

# Probabilistic Programming Languages

Guillaume Baudart

*MPRI 2025-2026*

Warm-up: Rejection sampling

---

Probabilistic Programming Languages

# Rejection sampling (hard)

*basic.ml*

```
module Rejection_sampling_hard : sig
  val sample : 'a Distribution.t → 'a
  val assume : bool → unit
  val infer : ?n:int → ('a → 'b) → 'a → 'b Distribution.t
end = struct ... end
```

## Inference algorithm

- Run the model to get a sample
- `sample` : draw a value from a distribution
- `assume` : accept / reject a sample
- If a sample is rejected, re-run the model to get another sample

## Hard conditioning

- `val observe : 'a Distribution.t → 'a → unit`
- Assume that a value was sampled from a distribution (??)

# Importance sampling

*basic.ml*

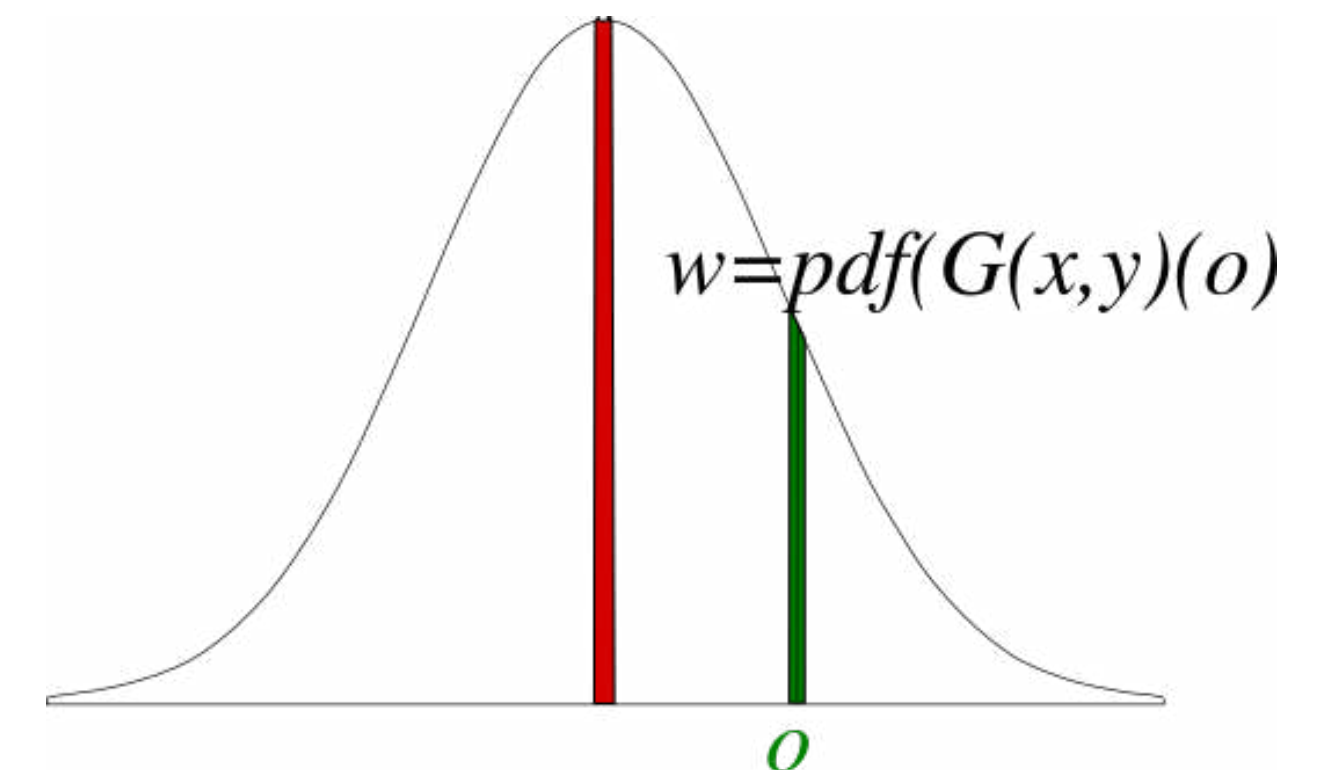
```
module Importance_sampling : sig
  type prob
  val sample : prob → 'a Distribution.t → 'a
  val factor : prob → float → unit
  val infer : ?n:int → (prob → 'a → 'b) → 'a → 'b Distribution.t
end = struct ... end
```

## Inference algorithm

- Run a set of  $n$  independent executions
- `sample`: draw a sample from a distribution
- `factor`: associate a score to the current execution
- Gather output values and score to approximate the posterior distribution

## Likelihood weighting

- `observe d x := factor (logpdf d x)`



# Example: Noisy position

```
open Basic.Importance_sampling

let gauss obs =
  let x = sample (gaussian ~mu:0.0 ~sigma:10.0) in
  let y = sample (gaussian ~mu:0.0 ~sigma:10.0) in
  List.iter
    (fun (xo, yo) →
      observe (gaussian ~mu:x ~sigma:1.0) xo;
      observe (gaussian ~mu:y ~sigma:1.0) yo )
    obs;
  (x, y)

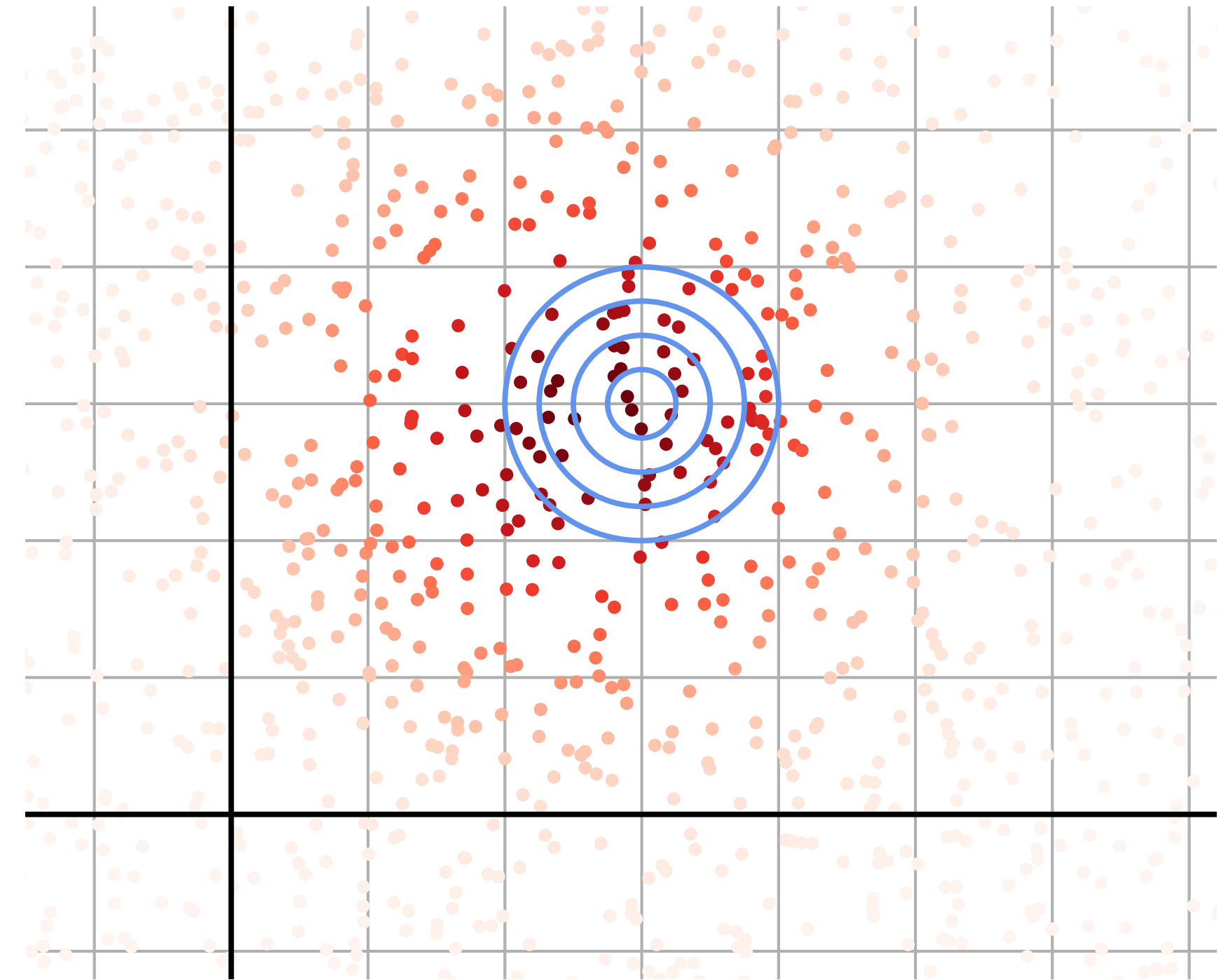
let _ =
  let dist = infer gauss data in
  plot dist
```

# Example: Noisy position

```
open Basic.Importance_sampling
```

```
let gauss obs =  
  let x = sample (gaussian ~mu:0.0 ~sigma:10.0) in  
  let y = sample (gaussian ~mu:0.0 ~sigma:10.0) in  
  List.iter  
    (fun (xo, yo) →  
      observe (gaussian ~mu:x ~sigma:1.0) xo;  
      observe (gaussian ~mu:y ~sigma:1.0) yo )  
    obs;  
  (x, y)  
  
let _ =  
  let dist = infer gauss data in  
  plot dist
```

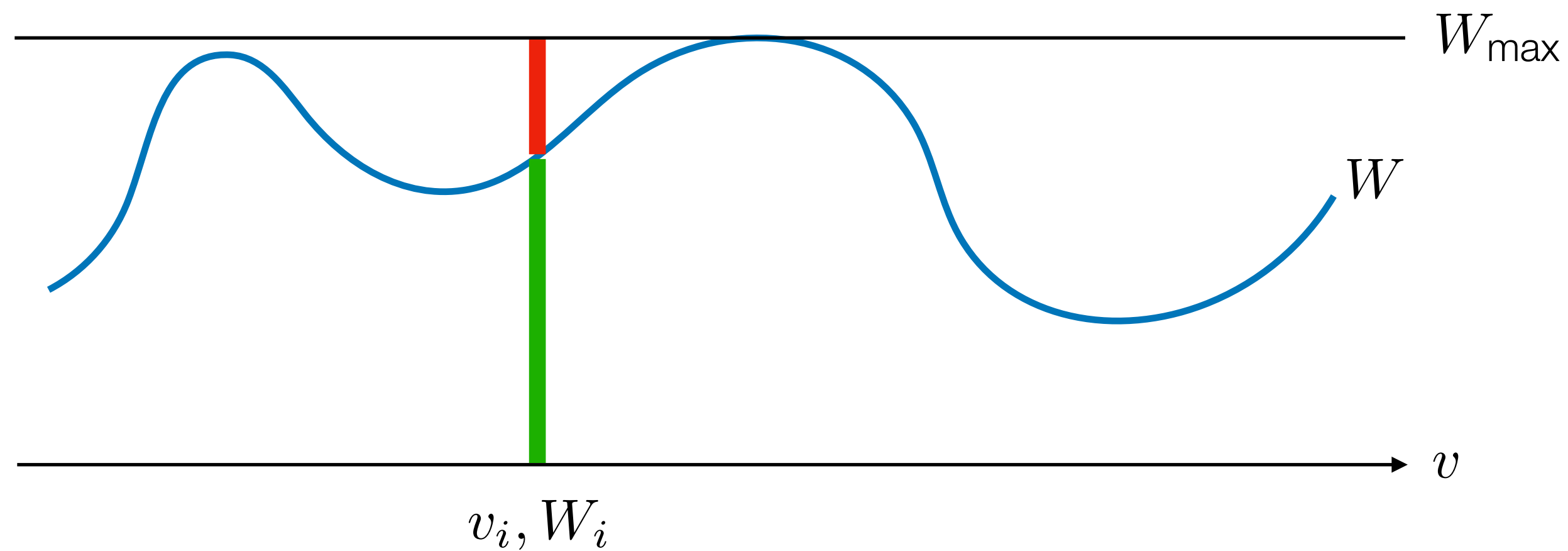
10 000 particles



# Weighted rejection sampling

Adapt rejection sampling to soft conditioning

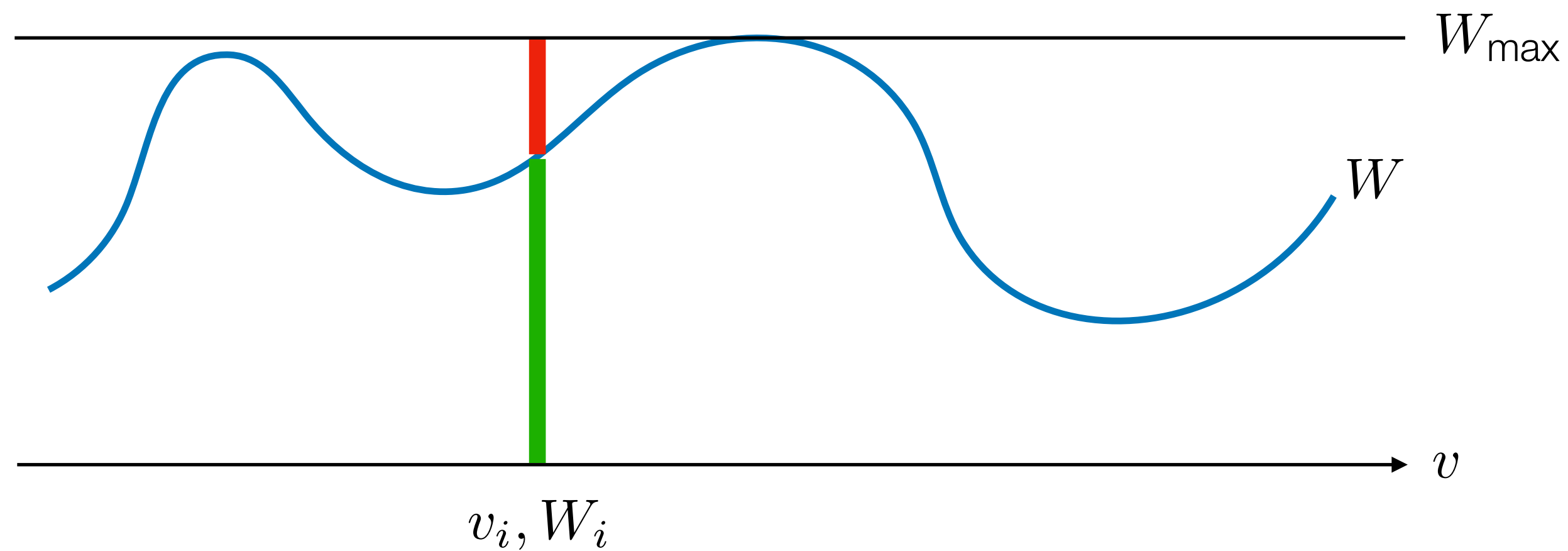
- Execute the sampler to get a pair  $(v_i, W_i)$
- Suppose  $W_{\max}$  is known
- Accept the sample with probability  $W_i/W_{\max}$  or retry



# 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



But  $W_{\max}$  is not known...



Try it in BYO-PPL!

# Rejection sampling

*basic.ml*

```
module Rejection_sampling = struct
  include Importance_sampling

  let infer ?(n = 1000) ?(max_score = 0.) model data =
    let rec gen i =
      let prob = { score = 0. } in
      let value = model prob data in
      let alpha = exp (min 0. (prob.score -. max_score)) in
      let u = Random.float 1. in
      if u ≤ alpha then value else gen i
    in
    let samples = List.init n gen in
    Distribution.empirical ~samples
end
```

(\* reset the score \*)  
(\* run the model \*)  
  
(\* accept / reject \*)

# The curse of dimensionality

Problem becomes harder as the dimension increases

Basic inference: importance sampling

- Performances decrease exponentially when the dimension increases
- Only use for low-dimension models

How to mitigate this problem?

- Make assumptions about the posterior distributions
- Break the problem into simpler, smaller problems





# The curse of dimensionality

Problem becomes harder as the dimension increases

Basic inference: importance sampling

- Performances decrease exponentially when the dimension increases
- Only use for low-dimension models

How to mitigate this problem?

- Make assumptions about the posterior distributions
- Break the problem into simpler, smaller problems

17h45mn



# Markov Chain Monte Carlo

---

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

# Metropolis Hastings

# Metropolis Hastings

## Trace

- $X$ : set of random variables (**sample**)
- $P(X)$ : prior distribution of  $X$
- A trace characterize one posible execution
- $W$ : score of the execution (same as importance sampling)



# Metropolis Hastings

## Trace

- $X$ : set of random variables (**sample**)
- $P(X)$ : prior distribution of  $X$
- A trace characterize one possible execution
- $W$ : score of the execution (same as importance sampling)

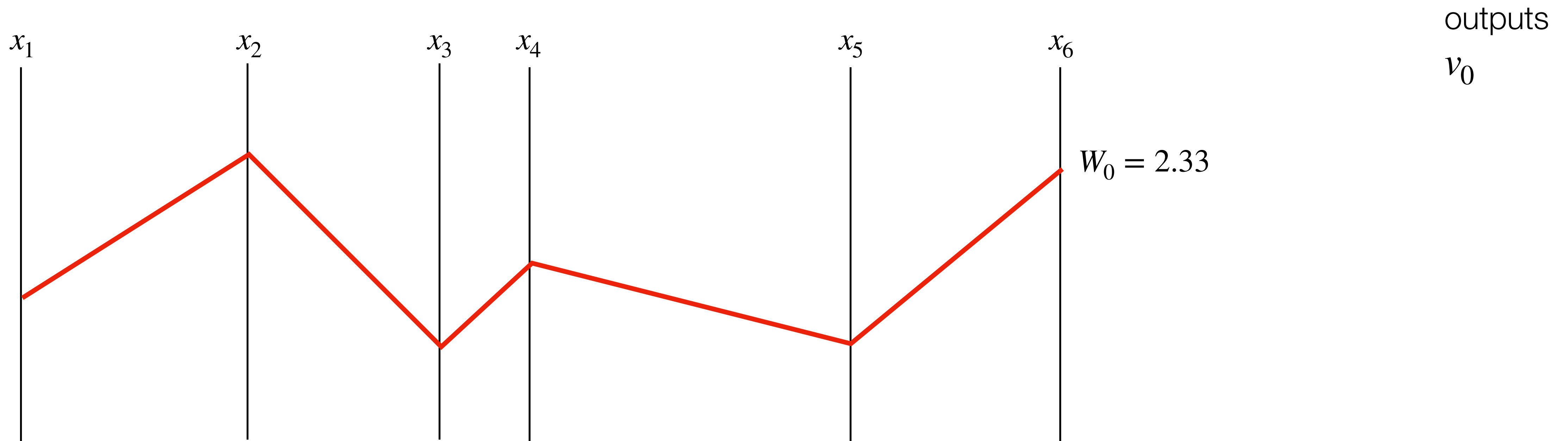
## Metropolis-Hastings algorithm

- Initialization: draw  $X_0$  at random to get a pair  $(v_0, W_0)$ .
- At each step:
  1. Draw a *candidate*  $X' \sim Q(X' | X_i)$  to get  $(v', W')$
  2. Acceptance rate:  $\alpha = \frac{P(X') W' Q(X_i | X')}{P(X_i) W_i Q(X' | X_i)}$ .
  3. Draw  $u \sim U(0, 1)$ .
  4. If  $u \leq \alpha$  (*accept*)  $\begin{cases} X_{i+1} = X' \\ v_{i+1} = v' \\ W_{i+1} = W' \end{cases}$  else (*reject*)  $\begin{cases} X_{i+1} = X_i \\ v_{i+1} = v_i \\ W_{i+1} = W_i \end{cases}$

# Multi-sites Metropolis Hastings

## Markov chain on execution traces

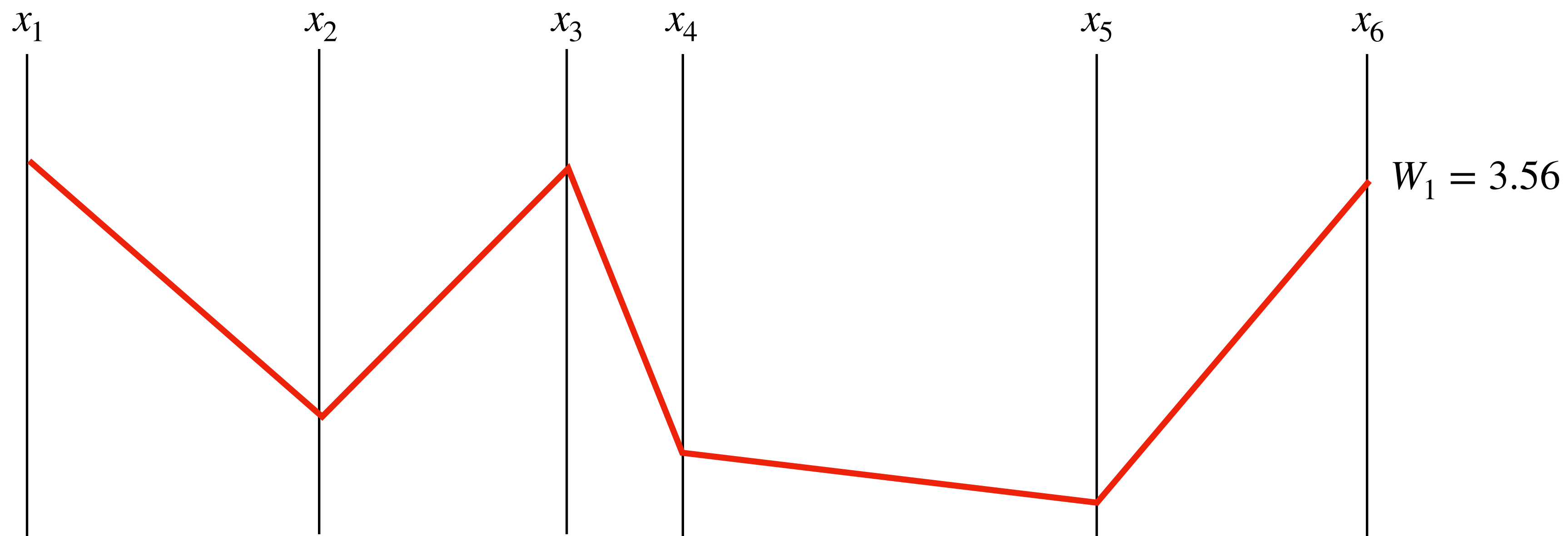
- Execute the sampler to get a candidate  $X'$  and the associated value and score  $(v_i, W_i)$
- If  $W' \geq W_i$  accept the candidate (and the associated value)
- Else accept the candidate with probability  $W'/W_i$
- Otherwise keep the previous trace  $X_i$



