Probabilistic Programming Languages

Guillaume Baudart
Christine Tasson

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MCMC Metropolis-Hastings

Probabilistic Programming Languages

Markov Chain Monte Carlo (MCMC)

Main idea

- Create a Markov chain that converge to the posterior distribution
- Iterate the process until convergence
- Generate samples to approximate the distribution

Pros

- Faster convergence
- Better results for high-dimensional models
- Advanced state-of-the-art optimizations (e.g., HMC, NUTS).

Cons

- Convergences?
- Traps: multimodal, funnel
- Samples correlation

Reminder: Rejection Sampling

coin.ml

```
let coin prob data =
  let z = sample prob (uniform ~a:0. ~b:1.) in
  List.iter (observe prob (bernoulli ~p:z)) data;
  z

let _ =
  let d = infer coin [ 1; 1; 0; 0; 0; 0; 0; 0; 0; 0 ] in
  plot d
```

Executing the model generates one sample

- `sample`: draw from a distribution
- `assume`/`observe`: hard conditioning, reject invalid samples
- Terminates with n valid samples

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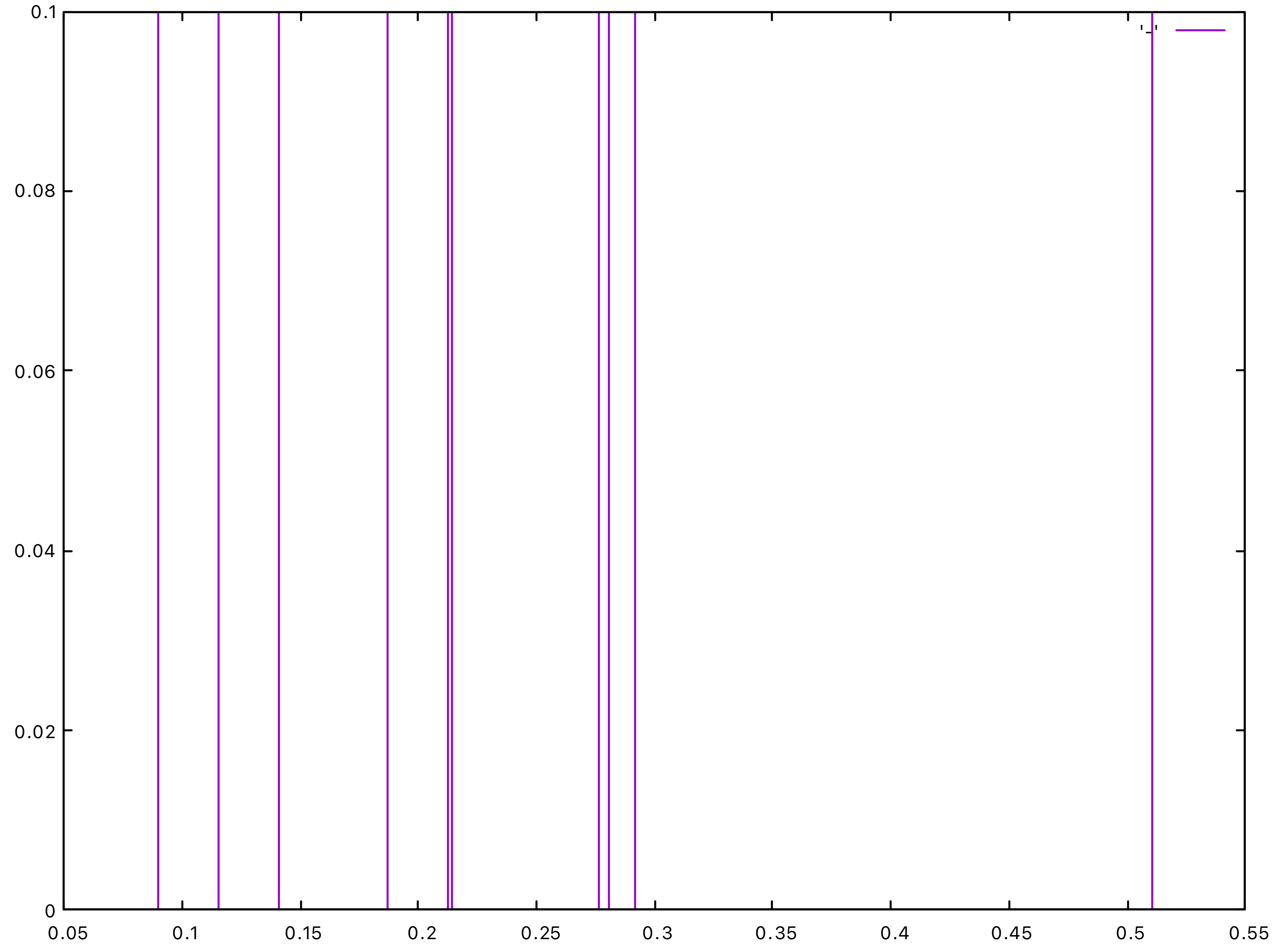
10 particles



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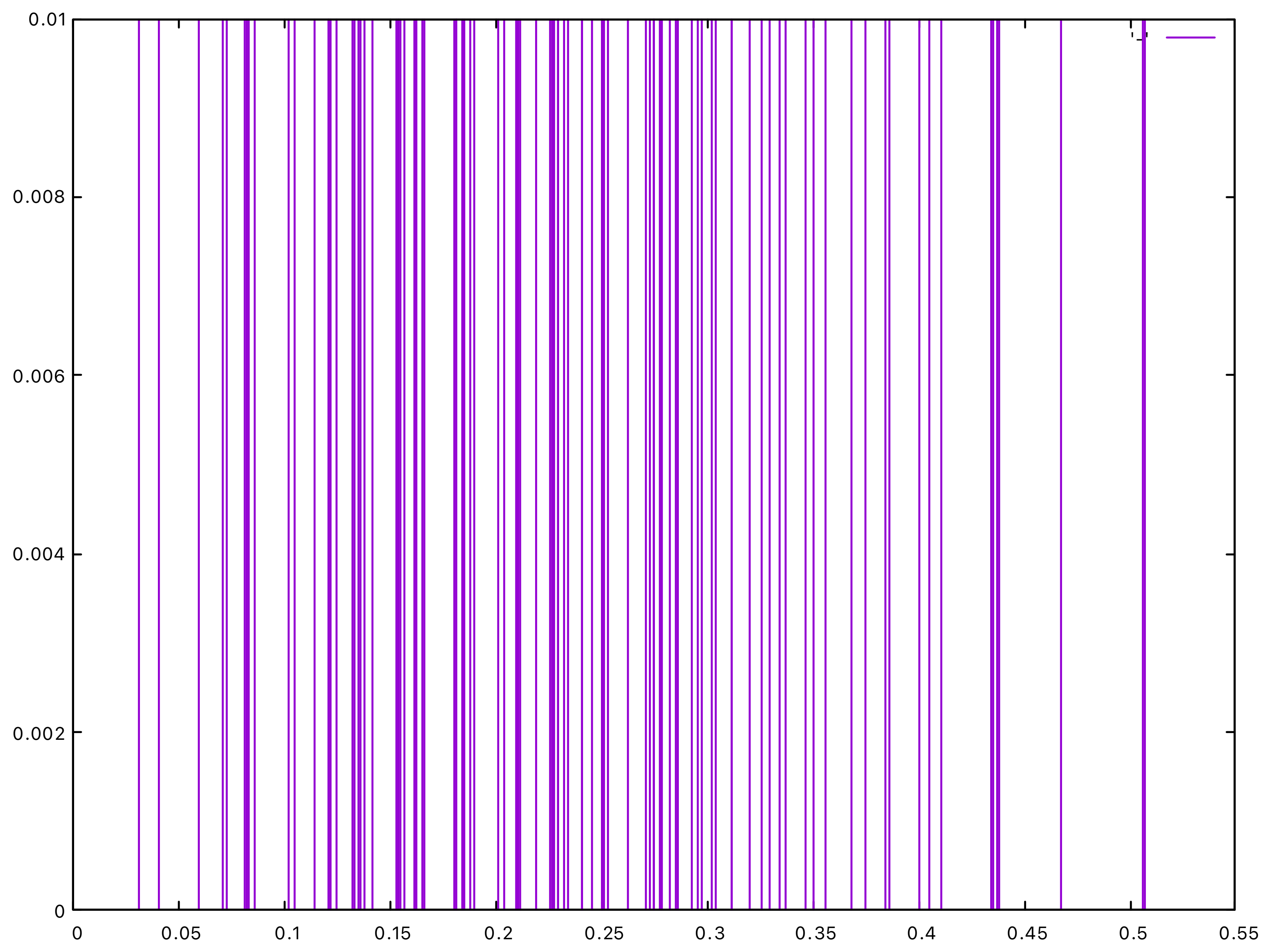

