Introduction to Probabilistic Programming

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Probabilistic programming languages

Probabilistic programming languages

General purpose programming languages extended with probabilistic constructs

- `x = sample(d)`: introduce a random variable `x` of distribution `d`
- `observe(d, y)`: condition on the fact that `y` was sampled from `d`
- `infer(m, y)`: compute posterior distribution of `m` given `y`

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Multiple examples:

- Church, Anglican (lisp, clojure), 2008
- WebPPL (javascript), 2014
- Pyro/NumPyro (python), 2017/2019
- Gen (julia), 2018
- ProbZelus (Zelus), 2019
- ...

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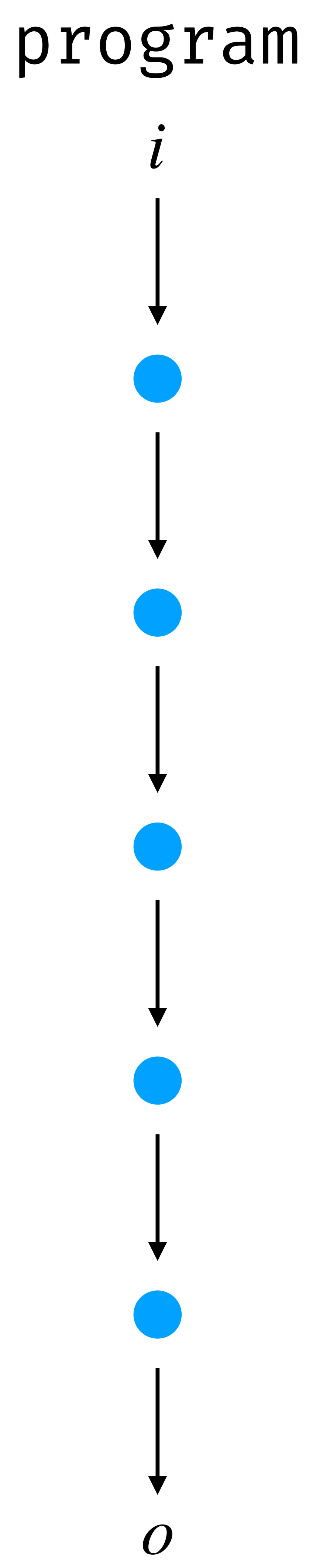
More and more, incorporating new ideas:

- New inference techniques, e.g., stochastic variational inference (SVI)
- Interaction with neural nets (deep probabilistic programming)

`infer :` $(\alpha \to \beta) \to \alpha \to \beta$ `dist`

$\texttt{infer} : (\alpha \to \beta) \to \alpha \to \beta\ \texttt{dist}$



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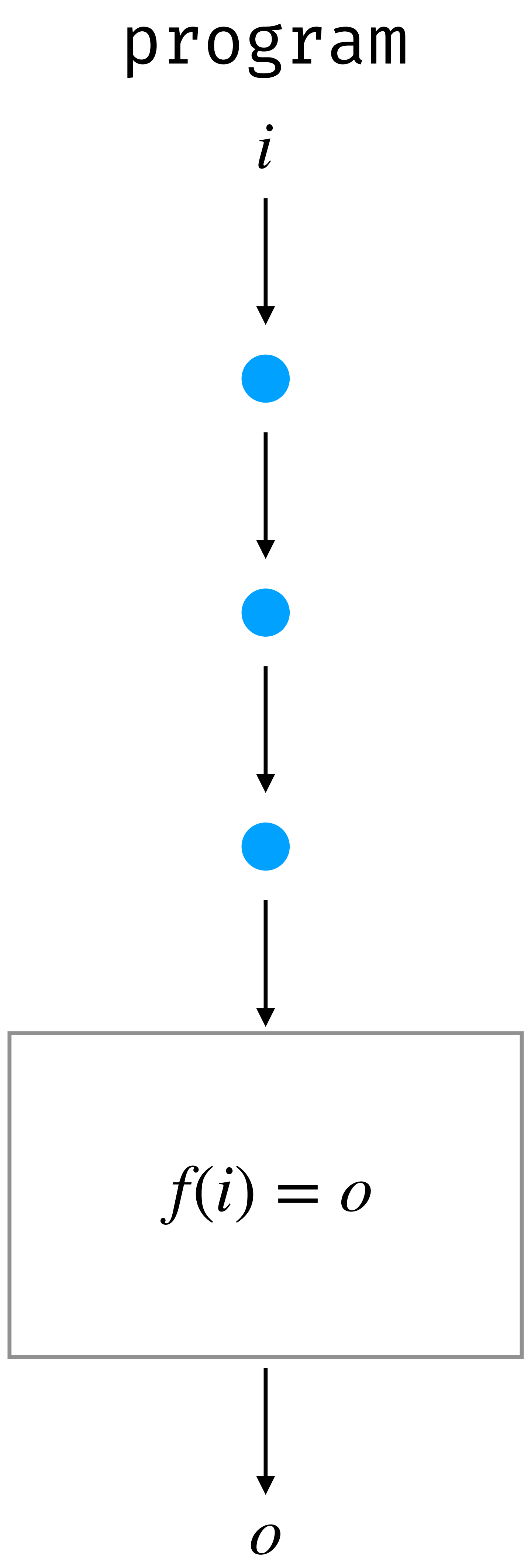
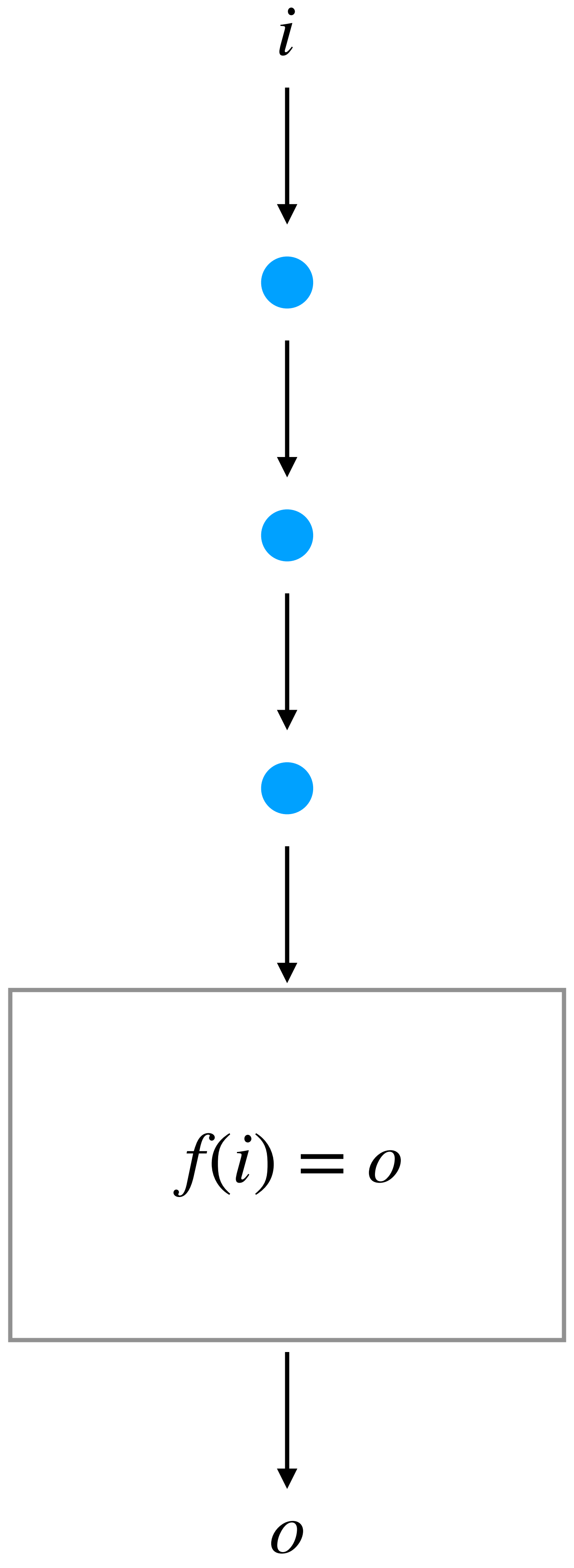