# Multi-sites Metropolis Hastings

## Markov chain on execution traces

- Execute the sampler to get a candidate  $X'$  and the associated value and score  $(v_i, W_i)$
- If  $W' \geq W_i$  accept the candidate (and the associated value)
- Else accept the candidate with probability  $W'/W_i$
- Otherwise keep the previous trace  $X_i$



outputs

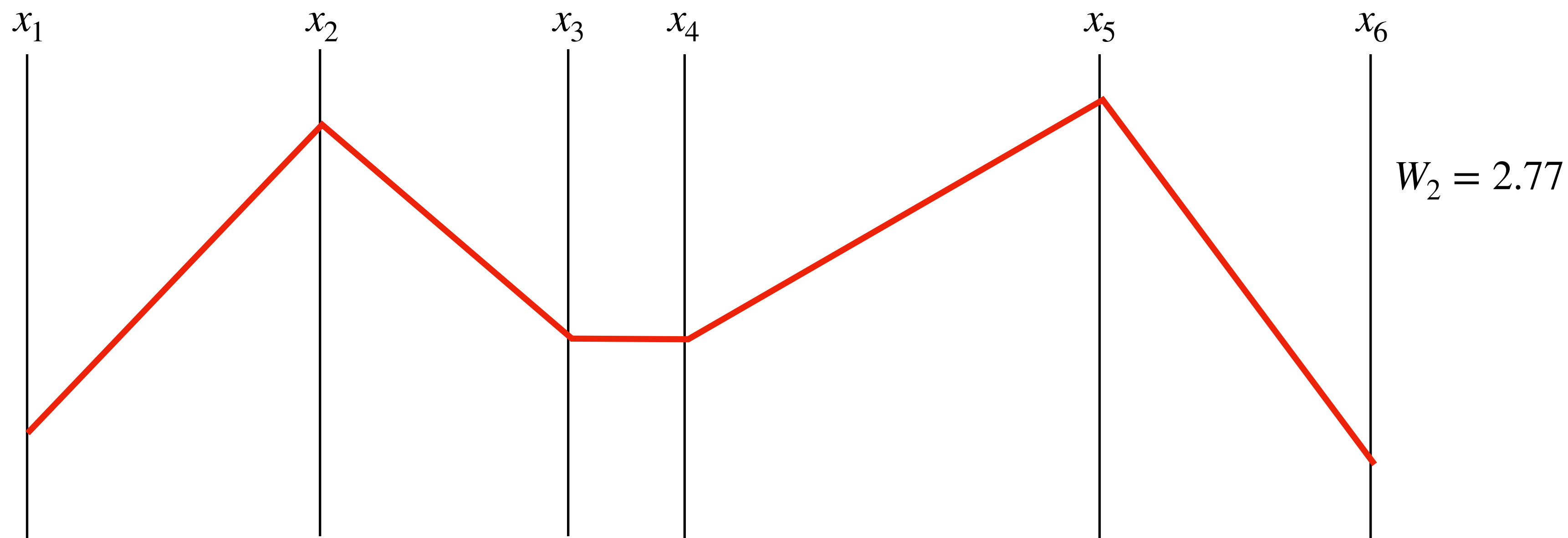
$v_0$

$v_1$

# Multi-sites Metropolis Hastings

## Markov chain on execution traces

- Execute the sampler to get a candidate  $X'$  and the associated value and score  $(v_i, W_i)$
- If  $W' \geq W_i$  accept the candidate (and the associated value)
- Else accept the candidate with probability  $W'/W_i$
- Otherwise keep the previous trace  $X_i$



outputs

$v_0$

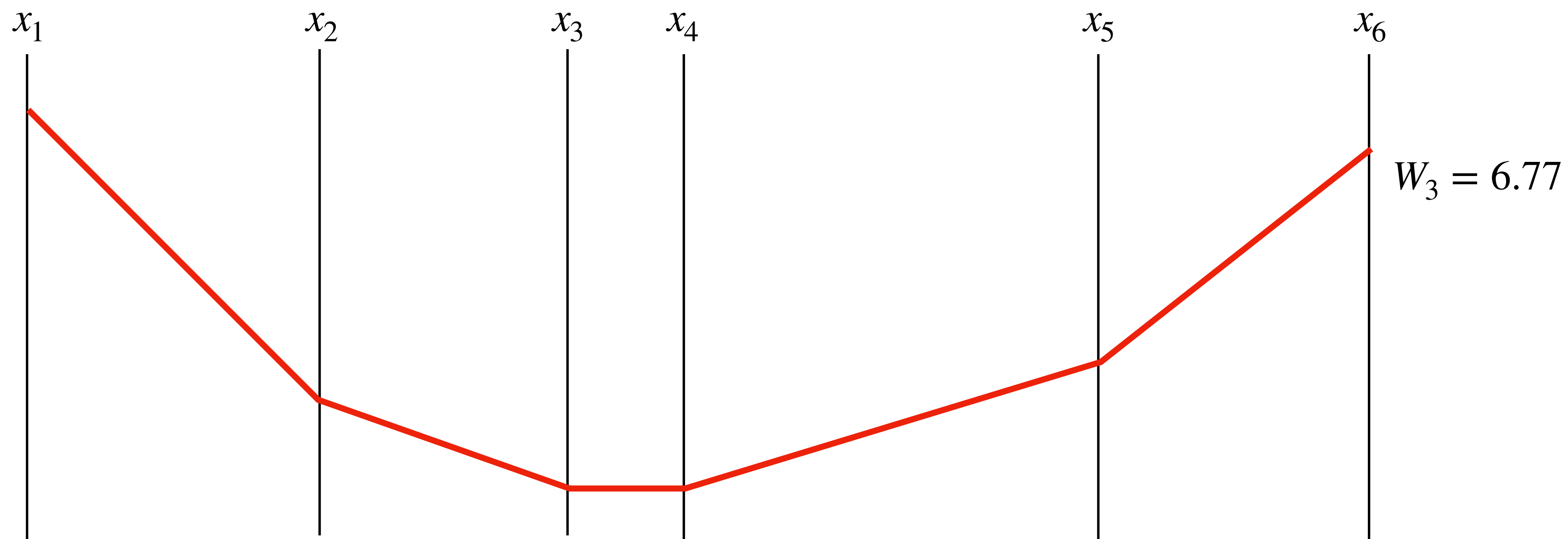
$v_1$

$v_1$

# Multi-sites Metropolis Hastings

## Markov chain on execution traces

- Execute the sampler to get a candidate  $X'$  and the associated value and score  $(v_i, W_i)$
- If  $W' \geq W_i$  accept the candidate (and the associated value)
- Else accept the candidate with probability  $W'/W_i$
- Otherwise keep the previous trace  $X_i$



outputs

$v_0$

$v_1$

$v_1$

$v_3$

...

# Multi-sites Metropolis Hastings: acceptance

Re-execute the entire trace

- Draw proposal from priors  $Q(X' | X_i) = P(X')$
- Resample all variables in  $X_i$  at each iteration

$$\begin{aligned}\alpha &= \frac{P(X') W' Q(X_i | X')}{P(X_i) W_i Q(X' | X_i)} \\ &= \frac{P(X') W' P(X_i)}{P(X_i) W_i P(X')} \\ &= \frac{W'}{W_i}\end{aligned}$$

# Multi-sites Metropolis Hastings: acceptance

Re-execute the entire trace

- Draw proposal from priors  $Q(X' | X_i) = P(X')$
- Resample all variables in  $X_i$  at each iteration

$$\begin{aligned}\alpha &= \frac{P(X') W' Q(X_i | X')}{P(X_i) W_i Q(X' | X_i)} \\ &= \frac{P(X') W' P(X_i)}{P(X_i) W_i P(X')} \\ &= \frac{W'}{W_i}\end{aligned}$$

## Markov chain on execution traces

- Execute the sampler to get a candidate  $X'$  and the associated value and score  $(v_i, W_i)$
- If  $W' \geq W_i$  accept the candidate (and the associated value)
- Else accept the candidate with probability  $W'/W_i$
- Otherwise keep the previous trace  $X_i$

Try it in BYO-PPL!



# Multi-sites Metropolis Hastings

*basic.ml*

```
module Simple_metropolis = struct
  include Importance_sampling

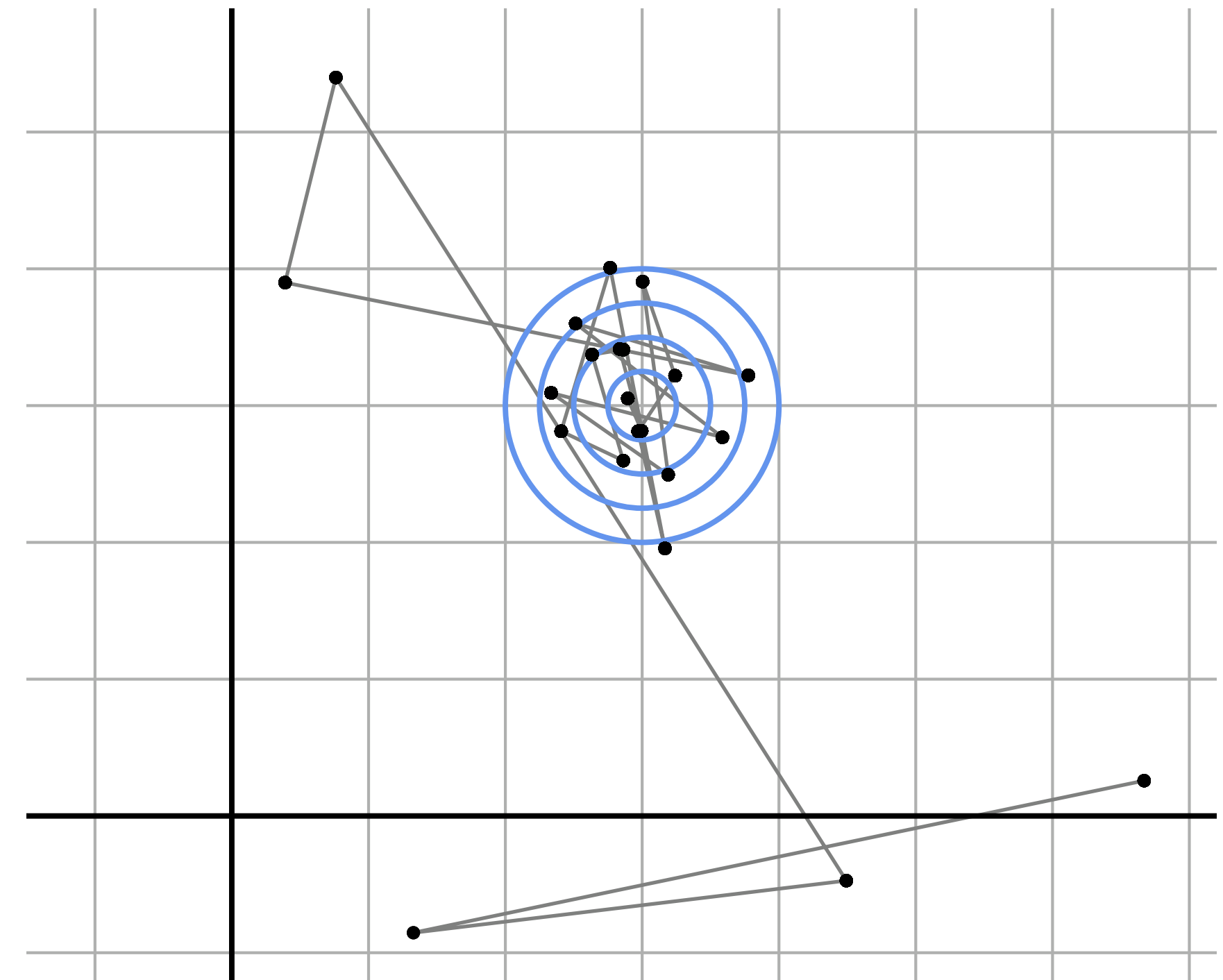
  let infer ?(n = 1000) model data =
    let rec gen n samples old_score old_value =
      if n = 0 then samples (* return the list of samples *)
      else
        let prob = { score = 0. } in (* reset prob *)
        let new_value = model prob data in (* generate candidate *)
        let alpha = exp (min 0. (prob.score -. old_score)) in
        let u = Random.float 1.0 in
        if not (u < alpha) then
          gen (n - 1) (old_value :: samples) old_score old_value (* reject *)
        else gen (n - 1) (new_value :: samples) prob.score new_value (* accept *)
    in
    let prob = { score = 0. } in
    let first_value = model prob data in (* generate first trace *)
    let samples = gen n [] prob.score first_value in (* generate samples *)
    Distribution.empirical ~samples
end
```

# Example: Noisy position

```
open Basic.Simple_metropolis
```

```
let gauss obs =  
  let x = sample (gaussian ~mu:0.0 ~sigma:10.0) in  
  let y = sample (gaussian ~mu:0.0 ~sigma:10.0) in  
  List.iter  
    (fun (xo, yo) →  
      observe (gaussian ~mu:x ~sigma:1.0) xo;  
      observe (gaussian ~mu:y ~sigma:1.0) yo )  
    obs;  
  (x, y)  
  
let _ =  
  let dist = infer gauss data in  
  plot dist
```

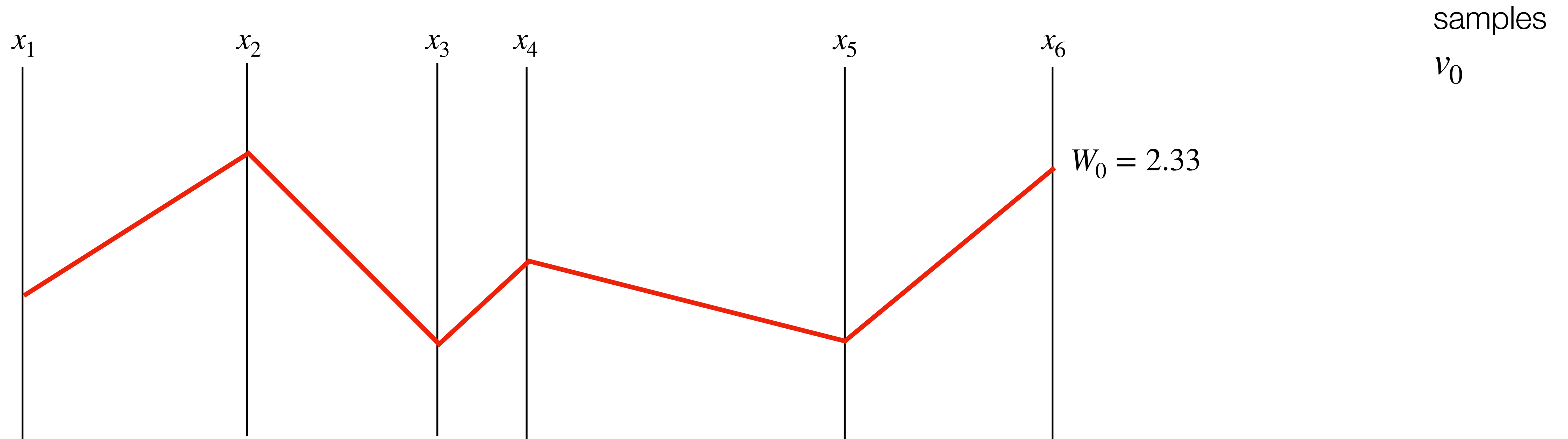
7000 samples



# Single-site Metropolis Hastings

Reuse most of the previous trace (i.e., sampled values)

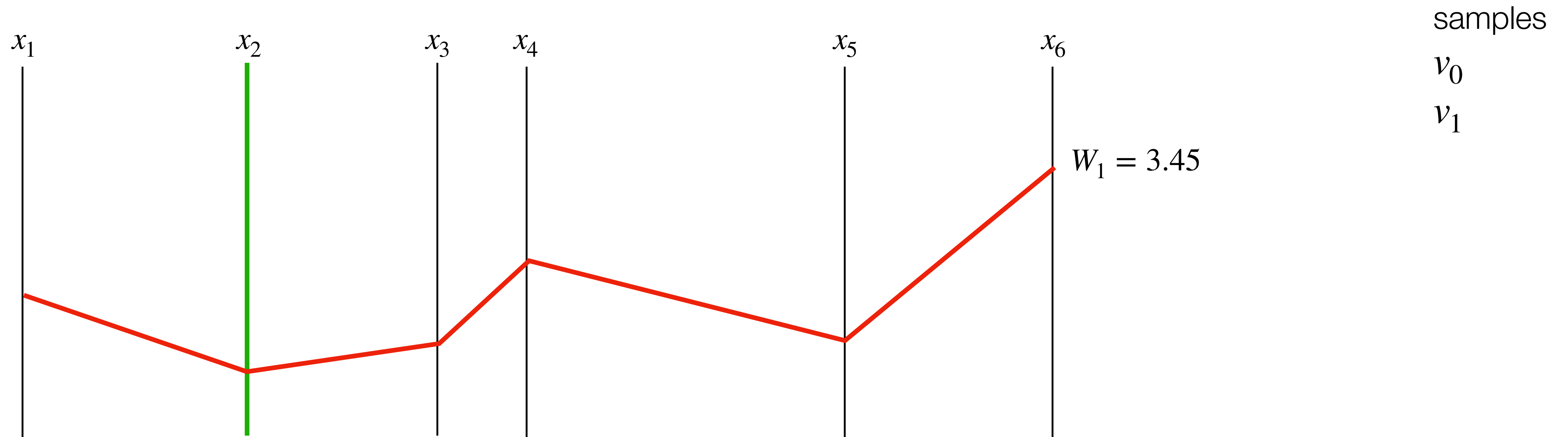
- Choose one random variable  $x_{\text{regen}}$  to resample to obtain a new execution
- Accept the trace with probability  $\alpha$
- Otherwise use the previous trace



# Single-site Metropolis Hastings

Reuse most of the previous trace (i.e., sampled values)

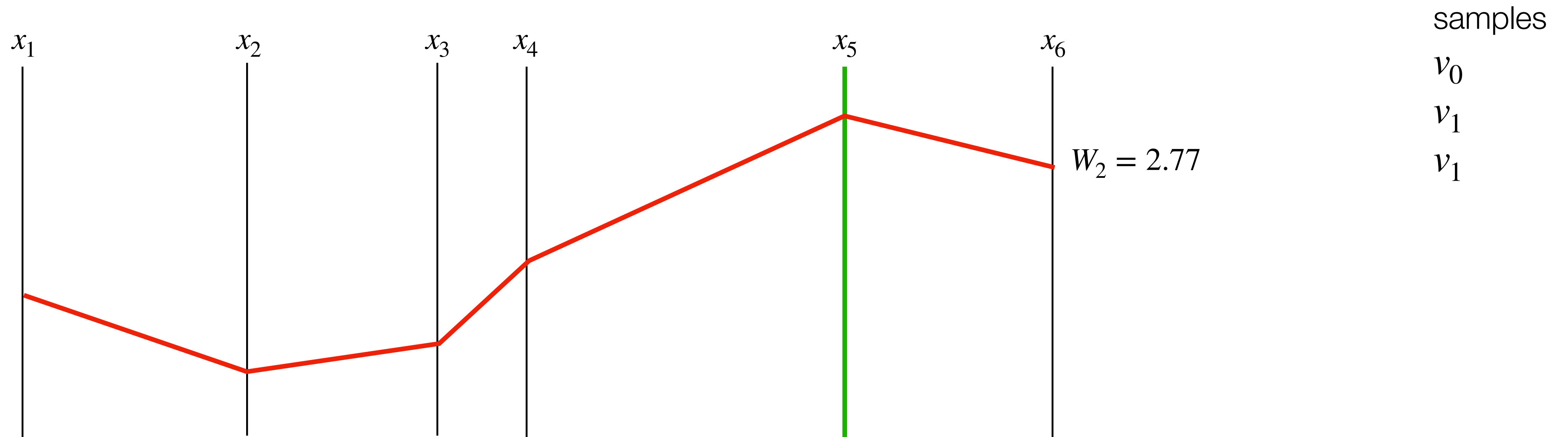
- Choose one random variable  $x_{\text{regen}}$  to resample to obtain a new execution
- Accept the trace with probability  $\alpha$
- Otherwise use the previous trace



# Single-site Metropolis Hastings

Reuse most of the previous trace (i.e., sampled values)

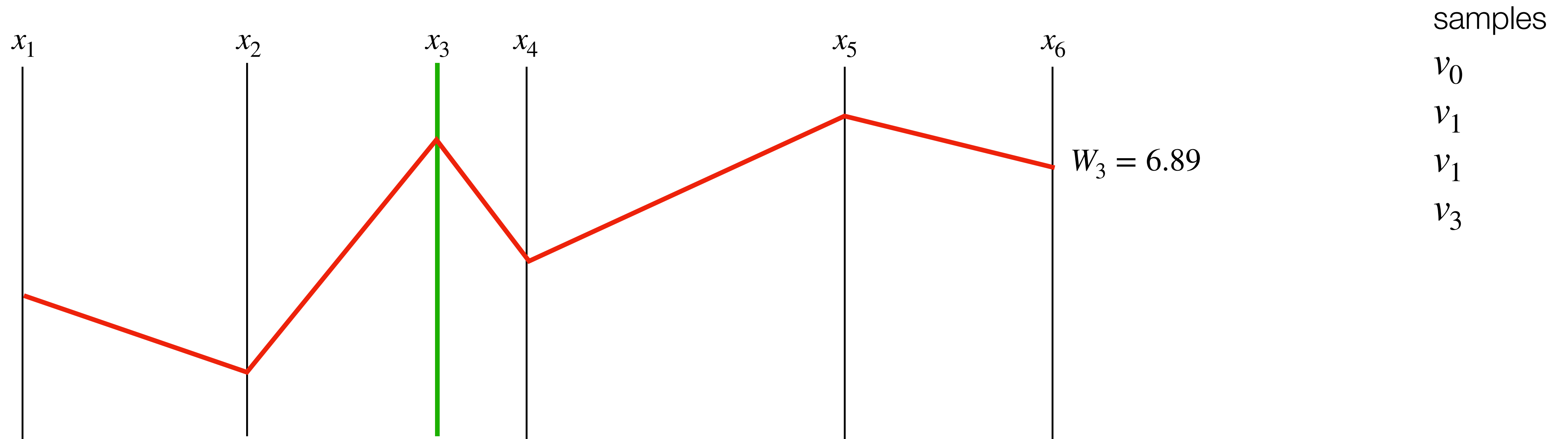
- Choose one random variable  $x_{\text{regen}}$  to resample to obtain a new execution
- Accept the trace with probability  $\alpha$
- Otherwise use the previous trace



# Single-site Metropolis Hastings

Reuse most of the previous trace (i.e., sampled values)

- Choose one random variable  $x_{\text{regen}}$  to resample to obtain a new execution
- Accept the trace with probability  $\alpha$
- Otherwise use the previous trace



# Single-site Metropolis Hastings: acceptance

# Single-site Metropolis Hastings: acceptance

## Notations

- For  $x \in X$ ,  $w(x)$ : density of sample  $x$  (same as **observe**)
- $C = (X' \cap X - \{x_{\text{regen}}\})$ : *cache*, i.e., reused variables between  $X$  and  $X'$

$$P(X) = \prod_{x \in X} w(x) \quad \text{prior distribution}$$

$$Q(X' \mid X) = \frac{1}{|X|} \prod_{x \in (X' - C)} w'(x) \quad \text{choice of } X' \text{ from } X$$