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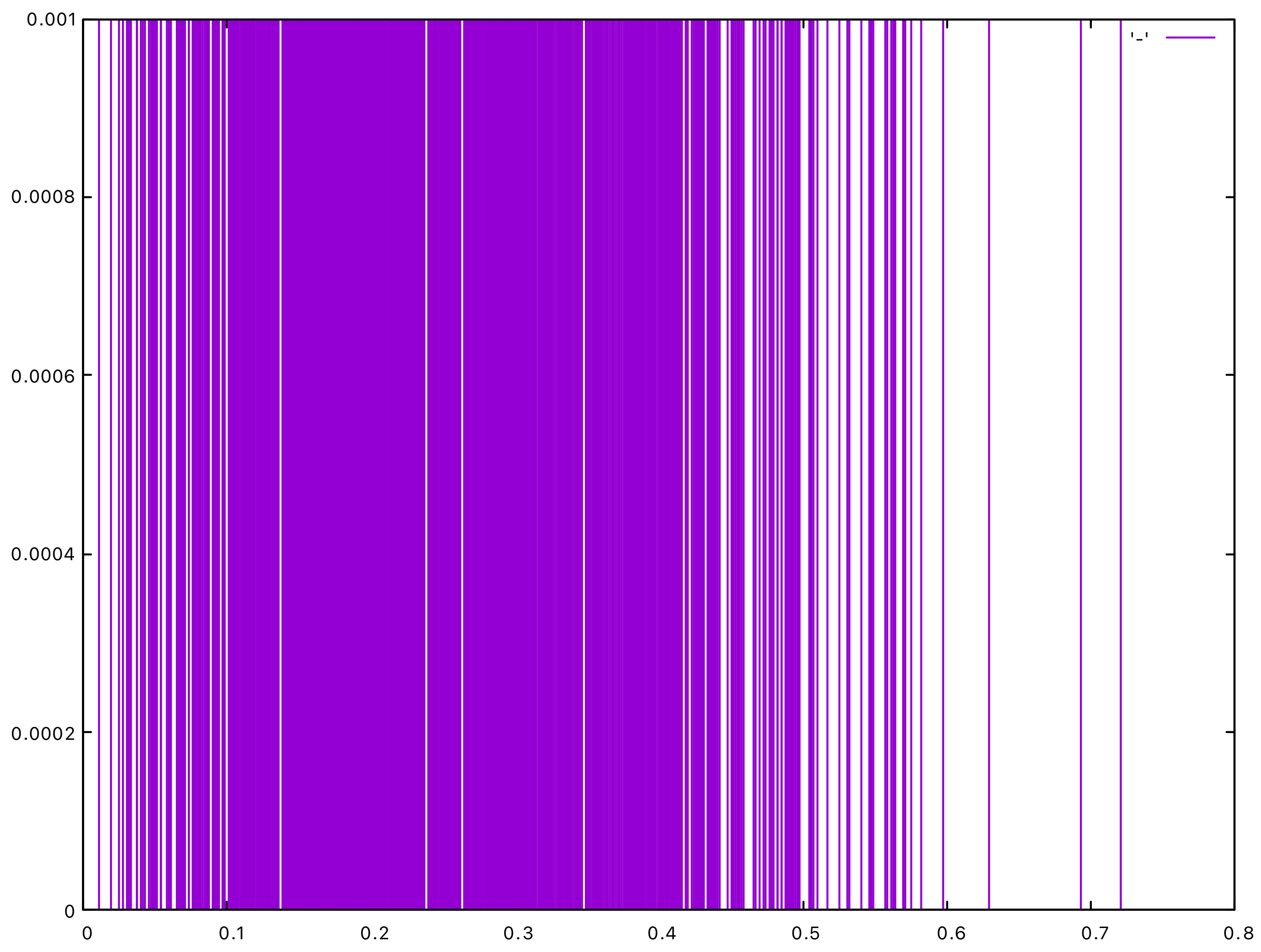
1000 particles



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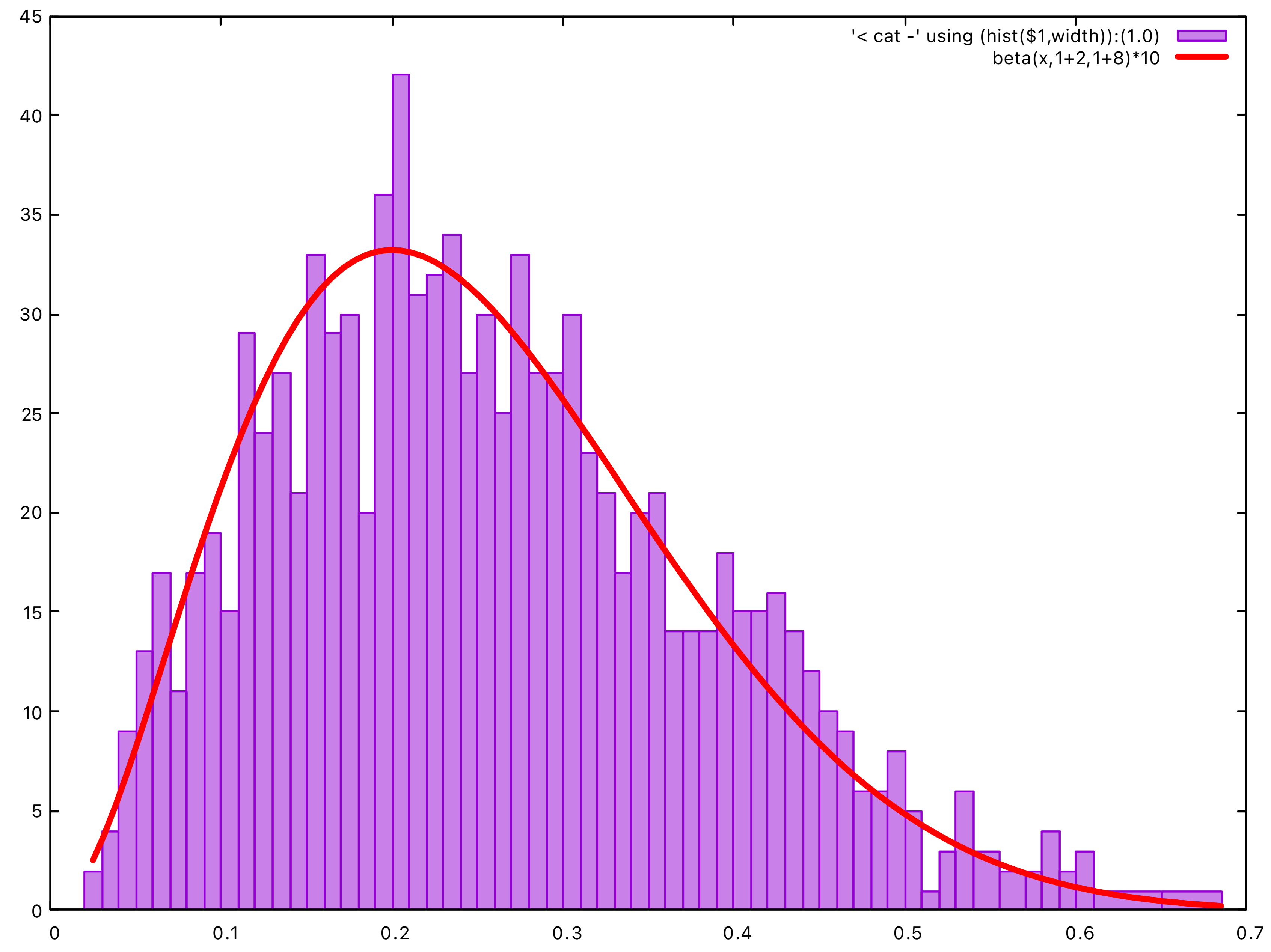

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Weighted Rejection Sampling

Adapt rejection sampling to soft conditioning

- Execute the sampler to get a pair (v_i, w_i)
- Suppose $w_{\max}$ is known
- Accept the sample with probability $w_i / w_{\max}$ or retry

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- Suppose $w_{\max}$ is known
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But $w_{\max}$ is not known...

Execution Trace

Consider a program execution with

- $X = x_0, \ldots, x_n$: set of random variables sampled at step i : the trace
- $Y = y_0, \ldots, y_m$: set of random variables observed at step i.