$\texttt{infer} : (\alpha \to \beta) \to \alpha \to \beta\ \texttt{dist}$

`program`



`sample`

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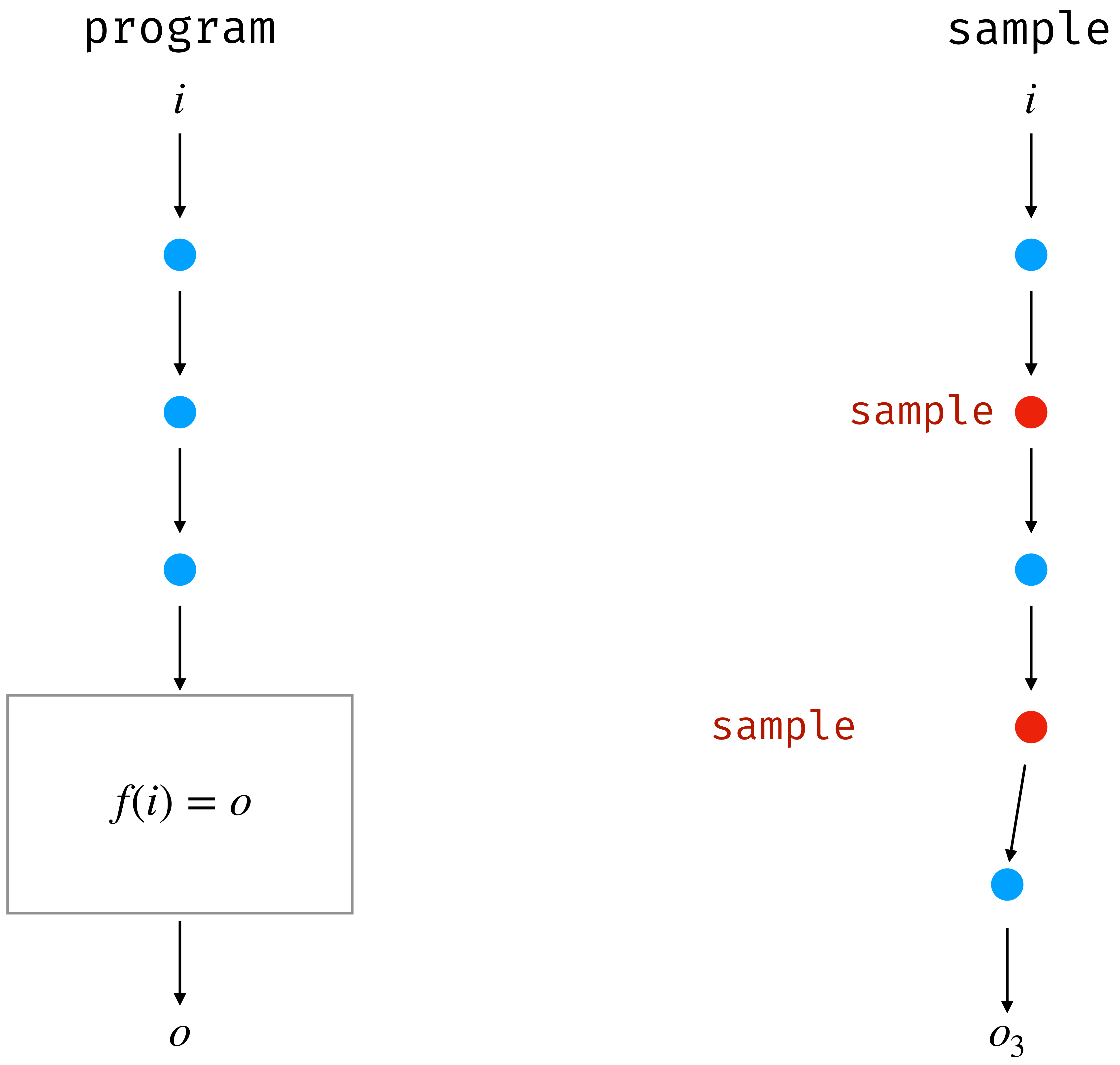
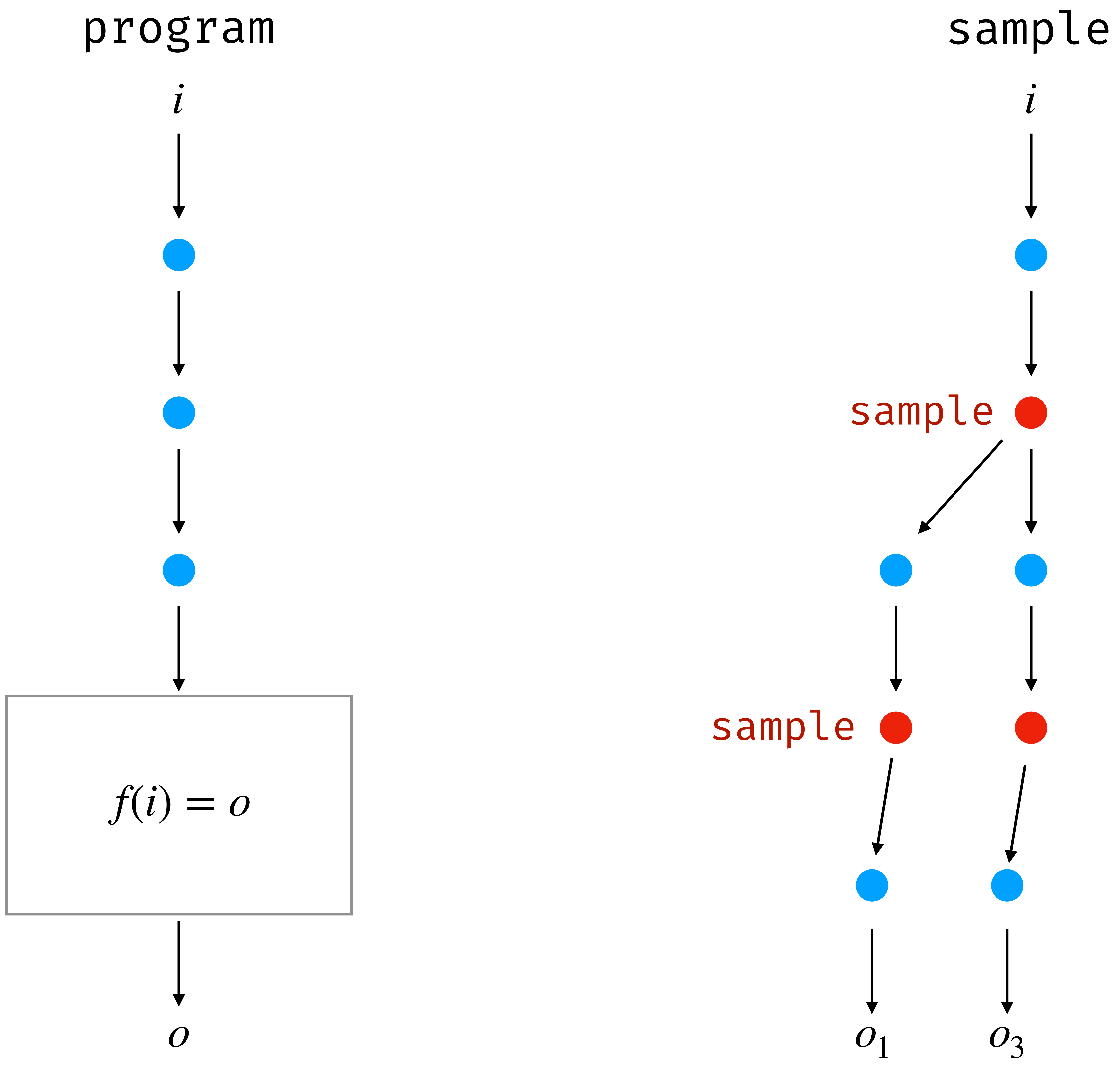


infer : $(\alpha \to \beta) \to \alpha \to \beta$ dist



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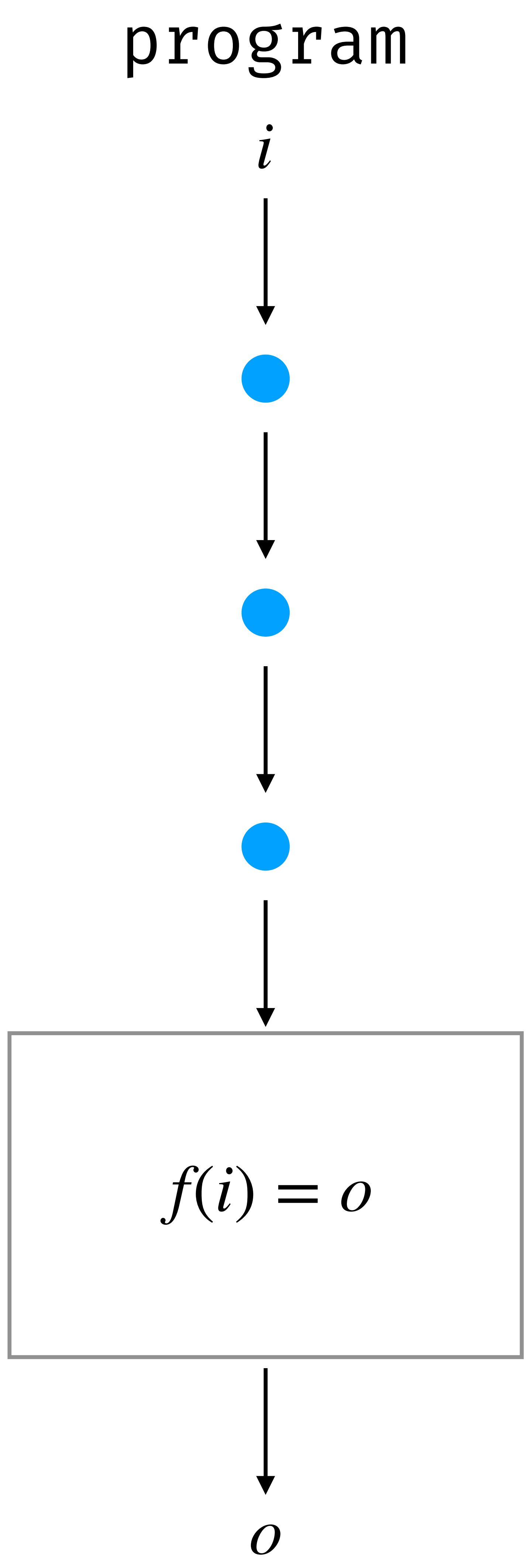