# Single-site Metropolis Hastings: acceptance

## Notations

- For  $x \in X$ ,  $w(x)$ : density of sample  $x$  (same as **observe**)
- $C = (X' \cap X - \{x_{\text{regen}}\})$ : *cache*, i.e., reused variables between  $X$  and  $X'$

$$P(X) = \prod_{x \in X} w(x) \quad \text{prior distribution}$$

$$Q(X' \mid X) = \frac{1}{|X|} \prod_{x \in (X' - C)} w'(x) \quad \text{choice of } X' \text{ from } X$$

$$\begin{aligned} \alpha &= \frac{P(X') W' Q(X_i \mid X')}{P(X_i) W_i Q(X' \mid X_i)} \\ &= \frac{\prod_{x \in X'} w'(x) W' |X_i| \prod_{x \in (X_i - C)} w(x)}{\prod_{x \in X_i} w(x) W_i |X'| \prod_{x \in (X' - C)} w'(x)} \\ &= \frac{|X_i| W' \prod_{x \in C} w'(x)}{|X'| W_i \prod_{x \in C} w(x)} \end{aligned}$$

# Single-site Metropolis Hastings: acceptance

## Notations

- For  $x \in X$ ,  $w(x)$ : density of sample  $x$  (same as **observe**)
- $C = (X' \cap X - \{x_{\text{regen}}\})$ : *cache*, i.e., reused variables between  $X$  and  $X'$

$$P(X) = \prod_{x \in X} w(x) \quad \text{prior distribution}$$

$$Q(X' \mid X) = \frac{1}{|X|} \prod_{x \in (X' - C)} w'(x) \quad \text{choice of } X' \text{ from } X$$

$$\begin{aligned} \alpha &= \frac{P(X') W' Q(X_i \mid X')}{P(X_i) W_i Q(X' \mid X_i)} \\ &= \frac{\prod_{x \in X'} w'(x) W' |X_i| \prod_{x \in (X_i - C)} w(x)}{\prod_{x \in X_i} w(x) W_i |X'| \prod_{x \in (X' - C)} w'(x)} \\ &= \frac{|X_i| W' \prod_{x \in C} w'(x)}{|X'| W_i \prod_{x \in C} w(x)} \end{aligned}$$

Reused variables are treated as observations

# Single-site Metropolis Hastings

Rerun (part of) the trace

- Assign a unique name to each random variable sample
- Can be added by a compiler: addressing transform
- Store sample and score in a table (cache)

```
let gauss obs =  
  let x = sample (gaussian ~mu:0.0 ~sigma:10.0) "x" in  
  let y = sample (gaussian ~mu:0.0 ~sigma:10.0) "y" in  
  List.iter  
    (fun (xo, yo) →  
      observe (gaussian ~mu:x ~sigma:1.0) xo;  
      observe (gaussian ~mu:y ~sigma:1.0) yo )  
    obs;  
  (x, y)
```

# Single-site Metropolis Hastings

*MetropolistHasting*

```
module Metropolis_hastings = struct
  type 'a sample_site = { x_value : 'a; x_score : float }
  type 'a prob = {
    mutable score : float;                                (* current score *)
    x_store : (string, 'a sample_site) Hashtbl.t;        (* sample store (trace) *)
    cache : (string, 'a sample_site) Hashtbl.t;           (* cache *)
  }

  let sample prob d name =
    let x_value =
      match Hashtbl.find_opt prob.cache name with
      | Some { x_value; _ } → x_value                      (* reuse if possible *)
      | None → Distribution.draw d                         (* otherwise draw a sample *)
    in
    let x_score = Distribution.logpdf d x_value in
    Hashtbl.add prob.x_store name { x_value; x_score };   (* store sample site *)
    x_value
```

# Single-site Metropolis Hastings

*MetropolistHasting*

```
let mh cache old_score old_x_store score x_store =  
  let l_alpha = log (length old_x_store) -. log (length x_store) in  
  let l_alpha = l_alpha +. score -. old_score in  
  let dom = intersect cache x_store in  
  let l_alpha = List.fold_left  
    (fun l_alpha x →  
      let { x_score; _ } = Hashtbl.find x_store x in  
      let { x_score = old_x_score; _ } = Hashtbl.find old_x_store x in  
      l_alpha +. x_score -. old_x_score)  
    dom l_alpha  
  in  
  exp (min 0. l_alpha)
```

$$\alpha = \frac{|X_i|}{|X'|} \frac{W'}{W_i} \frac{\prod_{x \in C} w'(x)}{\prod_{x \in C} w(x)}$$

# Single-site Metropolis Hastings

*MetropolistHasting*

```
let infer ?(n = 1000) model data =  
  let rec gen n samples old_score old_value old_x_store =  
    [ ... ]  
  in  
  
  let prob = { score = 0.; x_store = empty; cache = empty } in  
  let first_value = model prob data in (* generate first trace *)  
  let samples = gen n [] prob.score first_value prob.x_store in (* generate samples *)  
  Distribution.empirical ~samples  
end
```

# Single-site Metropolis Hastings

*MetropolistHasting*

```
let infer ?(n = 1000) model data =  
  let rec gen n samples old_score old_value old_x_store =  
    [ ... ]  
  in  
  
  let prob = { score = 0.; x_store = empty; cache = empty} in  
  let first_value = model prob data in (* generate first trace *)  
  let samples = gen n [] prob.score first_value prob.x_store in (* generate samples *)  
  Distribution.empirical ~samples  
end
```

Same as multi-sites...

# Single-site Metropolis Hastings

*MetropolistHasting*

```
let rec gen n samples old_score old_value old_x_store =
  if n = 0 then samples (* return the list of samples *)
  else
    let regen = pick old_x_store in (* pick one sample *)
    let cache = Hashtbl.copy old_x_store in (* use previous store as cache *)
    Hashtbl.remove cache regen; (* force resampling for regen *)

    let prob = { score = 0.; x_store = empty; cache } in (* reset prob *)
    let new_value = model prob data in (* generate candidate *)
    let alpha = mh cache old_score old_x_store prob.score prob.x_store in
    let u = Random.float 1.0 in
    if not (u < alpha) then
      gen (n - 1) (old_value :: samples) old_score old_value old_x_store (* reject *)
    else gen (n - 1) (new_value :: samples) prob.score new_value prob.x_store (* accept *)
in
```



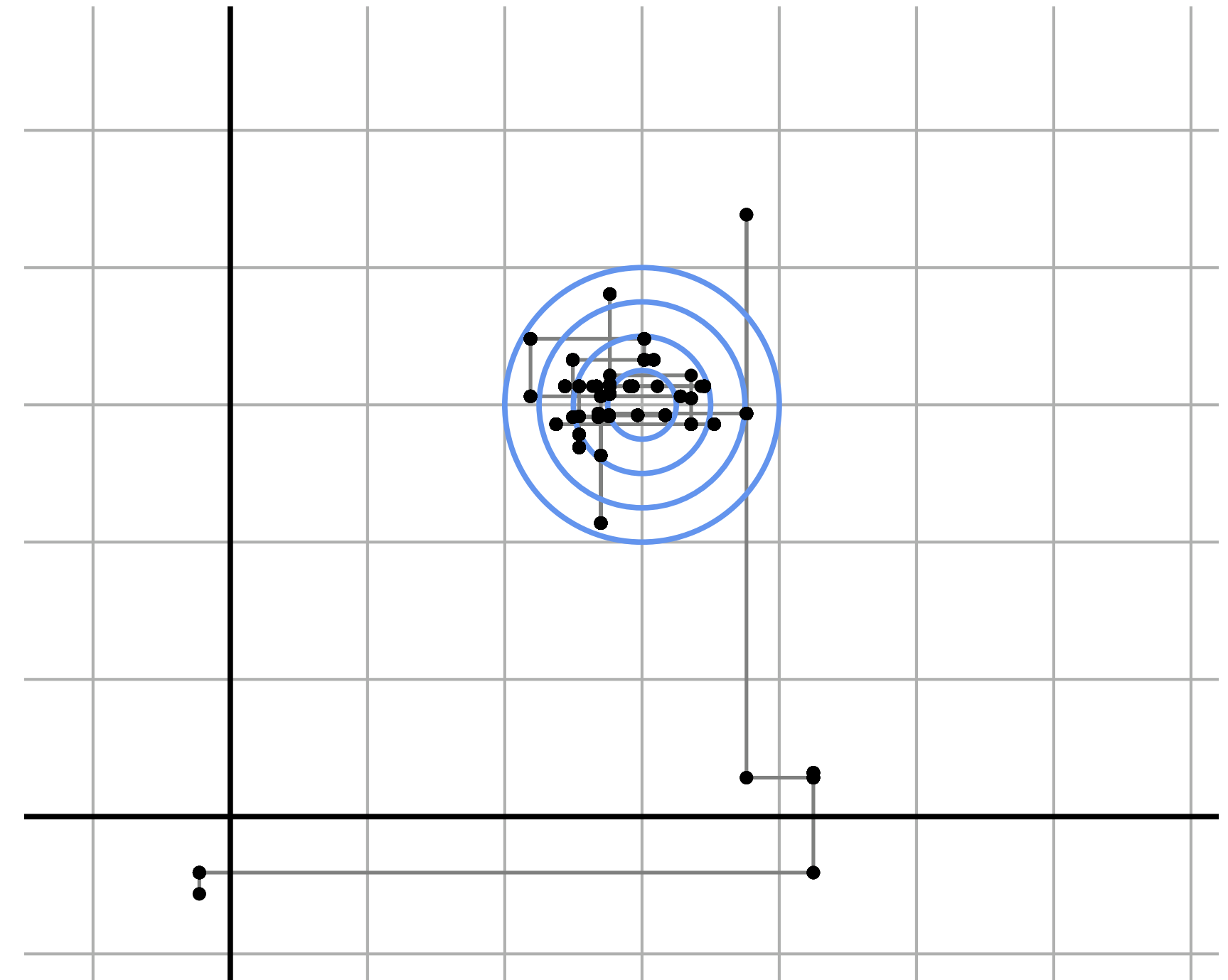
# Example: Noisy position

```
open Basic.Metropolis_hastings
```

```
let gauss obs =  
  let x = sample (gaussian ~mu:0.0 ~sigma:10.0) in  
  let y = sample (gaussian ~mu:0.0 ~sigma:10.0) in  
  List.iter  
    (fun (xo, yo) →  
      observe (gaussian ~mu:x ~sigma:1.0) xo;  
      observe (gaussian ~mu:y ~sigma:1.0) yo )  
    obs;  
  (x, y)
```

```
let _ =  
  let dist = infer gauss data in  
  plot dist
```

1000 samples



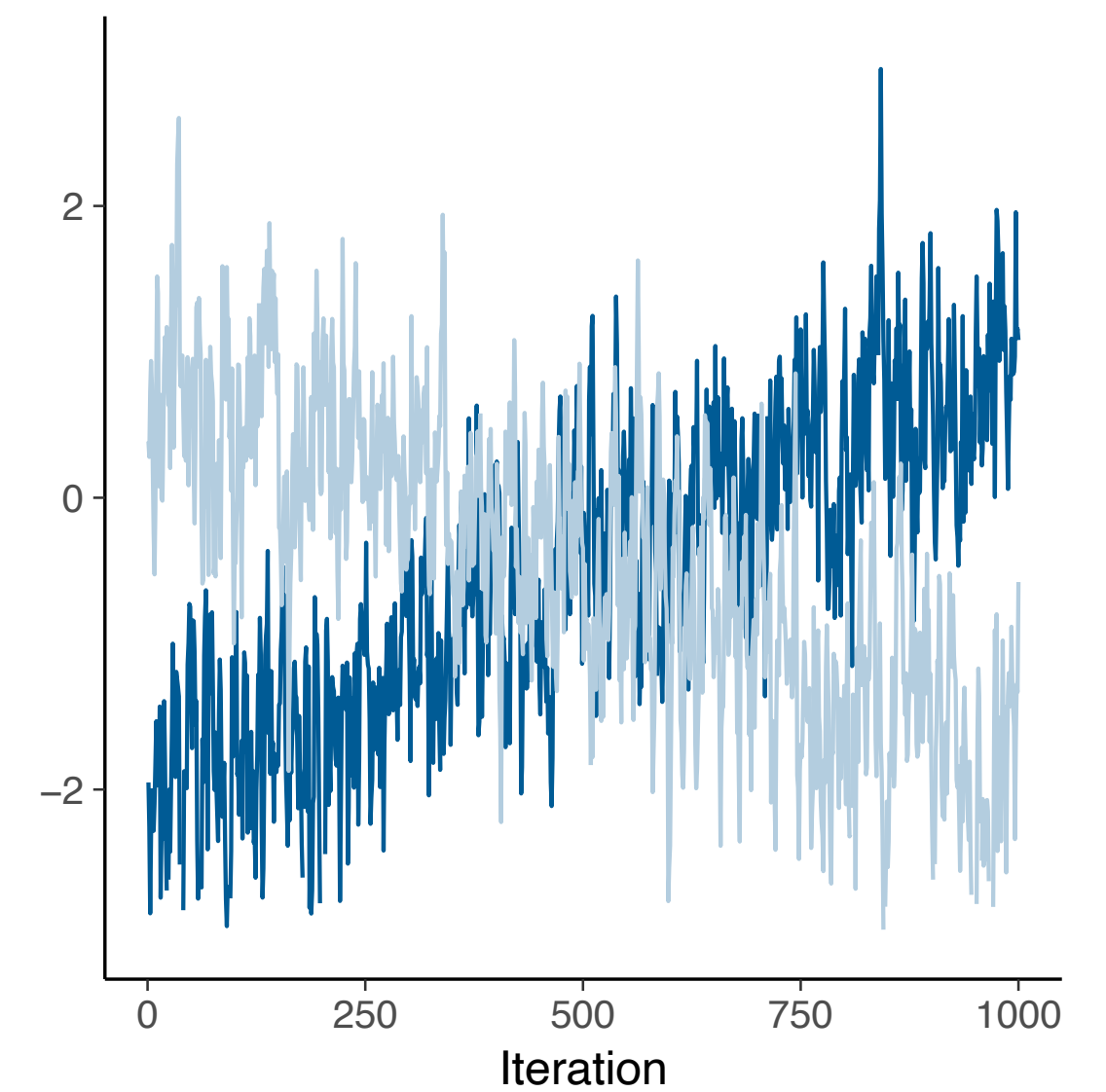
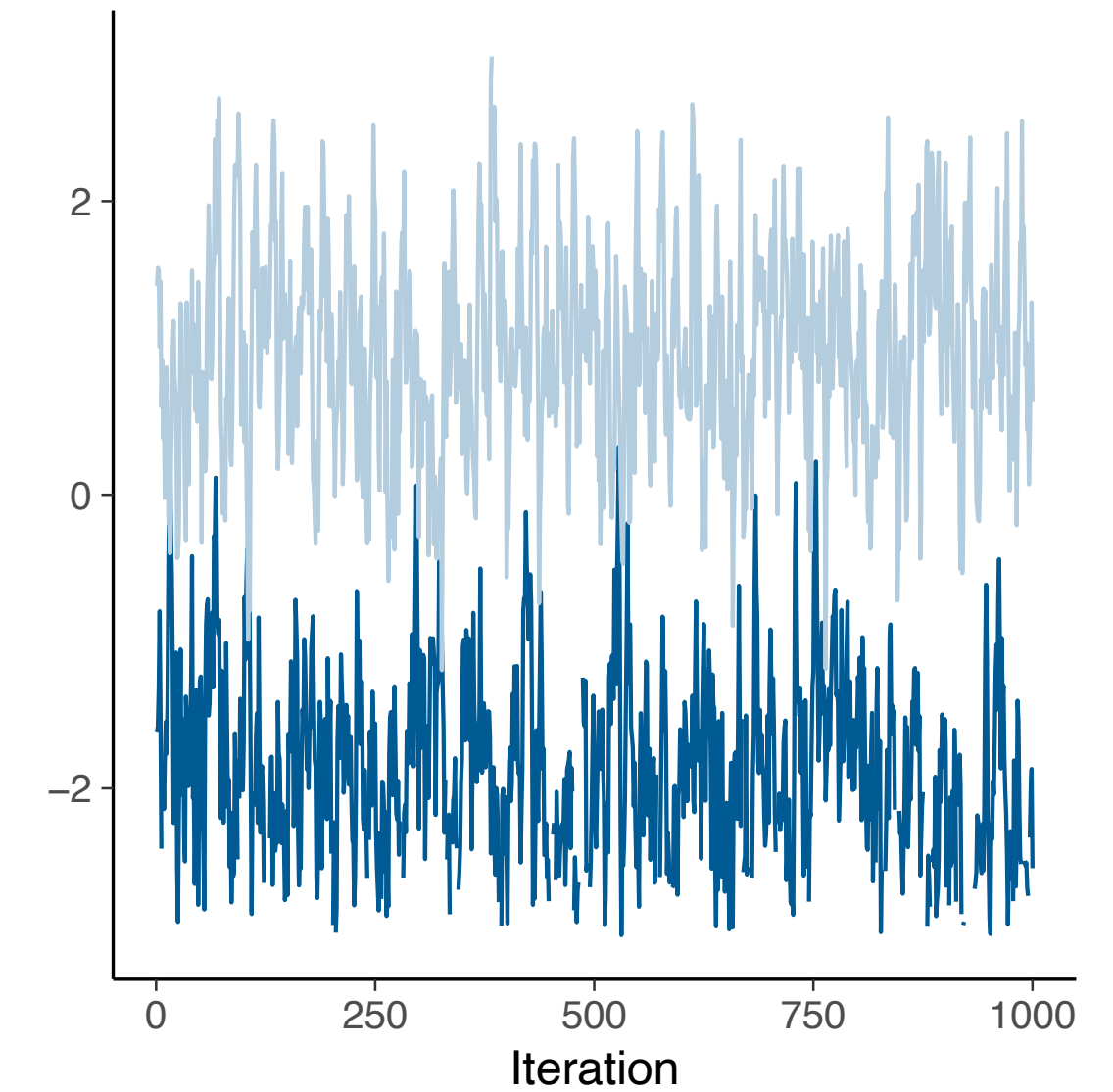
# Limitations

Convergence: theoretical conditions are complex

- Check experimentally: trace plot, R-hat (multi-chains)
- Solution: warmup, change initial conditions, reparameterization, ...

Sample correlation

- Diagnostic tools ESS (effective sample size)
- Solution: thinning, (keep one sample every  $n$ )



# Limitations

Convergence: theoretical conditions are complex

- Check experimentally: trace plot, R-hat (multi-chains)
- Solution: warmup, change initial conditions, reparameterization, ...

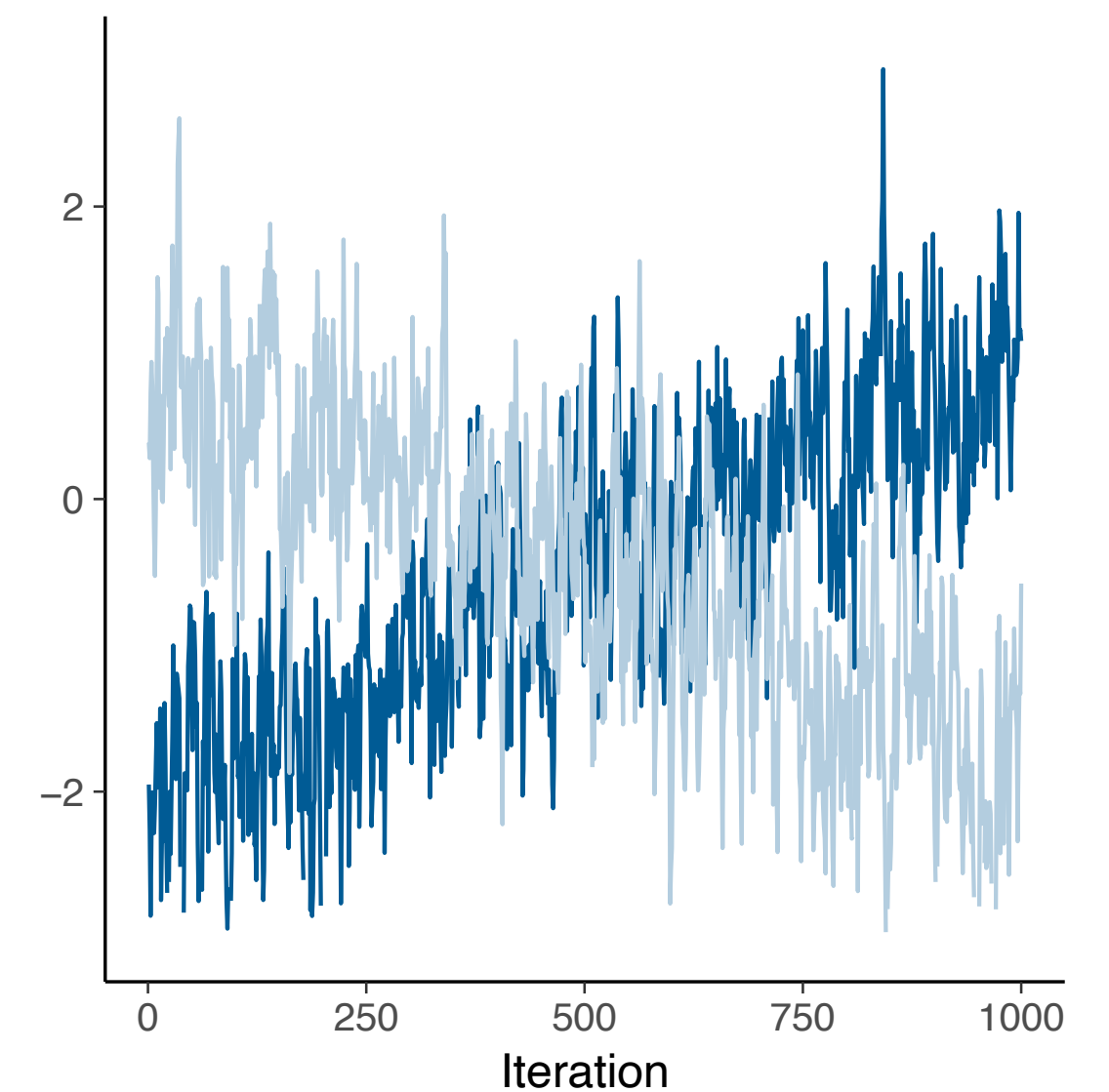
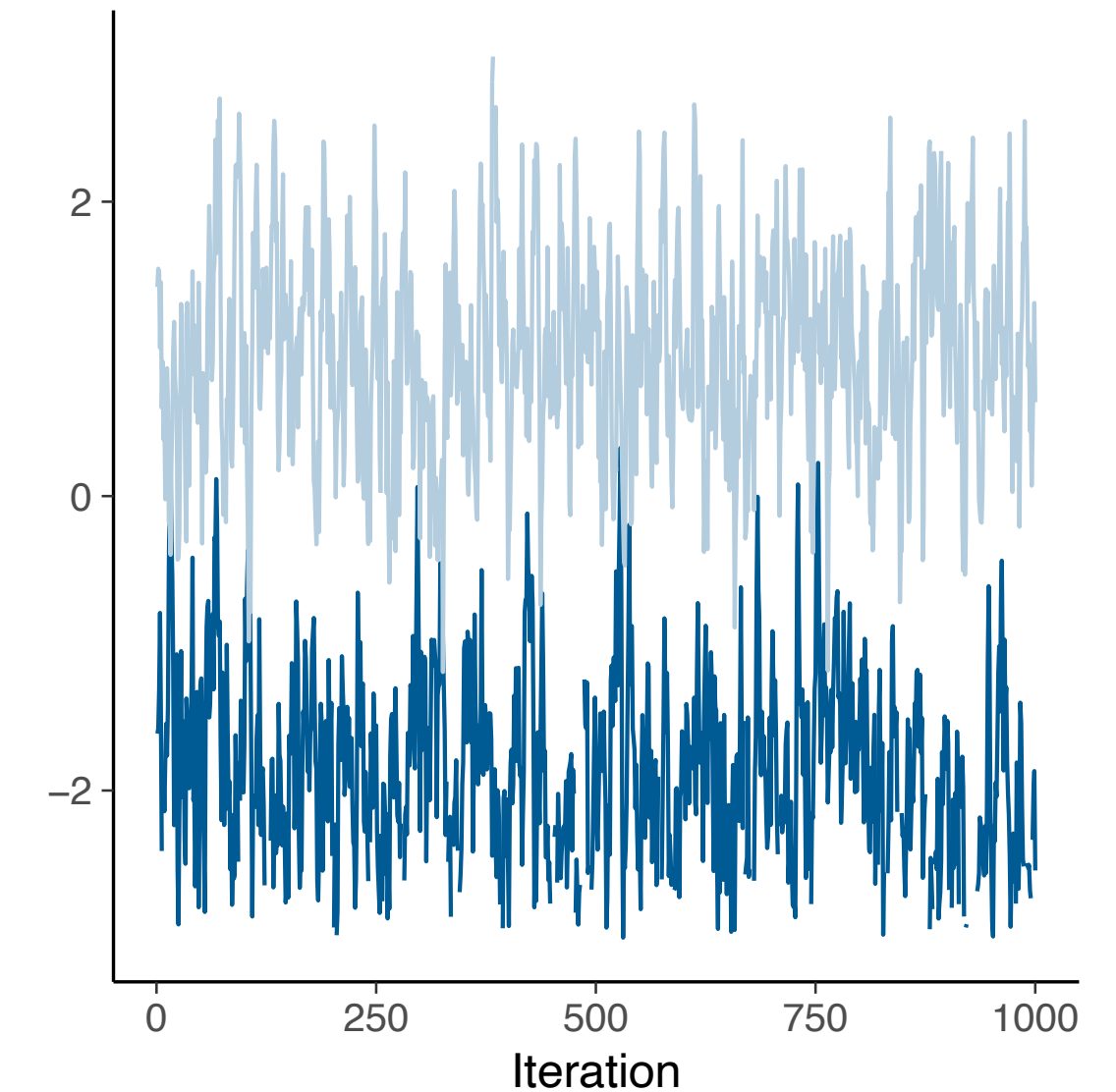
Sample correlation