Remarks

- Sets X and Y depend on the execution path
- We can only control X

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let bimodal y =
  let z = sample (bernoulli ~p:0.5) in
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    if z then sample (gaussian ~mu:-1. ~sigma:1.)
    else sample (gaussian ~mu:1. ~sigma:1.)
  in
  let () = observe (gaussian ~mu ~sigma:1.) y in
  z
```

Multi-Sites Metropolis Hastings

Markov chain on execution traces

- Execute the sampler to get a trace and associated score (X_i, w_i)
- If $w_i \geq w_{i-1}$ accept the trace (and the associated output)
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- Otherwise return the previous trace X_{i-1}

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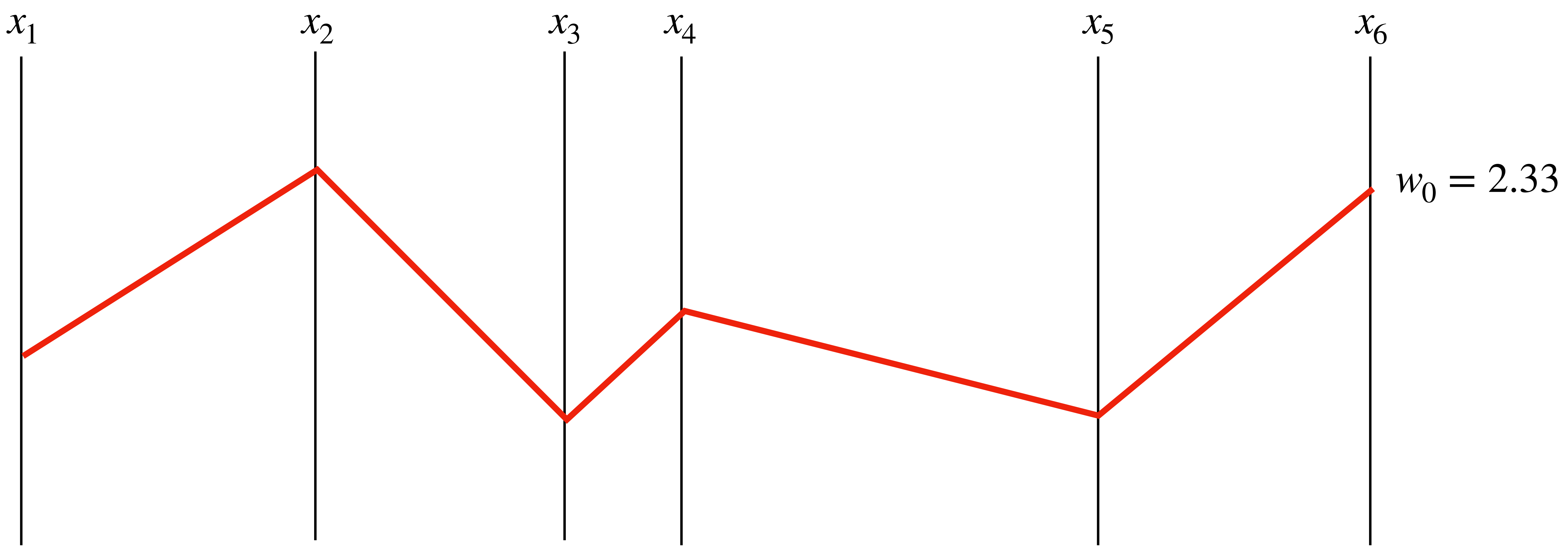

outputs

v_0

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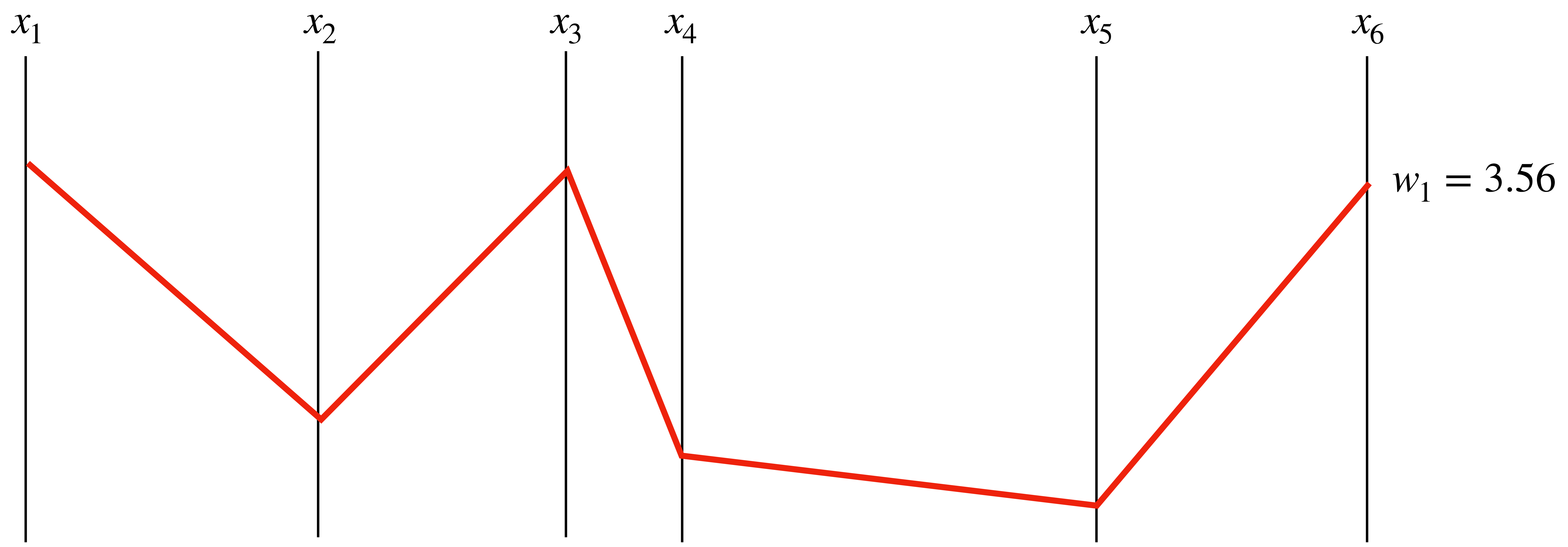

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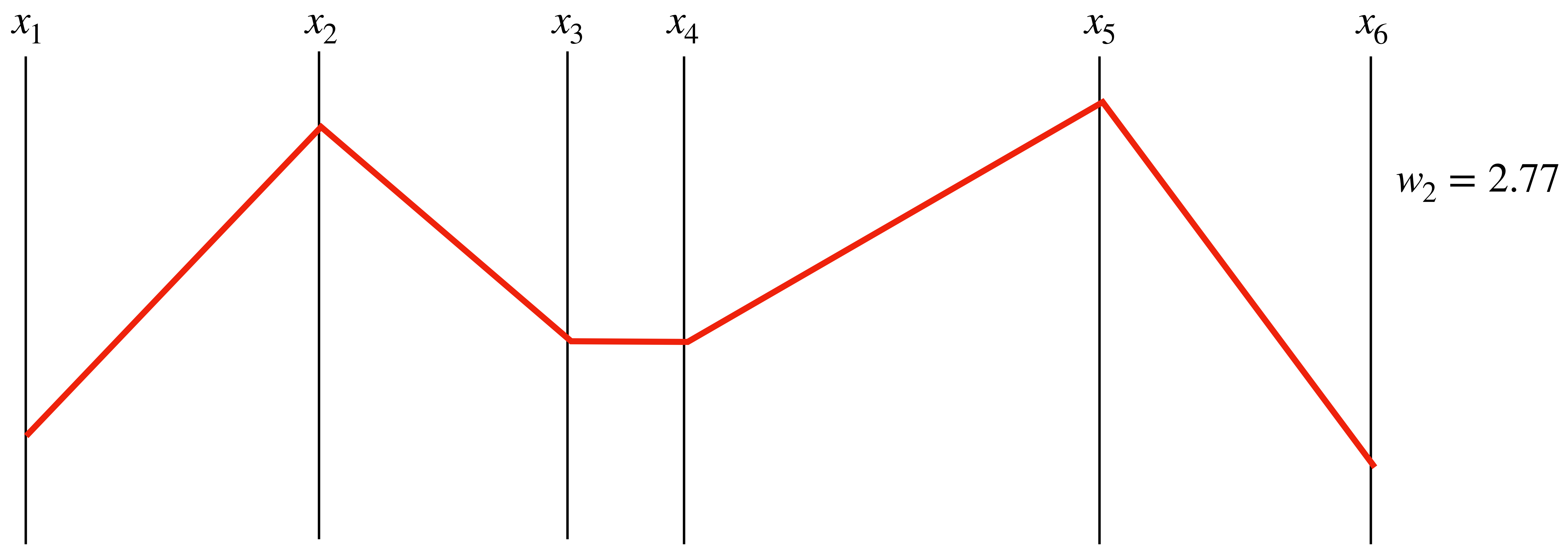

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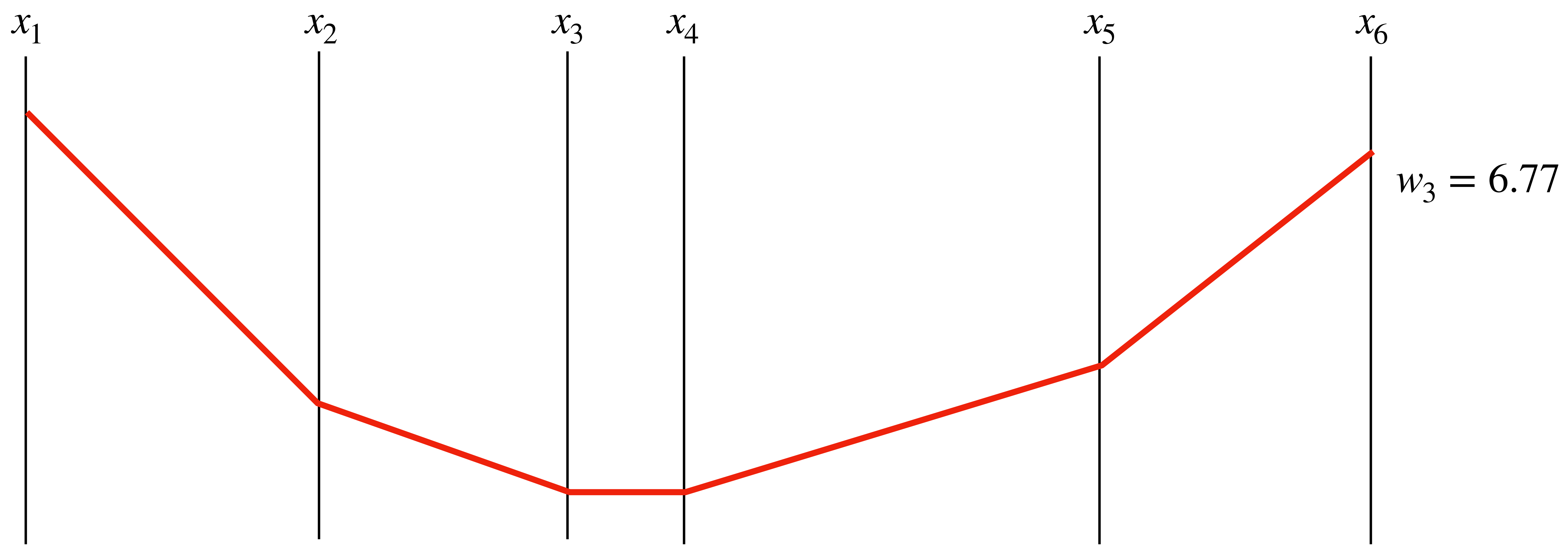

outputs

v_0

v_1

v_1

v_3

...

General Metropolis Hastings

More generally

- $X = x_0, \ldots, x_n$: set of random variables sampled at step i: the trace
- $Y = y_0, \ldots, y_m$: set of random variables observed at step i.
- Propose a new trace from a proposal distribution $q(X_i | X_{i-1})$
- Accept the trace with probability α, where

$$\alpha = \min\left(1, \frac{p(X_i, Y_i)}{p(X_{i-1}, Y_{i-1})} \frac{q(X_{i-1} \mid X_i)}{q(X_i \mid X_{i-1})}\right)$$

- Otherwise return the previous trace X_{i-1}

Multi-Sites Metropolis Hastings: Acceptation