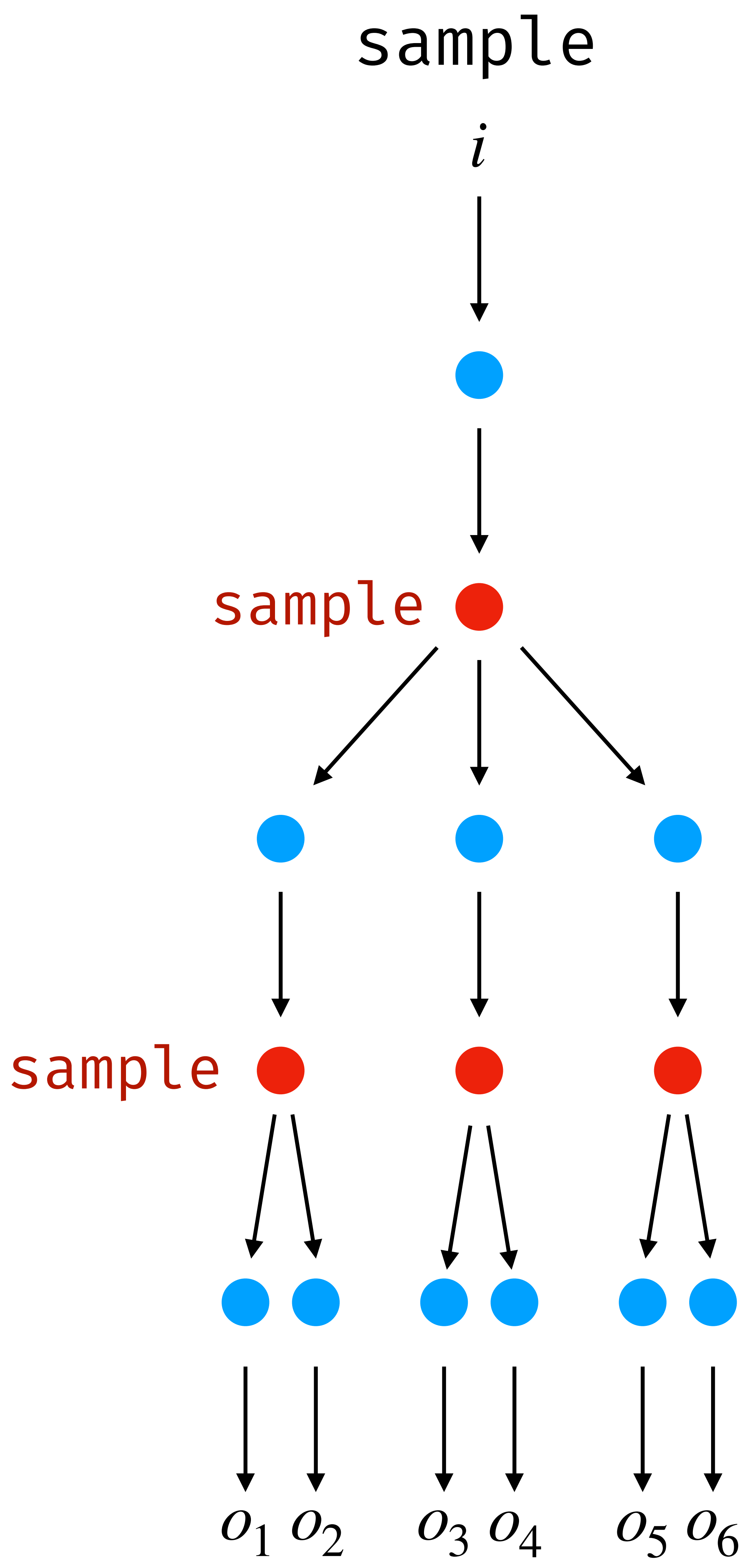

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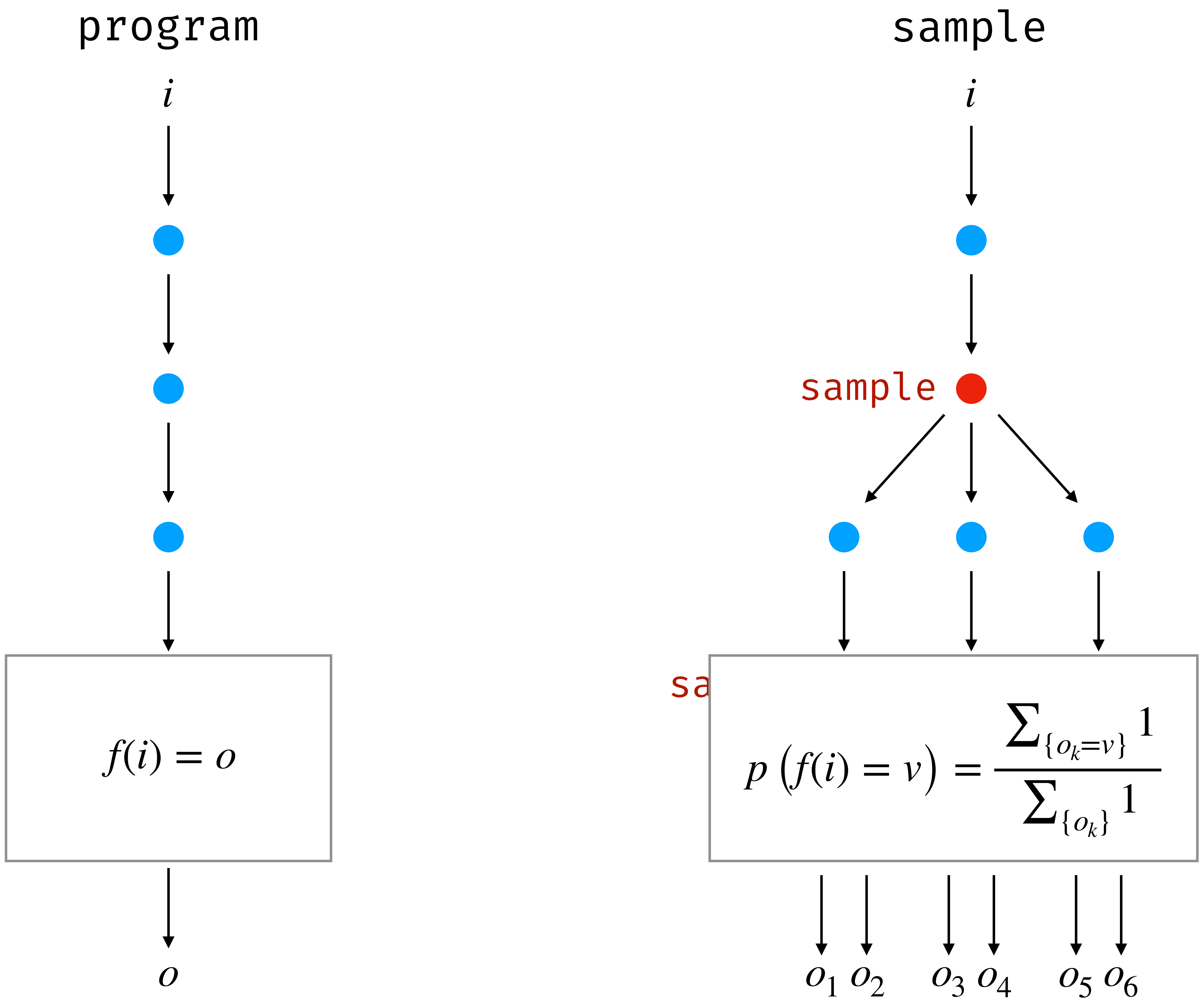

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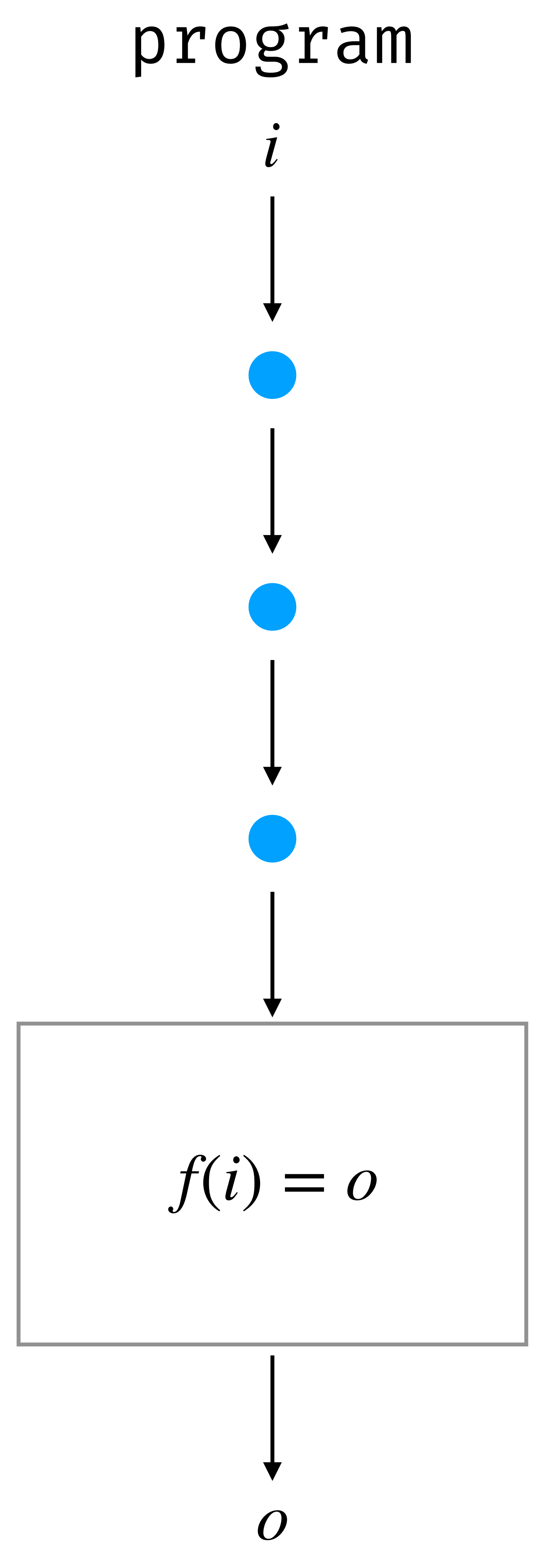

