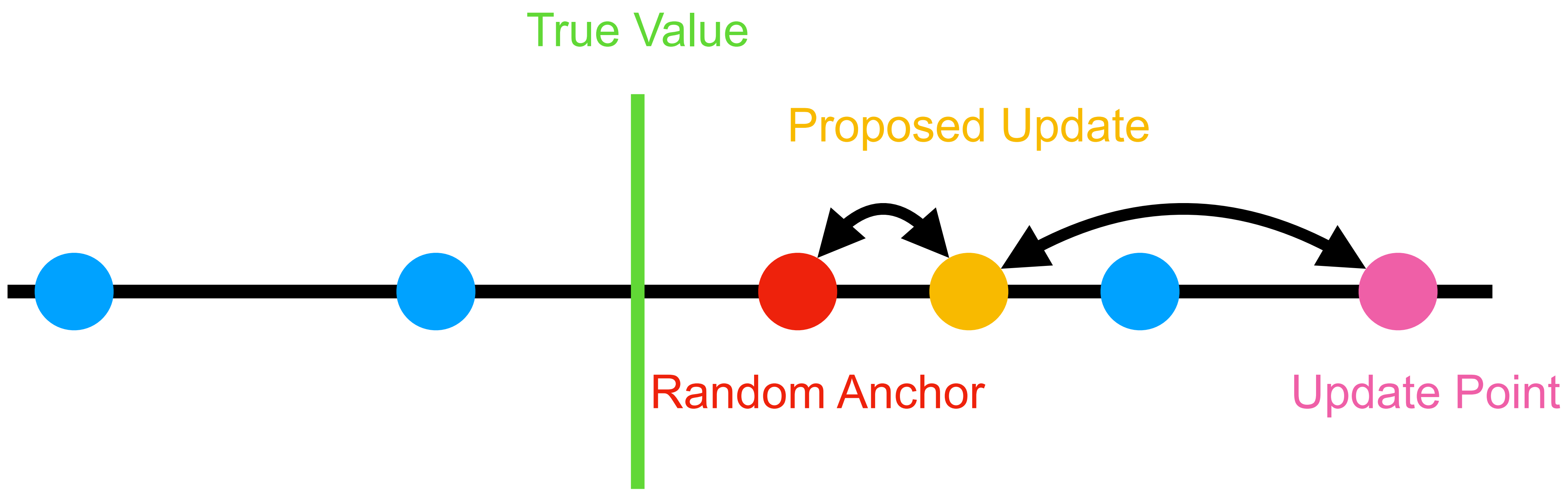
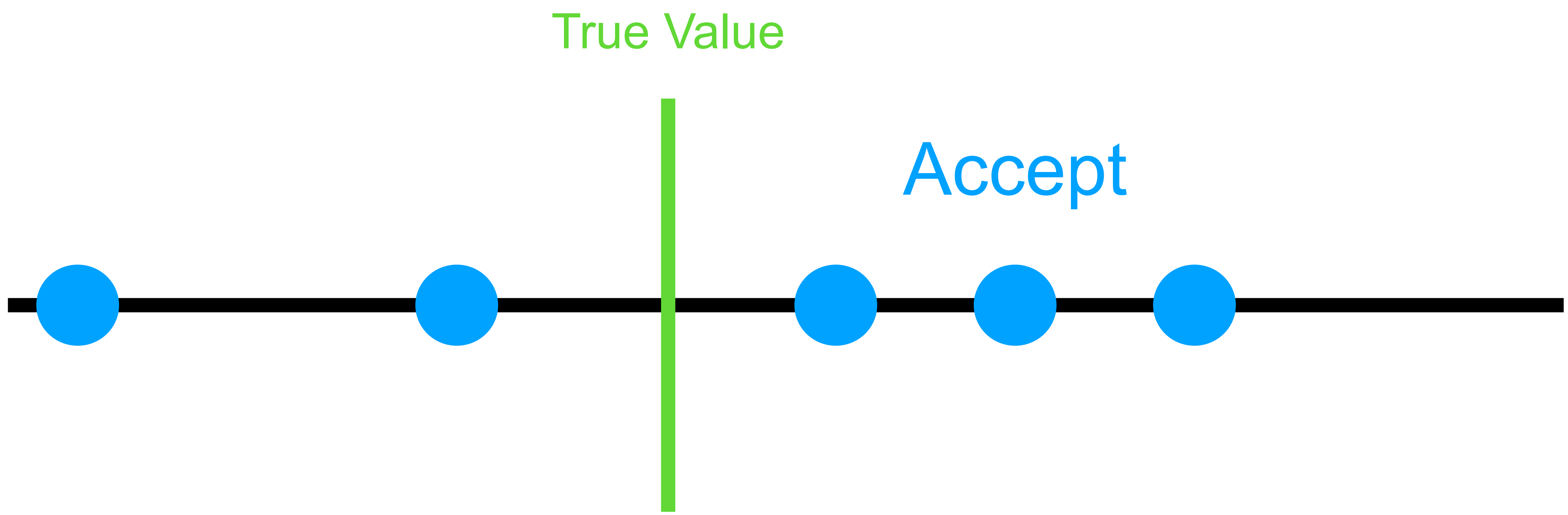
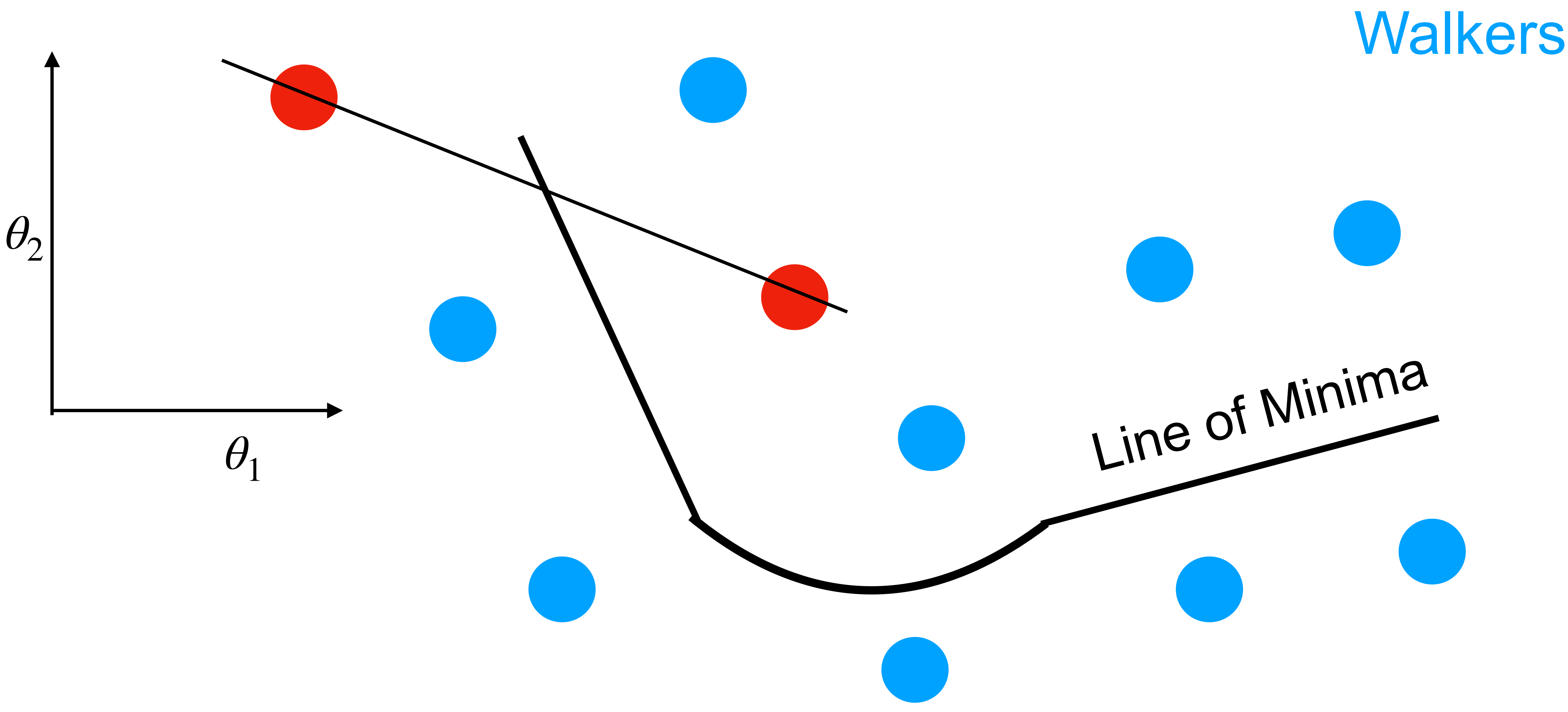