- Draw proposal from priors: $q(X_i \mid X_{i-1}) = p(X_i)$
- Resample all variable in X_i at each step

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\begin{aligned}
\frac{p(X_i, Y_i)}{p(X_{i-1}, Y_{i-1})} \frac{q(X_{i-1} \mid X_i)}{q(X_i \mid X_{i-1})} &= \frac{p(Y_i | X_i)\, p(X_i)}{p(Y_{i-1} \mid X_{i-1})\, p(X_{i-1})} \frac{q(X_{i-1} \mid X_i)}{q(X_i \mid X_{i-1})} \\
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&= \frac{p(Y_i | X_i)}{p(Y_{i-1} \mid X_{i-1}))} \\
&= \frac{w_i}{w_{i-1}}
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Reuse most of the previous trace (i.e., sampled values)

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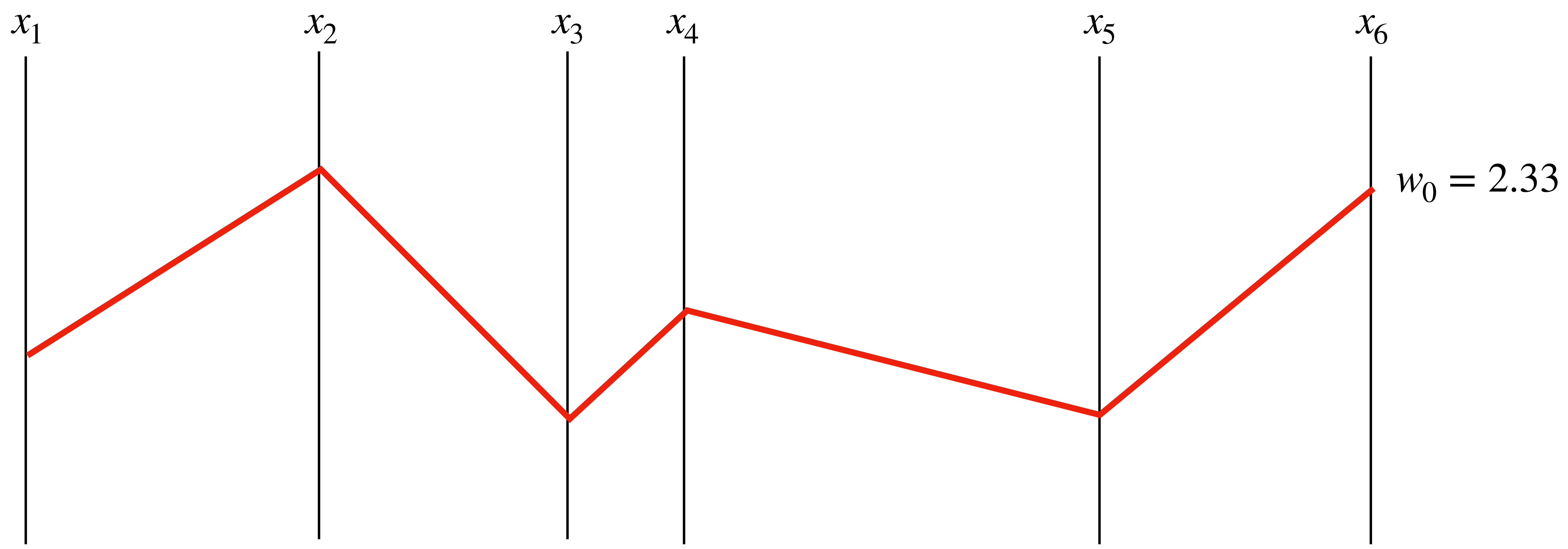

samples

v_0

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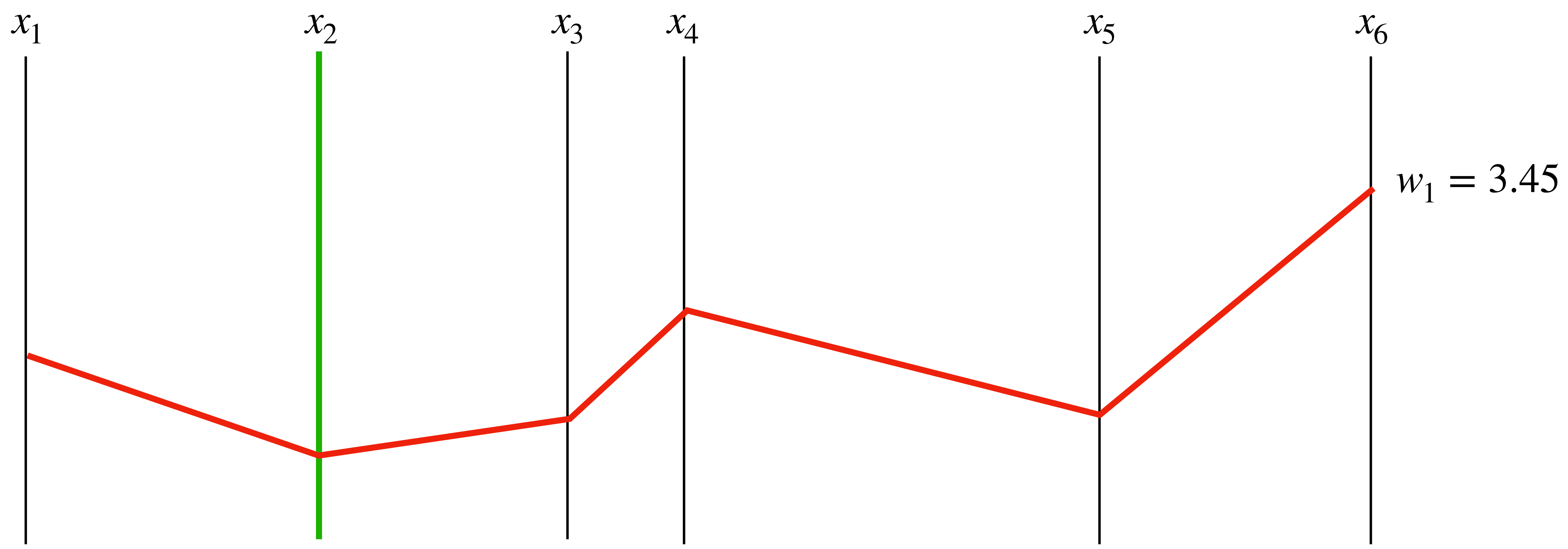

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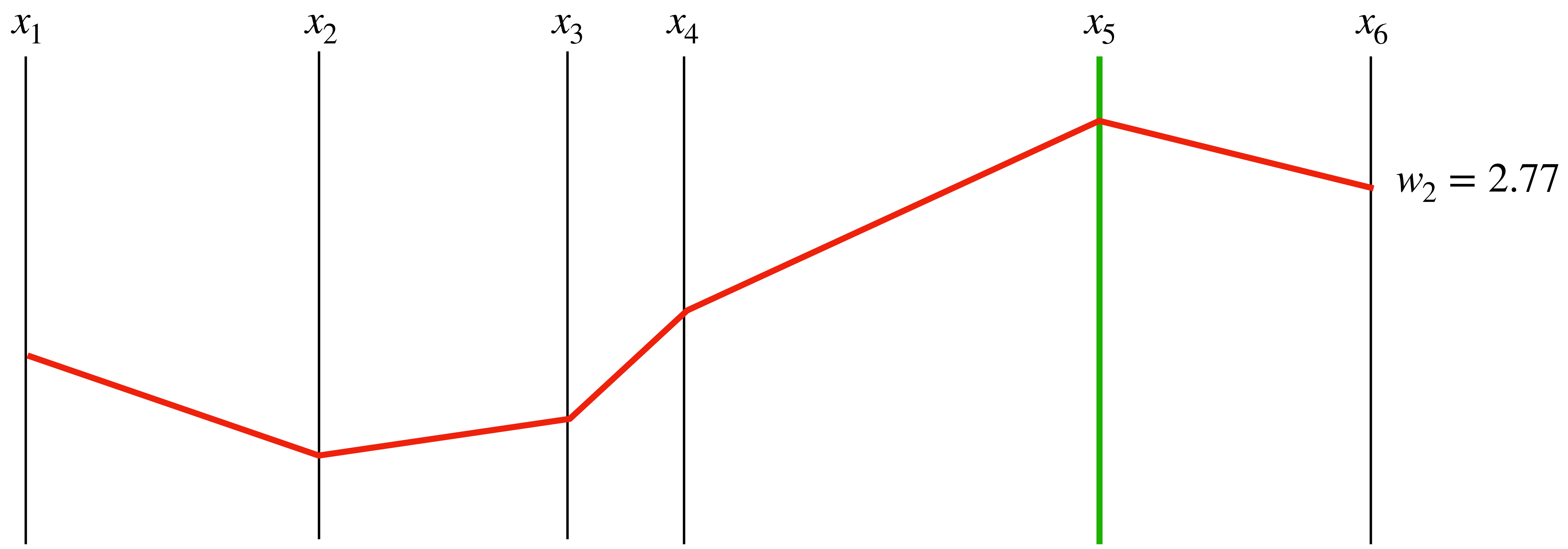

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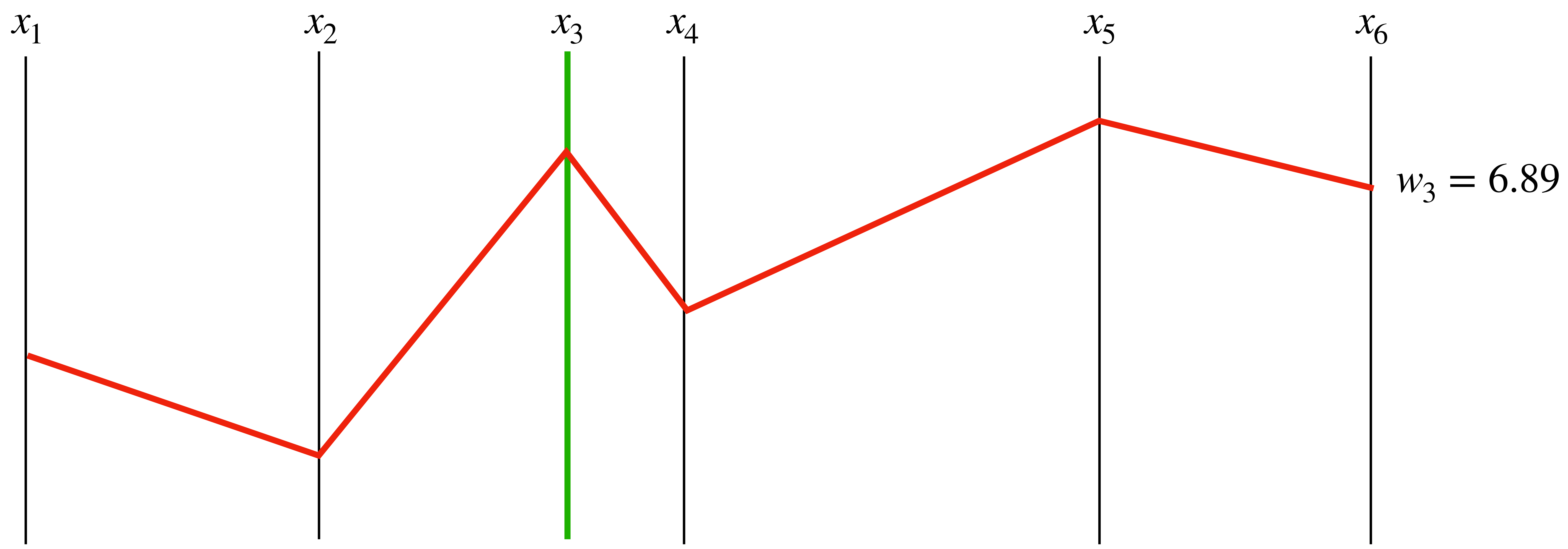

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v_0

v_1

v_1

v_3

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Track the likelihood of all random variable during execution

- `x = sample d → w(x) = (x, pdf d x)`
- `observe d y  → w(y) = (y, pdf d y)`

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```
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Track the likelihood of all random variable during execution

- `x = sample d → w(x) = (x, pdf d x)`
- `observe d y  → w(y) = (y, pdf d y)`   score (as in importance sampling)

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- Pick one variable x_0 at random in the trace