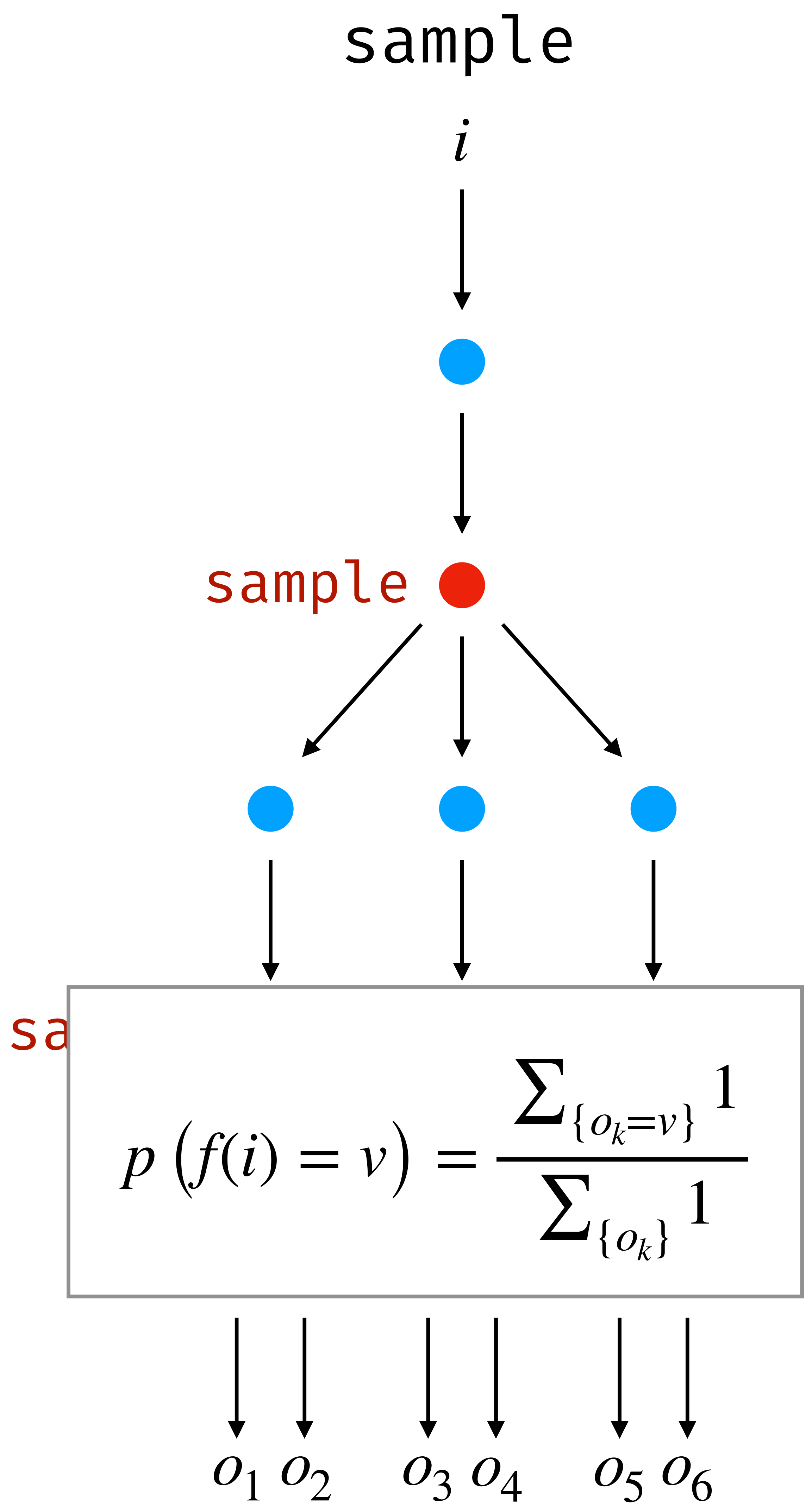

observe

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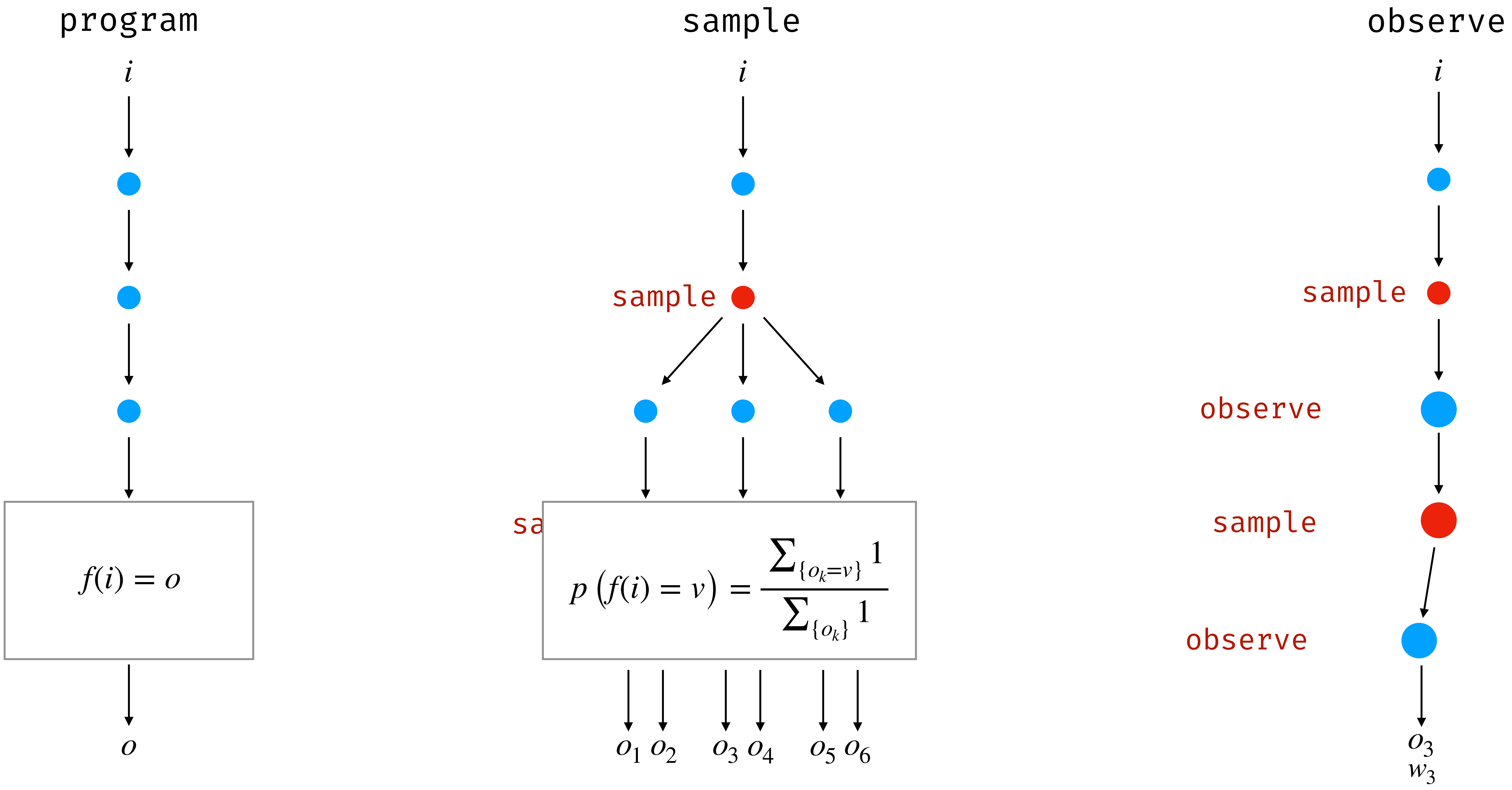