Example Fit



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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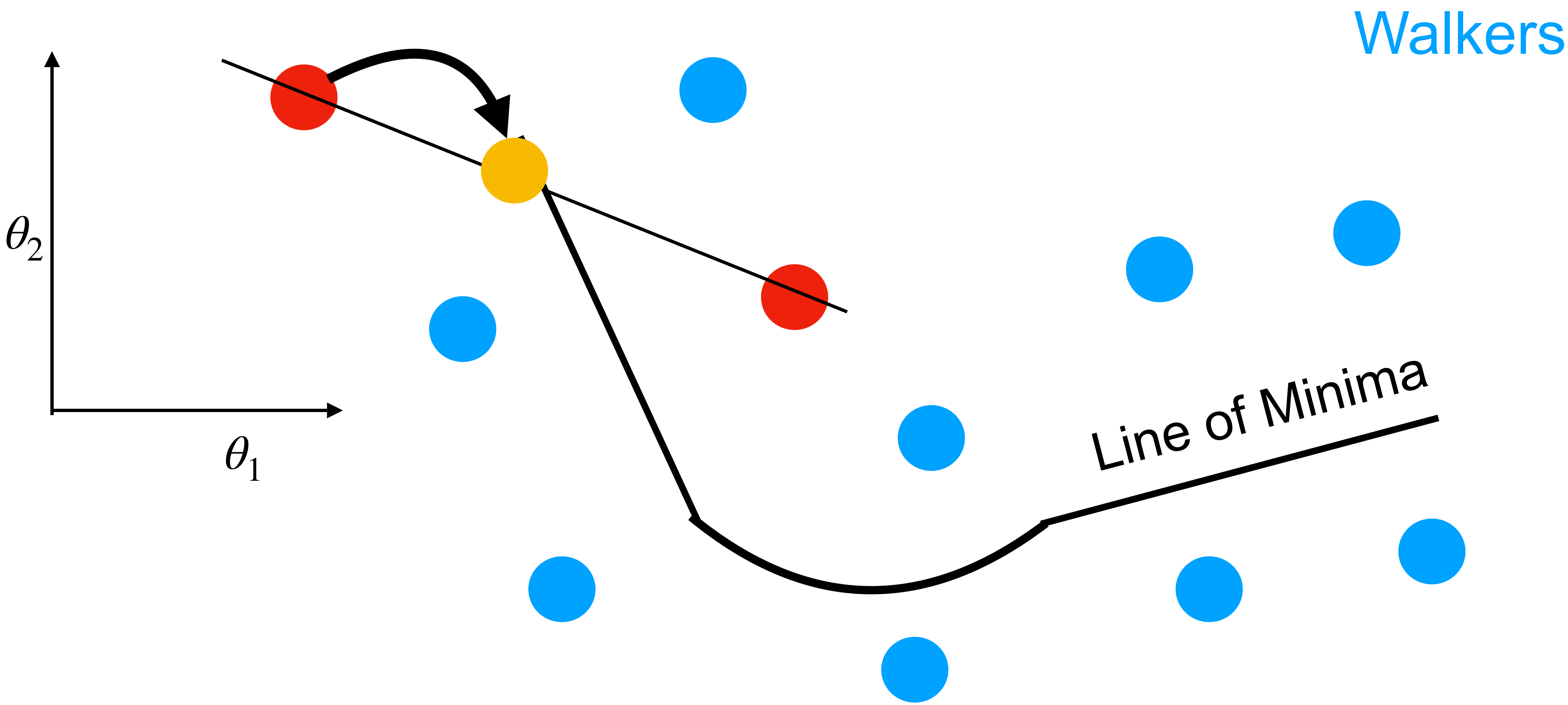