- Resample only this variable and all its dependencies $X = X^{\text{sample}} \cup X^{\text{reuse}}$

$$\frac{p(X_i, Y_i)}{p(X_{i-1}, Y_{i-1})} \frac{q(X_{i-1} \mid X_i)}{q(X_i \mid X_{i-1})} = \frac{p(X_i, Y_i)}{p(X_{i-1}, Y_{i-1})} \frac{q(X_{i-1} \mid X_i, x_0)\ q(x_0 \mid X_i)}{q(X_i \mid X_{i-1}, x_0)\ q(x_0 \mid X_{i-1})}$$

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(not necessarily independent)

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1/(n choices)

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$$q(X \mid X', x_0) = \prod_{x \in X^{\text{sample}}} w(x)$$

Resampled from the prior

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$$= \frac{|X_{i-1}|}{|X_i|} \frac{\prod_{x \in X_i} w(x) \ \prod_{y \in Y_i} w(y)}{\prod_{x \in X_i^{\text{sample}}} w(x)} \frac{\prod_{x \in X_{i-1}^{\text{sample}}} w(x)}{\prod_{x \in X_{i-1}} w(x) \ \prod_{y \in Y_{i-1}} w(y)}$$

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&= \underbrace{\frac{|X_{i-1}|}{|X_i|}}_{\text{choice } x_0} \underbrace{\frac{\prod_{x \in X_i^{\text{reuse}}} w(x)}{\prod_{x \in X_{i-1}^{\text{reuse}}} w(x)}}_{\text{reused}} \underbrace{\frac{\prod_{y \in Y_i} w(y)}{\prod_{y \in Y_{i-1}} w(y)}}_{\text{scores}}
\end{aligned}$$

Implementation

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Option 1

- CPS model
- Pick x_0 at random
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- Resample only when needed

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Warning: Memoization naming scheme
Different variable may have the same name...

Limitations

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Convergence

- Theoretical conditions are complex
- Must be checked experimentally