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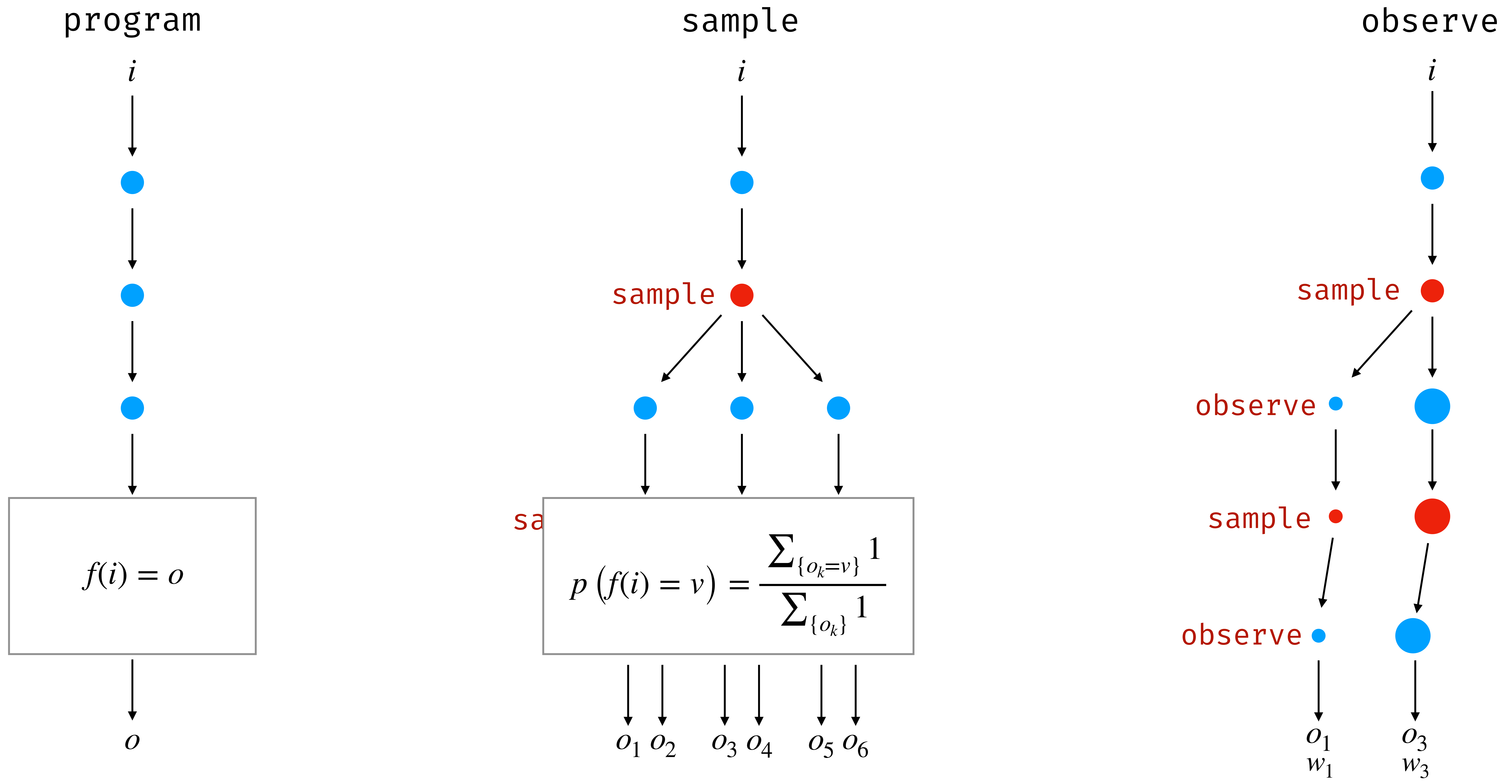

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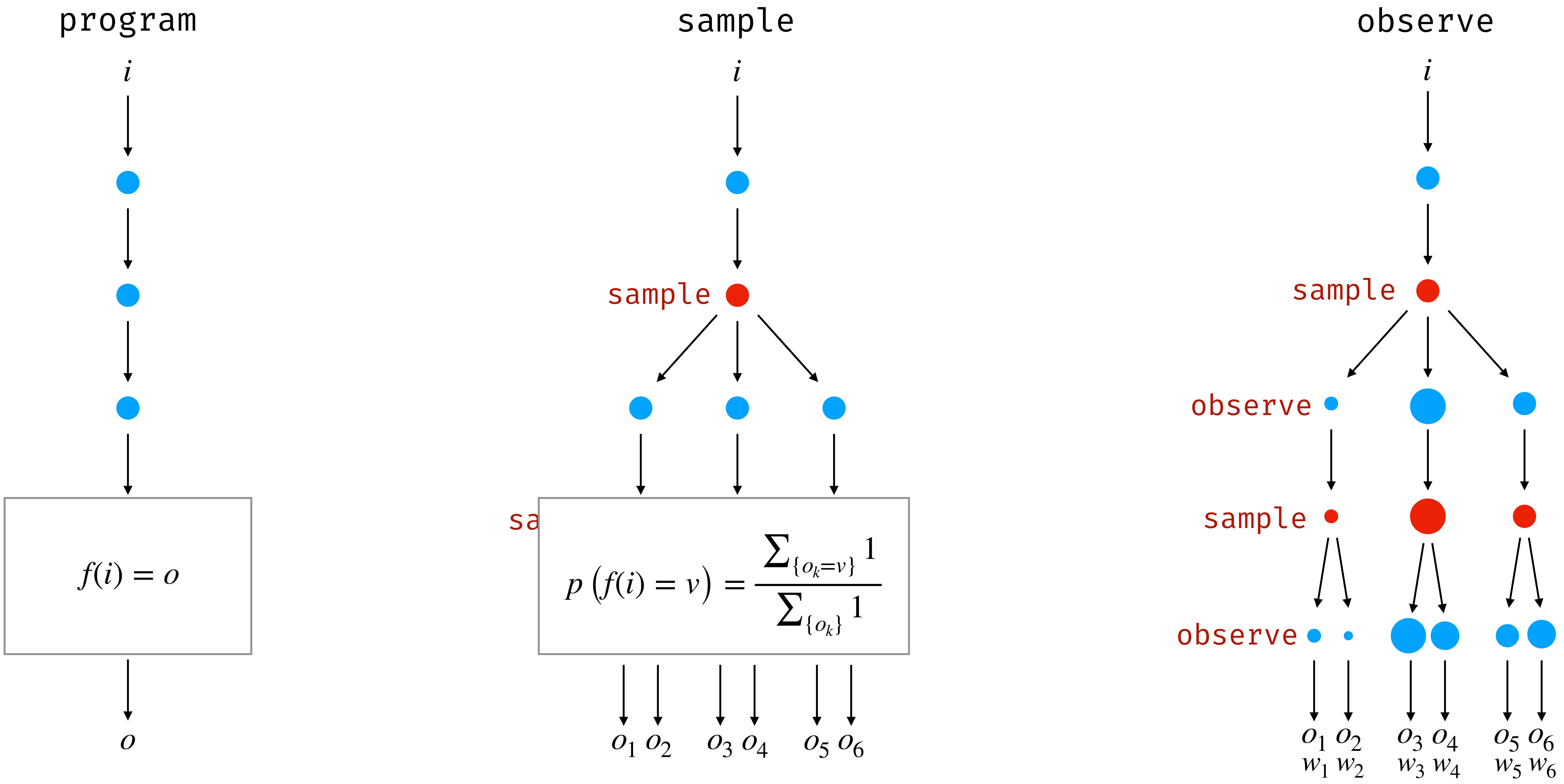

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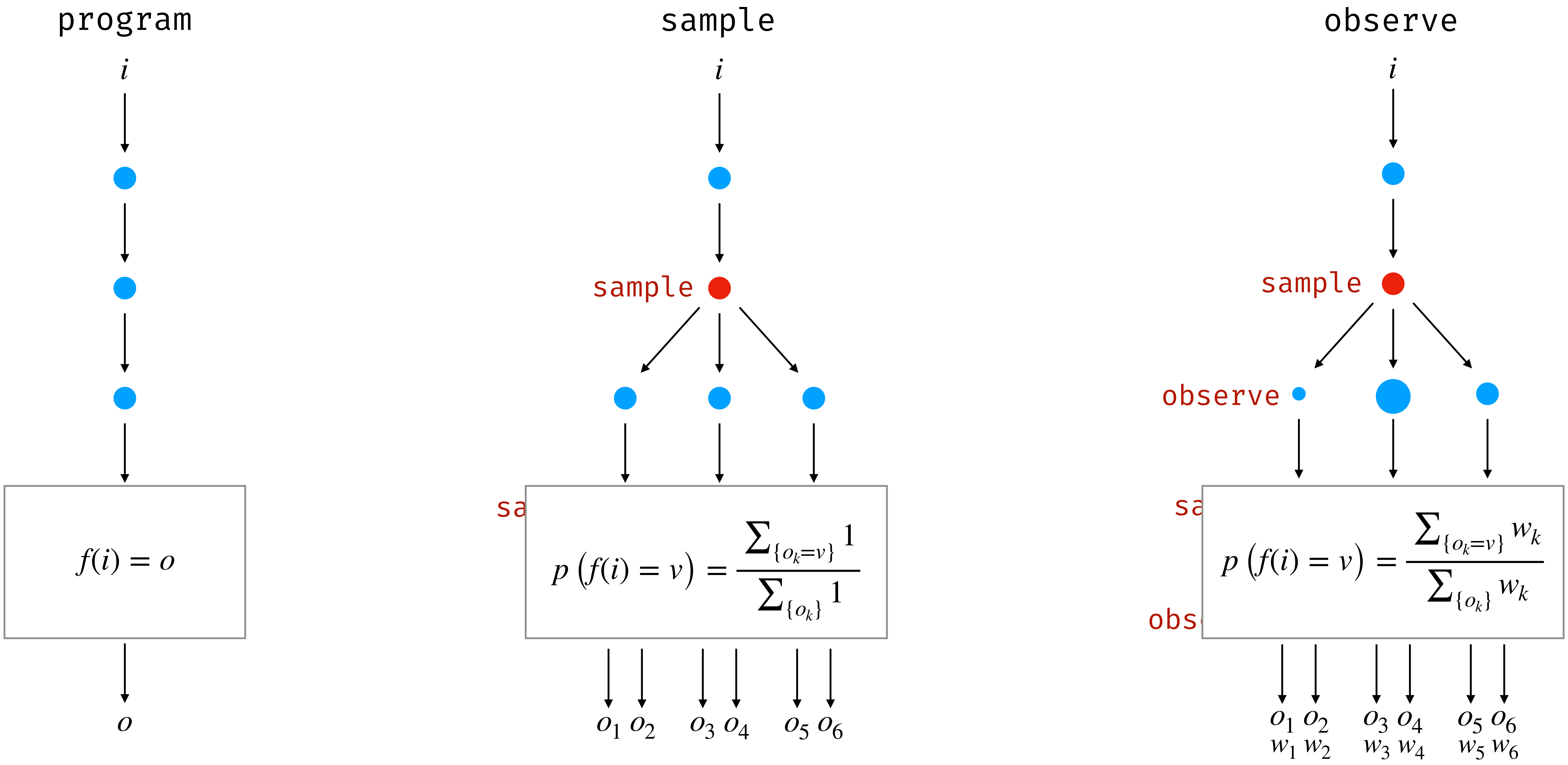