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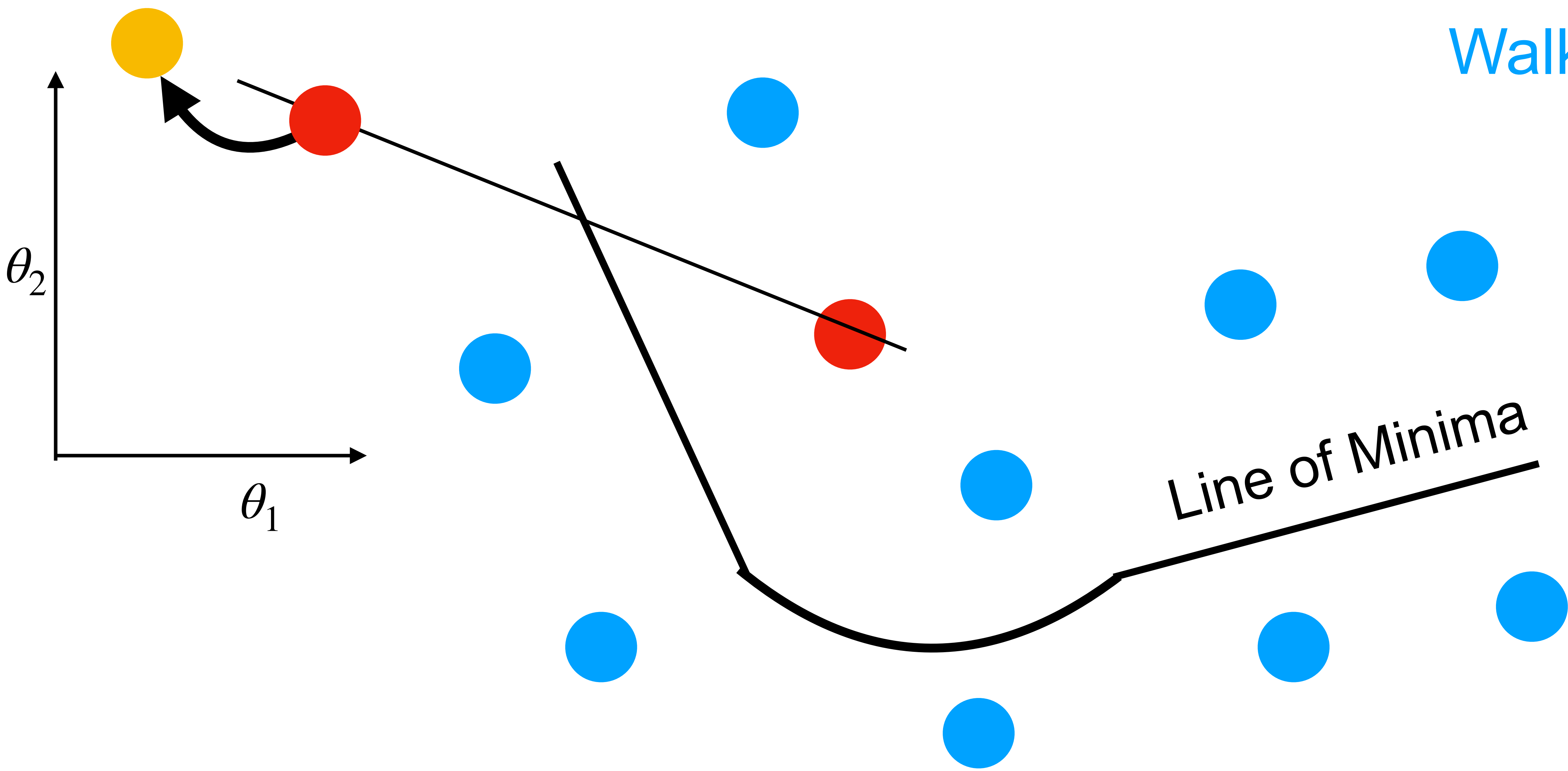

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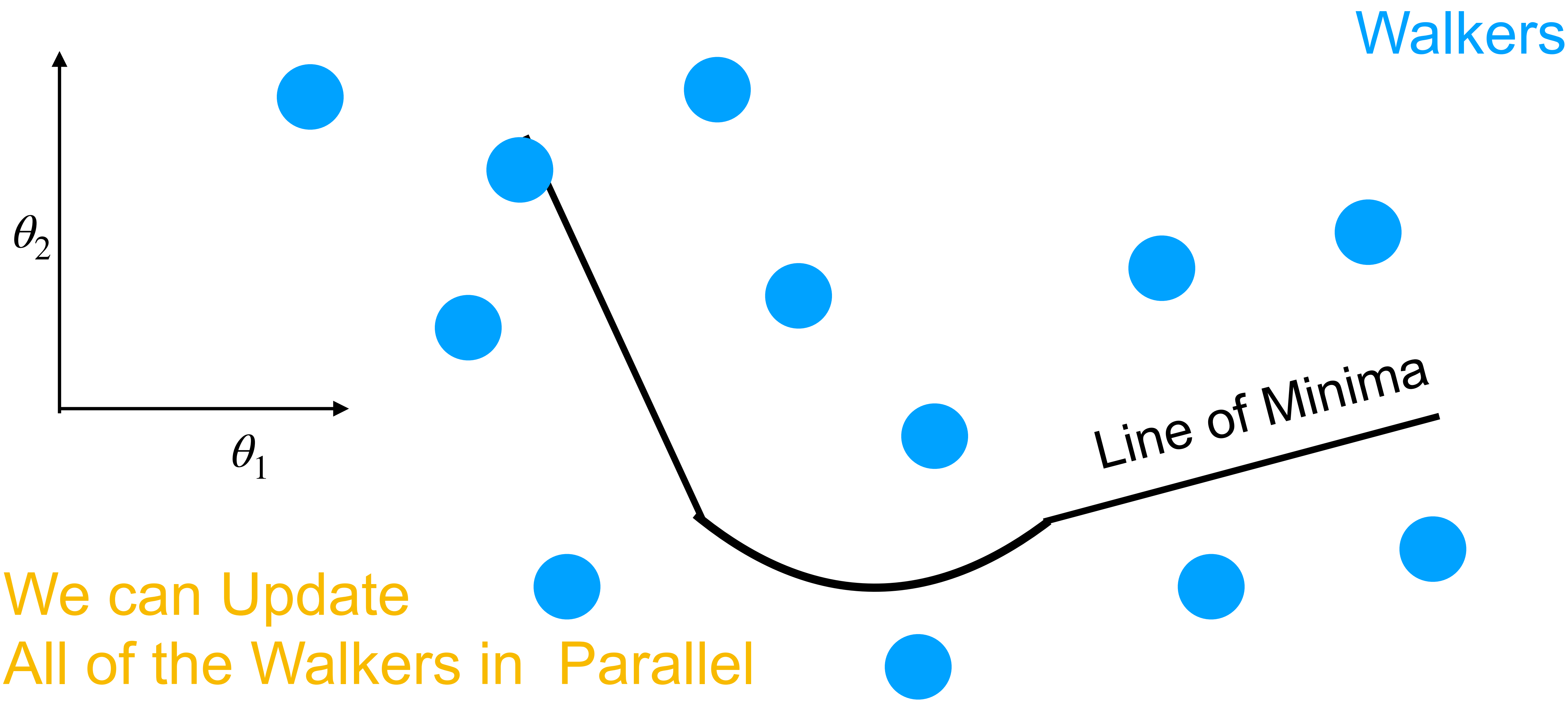