- Diagnostic tools ESS (effective sample size)
- Solution: thinning, (keep one sample every  $n$ )

Model: gauss

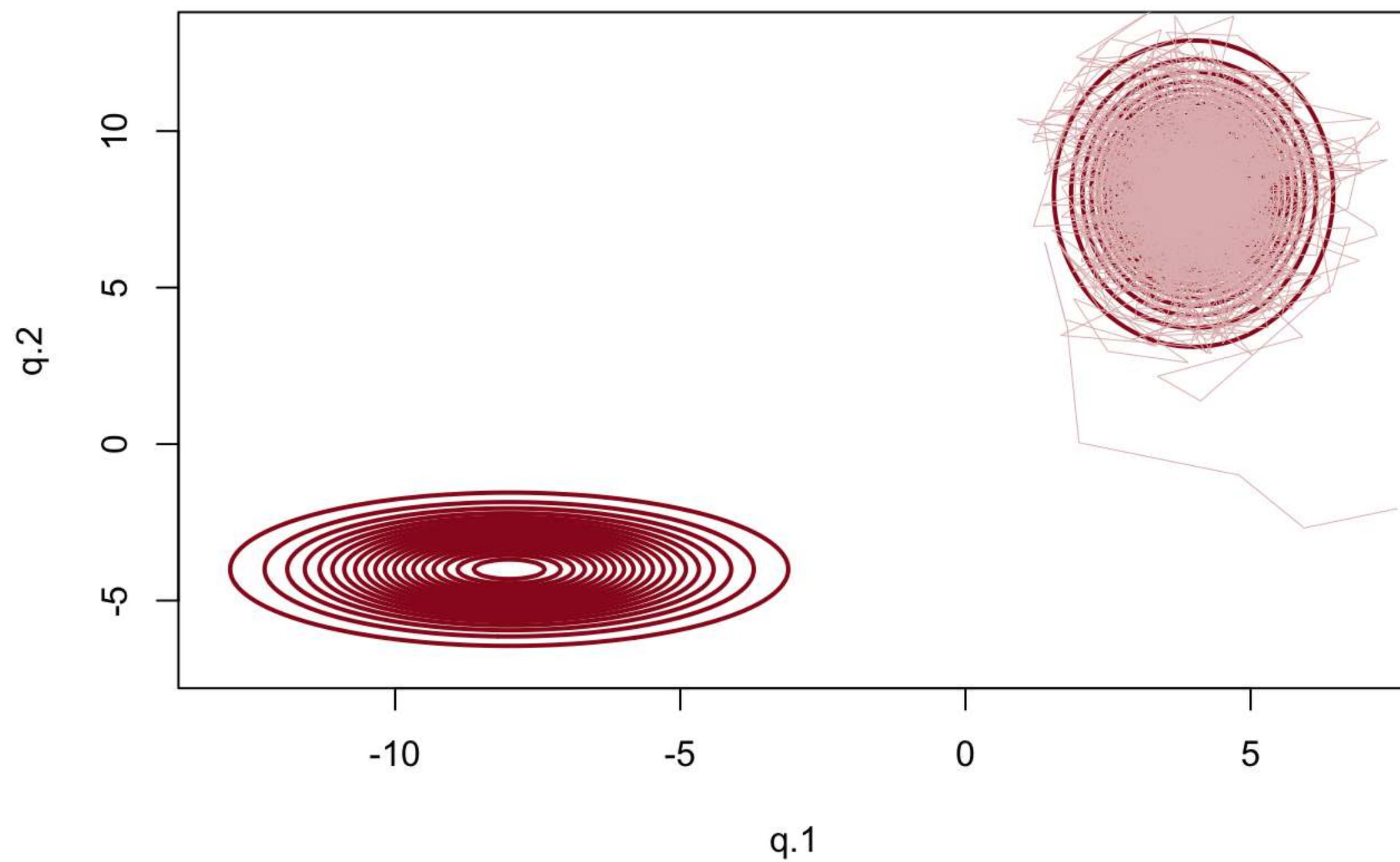
chains=4, num\_particles=1000, warmups=1000

	mean	sd	ess_bulk	r_hat
x	2.793	0.373	21.0	1.23
y	3.028	0.335	43.0	1.08



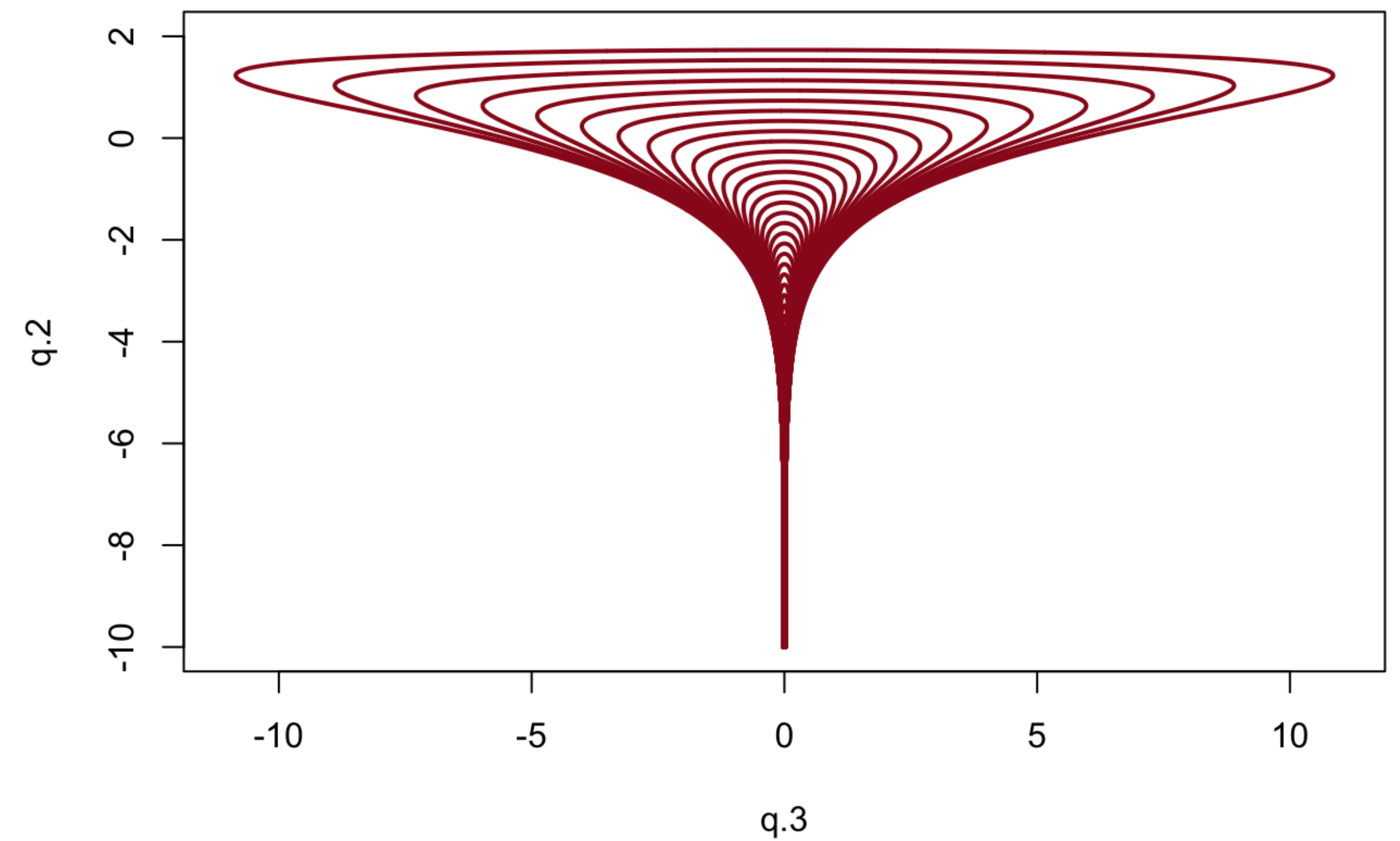
# Pathological models

**Metastable Target Density**



Multimodal distribution

**Funnel Target Density**



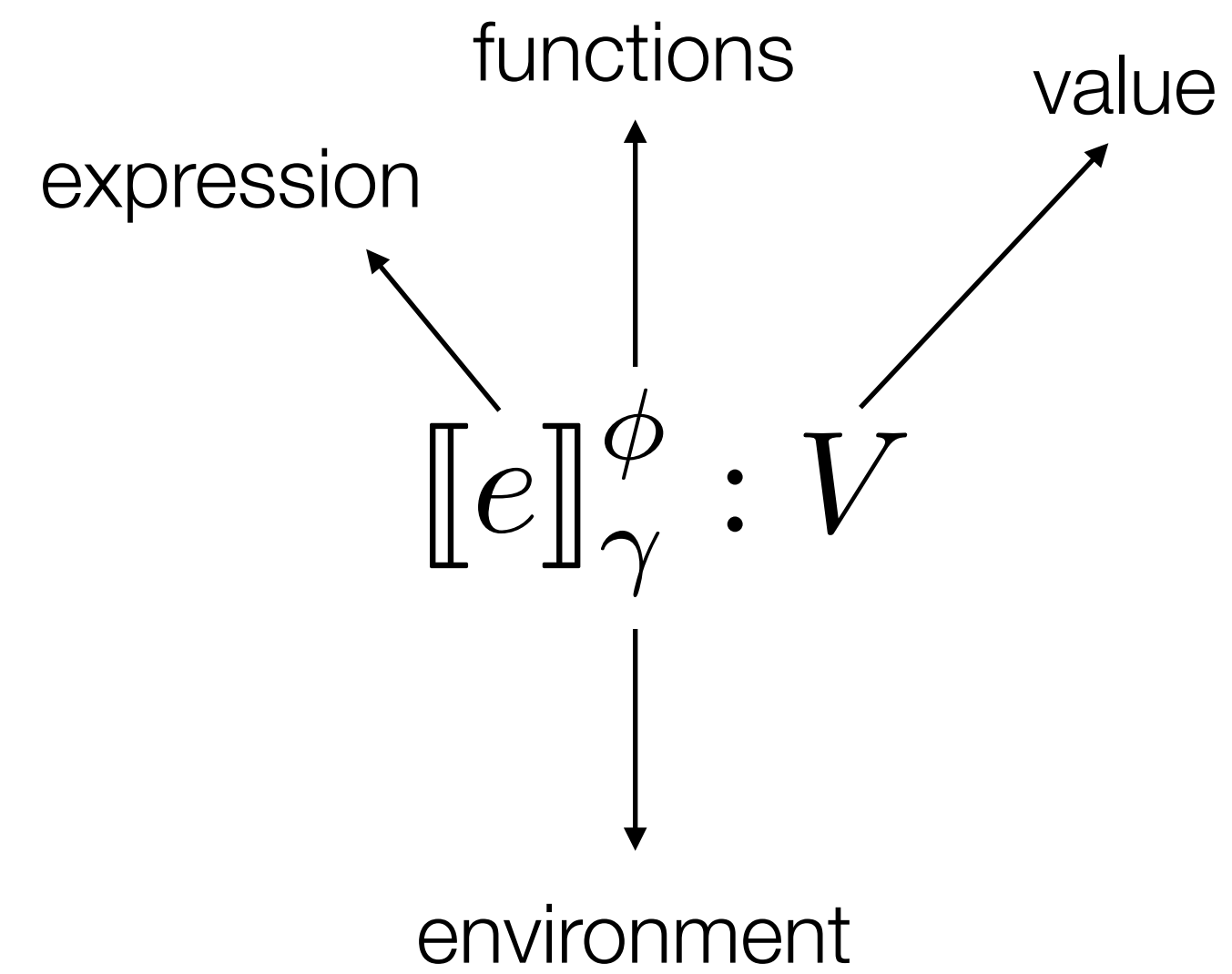
Neal's funnel

# Density semantics

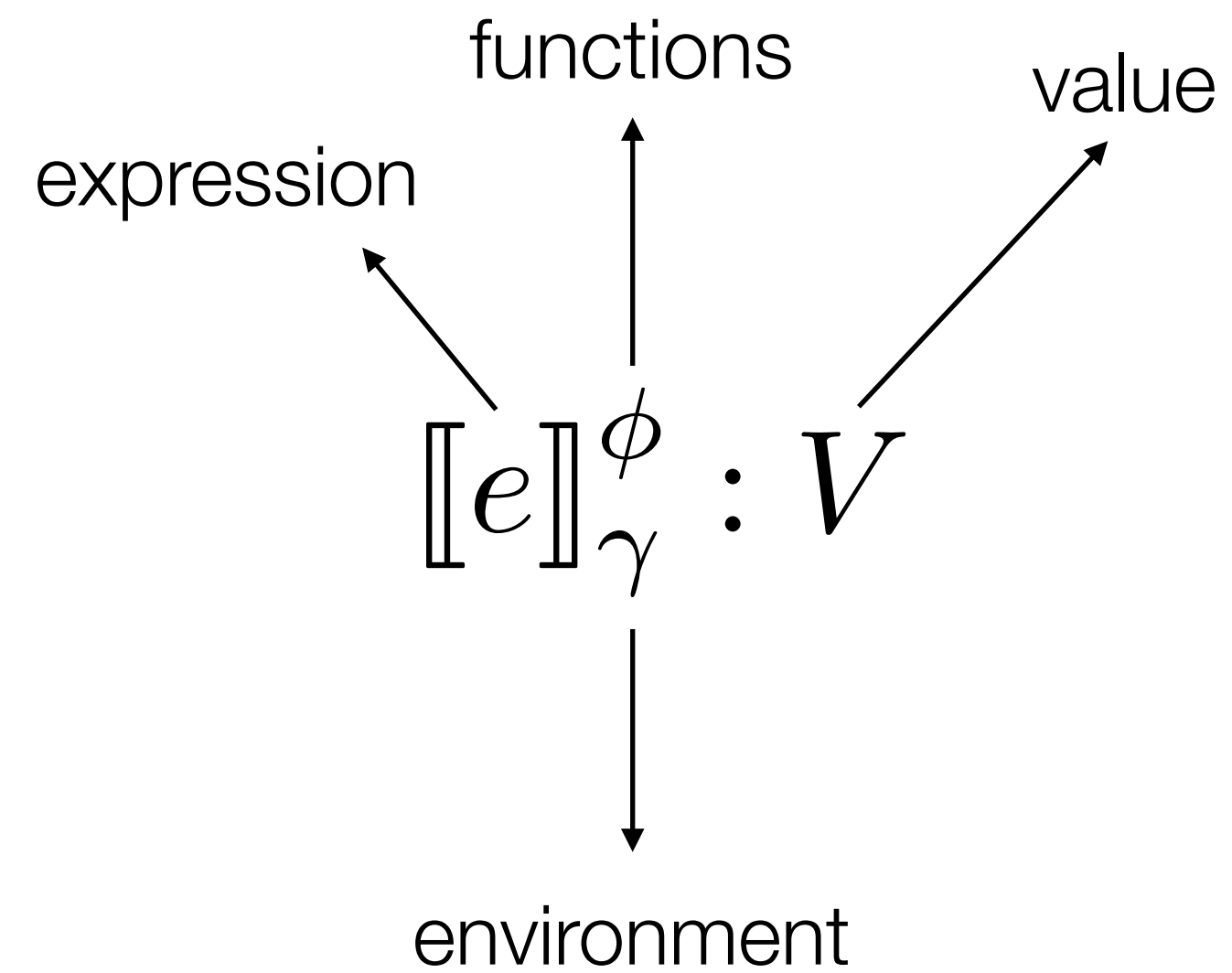
---

## Probabilistic Programming Languages

# Reminders: deterministic semantics



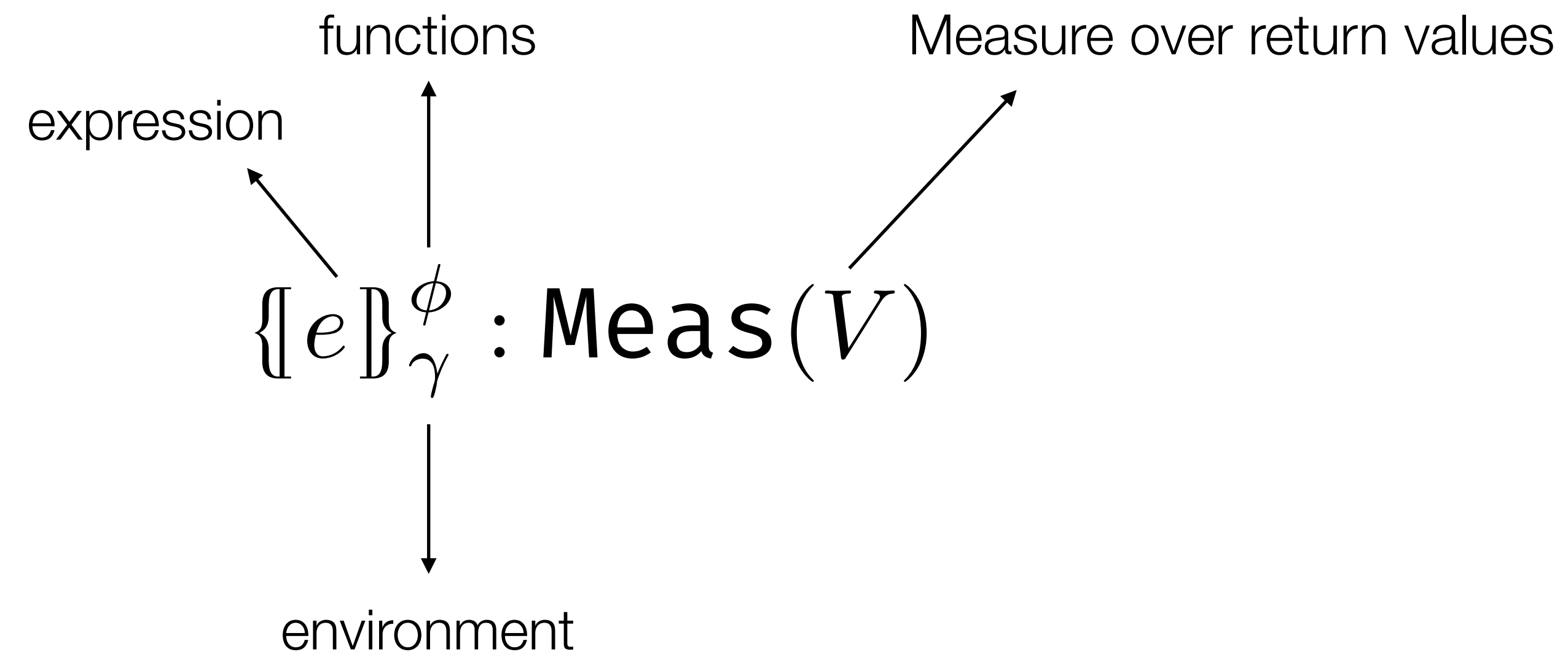
# Reminders: deterministic semantics



Example:

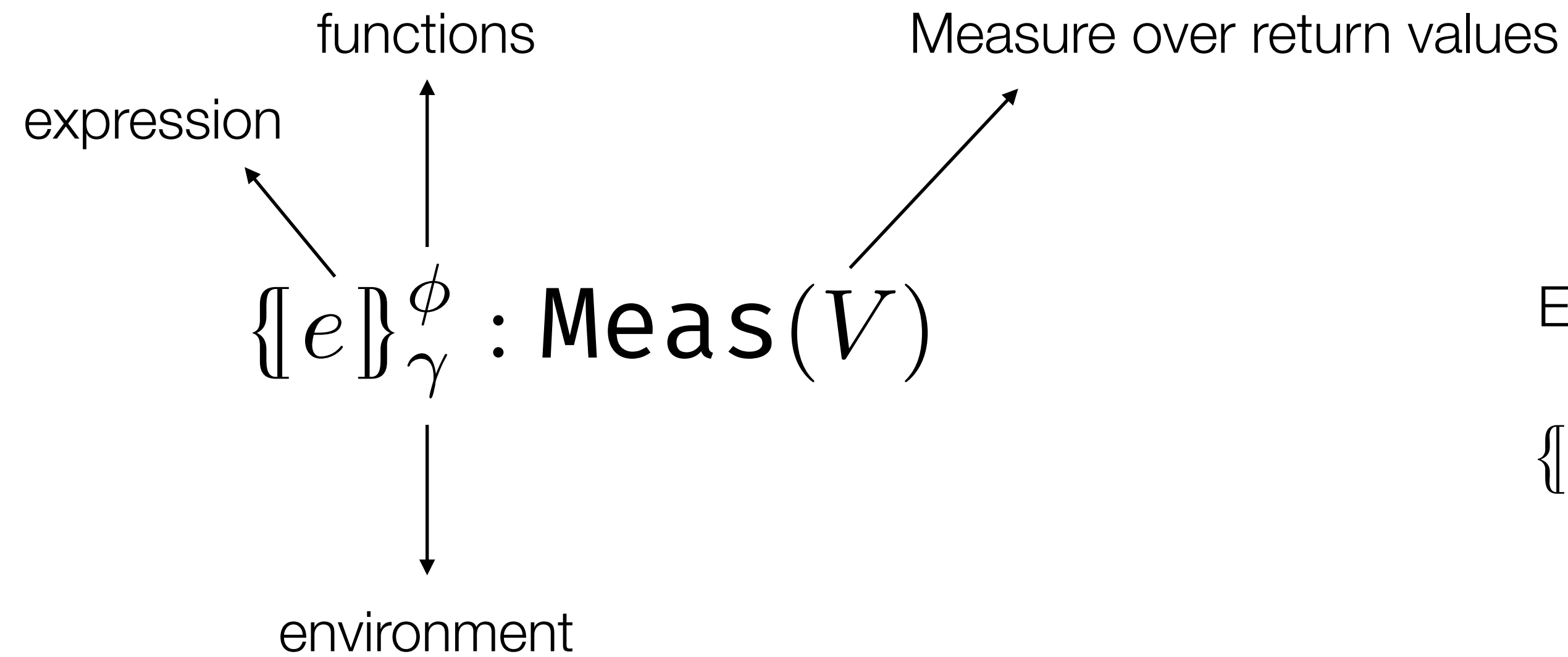
$$\begin{aligned} \llbracket \text{let } y = 40 \text{ in } x + y \rrbracket_{[x \leftarrow 2]}^\emptyset &= \llbracket x + y \rrbracket_{[x \leftarrow 2, y \leftarrow 40]}^\emptyset \\ &= 42 \end{aligned}$$

# Reminders: kernel semantics





# Reminders: kernel semantics

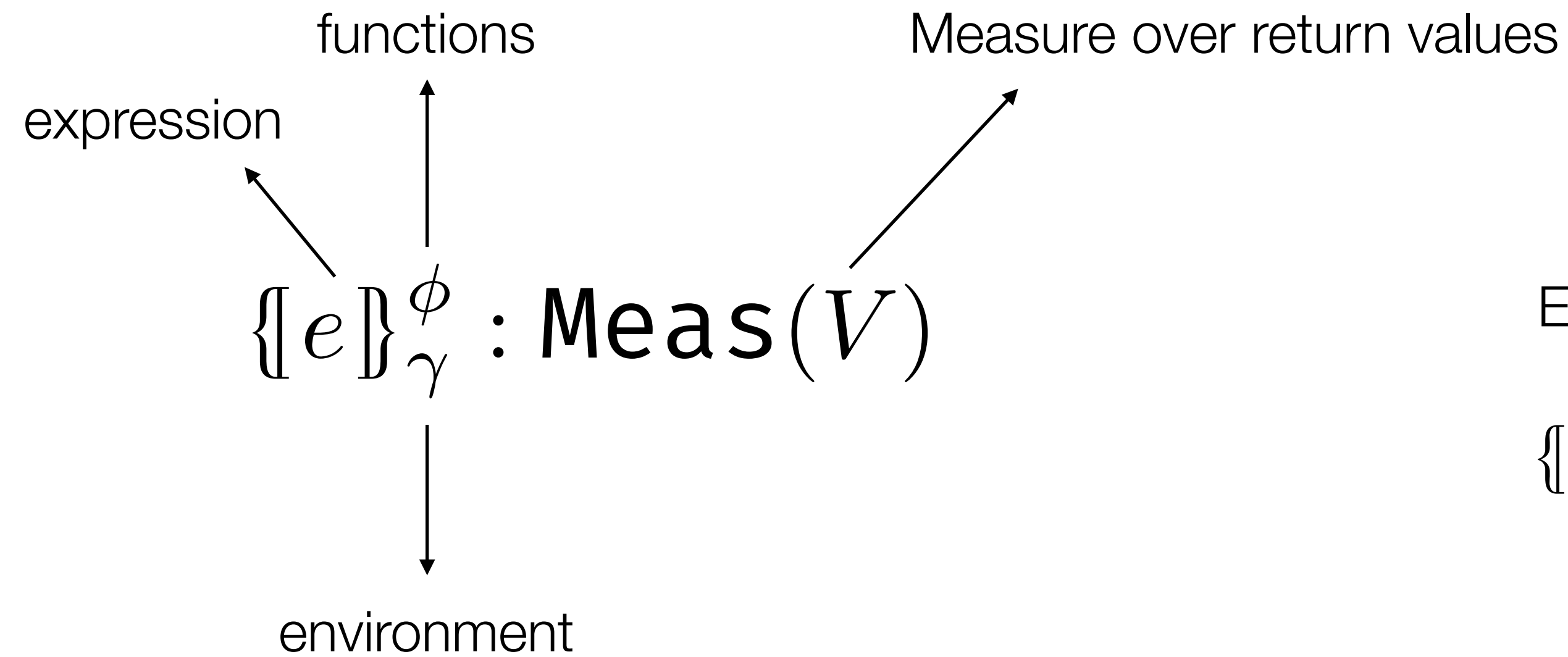


Example:

$$\{\text{sample}(\mathcal{N}(0, 1))\}_{\emptyset}^{\emptyset}(\mathbb{R}^+) = 0.5$$

# Reminders: kernel semantics

Unnormalized measure

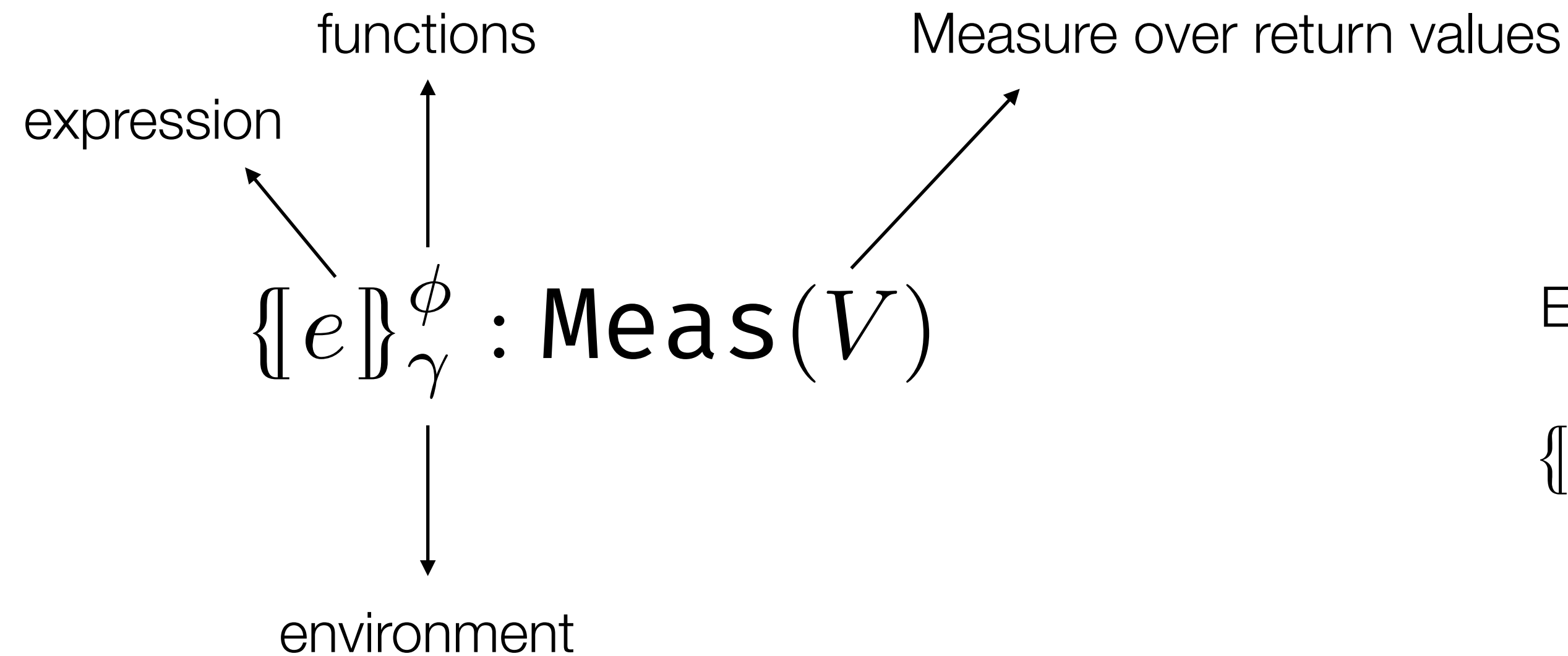


Example:

$$\{\text{sample}(\mathcal{N}(0, 1))\}_{\emptyset}^{\emptyset}(\mathbb{R}^+) = 0.5$$

# Reminders: kernel semantics

Unnormalized measure



Example:

$$\{\text{sample}(\mathcal{N}(0, 1))\}_{\emptyset}^{\emptyset}(\mathbb{R}^+) = 0.5$$

$$\llbracket \text{infer}(e) \rrbracket_{\gamma}^{\phi} = \frac{\{e\}_{\gamma}^{\phi}}{\{e\}_{\gamma}^{\phi}(\llbracket \text{typeOf}(e) \rrbracket)}$$

# Density semantics

## Key idea

- A model is a function  $f : R \rightarrow t \times \mathbb{R}^+$
- Associate a value  $v(r)$  and a score  $W(r)$  to parameters (random variables)
- Deterministic function *given an oracle* for the parameters

Interpretation close to our weighted samplers for approximate inference

## Back to measure

- $\rho$ : uniform distributions on parameters
- We get a measure by integrating  $f$  along  $\rho$

$$\mu(U) = \int \rho(dr) W(r) \delta_{v(r)}(U)$$

# Density semantics

## Key idea

- A model is a function  $f : R \rightarrow t \times \mathbb{R}^+$
- Associate a value  $v(r)$  and a score  $W(r)$  to parameters (random variables)
- Deterministic function *given an oracle* for the parameters

Interpretation close to our weighted samplers for approximate inference

## Back to measure

- $\rho$ : uniform distributions on parameters
- We get a measure by integrating  $f$  along  $\rho$

$$\mu(U) = \int \rho(dr) W(r) \delta_{v(r)}(U)$$

Problem: random variables can change between two executions

```
let c = sample (bernoulli ~p:0.5)
if c then let x = sample (gaussian ~mu:0. ~sigma:1.) in ...
```

# Measure over parameters

# Measure over parameters

## Key ideas

- Map random elements in  $[0, 1]$  to samples using inverse transform sampling
- Pass random elements as argument to the semantics

## Inverse transform sampling

- Draw a sample  $u \sim \text{Uniform}(0, 1)$
- Compute sample value  $x = \text{icdf}(\mu)(u)$
- $\text{icdf}(\mu)$ : generalized inverse of the cumulative distribution function

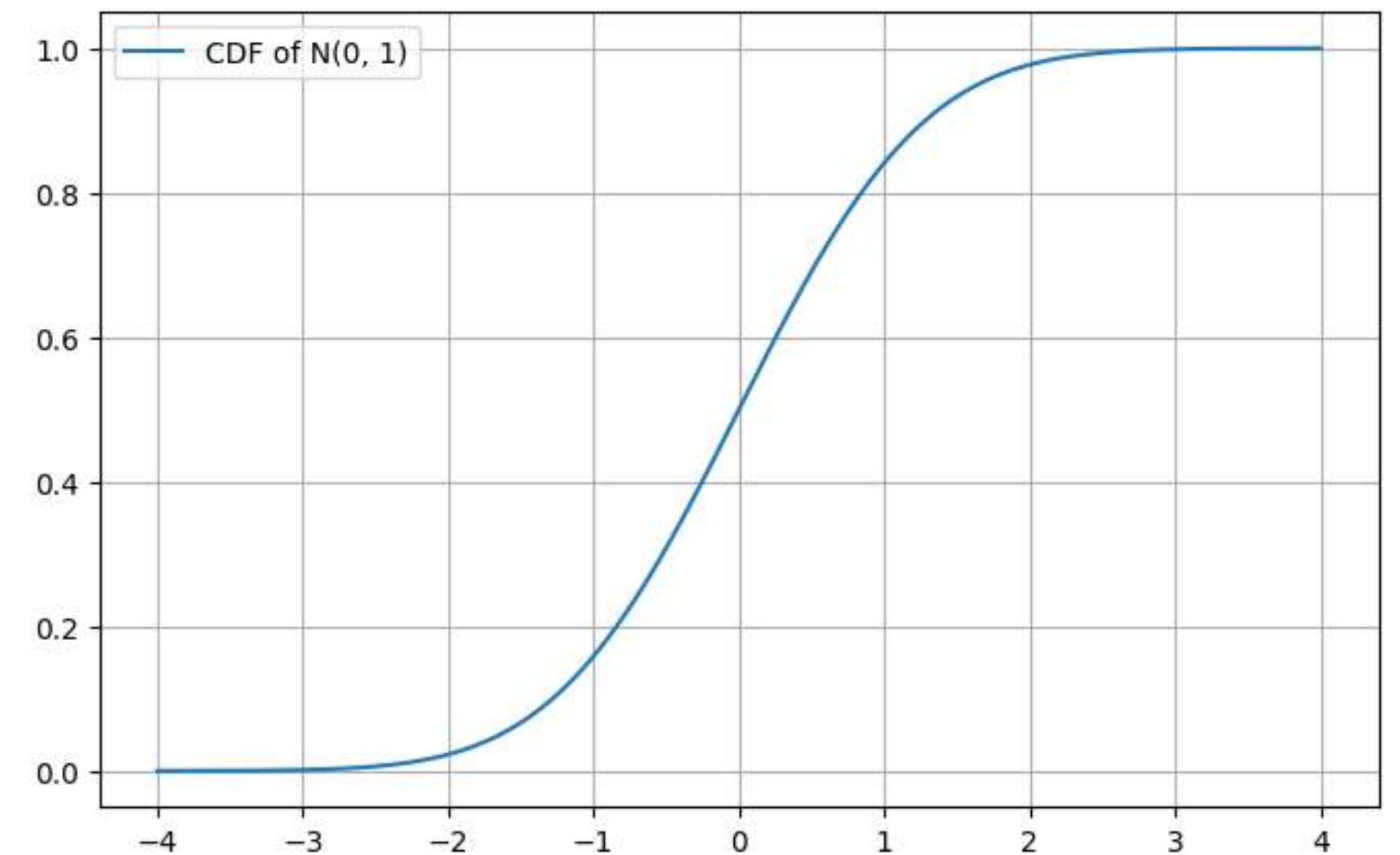
# Measure over parameters

## Key ideas

- Map random elements in  $[0, 1]$  to samples using inverse transform sampling
- Pass random elements as argument to the semantics

## Inverse transform sampling

- Draw a sample  $u \sim \text{Uniform}(0, 1)$
- Compute sample value  $x = \text{icdf}(\mu)(u)$
- $\text{icdf}(\mu)$ : generalized inverse of the cumulative distribution function





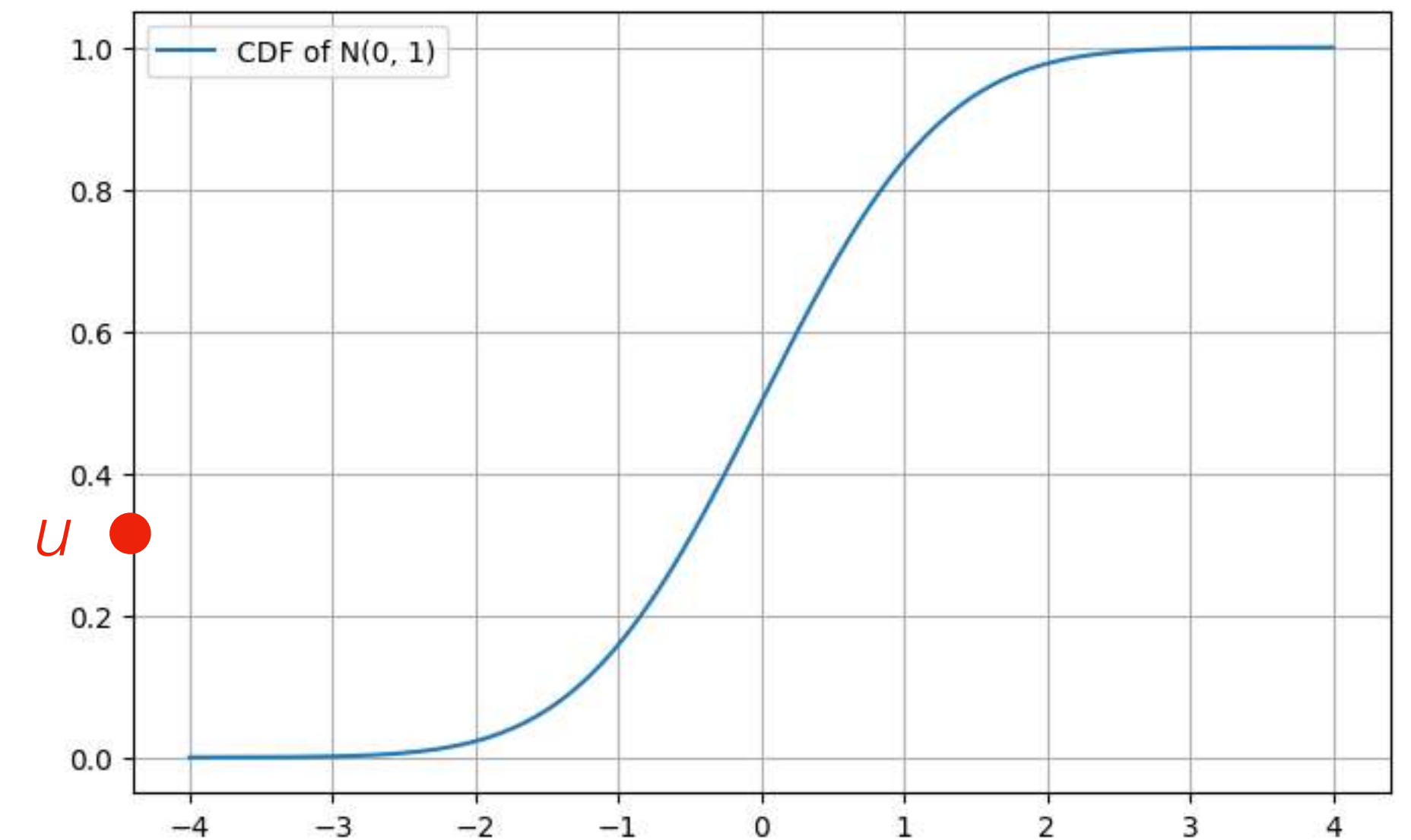
# Measure over parameters

## Key ideas

- Map random elements in  $[0, 1]$  to samples using inverse transform sampling
- Pass random elements as argument to the semantics

## Inverse transform sampling

- Draw a sample  $u \sim \text{Uniform}(0, 1)$
- Compute sample value  $x = \text{icdf}(\mu)(u)$
- $\text{icdf}(\mu)$ : generalized inverse of the cumulative distribution function



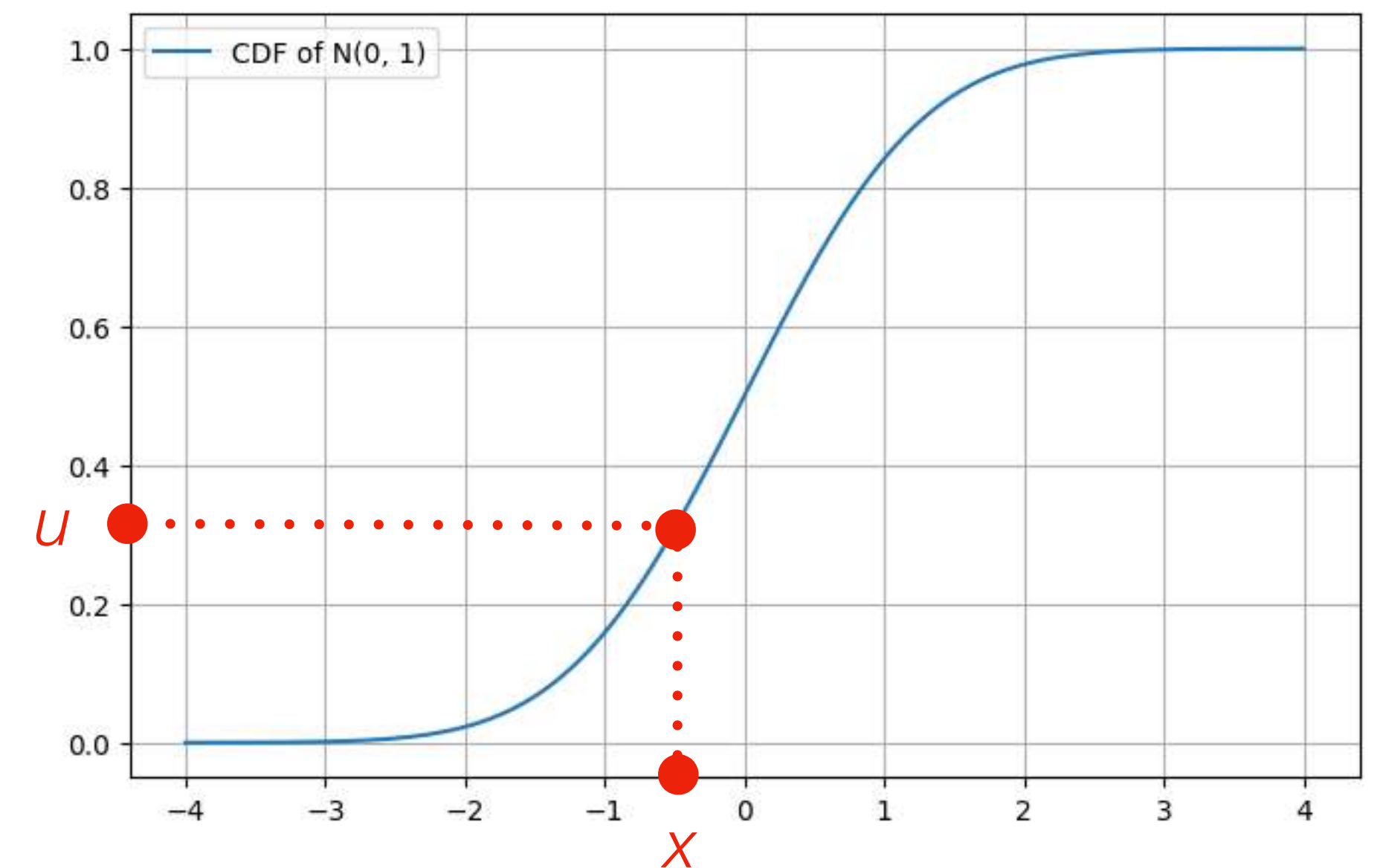
# Measure over parameters

## Key ideas

- Map random elements in  $[0, 1]$  to samples using inverse transform sampling
- Pass random elements as argument to the semantics