Bayesian reasoning

$$p(x \mid y_1, \ldots, y_n) = \frac{p(x)\ p(y_1, \ldots, y_n \mid x)}{p(y_1, \ldots, y_n)}$$ (Bayes' theorem)

$$\propto p(x)\ p(y_1, \ldots, y_n \mid x)$$ (Data are constants)

Thomas Bayes (1701-1761)

https://en.wikipedia.org/wiki/Thomas_Bayes

Bayesian reasoning

Bayesian Inference: learn parameters from data

- Latent parameter x
- Observed data $y_1, \ldots, y_n$

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$$\propto p(x)\, p(y_1, \ldots, y_n \mid x) \qquad \text{(Data are constants)}$$

prior *likelihood*

```
def model(y1, … , yn):
  x = sample prior
  observe ((likelihood x), (y1, … , yn))
  return x

infer(model, (y1, … , yn))
```

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More general than classic Bayesian Reasoning

```
def weird() =
  b = sample(Bernoulli(0.5))
  mu = 0.5 if (b = 1) else 1.0
  theta = sample(Gaussian(mu, 1.0))
  if theta > 0.:
    observe (Gaussian(mu, 0.5), theta)
    return theta
  else:
    return weird ()
```

Probabilistic programming

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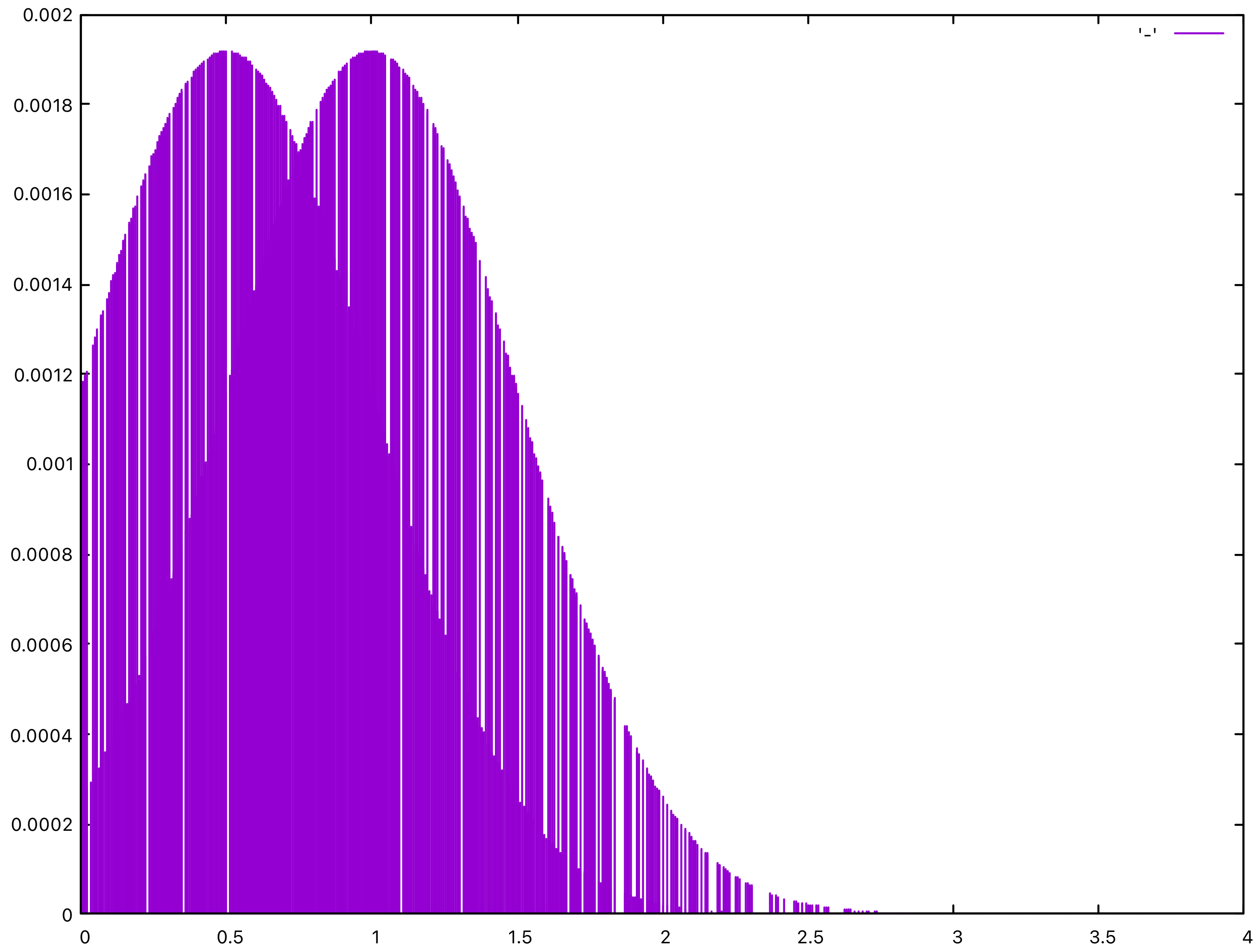

Outline

For a given inference algorithm, how to implement `sample`, `assume`, `factor`, `observe`, and `infer`?

I - Approximate inference

- Importance sampling
- Markov Chain Monte Carlo (MCMC) with Metropolis-Hastings

II - Labs: Introduction to Sequential Monte Carlo methods

- State-space models
- Resampling

III - Density semantics

- Weighted samplers
- Measures on oracles

Part I. Approximate Inference

Introduction to Probabilistic Programming

Interpreter and handlers

Interpretation of the probabilistic constructs depends on the inference

- 1 inference = 1 `Handler` class
- Implement methods `sample`, `factor`, `infer`, ...
- Handlers are context managers

```
def model(data): [...]

with ImportanceSampling(num_particles=1000):
   dist = infer(model, data)

with MetropolisHastings(num_samples=1000):
   dist = infer(model, data)
```

Interpreter and handlers


```
class Handler: [...]

  def __init__(self, *args, **kwargs) → T: pass

  def sample(self, dist: Distribution[T]) → T: pass

  def assume(self, p: bool) → None: pass

  def factor(self, weight: float) → None: pass

  def observe(self, dist: Distribution[T], value: T) → None: pass

  def infer(self, model: Callable[P, T], data: P) → Distribution[T]: pass
```

Importance sampling

Importance sampling

Inference algorithm

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

$$p_i = \frac{W_i}{\sum_{1 \le i \le n} W_i}$$

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Conditioning

- `assume(p)`: sets the score to 0 if `p` is false
- `observe(d,v)`: multiply the score by the likelihood of `d` at `v` (density function of `d`)

Importance sampling

0

```
def model(data):
  ...
  x = sample ...
  ...
  factor ...
  ...
  return output
```

1

```
def model(data):
  ...
  x = sample ...
  ...
  factor ...
  ...
  return output
```

2

```
def model(data):
  ...
  x = sample ...
  ...
  factor ...
  ...
  return output
```