- Diagnostic tools: trace plot, R-hat (multi-chains)
- Solution: warmup, change initial conditions, reparameterization, ...

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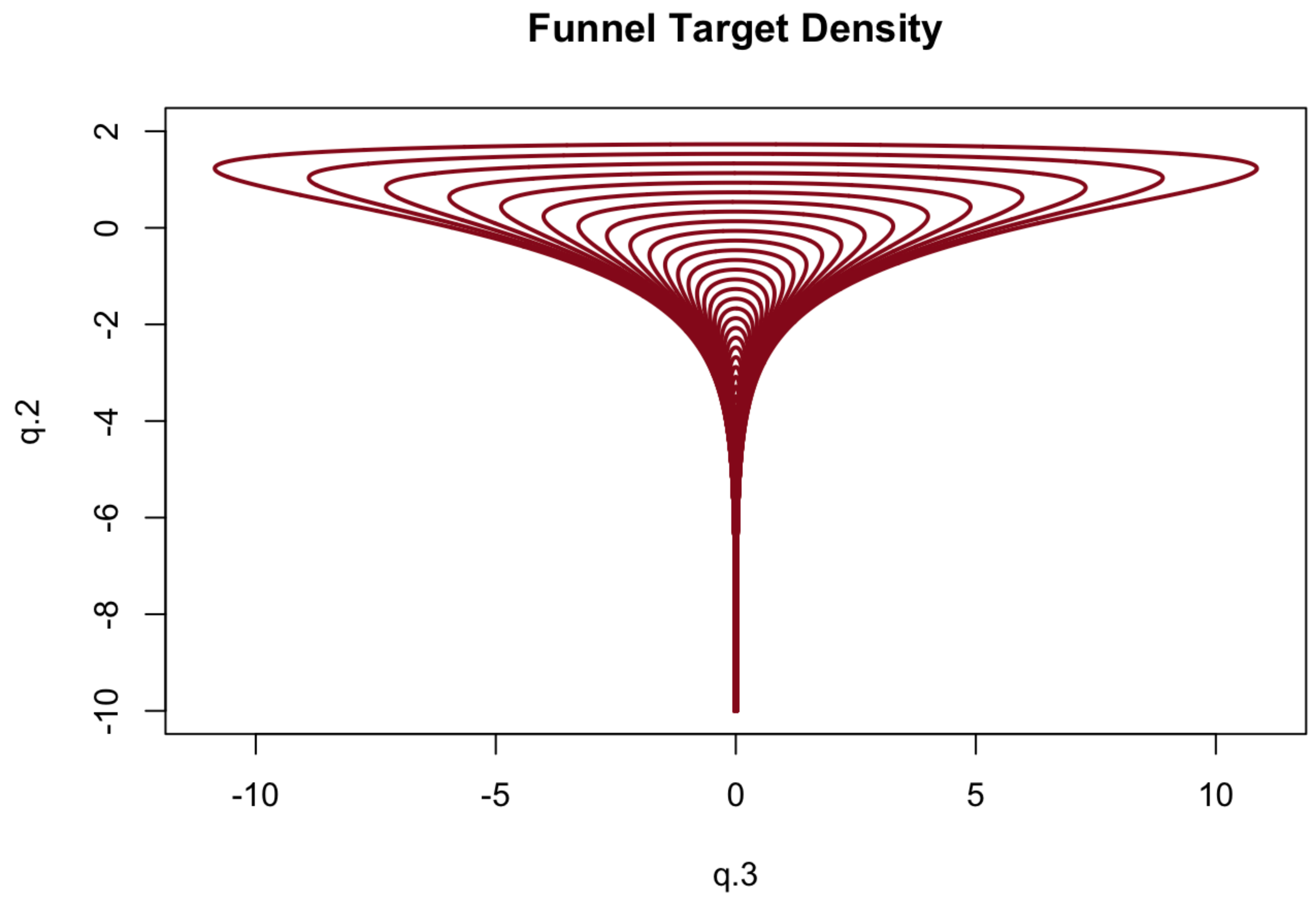
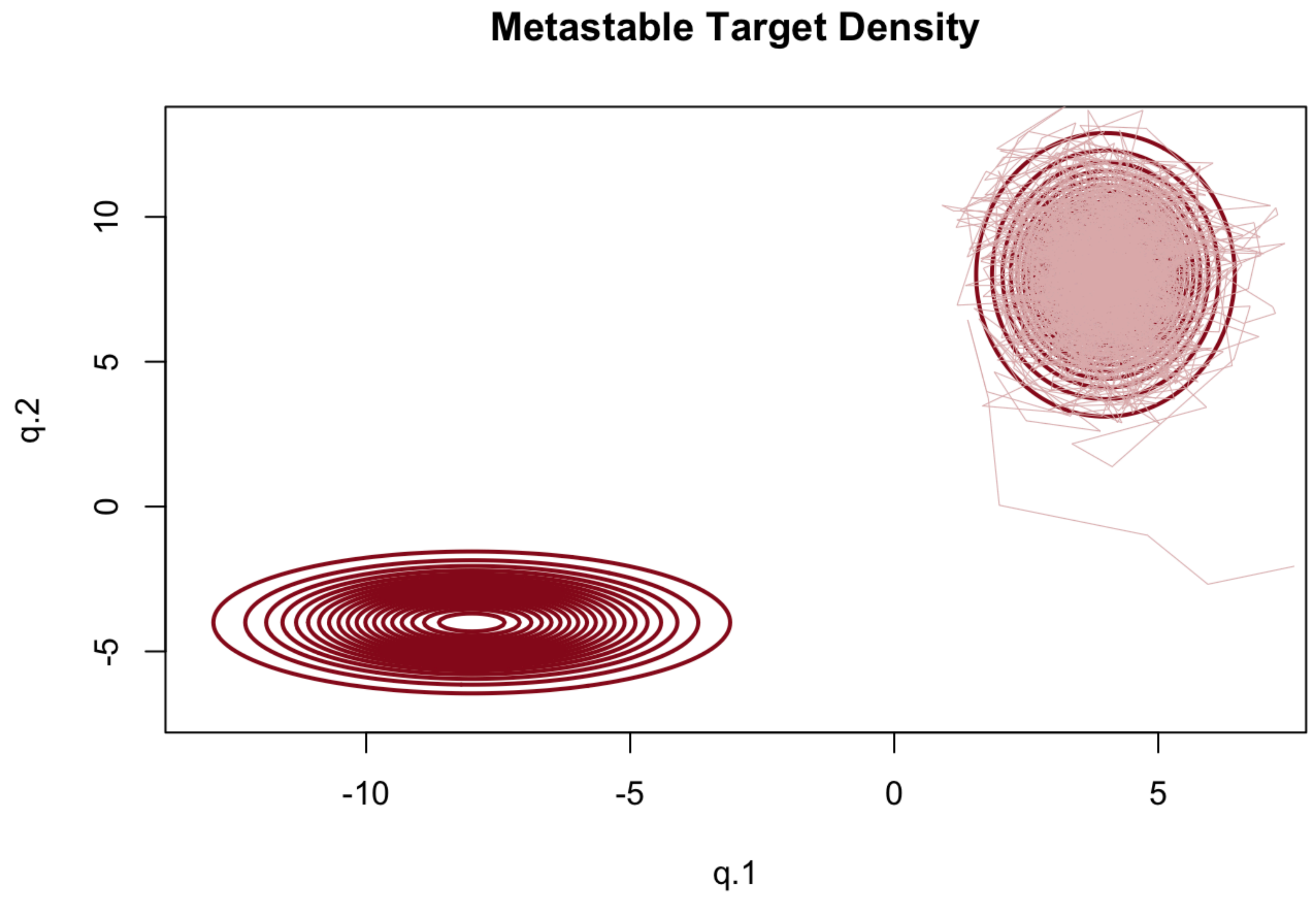
Pathological models

- Multimodal distribution
- Neal's Funnel





https://betanalpha.github.io/assets/case_studies/markov_chain_monte_carlo.html

Advanced Inference

Probabilistic Programming Languages

Hamiltonian Monte-Carlo (HMC)

Hamiltonian Monte-Carlo (HMC)

Analogy: Particle in an energy field

- Program define a density of the form $p(X) \propto \exp(-U(X))$
- On continuous spaces U can be interpreted as an energy
- Low energy wells correspond to high probability regions
- HMC simulate the trajectory of a particle in this energy field

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Hamiltonian dynamic

- M: Mass matrix
- P: Momentum
- $K(P) = \frac{1}{2} P^T M P$

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$$\overset{\text{hamiltonian}}{\uparrow \atop H(X,P)} = \underset{\text{kinetic energy}}{K(P) \atop \downarrow} + \overset{\text{potential energy}}{\uparrow \atop U(X)}$$

Hamiltonian Monte-Carlo (HMC)

$$\underbrace{H(X,P)}_{\text{hamiltonian}} = \underbrace{K(P)}_{\text{kinetic energy}} + \underbrace{U(X)}_{\text{potential energy}}$$

Hamiltonian Monte-Carlo (HMC)

Energy conservation

$$\frac{dH}{dt} = (\nabla_P H)^T \frac{dP}{dt} + (\nabla_X H)^T \frac{dX}{dt} = 0$$

hamiltonian

potential energy

$$H(X, P) = K(P) + U(X)$$

kinetic energy

Hamiltonian Monte-Carlo (HMC)

Energy conservation

$$\frac{dH}{dt} = (\nabla_P H)^T \frac{dP}{dt} + (\nabla_X H)^T \frac{dX}{dt} = 0$$