## Inverse transform sampling

- Draw a sample  $u \sim \text{Uniform}(0, 1)$
- Compute sample value  $x = \text{icdf}(\mu)(u)$
- $\text{icdf}(\mu)$ : generalized inverse of the cumulative distribution function



# Measure over parameters

## Key ideas

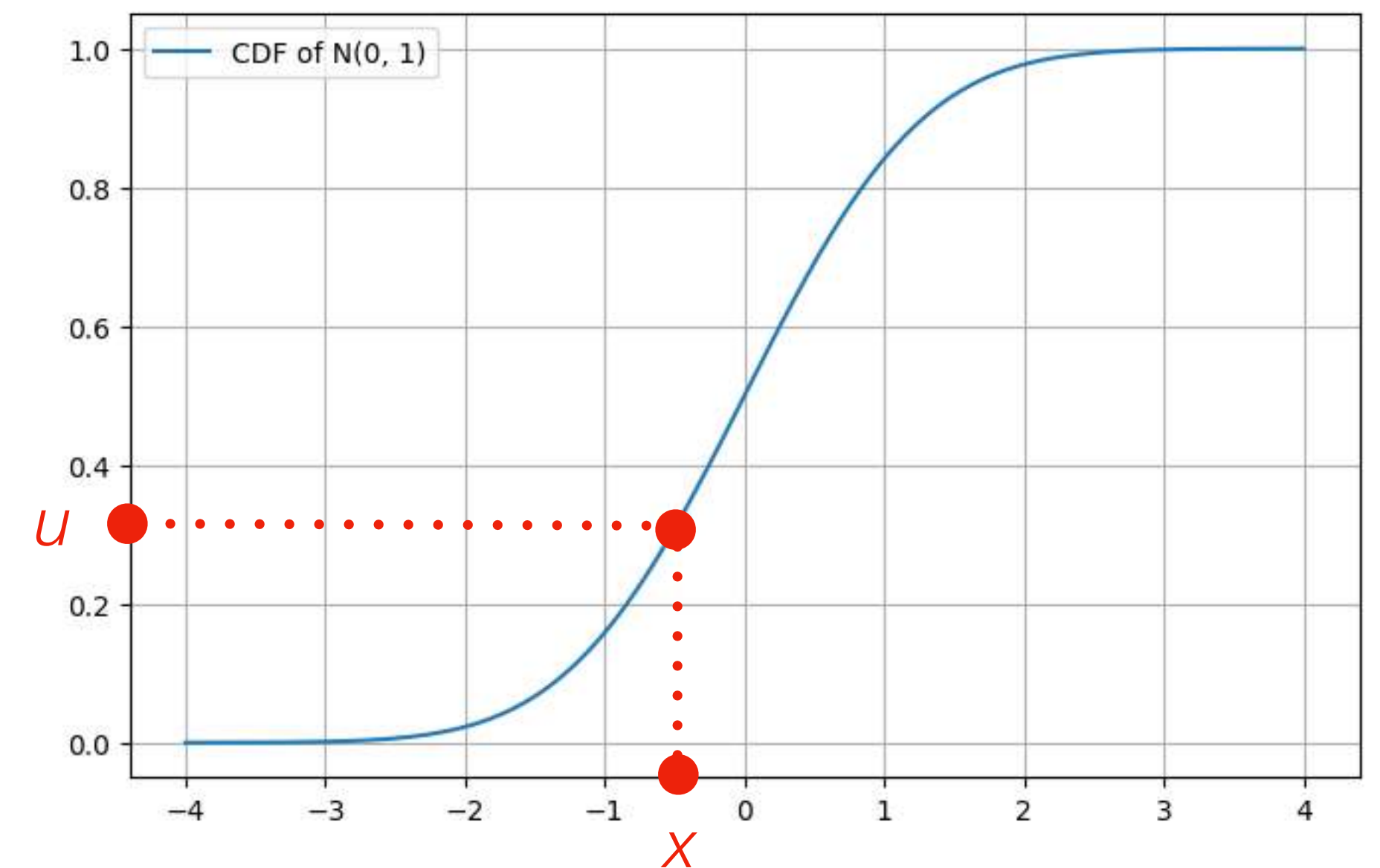
- Map random elements in  $[0, 1]$  to samples using inverse transform sampling
- Pass random elements as argument to the semantics

## Inverse transform sampling

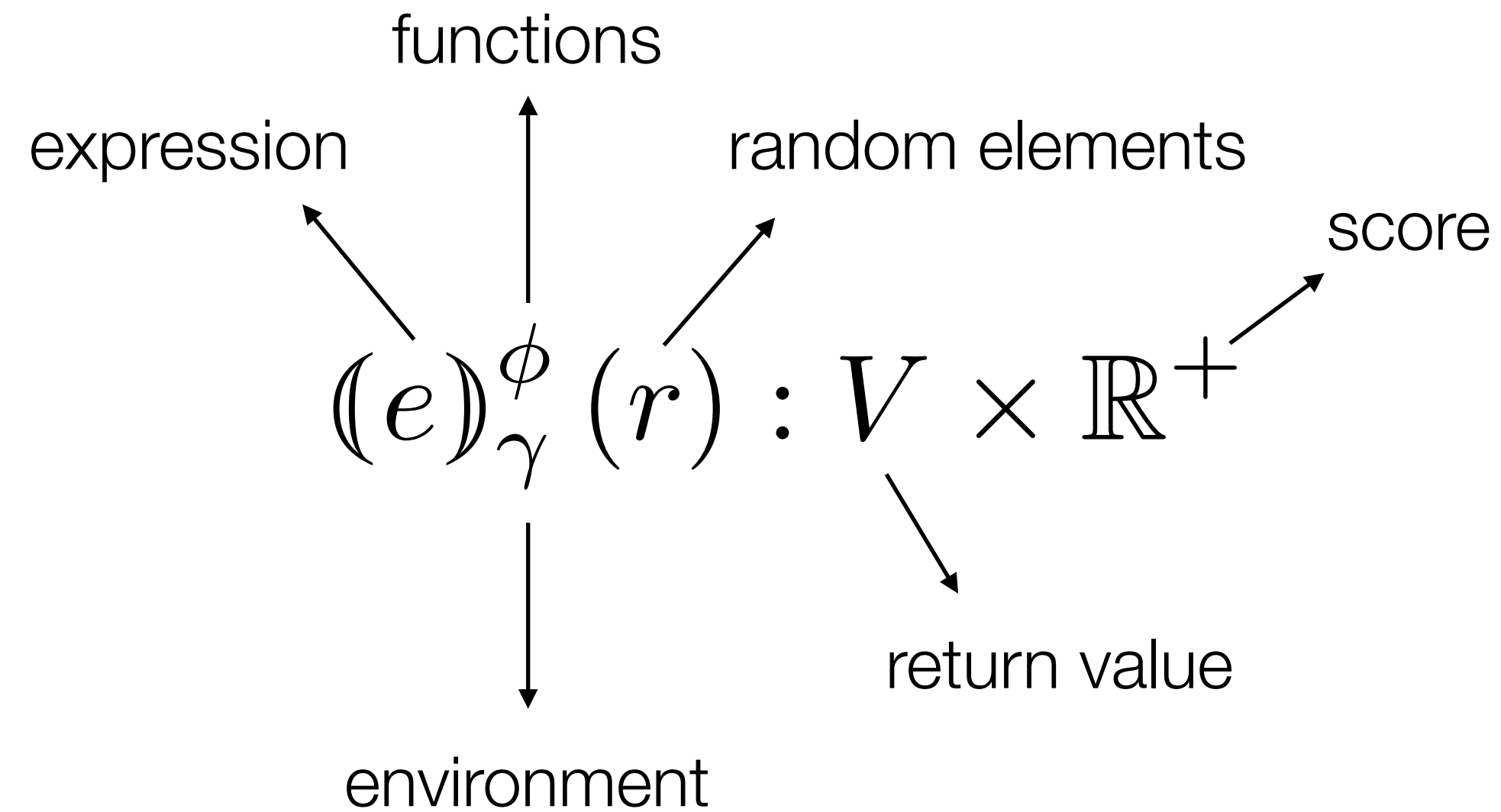
- Draw a sample  $u \sim \text{Uniform}(0, 1)$
- Compute sample value  $x = \text{icdf}(\mu)(u)$
- $\text{icdf}(\mu)$ : generalized inverse of the cumulative distribution function

## Uniform measure over parameters

- Use the Lebesgue measure  $\lambda$  over  $[0, 1]$  for each random element
- Product space across all possible parameters (cube)

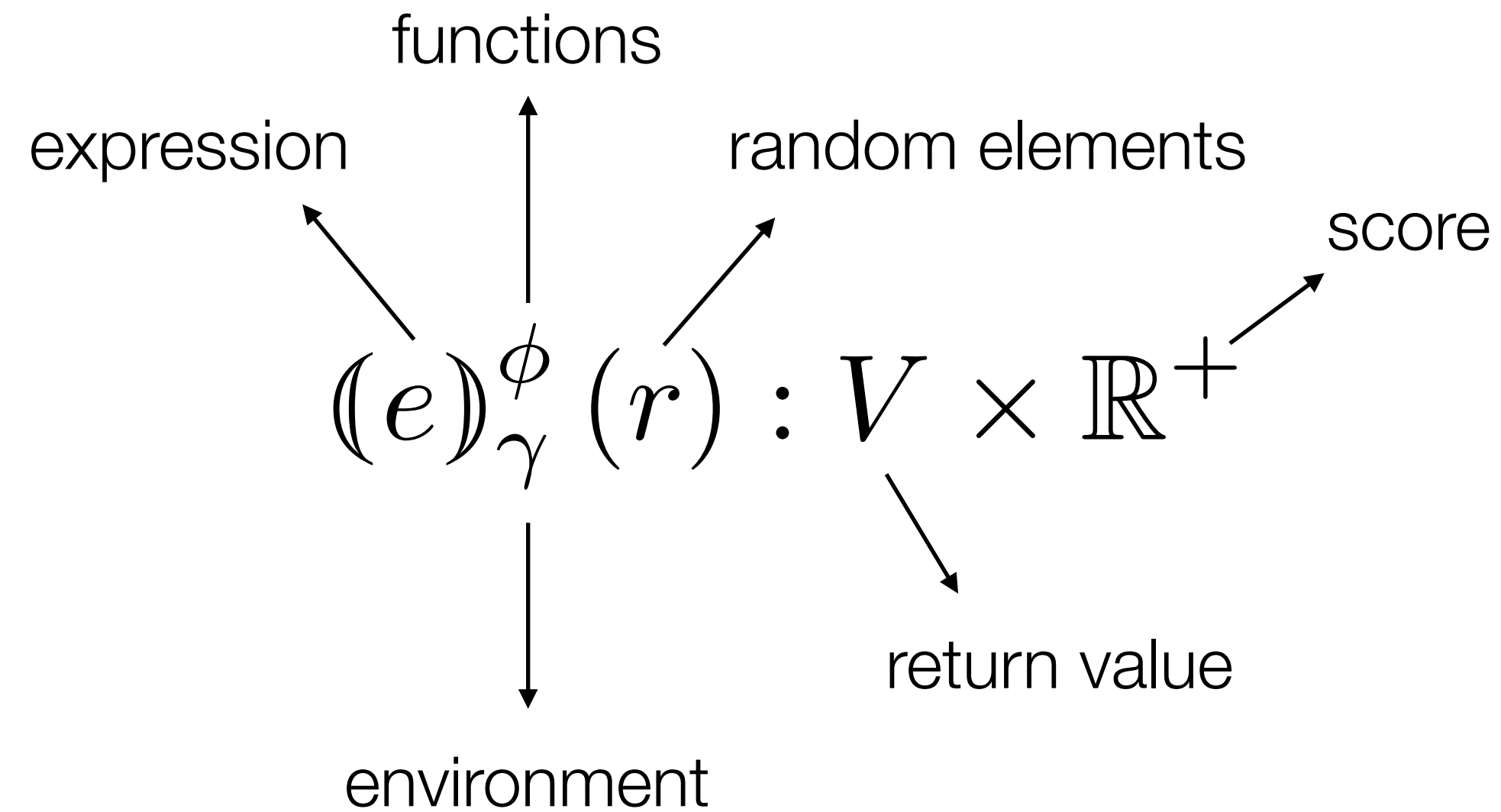


# Density semantics



$$\llbracket \text{infer}(e) \rrbracket_{\gamma}^{\phi}(U) = \begin{cases} \frac{\mu(U)}{\mu(\top)} & \text{with } \begin{cases} \mu(U) = \int \rho(dr) W(r) \delta_{v(r)}(U) \\ v(r), W(r) = ((e))_{\gamma}^{\phi}(r) \end{cases} \\ \text{Error} & \text{otherwise} \end{cases} \quad \text{if } 0 < \mu(\top) < \infty$$

# Density semantics



Example:

$$((\text{sample}(\mathcal{N}(0, 1)))_{\gamma}^{\phi}(r) = \text{icdf}(\mathcal{N}(0, 1))(r)$$

$$\llbracket \text{infer}(e) \rrbracket_{\gamma}^{\phi}(U) = \begin{cases} \frac{\mu(U)}{\mu(\top)} & \text{with } \begin{cases} \mu(U) = \int \rho(dr) W(r) \delta_{v(r)}(U) \\ v(r), W(r) = ((e))_{\gamma}^{\phi}(r) \end{cases} \\ \text{Error} & \text{otherwise} \end{cases} \quad \text{if } 0 < \mu(\top) < \infty$$

# Density semantics

# Density semantics

Remember: sampler semantics

- Expressions are interpreted as weighted samplers in log space
- Given an environment  $\phi, \gamma$ , and random elements  $r$ ,  $((e)_{\gamma}^{\phi}(r) = v, W$
- $((e)^{\phi} : \Gamma \times R \rightarrow V \times \mathbb{R}^+$
- Parameters are now inputs

# Density semantics

## Remember: sampler semantics

- Expressions are interpreted as weighted samplers in log space
- Given an environment  $\phi, \gamma$ , and random elements  $r$ ,  $\llbracket e \rrbracket_{\gamma}^{\phi}(r) = v, W$
- $\llbracket e \rrbracket^{\phi} : \Gamma \times R \rightarrow V \times \mathbb{R}^+$
- Parameters are now inputs

$$\llbracket c \rrbracket_{\gamma}^{\phi}(\emptyset) = c, 1$$

$$\llbracket x \rrbracket_{\gamma}^{\phi}(\emptyset) = \gamma(x), 1$$

$$\llbracket \text{sample}(e) \rrbracket_{\gamma}^{\phi}(r) = \text{icdf}(\llbracket e \rrbracket_{\gamma}^{\phi})(r), 1$$

$$\llbracket \text{factor}(e) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \llbracket e \rrbracket_{\gamma}^{\phi}$$

$$\llbracket \text{observe}(e_1, e_2) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \text{pdf}(\llbracket e_1 \rrbracket_{\gamma}^{\phi})(\llbracket e_2 \rrbracket_{\gamma}^{\phi})$$

$$\begin{aligned} \llbracket \text{let } x = e_1 \text{ in } e_2 \rrbracket_{\gamma}^{\phi}(r_1, r_2) &= \text{let } v_1, W_1 = \llbracket e_1 \rrbracket_{\gamma}^{\phi}(r_1) \text{ in} \\ &\quad \text{let } v_2, W_2 = \llbracket e_2 \rrbracket_{\gamma+[x \leftarrow v_1]}^{\phi}(r_2) \text{ in} \\ &\quad v_2, W_1 \times W_2 \end{aligned}$$



# Density semantics

Remember: sampler semantics

- Expressions are interpreted as weighted samplers in log space
- Given an environment  $\phi, \gamma$ , and random elements  $r$ ,  $\llbracket e \rrbracket_{\gamma}^{\phi}(r) = v, W$
- $\llbracket e \rrbracket^{\phi} : \Gamma \times R \rightarrow V \times \mathbb{R}^+$
- Parameters are now inputs

$$\llbracket c \rrbracket_{\gamma}^{\phi}(\emptyset) = c, 1$$

$$\llbracket x \rrbracket_{\gamma}^{\phi}(\emptyset) = \gamma(x), 1$$

$$\llbracket \text{sample}(e) \rrbracket_{\gamma}^{\phi}(r) = \text{icdf}(\llbracket e \rrbracket_{\gamma}^{\phi})(r), 1$$

$$\llbracket \text{factor}(e) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \llbracket e \rrbracket_{\gamma}^{\phi}$$

$$\llbracket \text{observe}(e_1, e_2) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \text{pdf}(\llbracket e_1 \rrbracket_{\gamma}^{\phi})(\llbracket e_2 \rrbracket_{\gamma}^{\phi})$$

$$\begin{aligned} \llbracket \text{let } x = e_1 \text{ in } e_2 \rrbracket_{\gamma}^{\phi}(r_1, r_2) &= \text{let } v_1, W_1 = \llbracket e_1 \rrbracket_{\gamma}^{\phi}(r_1) \text{ in} \\ &\quad \text{let } v_2, W_2 = \llbracket e_2 \rrbracket_{\gamma+[x \leftarrow v_1]}^{\phi}(r_2) \text{ in} \\ &\quad v_2, W_1 \times W_2 \end{aligned}$$

Random elements: program structure

Deterministic expression:  $\emptyset$

# Density semantics

Remember: sampler semantics

- Expressions are interpreted as weighted samplers in log space
- Given an environment  $\phi, \gamma$ , and random elements  $r$ ,  $\llbracket e \rrbracket_{\gamma}^{\phi}(r) = v, W$
- $\llbracket e \rrbracket^{\phi} : \Gamma \times R \rightarrow V \times \mathbb{R}^+$
- Parameters are now inputs

$$\llbracket c \rrbracket_{\gamma}^{\phi}(\emptyset) = c, 1$$

$$\llbracket x \rrbracket_{\gamma}^{\phi}(\emptyset) = \gamma(x), 1$$

$$\llbracket \text{sample}(e) \rrbracket_{\gamma}^{\phi}(r) = \text{icdf}(\llbracket e \rrbracket_{\gamma}^{\phi})(r), 1$$

$$\llbracket \text{factor}(e) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \llbracket e \rrbracket_{\gamma}^{\phi}$$

$$\llbracket \text{observe}(e_1, e_2) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \text{pdf}(\llbracket e_1 \rrbracket_{\gamma}^{\phi})(\llbracket e_2 \rrbracket_{\gamma}^{\phi})$$

$$\begin{aligned} \llbracket \text{let } x = e_1 \text{ in } e_2 \rrbracket_{\gamma}^{\phi}(r_1, r_2) &= \text{let } v_1, W_1 = \llbracket e_1 \rrbracket_{\gamma}^{\phi}(r_1) \text{ in} \\ &\quad \text{let } v_2, W_2 = \llbracket e_2 \rrbracket_{\gamma+[x \leftarrow v_1]}^{\phi}(r_2) \text{ in} \\ &\quad v_2, W_1 \times W_2 \end{aligned}$$

Random elements: program structure

Deterministic expression:  $\emptyset$

Sub-expressions: nested tuples

# Density semantics

Remember: sampler semantics

- Expressions are interpreted as weighted samplers in log space
- Given an environment  $\phi, \gamma$ , and random elements  $r$ ,  $\llbracket e \rrbracket_{\gamma}^{\phi}(r) = v, W$
- $\llbracket e \rrbracket^{\phi} : \Gamma \times R \rightarrow V \times \mathbb{R}^+$
- Parameters are now inputs

$$\llbracket c \rrbracket_{\gamma}^{\phi}(\emptyset) = c, 1$$

$$\llbracket x \rrbracket_{\gamma}^{\phi}(\emptyset) = \gamma(x), 1$$

$$\llbracket \text{sample}(e) \rrbracket_{\gamma}^{\phi}(r) = \text{icdf}(\llbracket e \rrbracket_{\gamma}^{\phi})(r), 1$$

$$\llbracket \text{factor}(e) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \llbracket e \rrbracket_{\gamma}^{\phi}$$

$$\llbracket \text{observe}(e_1, e_2) \rrbracket_{\gamma}^{\phi}(\emptyset) = (), \text{pdf}(\llbracket e_1 \rrbracket_{\gamma}^{\phi})(\llbracket e_2 \rrbracket_{\gamma}^{\phi})$$

$$\begin{aligned} \llbracket \text{let } x = e_1 \text{ in } e_2 \rrbracket_{\gamma}^{\phi}(r_1, r_2) &= \text{let } v_1, W_1 = \llbracket e_1 \rrbracket_{\gamma}^{\phi}(r_1) \text{ in} \\ &\quad \text{let } v_2, W_2 = \llbracket e_2 \rrbracket_{\gamma+[x \leftarrow v_1]}^{\phi}(r_2) \text{ in} \\ &\quad v_2, W_1 \times W_2 \end{aligned}$$

Random elements: program structure

Deterministic expression:  $\emptyset$

Sub-expressions: nested tuples

must know the structure of the program...

# Exercises

What is the density semantics of the following programs?

```
let my_gaussian (mu, sigma) =  
  let x = sample (gaussian (mu, sigma)) in  
  x
```

```
let my_beta (a, b) =  
  let x = sample (uniform (0., 1.)) in  
  let () = observe (beta (a, b), x) in  
  x
```

```
let coin (x1, ..., xn) =  
  let z = sample (uniform (0., 1.)) in  
  observe (bernoulli (z), x1); ... ; observe (bernoulli (z), xn);  
  z
```

# Semantics equivalence

*Theorem. For an expression  $e$ , the density semantics of  $e$  is the density of the measure defined by the kernel semantics.*

$$\llbracket e \rrbracket_{\gamma}^{\phi}(U) = \int \rho(dr) W(r) \delta_{v(r)}(U) \quad \text{where } v(r), W(r) = \llbracket e \rrbracket_{\gamma}^{\phi}(r)$$

*Proof.* By induction... (see notes)



# Semantics equivalence

*Theorem. For an expression  $e$ , the density semantics of  $e$  is the density of the measure defined by the kernel semantics.*

$$\llbracket e \rrbracket_{\gamma}^{\phi}(U) = \int \rho(dr) W(r) \delta_{v(r)}(U) \quad \text{where } v(r), W(r) = \llbracket e \rrbracket_{\gamma}^{\phi}(r)$$

*Proof.* By induction... (see notes)

□

The kernel and density semantics define the same object

Advanced inference: HMC, SVI

---

Probabilistic Programming Languages

# Hamiltonian Monte-Carlo (HMC)



# Hamiltonian Monte-Carlo (HMC)

Preferred inference algorithm for Stan

# Hamiltonian Monte-Carlo (HMC)

Preferred inference algorithm for Stan

Analogy: Particle in an energy field

- Program define a density of the form  $\exp(-U(X))$
- 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

Hamiltonian Dynamics

- $M$ : mass matrix
- $P$ : momentum

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

# Hamiltonian Monte-Carlo (HMC)

Preferred inference algorithm for Stan

Analogy: Particle in an energy field

- Program define a density of the form  $\exp(-U(X))$
- 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

Hamiltonian Dynamics

- $M$ : mass matrix
- $P$ : momentum

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

The diagram illustrates the components of the Hamiltonian. The equation  $H(X, P) = K(P) + U(X)$  is centered. An upward arrow from  $H(X, P)$  points to the label "hamiltonian". A downward arrow from  $K(P)$  points to the label "kinetic energy". An upward arrow from  $U(X)$  points to the label "potential energy".

$$\begin{array}{ccc} \text{hamiltonian} & & \text{potential energy} \\ \uparrow & & \uparrow \\ H(X, P) = K(P) + U(X) \\ \downarrow & & \\ \text{kinetic energy} & & \end{array}$$

# Hamiltonian Monte-Carlo (HMC)

Energy conservation

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

Hamiltonian dynamics

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

The diagram illustrates the decomposition of the Hamiltonian function  $H(X, P)$  into its components. The equation  $H(X, P) = K(P) + U(X)$  is centered. An upward arrow from  $H(X, P)$  points to the label "hamiltonian". A downward arrow from  $K(P)$  points to the label "kinetic energy". An upward arrow from  $U(X)$  points to the label "potential energy".

$$\begin{array}{ccc} \text{hamiltonian} & & \text{potential energy} \\ \uparrow & & \uparrow \\ H(X, P) = K(P) + U(X) \\ \downarrow & & \\ \text{kinetic energy} & & \end{array}$$

# Hamiltonian Monte-Carlo (HMC)

# Hamiltonian Monte-Carlo (HMC)

Generate samples  $(X, P)$  from the density  $\exp(-H(X, P))$

- At each iteration
- Sample an initial momentum  $P_0 \sim \mathcal{N}(0, M)$
- Solve the Hamiltonian dynamics (discretized)
- Perform a Metropolis Hastings update with probability  $\alpha$

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

If the hamiltonian is preserved: accept with probability 1.