Speeding up MCMC

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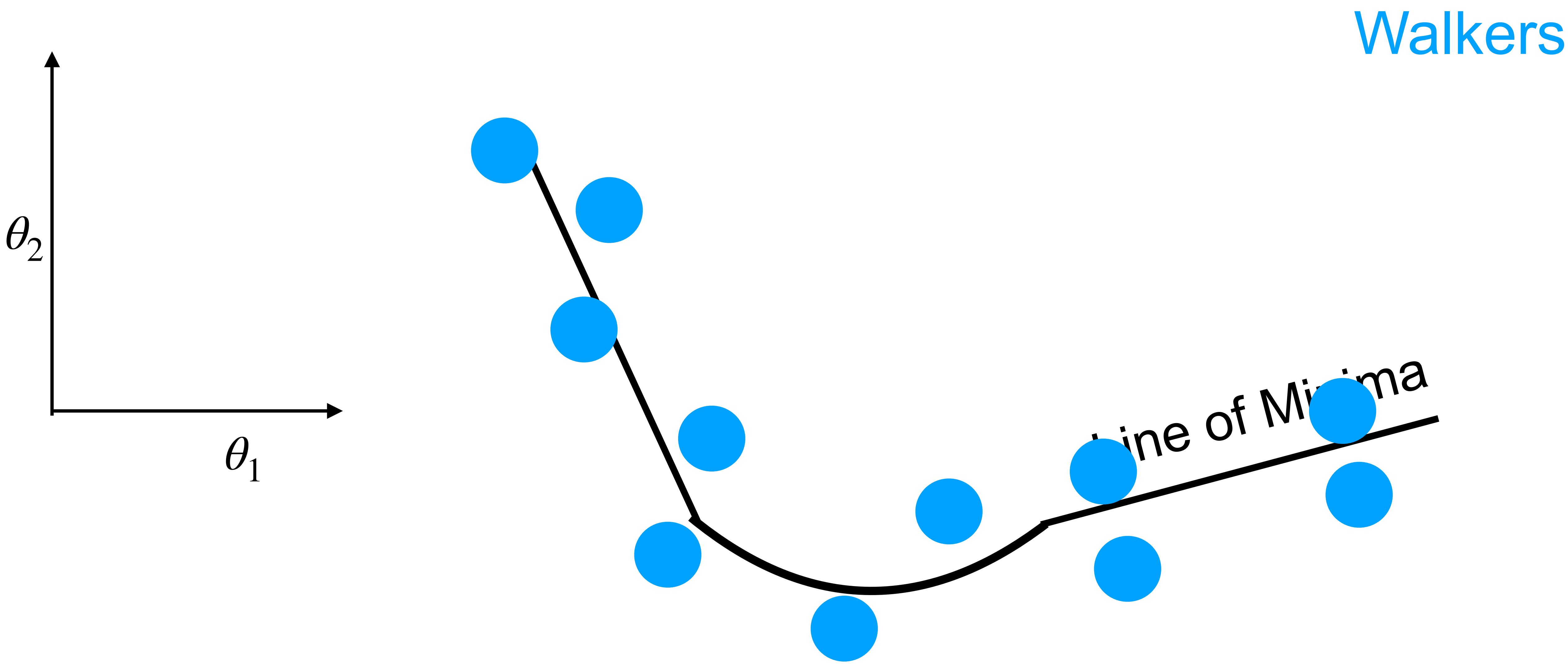


Visualizing in Bayes

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

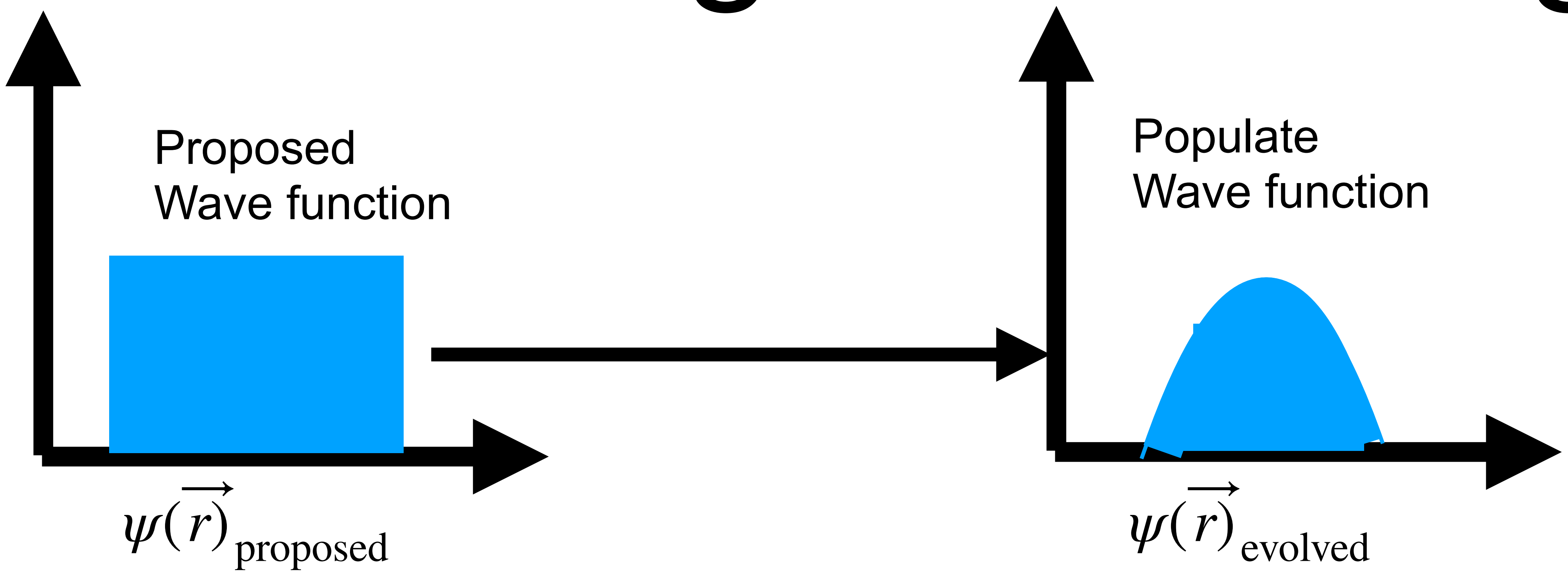
$$\sum_j p_j(\vec{r}\,|\,\vec{\theta}) = \frac{\psi_j^*(\vec{r}\,|\,\vec{\theta})\psi_j(\vec{r}\,|\,\vec{\theta})}{\langle\psi\,|\,\psi\rangle}$$