Importance sampling

0
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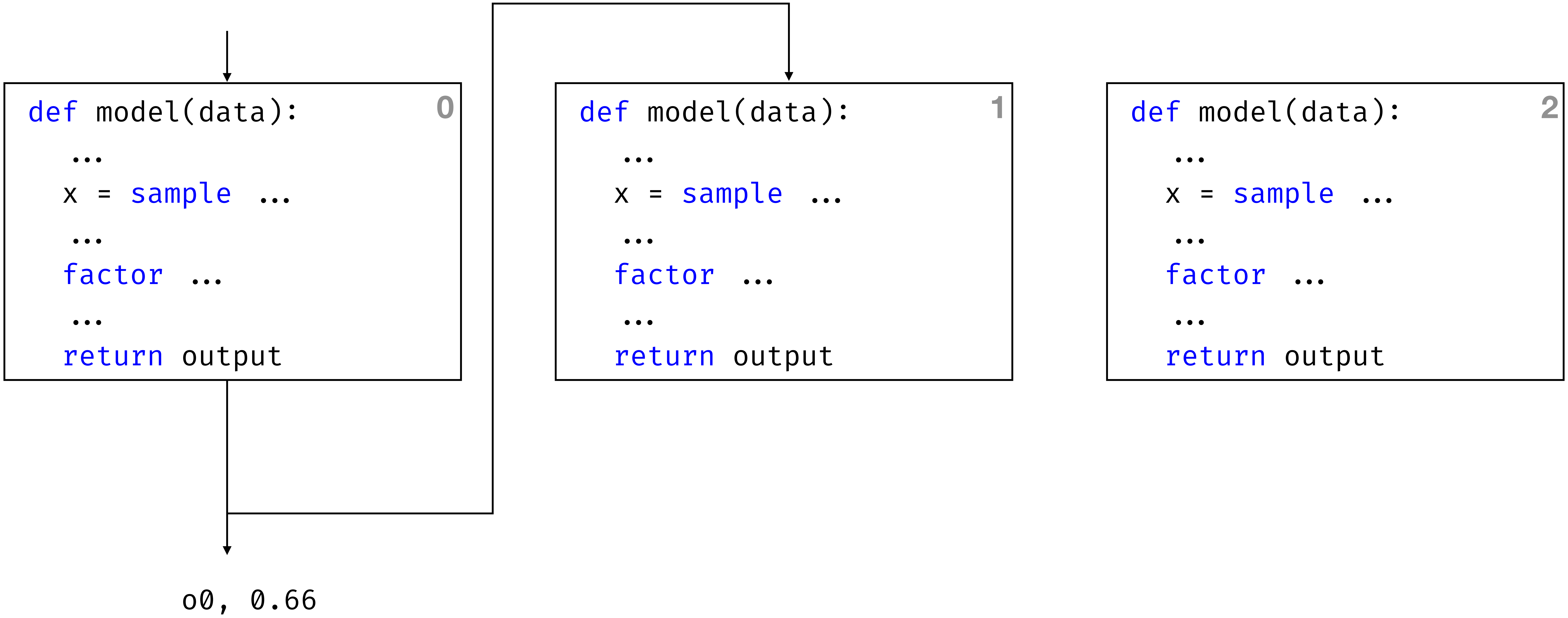
```

o0, 0.66

Importance sampling



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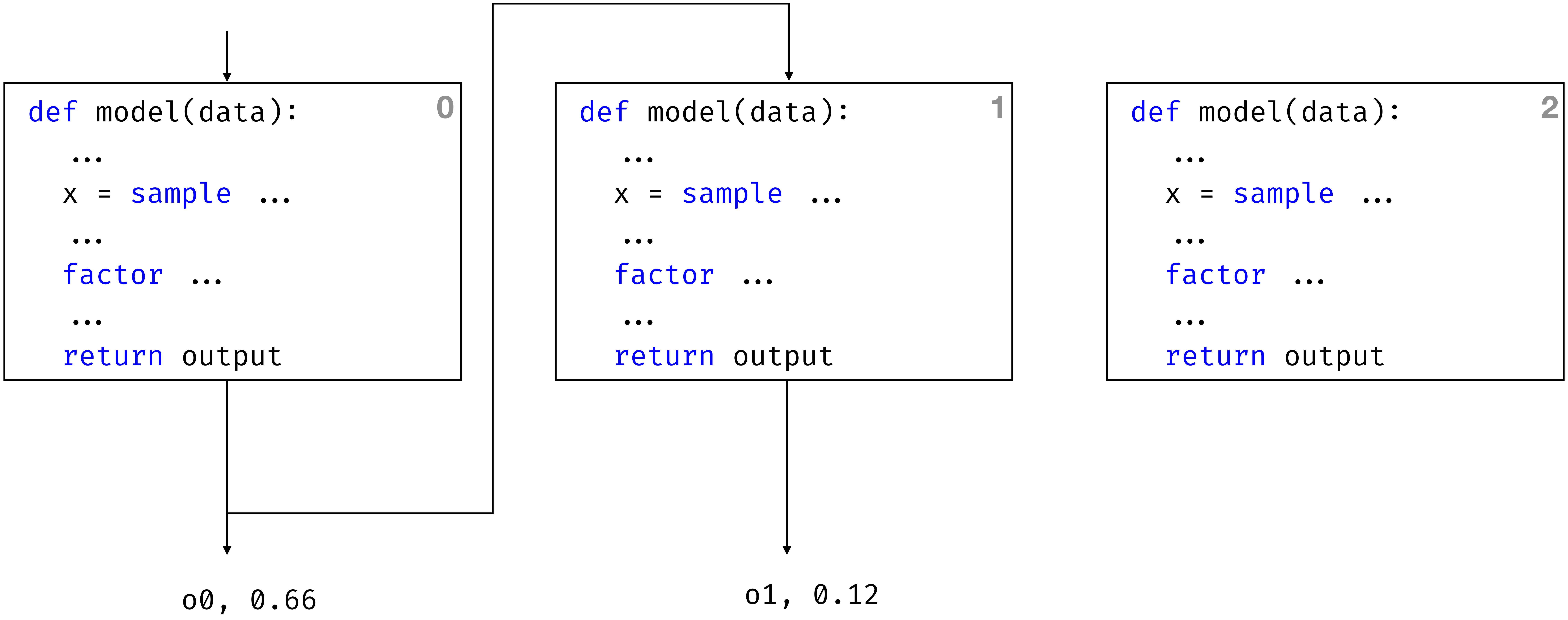

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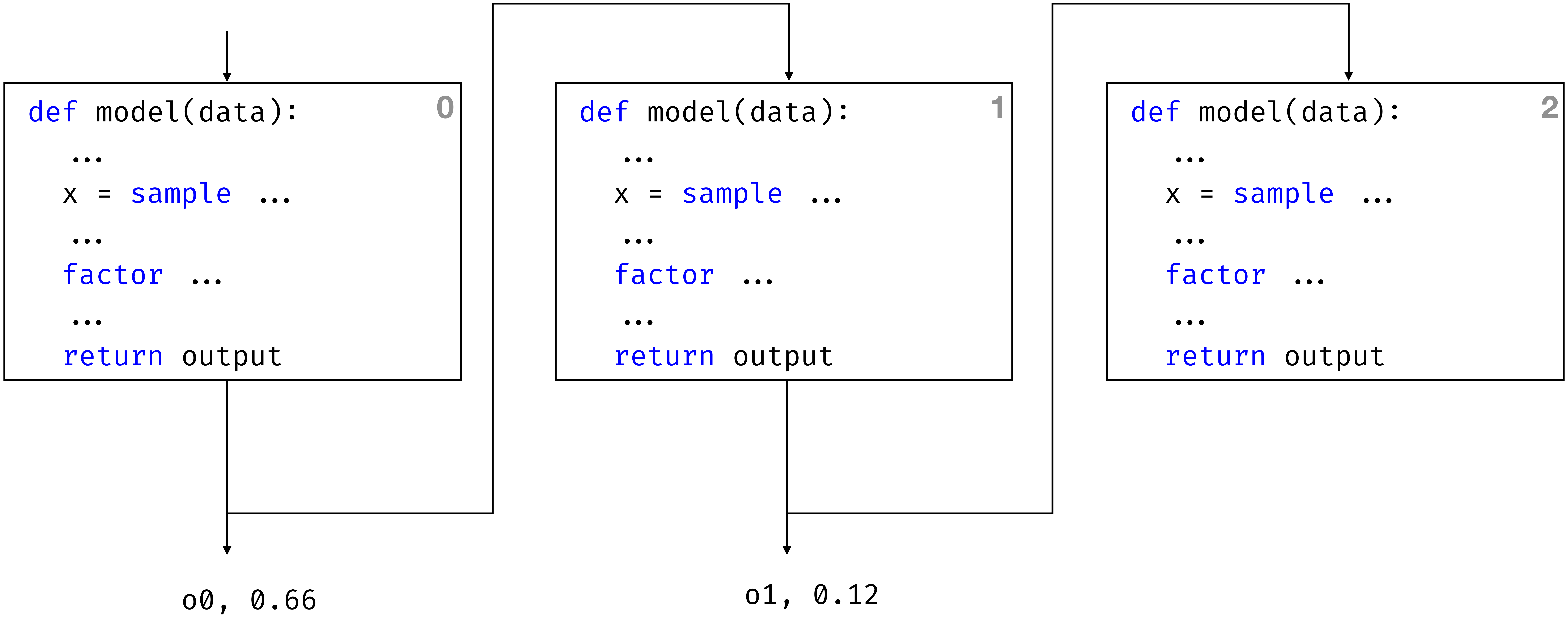

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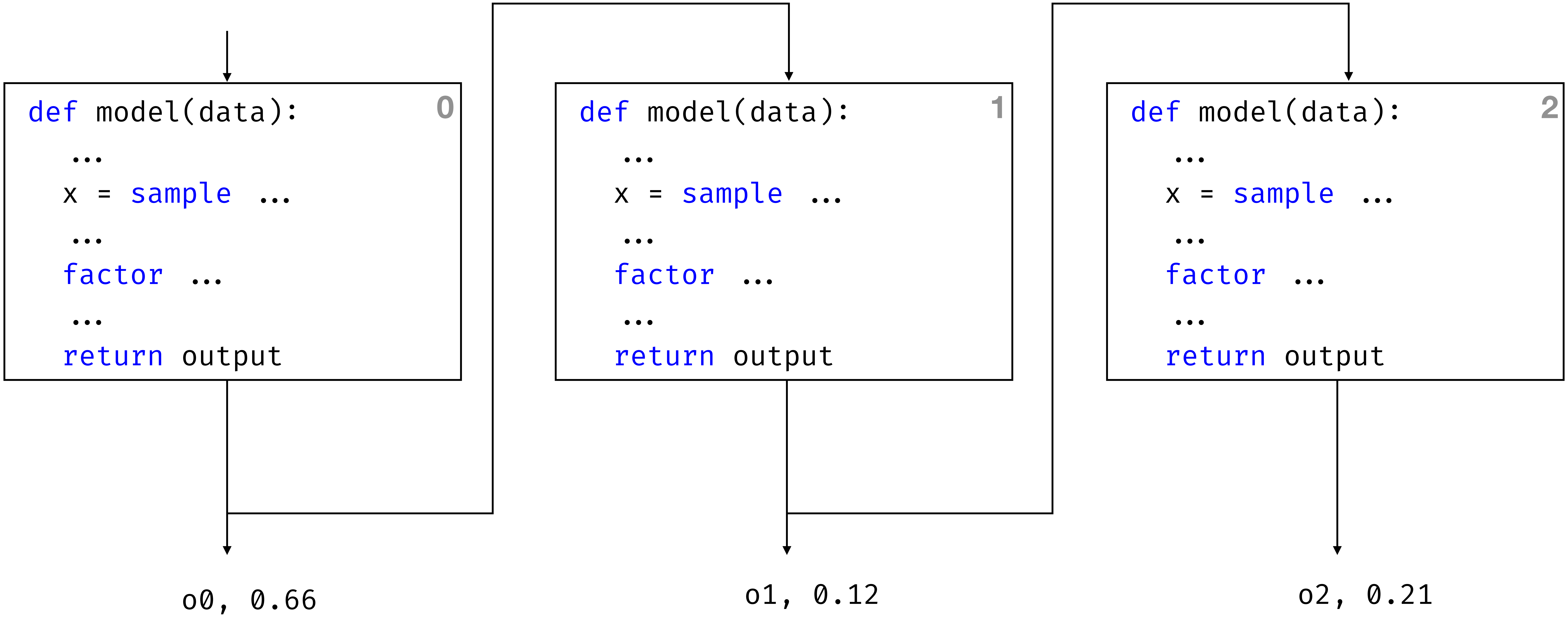

Importance sampling