- Problem: numerical approximations
- Solution: leapfrog integrator and reject using MH acceptance probability

# Hamiltonian Monte-Carlo (HMC)

Generate samples  $(X, P)$  from the density  $\exp(-H(X, P))$

- At each iteration
- Sample an initial momentum  $P_0 \sim \mathcal{N}(0, M)$
- Solve the Hamiltonian dynamics (discretized)
- Perform a Metropolis Hastings update with probability  $\alpha$

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

momentum can then be marginalized

If the hamiltonian is preserved: accept with probability 1.

- Problem: numerical approximations
- Solution: leapfrog integrator and reject using MH acceptance probability

# Hamiltonian Monte-Carlo (HMC)

```
let u x = let _, w = model data x in w
let k p = 0.5 * transpose p * inv m * p

let h x p = u x +. k p

let rec gen n values x =
  if n = 0 then values
  else
    let p = Distribution.draw mv_normal(0, m) in
    let x', p' = leapfrog (grad u) x p in
    let next_x = if Random.float 1. < exp(h x p -. h x' p') then x' else x in
    let next_value, _ = model data next_x in
    gen (n - 1) (next_value :: values) next_x
```



# Hamiltonian Monte-Carlo (HMC)

```
let u x = let _, w = model data x in w
let k p = 0.5 * transpose p * inv m * p

let h x p = u x +. k p

let rec gen n values x =
  if n = 0 then values
  else
    let p = Distribution.draw mv_normal(0, m) in
    let x', p' = leapfrog (grad u) x p in
    let next_x = if Random.float 1. < exp(h x p -. h x' p') then x' else x in
    let next_value, _ = model data next_x in
    gen (n - 1) (next_value :: values) next_x
```

Warning: pseudo-code

# Hamiltonian Monte-Carlo (HMC)

```
let u x = let _, w = model data x in w
let k p = 0.5 * transpose p * inv m * p

let h x p = u x +. k p

let rec gen n values x =
  if n = 0 then values
  else
    let p = Distribution.draw mv_normal(0, m) in
    let x', p' = leapfrog (grad u) x p in
    let next_x = if Random.float 1. < exp(h x p -. h x' p') then x' else x in
    let next_value, _ = model data next_x in
    gen (n - 1) (next_value :: values) next_x
```

autodiff magic!

Warning: pseudo-code

# Hamiltonian Monte-Carlo (HMC)

```
let u x = let _, w = model data x in w
let k p = 0.5 * transpose p * inv m * p
```

model is a function from parameters  
to (value, score), differentiable.

```
let h x p = u x +. k p
```

```
let rec gen n values x =
  if n = 0 then values
  else
    let p = Distribution.draw mv_normal(0, m) in
    let x', p' = leapfrog (grad u) x p in
    let next_x = if Random.float 1. < exp(h x p -. h x' p') then x' else x in
    let next_value, _ = model data next_x in
    gen (n - 1) (next_value :: values) next_x
```

autodiff magic!

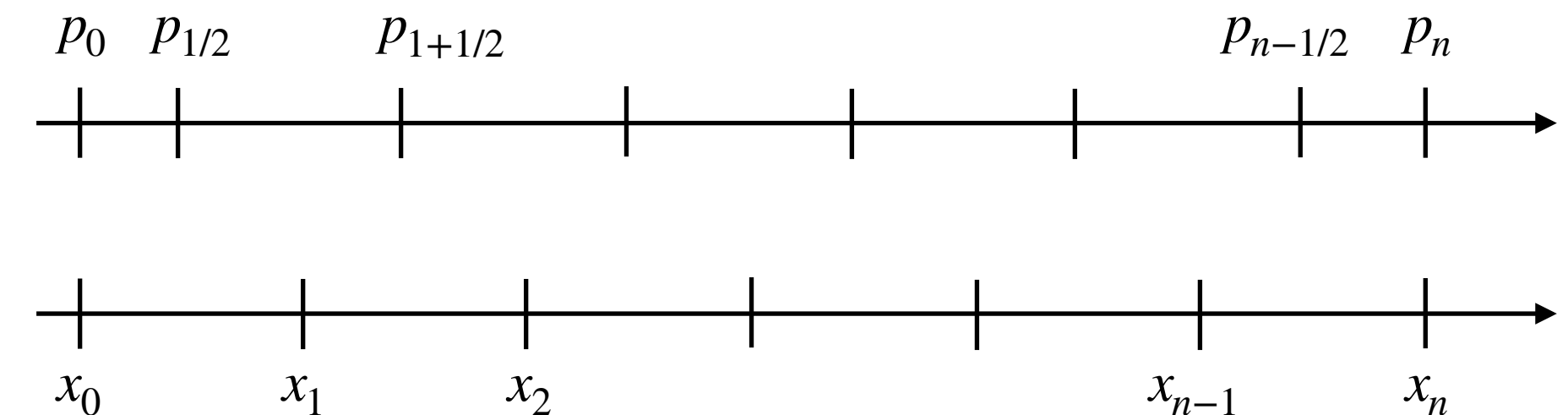
Warning: pseudo-code

# Leapfrog integration

```
let leapfrog u_grad x0 p0 =  
  let p = p0 - 0.5 * step_size * u_grad x0 in  
  let rec loop n x p =  
    if n = 0 then x, p  
    else  
      let x' = x + step_size * p in  
      let p' = p - step_size * u_grad x' in  
      loop (n-1) x' p'  
  in  
  let xt, pt = loop (path_len - 1) x0 p in  
  let x' = xt + step_size * pt in  
  let p' = pt - 0.5 * step_size * u_grad x' in  
  x', p'
```

(\* first half step for the momentum \*)

(\* last half step for the momentum \*)



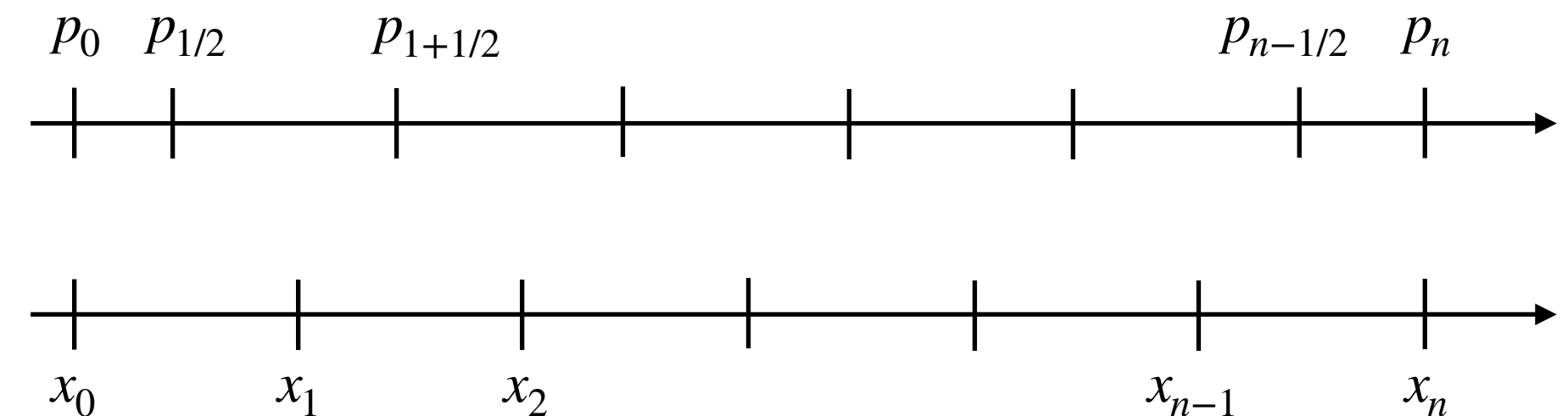
# Leapfrog integration

```
let leapfrog u_grad x0 p0 =  
  let p = p0 - 0.5 * step_size * u_grad x0 in  
  let rec loop n x p =  
    if n = 0 then x, p  
    else  
      let x' = x + step_size * p in  
      let p' = p - step_size * u_grad x' in  
      loop (n-1) x' p'  
  in  
  let xt, pt = loop (path_len - 1) x0 p in  
  let x' = xt + step_size * pt in  
  let p' = pt - 0.5 * step_size * u_grad x' in  
  x', p'
```

Warning: pseudo-code

(\* first half step for the momentum \*)

(\* last half step for the momentum \*)



# Stochastic Variational Inference (SVI)

$p(z|x)$



# Stochastic Variational Inference (SVI)

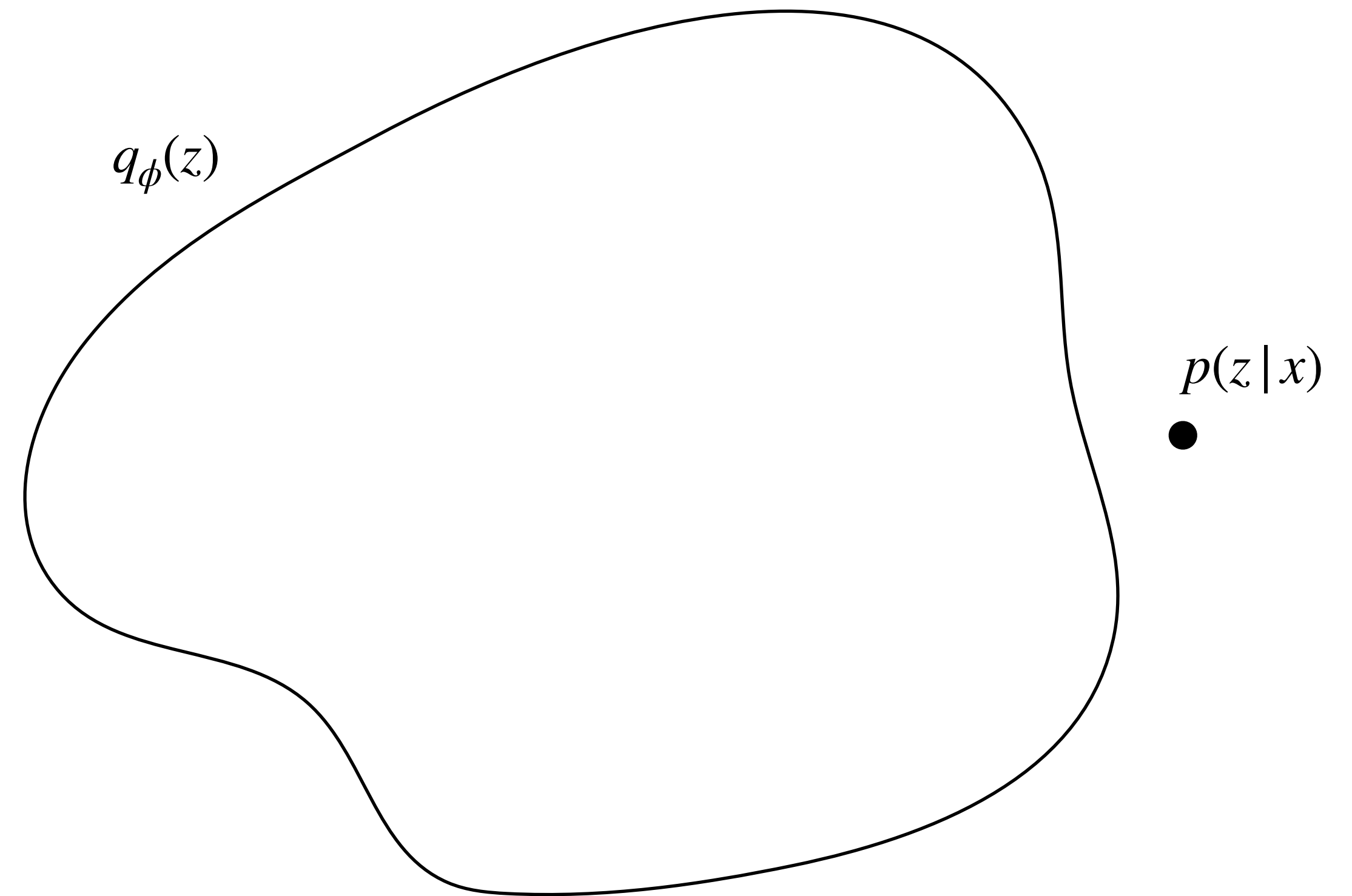
$$p(z \mid x) = \frac{p(x \mid z)p(z)}{p(x)} = \frac{p(x \mid z)p(z)}{\int_z p(x \mid z)p(z)dz}$$

$p(z \mid x)$



# Stochastic Variational Inference (SVI)

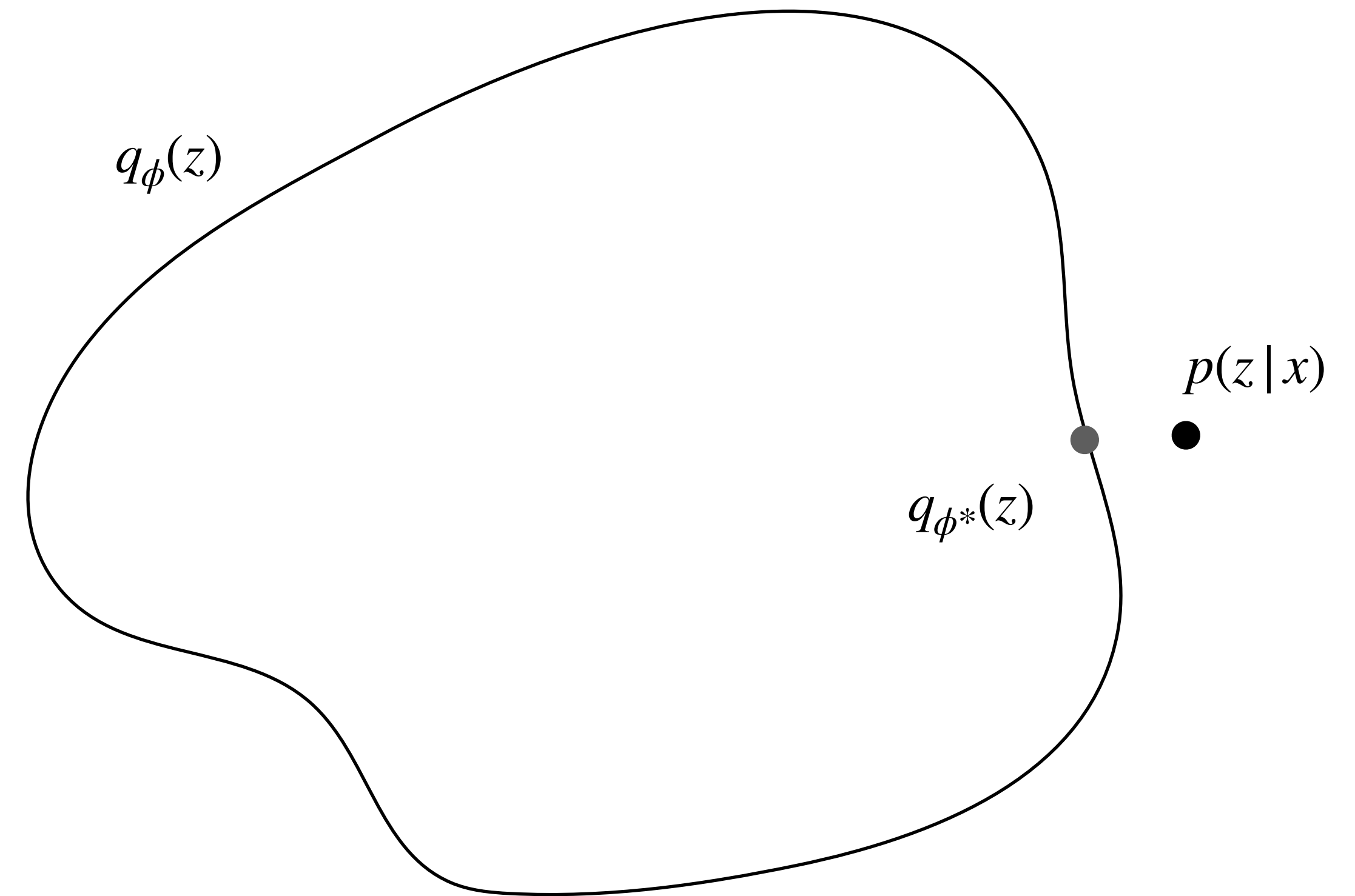
$$p(z | x) = \frac{p(x | z)p(z)}{p(x)} = \frac{p(x | z)p(z)}{\int_z p(x | z)p(z)dz}$$





# Stochastic Variational Inference (SVI)

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

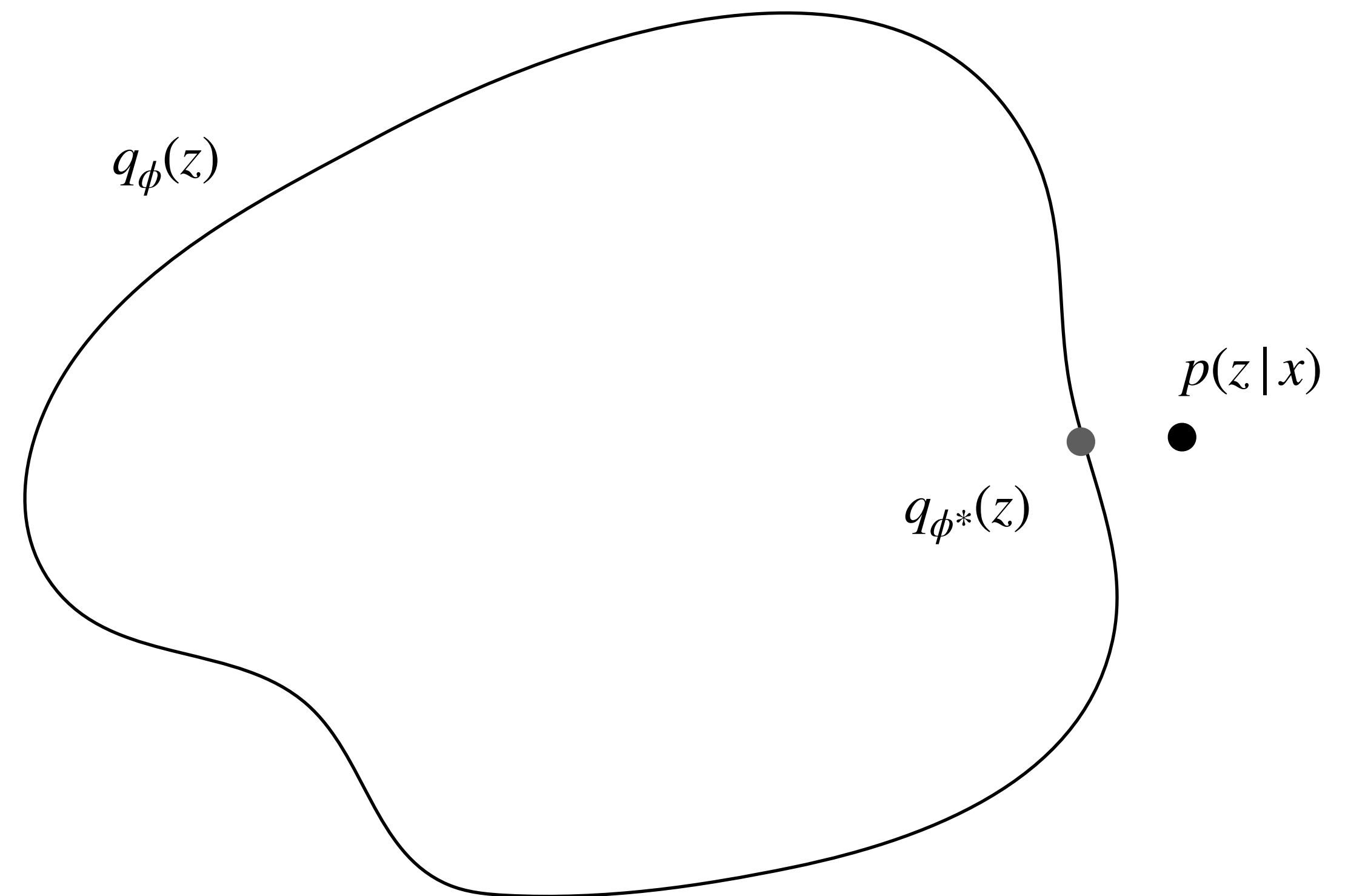


# Stochastic Variational Inference (SVI)

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

## Variational family

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



# Stochastic Variational Inference (SVI)

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

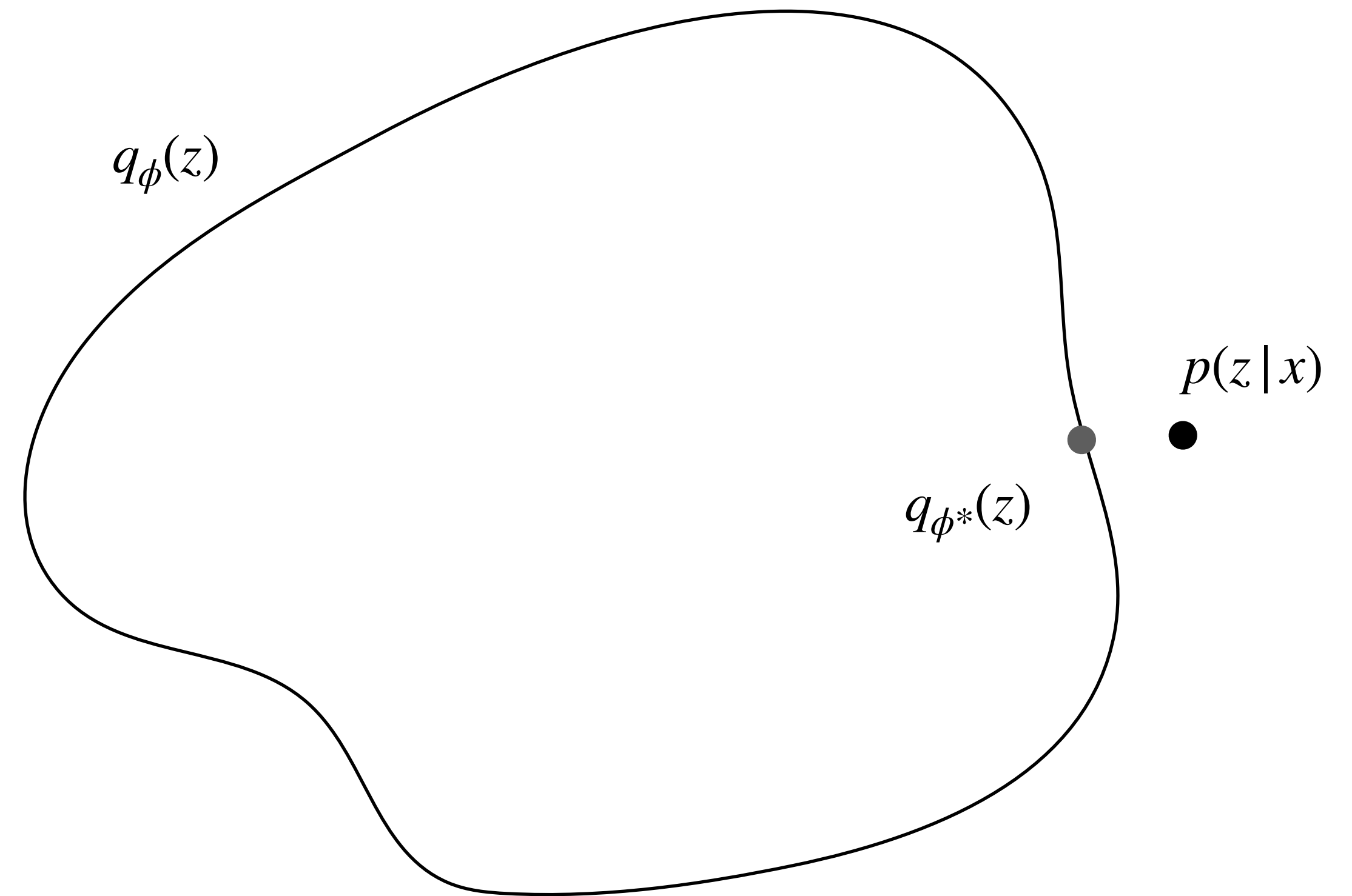
## Variational family

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

## Metrics: Kullback-Leibler divergence

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

- $KL(q \parallel p) \geq 0$  positive
- $KL(q \parallel p) = 0 \iff |x| \neq 0 \implies p(x) = q(x)$ , equal almost everywhere
- $KL(q \parallel p) \neq KL(p \parallel q)$  asymmetric
- No triangular inequality