We can define probability from wavefunction

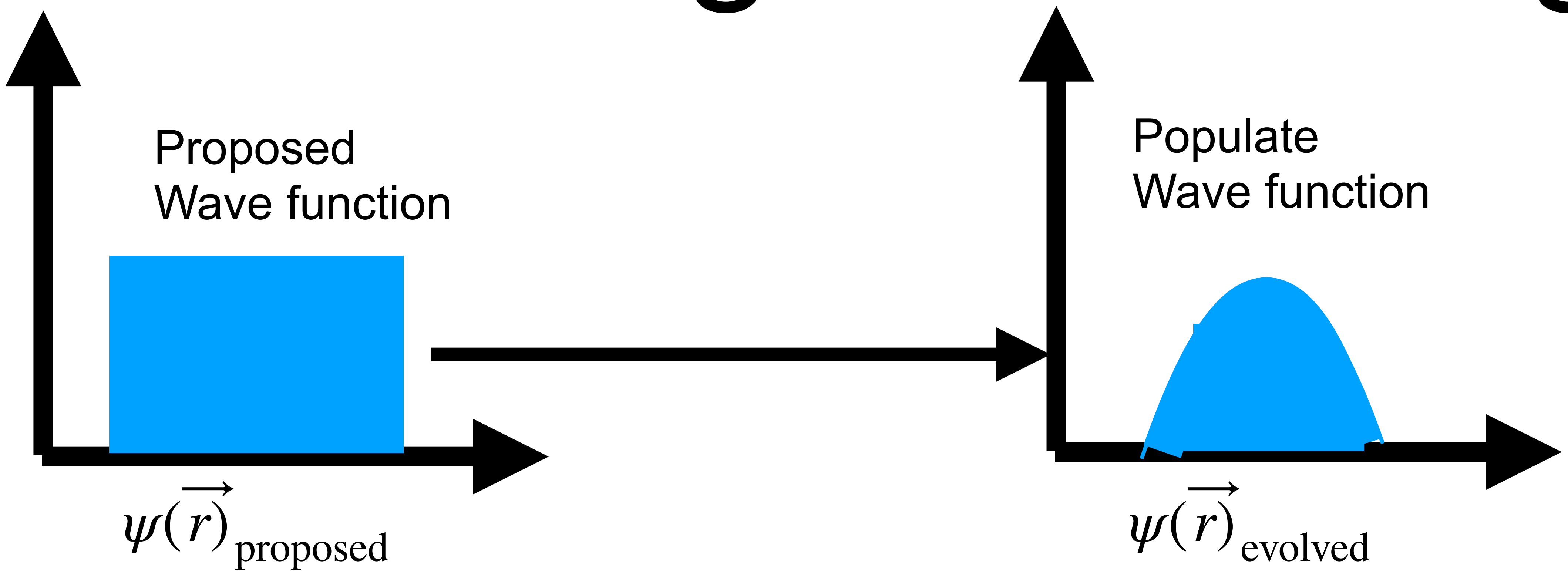
$$\sum_j w_{i+1}^j = \frac{p_j(\overrightarrow{r_{i+1}}\,|\,\vec{\theta})}{p_j(\overrightarrow{r_i}\,|\,\vec{\theta})}$$