Hamiltonian dynamics

$$\begin{cases} \dfrac{dX}{dt} = \nabla_P H(X, P) = M^{-1} P \\ \dfrac{dP}{dt} = \nabla_P H(X, P) = -\nabla_X U(X) \end{cases}$$

hamiltonian

potential energy

$$H(X, P) = K(P) + U(X)$$

kinetic energy

Hamiltonian Monte-Carlo (HMC)

Hamiltonian Monte-Carlo (HMC)

Generate samples from $p(X, P) \propto \exp(-H(X, P))$

- At each iteration
- Sample an initial momentum $P_i(0) \sim \mathcal{N}(0,\ M)$
- Solve the Hamiltonian dynamic (discretized)
- Perform a Metropolis Hastings update with probability α

$$\alpha = \min\left(1,\ \frac{\exp(-H(X_i, P_i))}{\exp(-H(X_{i-1}, P_{i-1}))}\right)$$

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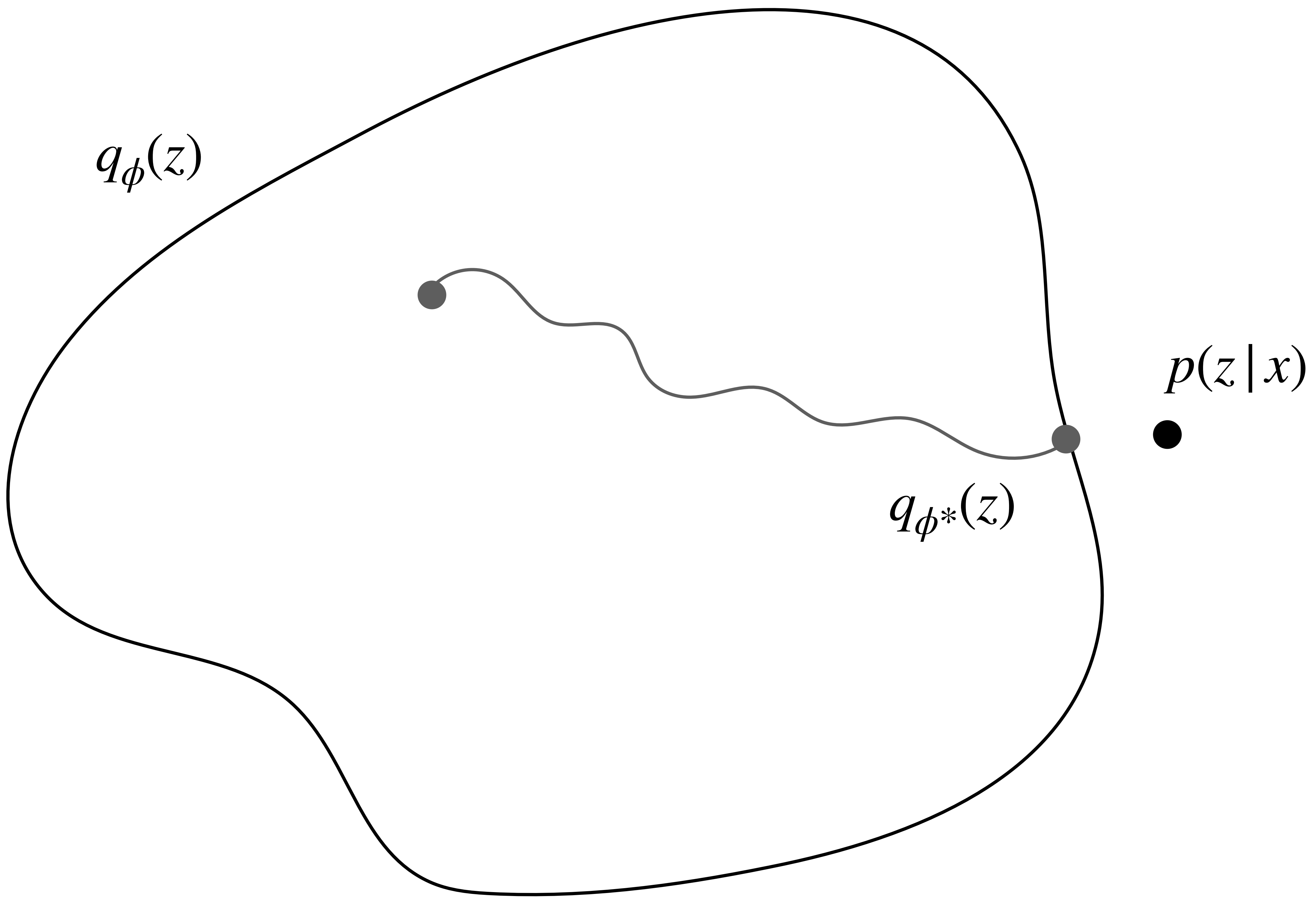
Parameter P can be marginalized

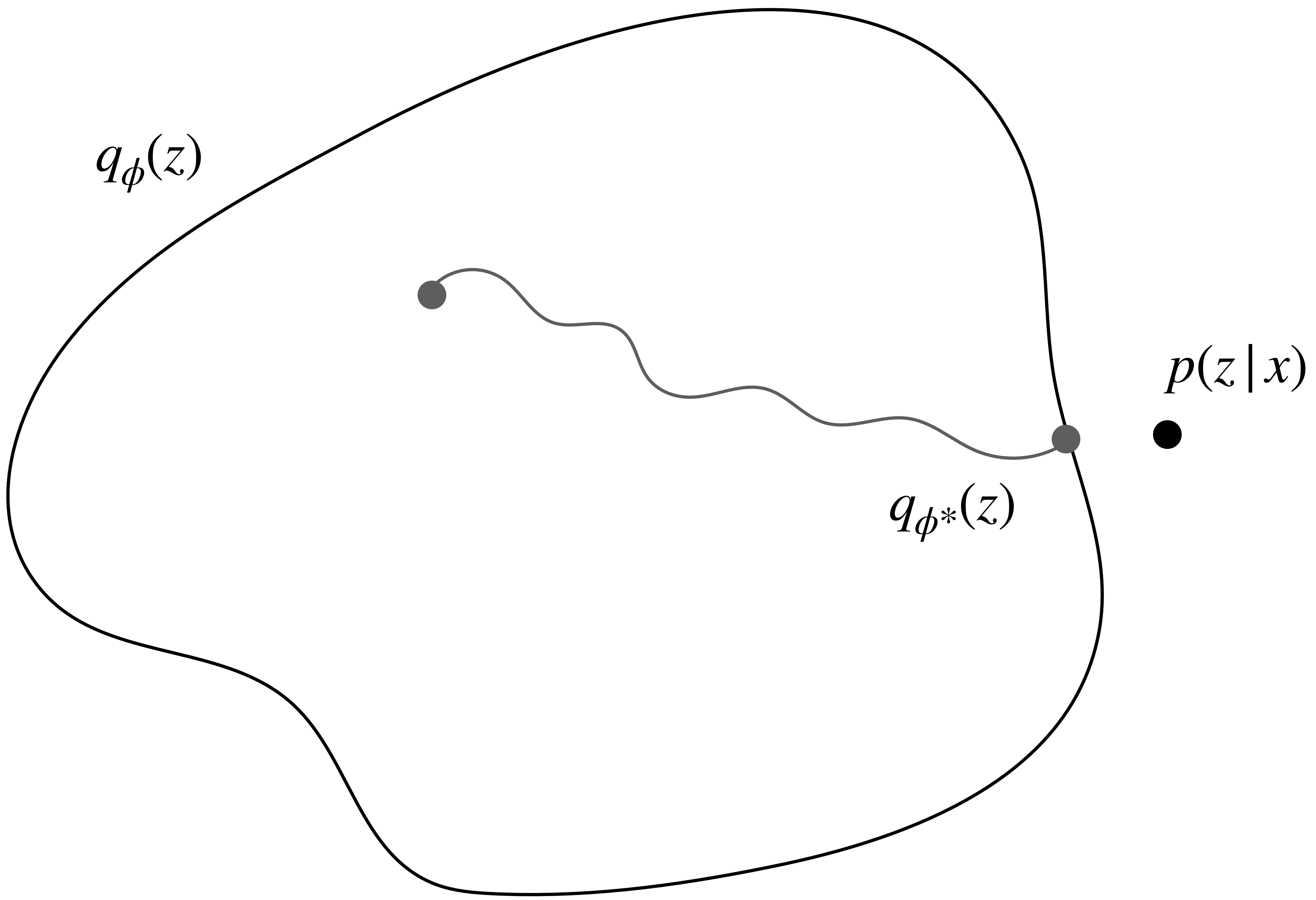
Stochastic Variational Inference (SVI)



Blei et al. 2017

Stochastic Variational Inference (SVI)

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)} = \frac{p(x|z)p(z)}{\int_z p(x|z)p(z)dz}$$



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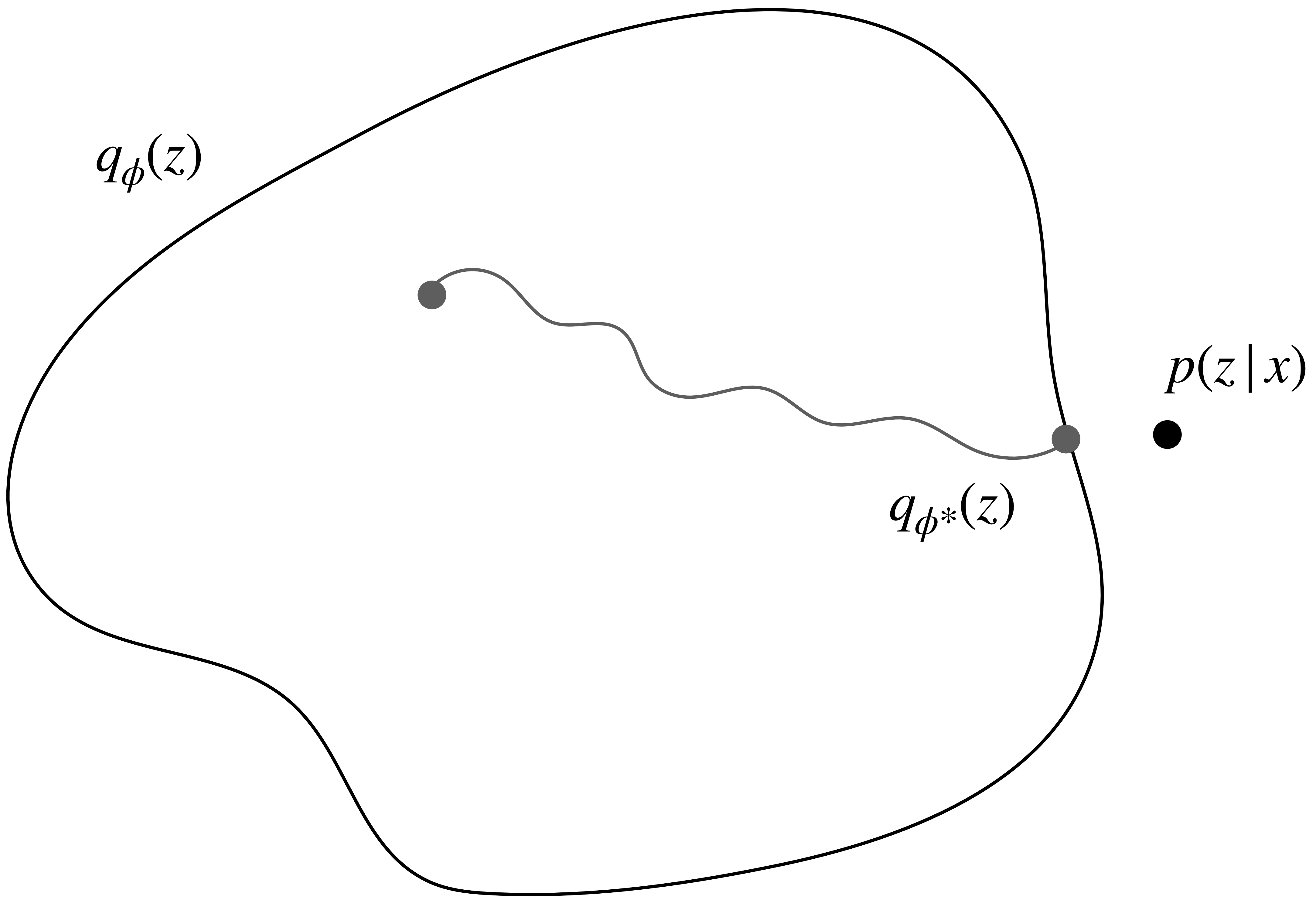
Variational family

- Parameterized by a parameter ϕ
- Find the closest member to the posterior $q_{\phi^*}(z)$
- Optimization problem



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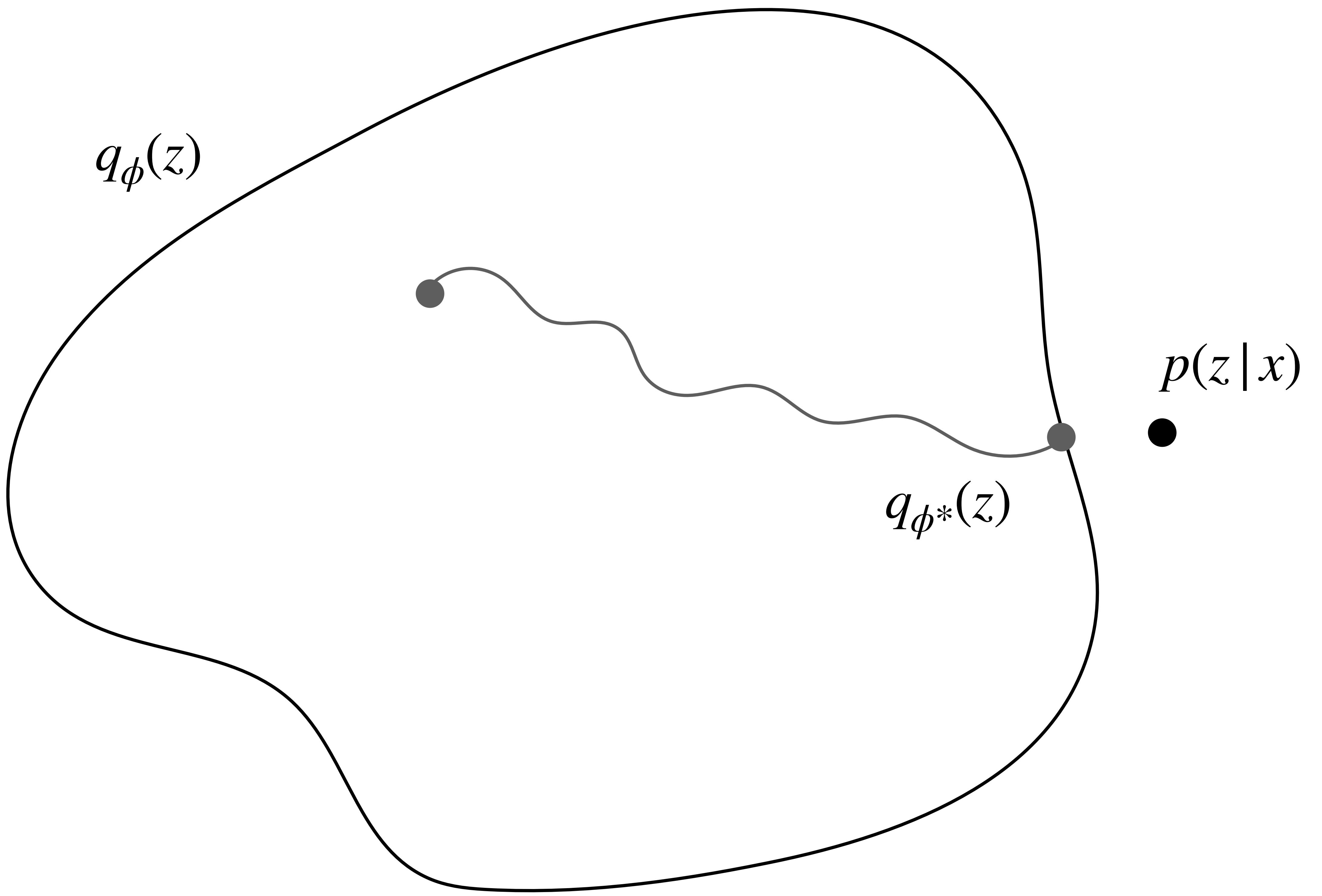
Metrics: Kullback-Leibler divergence

$$KL(q(x) \ || \ p(x)) = -\int q(x) \ \log \frac{p(x)}{q(x)} \ dx$$

- $KL(q \ || \ p) \geq 0$
- $KL(q \ || \ p) \neq KL(p \ || \ q)$



Blei et al. 2017

Stochastic Variational Inference (SVI)

$$
\begin{aligned}
KL(q_\phi(z) \mid\mid p(z|x)) &= -\int q_\phi(z) \log \frac{p(z|x)}{q_\phi(z)} \ dz \\