# Stochastic Variational Inference (SVI)

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

# Stochastic Variational Inference (SVI)

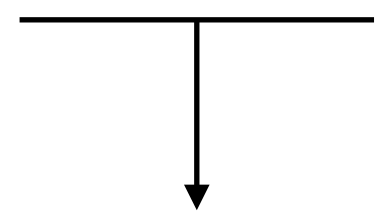
$$\begin{aligned} KL(q_\phi(z) \parallel p(z|x)) &= - \int q_\phi(z) \log \frac{p(z|x)}{q_\phi(z)} dz \\ &= - \int q_\phi(z) \log \frac{p(x, z)}{p(x)q_\phi(z)} dz \\ &= - \int q_\phi(z) \log \frac{p(x, z)}{q_\phi(z)} dz + \int q_\phi(z) \log p(x) dz \\ &= - \int q_\phi(z) \log \frac{p(x, z)}{q_\phi(z)}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

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

# Stochastic Variational Inference (SVI)

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

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



constant

# Stochastic Variational Inference (SVI)

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

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

↓

constant

↓

minimize





# Stochastic Variational Inference (SVI)

# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

Program your own guide

- Pyro (first versions)
- Sample the same variables in the guide and the model

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

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

# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

Program your own guide

- Pyro (first versions)
- Sample the same variables in the guide and the model

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

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

Approximate gradient ascent.

$$\nabla_{\phi} KL(q_{\phi}(z) \parallel p(z \mid x)) \longrightarrow \nabla_{\phi} \mathcal{L} = \nabla_{\phi} \int q_{\phi}(z) \log \frac{p(x, z)}{q_{\phi}(z)} dz$$

# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

Program your own guide

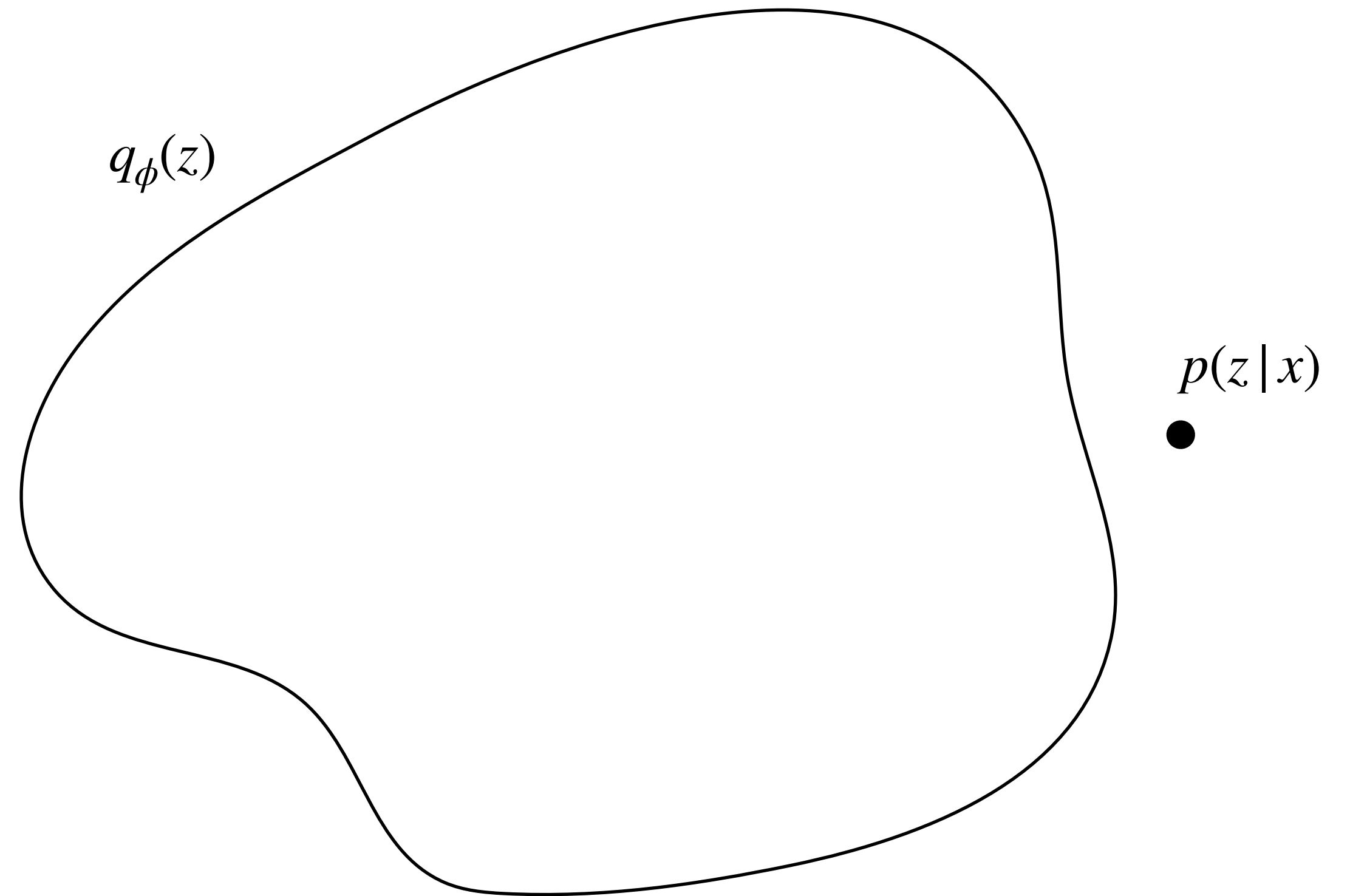
- Pyro (first versions)
- Sample the same variables in the guide and the model

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

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

Approximate gradient ascent.

$$\nabla_{\phi} KL(q_{\phi}(z) \parallel p(z \mid x)) \longrightarrow \nabla_{\phi} \mathcal{L} = \nabla_{\phi} \int q_{\phi}(z) \log \frac{p(x, z)}{q_{\phi}(z)} dz$$



# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

Program your own guide

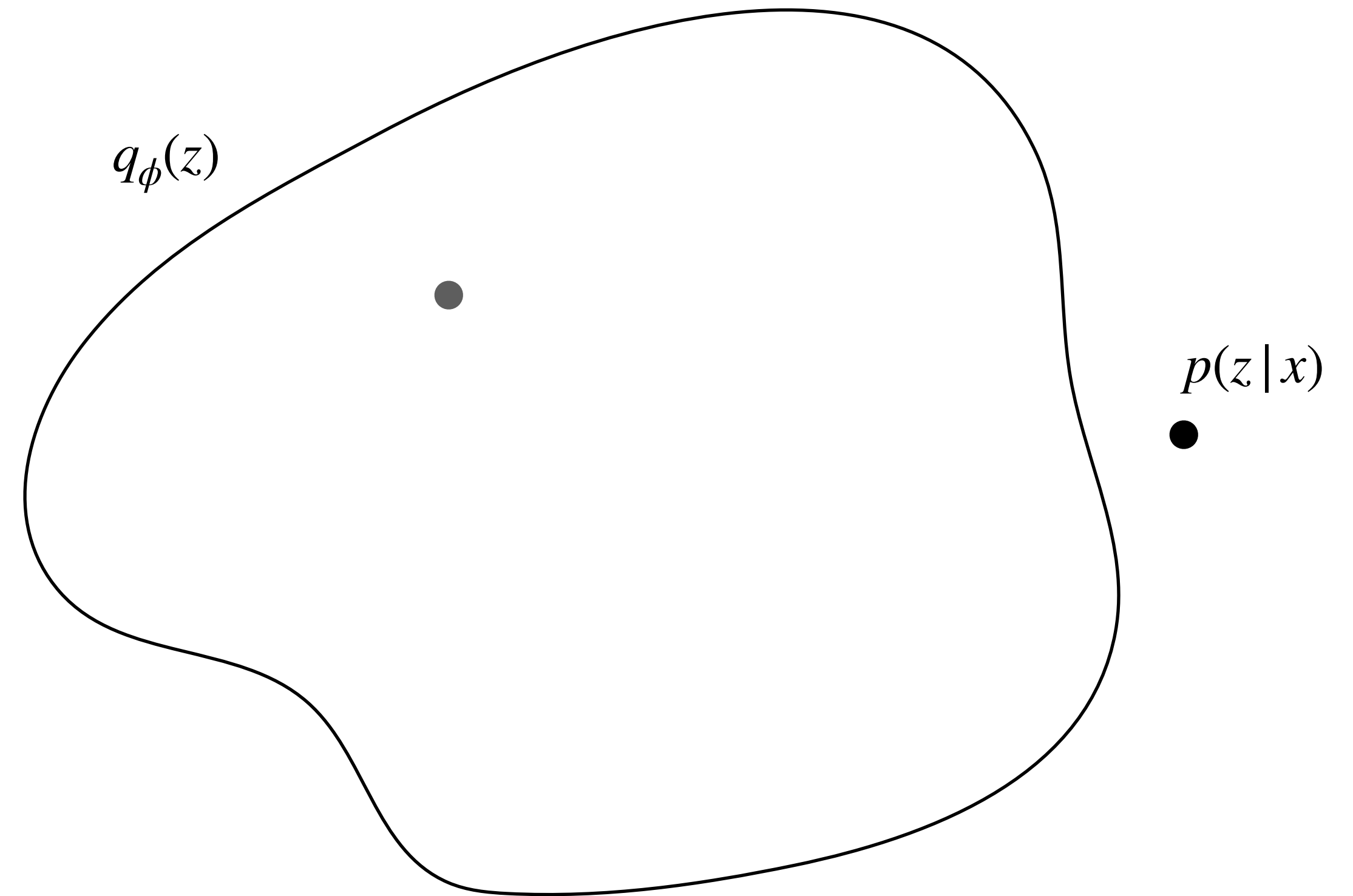
- Pyro (first versions)
- Sample the same variables in the guide and the model

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

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

Approximate gradient ascent.

$$\nabla_{\phi} KL(q_{\phi}(z) \parallel p(z \mid x)) \longrightarrow \nabla_{\phi} \mathcal{L} = \nabla_{\phi} \int q_{\phi}(z) \log \frac{p(x, z)}{q_{\phi}(z)} dz$$



# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

Program your own guide

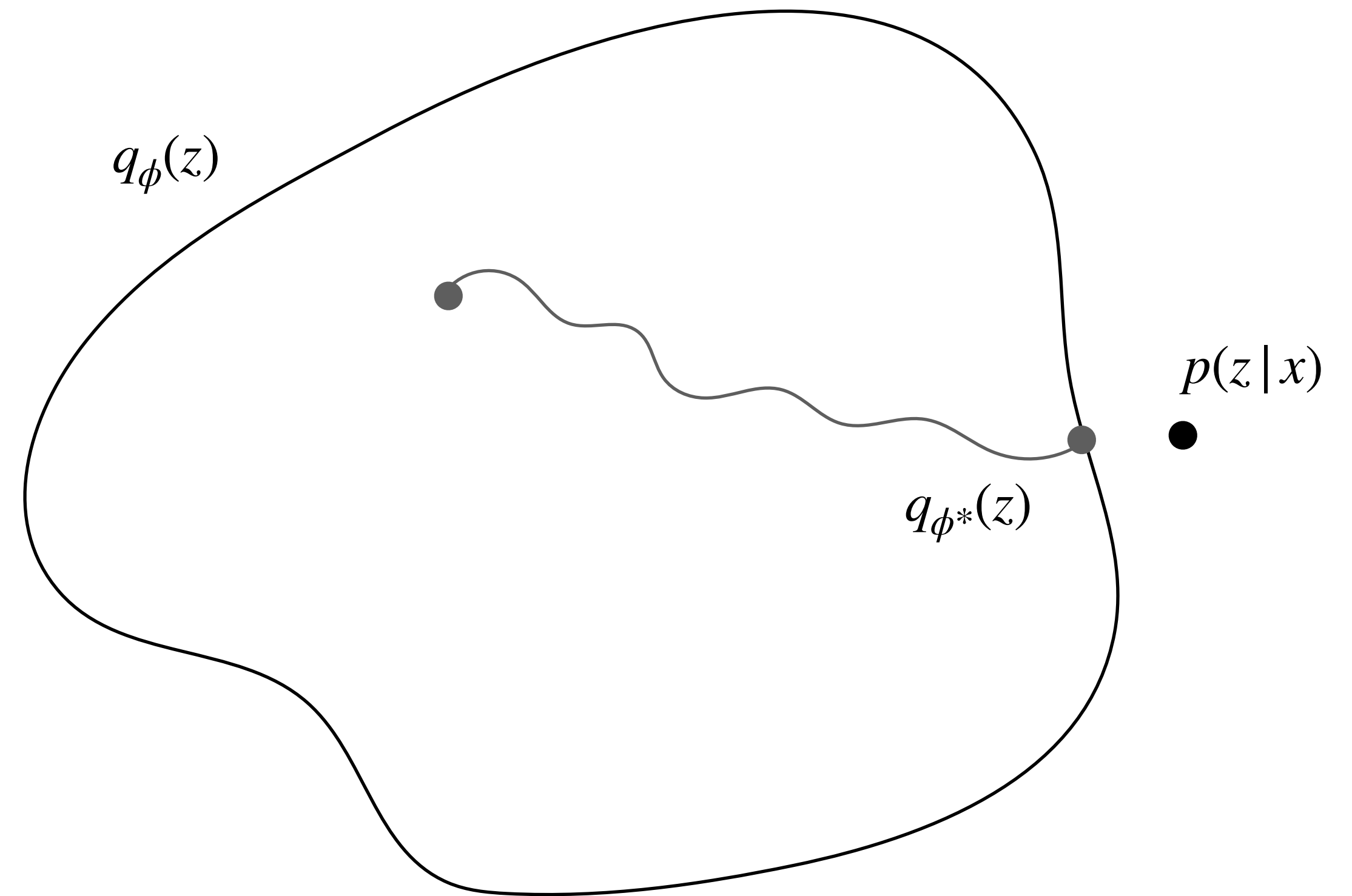
- Pyro (first versions)
- Sample the same variables in the guide and the model

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

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

Approximate gradient ascent.

$$\nabla_{\phi} KL(q_{\phi}(z) \parallel p(z \mid x)) \longrightarrow \nabla_{\phi} \mathcal{L} = \nabla_{\phi} \int q_{\phi}(z) \log \frac{p(x, z)}{q_{\phi}(z)} dz$$



# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

Program your own guide

- Pyro (first versions)
- Sample the same variables in the guide and the model

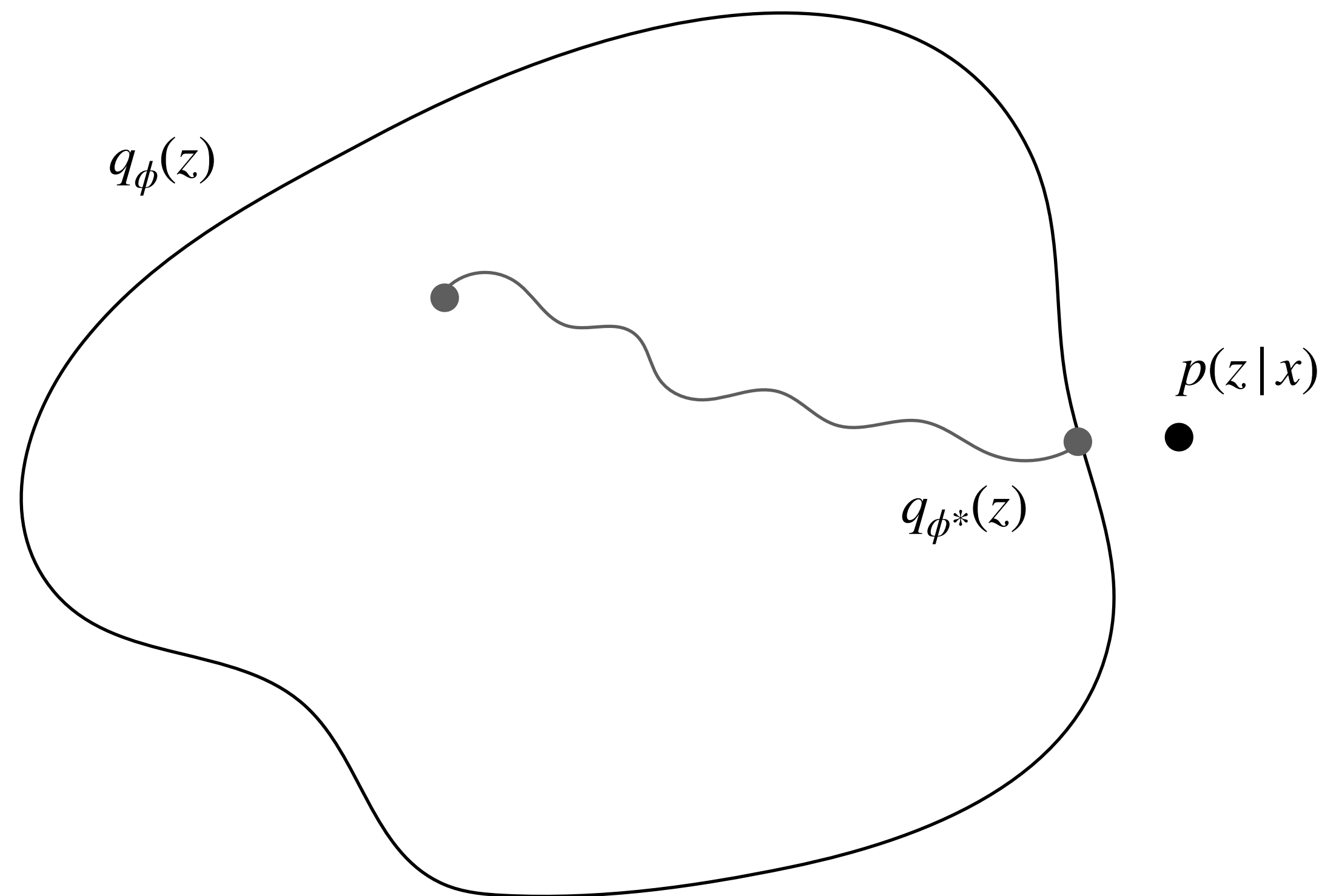
```
def model():  
    pyro.sample("z_1", ... )
```

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

Approximate gradient ascent.

$$\nabla_{\phi} KL(q_{\phi}(z) \parallel p(z \mid x)) \longrightarrow \nabla_{\phi} \mathcal{L} = \nabla_{\phi} \int q_{\phi}(z) \log \frac{p(x, z)}{q_{\phi}(z)} dz$$

autodiff magic!



# Stochastic Variational Inference (SVI)

How to solve the optimisation problem?

## Black-box variational inference

- Variational families with tractable solution
- Mean-field approximation  $q_\phi(z) = \prod_{i=1}^n \mathcal{N}(z_i | \mu_i, \sigma_i)$  where  $\phi = \{\mu_i, \sigma_i\}_{i \in [1, n]}$
- Full-rank approximation  $q_\phi(z) = \mathcal{N}(z | \mu, \Sigma)$  where  $\phi = (\mu, \Sigma)$

## Assumptions

- Independences between random variables
- Only use Gaussians distributions



# References

## An Introduction to Probabilistic Programming

Jan-Willem van de Meent, Brooks Paige, Hongseok Yang, Frank Wood

<https://arxiv.org/abs/1809.10756>

## Lightweight Implementations of Probabilistic Programming Languages Via Transformational Compilation

David Wingate Andreas Stuhlmüller Noah D. Goodman

AISTATS 2011

## Markov Chain Monte Carlo in Practice

Michael Bettancourt

[https://betanalpha.github.io/assets/case\\_studies/markov\\_chain\\_monte\\_carlo.html](https://betanalpha.github.io/assets/case_studies/markov_chain_monte_carlo.html)

## Variational Inference: A Review for Statisticians

David M. Blei, Alp Kucukelbir, Jon D. McAuliffe

<https://arxiv.org/abs/1601.00670>