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

Solving Schroedinger



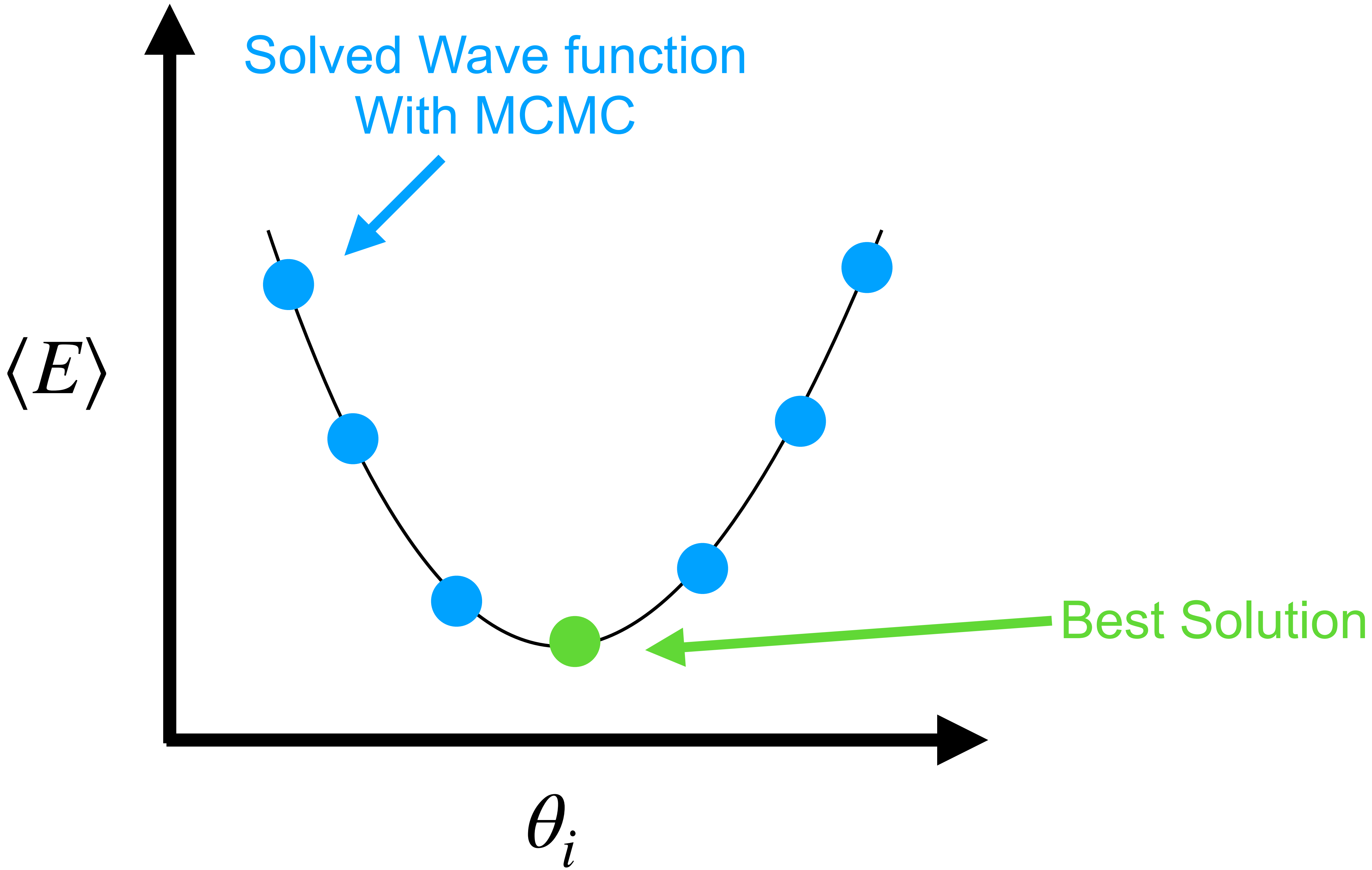
Solving Schroedinger



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

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

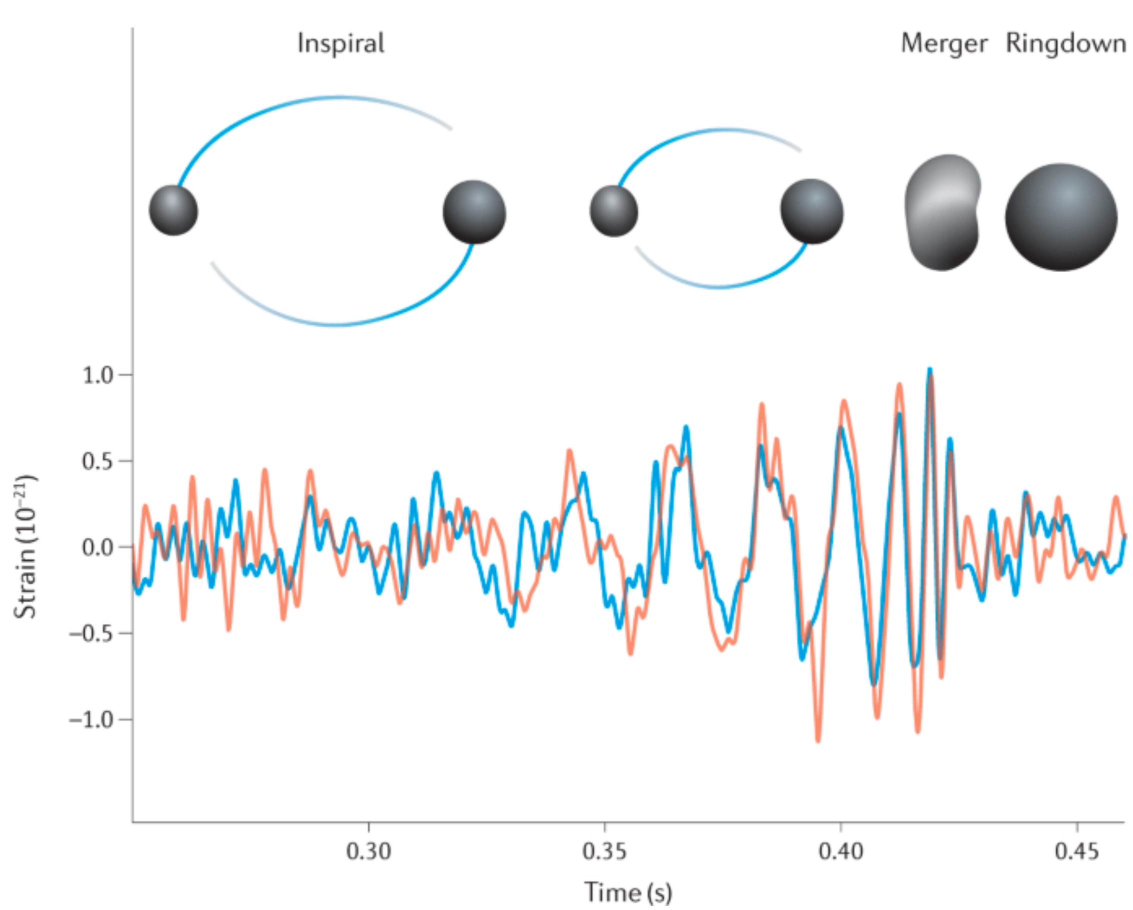
Solving Schroedinger

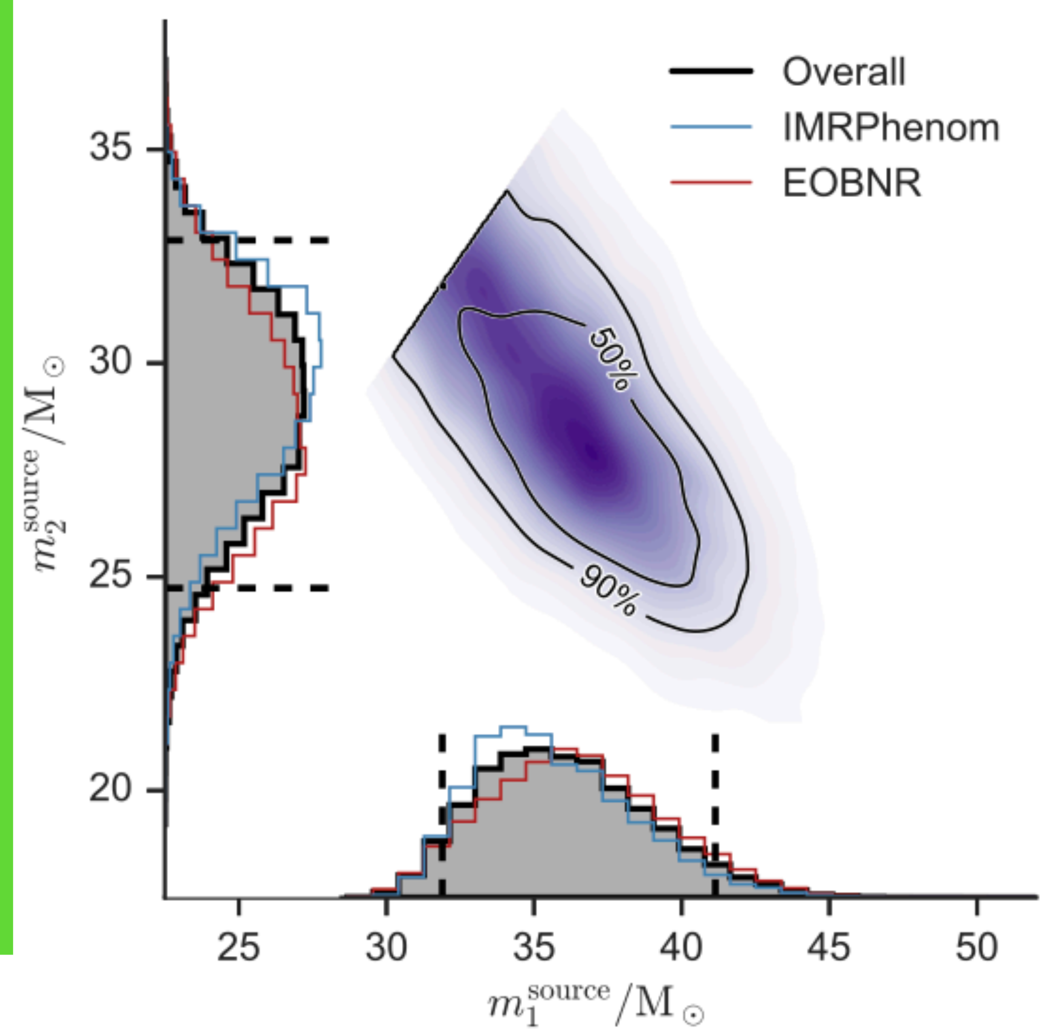


Our goal is to minimize the Energy given a wave functional form

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