&= -\int q_\phi(z) \log \frac{p(x,z)}{p(x) q_\phi(z)} \ dz \\
&= -\int q_\phi(z) \log \frac{p(x,z)}{q_\phi(z)} \ dz + \int q_\phi(z) \log p(x) \ dz \\
&= -\int q_\phi(z) \log \frac{p(x,z)}{q_\phi(z)} \ dz + \log p(x)
\end{aligned}
$$

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KL(q_\phi(z)\ ||\ p(z|x)) &= -\int q_\phi(z) \log \frac{p(z|x)}{q_\phi(z)}\ dz \\
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\log p(x) = KL(q_\phi(z)\ ||\ p(x,z)) + \int q_\phi(z)\ \log \frac{p(x,z)}{q_\phi(z)}\ dz
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$$

Stochastic Variational Inference (SVI)

$$\mathscr{L} = \int q_\phi(z) \ \log \frac{p(x,z)}{q_\phi(z)} \ dz$$

$$= \int q_\phi(z) \ \log \frac{p(x\,|\,z)p(z)}{q_\phi(z)} \ dz$$

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$$\underbrace{\log p(x)}_{\text{constant}} = \underbrace{KL(q_\phi(z)\ ||\ p(x,z))}_{\text{minimize}} + \underbrace{\int q_\phi(z)\ \log \frac{p(x,z)}{q_\phi(z)}\ dz}_{\text{maximize ELBO } \mathscr{L}}$$

Variational Family

Variational Family

Black-box variational inference

- Mean-field approximation $q_\phi(z) = \prod_{i=1}^{n} \mathcal{N}(z_i \mid \mu_i, \sigma_i)$ where $\phi = \{\mu_i, \sigma_i\}_{i \in [1,n]}$
- Full-rank approximation $q_\phi(z) = \mathcal{N}(z \mid \mu, \Sigma)$ where $\phi = (\mu, \Sigma)$
- Pyro autoguides

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Program your own guide

- Pyro (first versions)
- Must sample the same variables in the guide and the model
- Static analysis?

```
def model():
    pyro.sample("z_1", ...)

def guide():
    pyro.sample("z_1", ...)
```


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