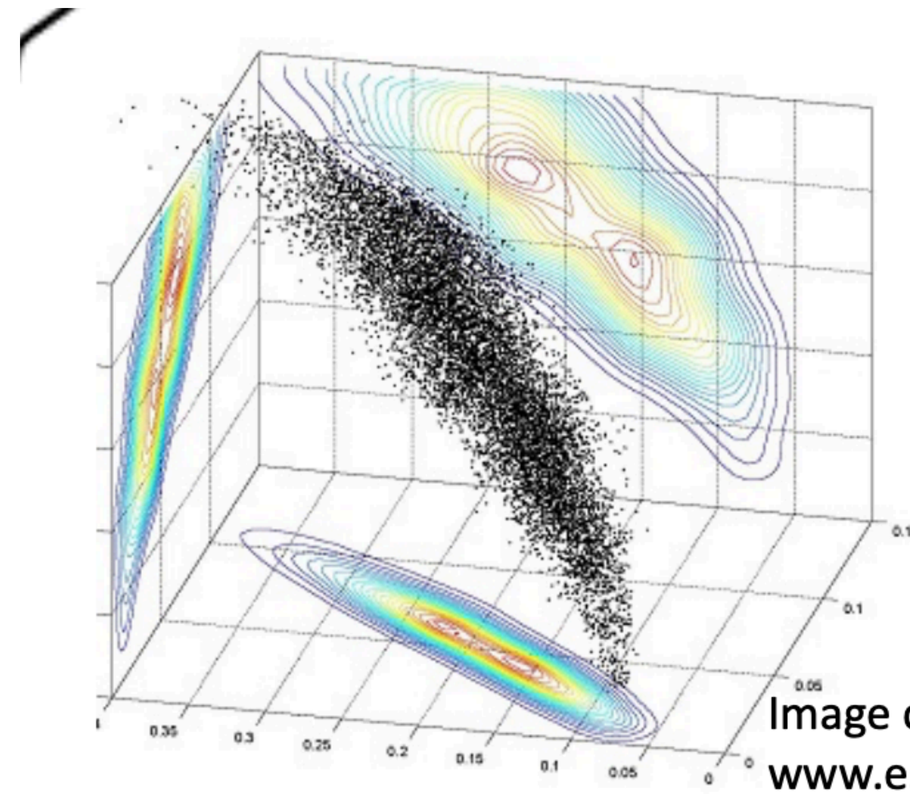


Image credit: www.essenceps.com

- 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

Visualizing in Bayes

Posterior probability of the model in light of the data

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Equilibrated Best Fit

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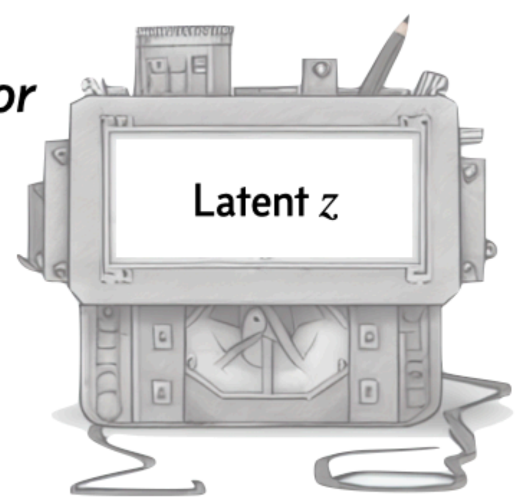
Simulation Based Inference

Simulation-based inference (SBI)

Simulator

Parameters θ →  → Observations x

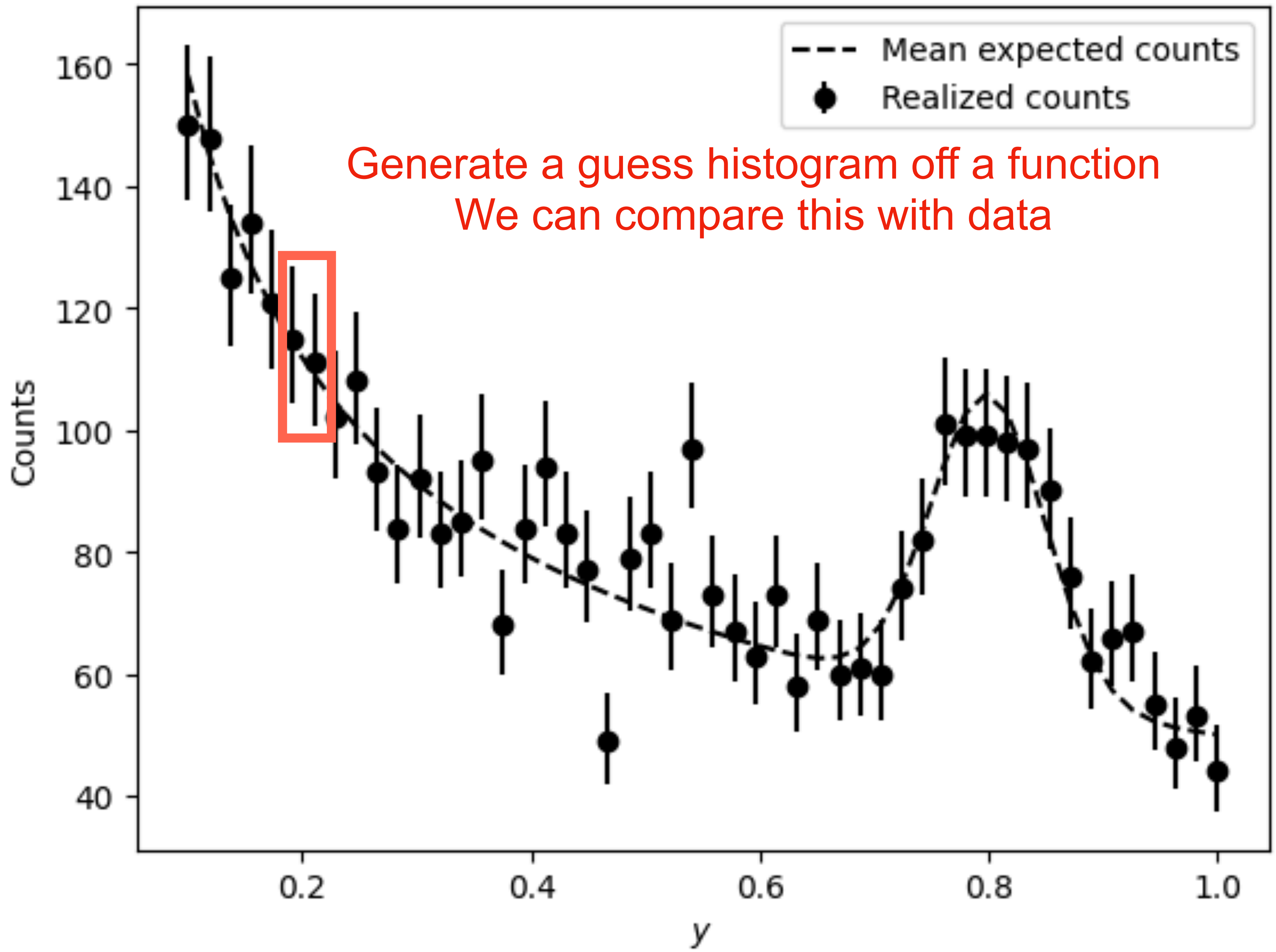
Prediction:

- Mechanistic forward model
- We can generate samples from a simulator $x \sim p(x \mid \theta)$

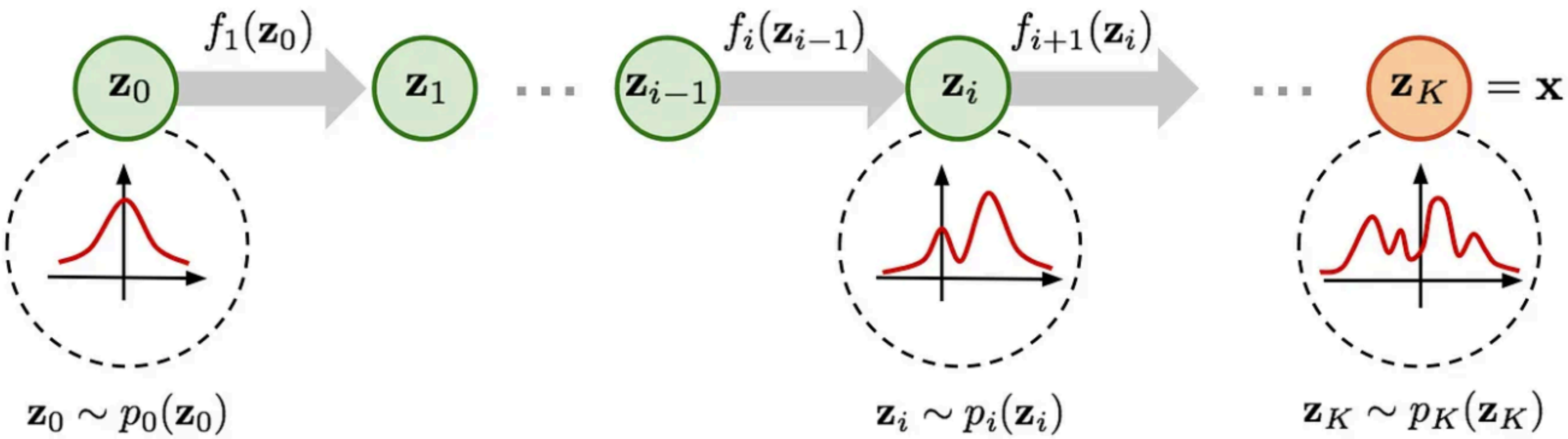
Inference:

- Likelihood $p(x \mid \theta) = \int \mathrm{d}z \, p(x, z \mid \theta)$ is intractable
- *Inference is challenging*

Poisson Fluctuation



Normalizing Flow



$$z \sim p_\theta(z) = N(z; 0, 1)$$

$$x = f_\theta(z) = f_K \circ \ldots f_2 \circ f_1(z)$$

each f_i is invertible

How Does it Work?

$$f : Z \to X,\ f\, is\, invertible$$

$$p_\theta(z)\, defined\, over\, z \in Z$$

$$p_\theta(x) \neq p_\theta(f_\theta^{-1}(x)))$$

Change of variable formula:

$$p_\theta(x) = p_\theta(f_\theta^{-1}(x))) \left| det(\frac{\partial f^{-1}(x))}{\partial x}) \right|$$

$$p_\theta(x) = p_\theta(z)) \left| det(\frac{\partial z}{\partial x}) \right|$$

$$\log\left(p_\theta(x)\right) = \log\left(p_\theta(z)\right) \ + \ \sum_{i=1}^{K} \log \left| det(\frac{\partial f_i^{-1}}{\partial z_i}) \right|$$

exact likelihood evalutation

Poisson flucutate a func

“Traditional” SBI: *Approximate Bayesian Computation*

[Rubin 1984]