```
class Importance_sampling(Handler):
  def __init__(self, num_particles: int = 1000) → None:
    self.num_particles = num_particles
    self.score: float = 0   # current score

  def sample(self, dist: Distribution[T]) → T:
    return dist.sample()   # draw sample

  def factor(self, weight: float) → None:
    self.score += weight   # update the score (log scale)

  def infer(self, model: Callable[P, T], data: P) → Distribution[T]:
    samples: List[Tuple[T, float]] = []
    for _ in range(self.num_particles):   # run num_particles executions
      self.score = 0   # reset the score
      samples.append((model(data), self.score)) # store value and score
    return Categorical(samples)
```

Example: bias of a coin

```python
from mu_ppl import *

def coin(obs: List[int]) -> float:
  p = sample(Uniform(0, 1))
  for o in obs:
    observe(Bernoulli(p), o)
  return p

with ImportanceSampling(num_particles=10000):
  dist = infer(coin, [0, 0, 0, 0, 0, 0, 0, 0, 1, 1])
  viz(dist)
```

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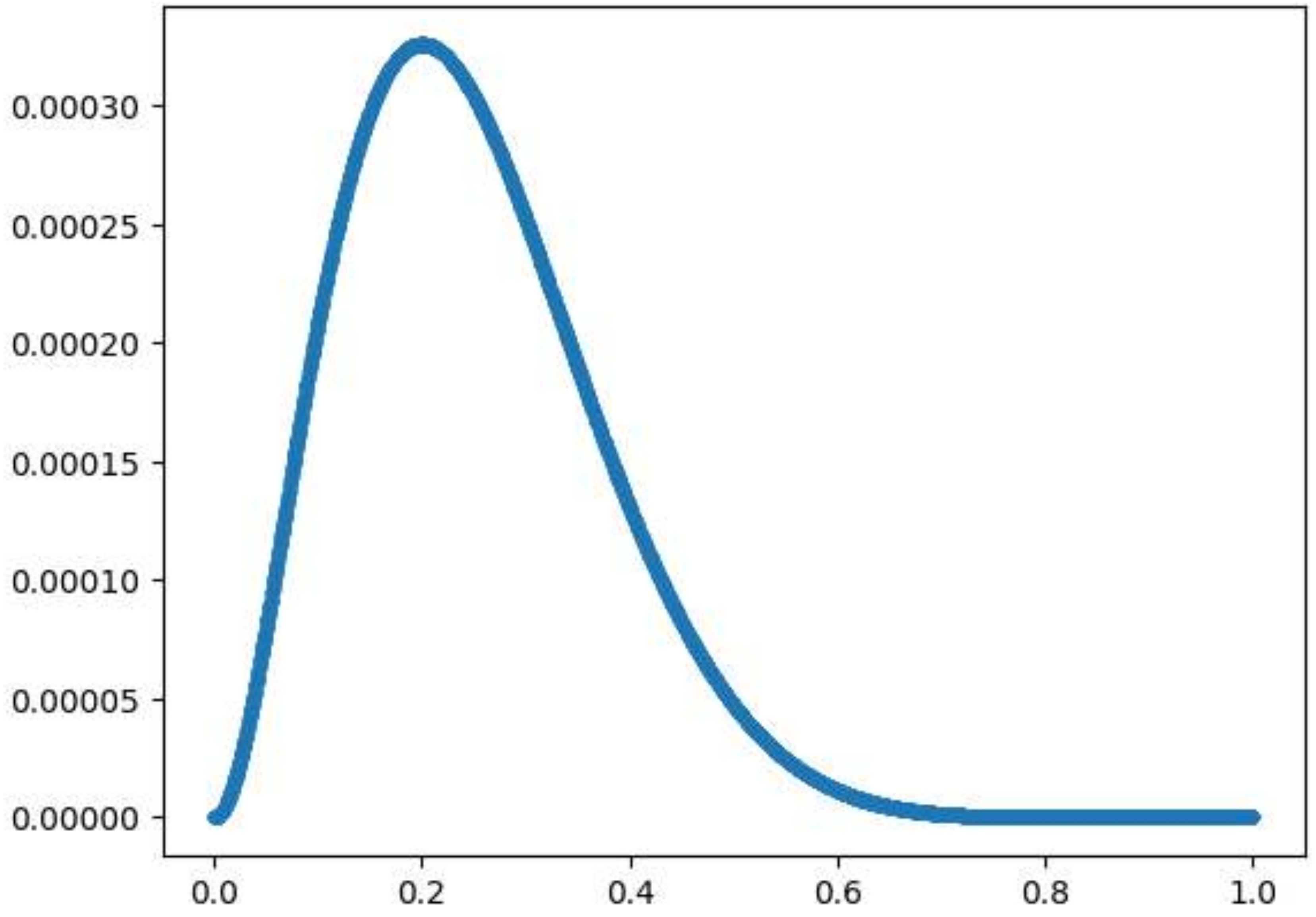

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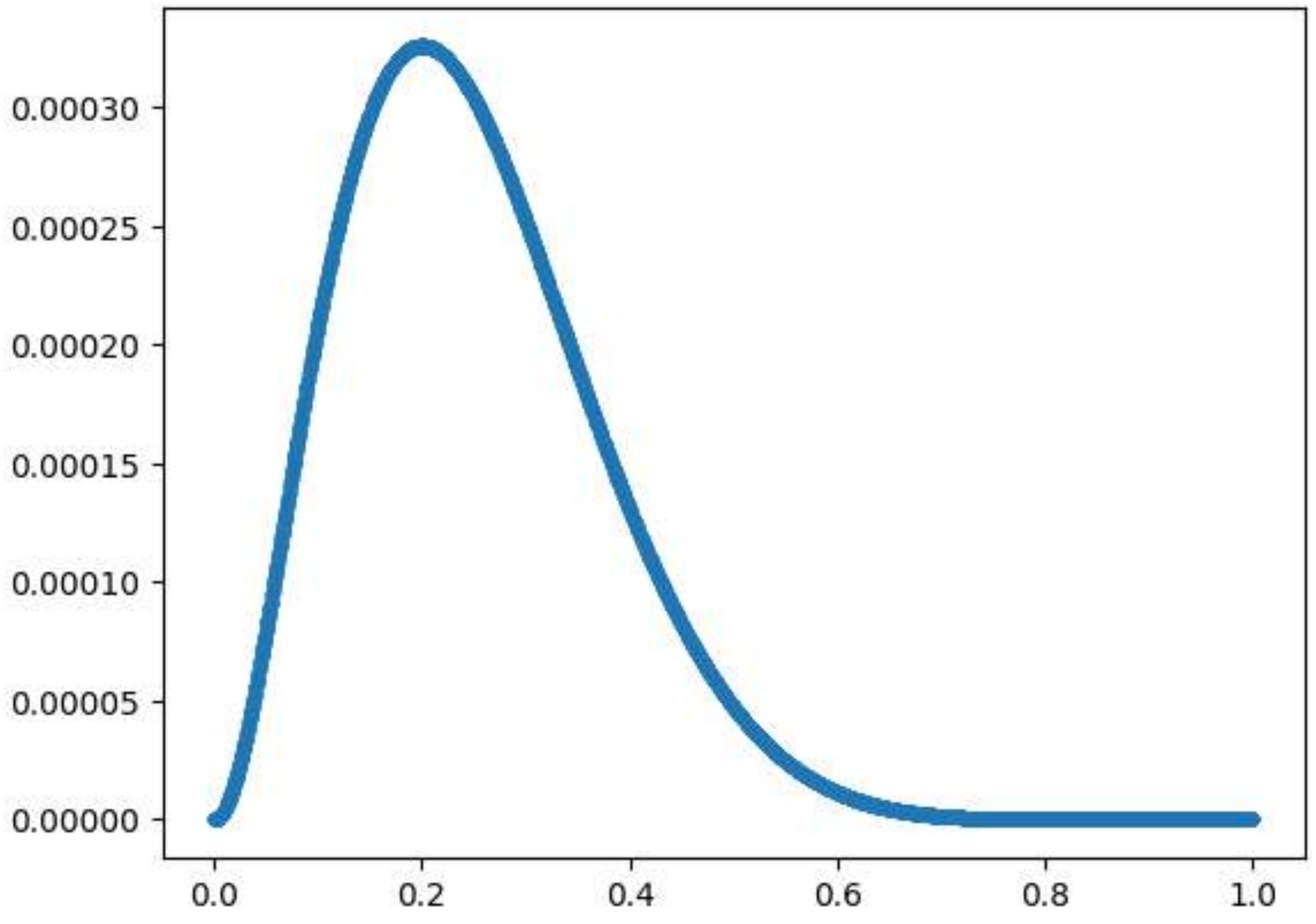
Exact solution: Beta(#heads + 1, #tails + 1)



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

Sven Sachsalber, *Looking for a needle in the Haystack*, 2014

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17h45mn

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Markov Chain Monte Carlo (MCMC)

Main idea

- Create a Markov chain over executions that converges to the posterior distribution
- Iterate the process until convergence
- Then, each iteration generates a valid sample
- Accumulate samples to approximate the posterior 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

Example: bias of a coin

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def coin(obs: List[int]) → float:
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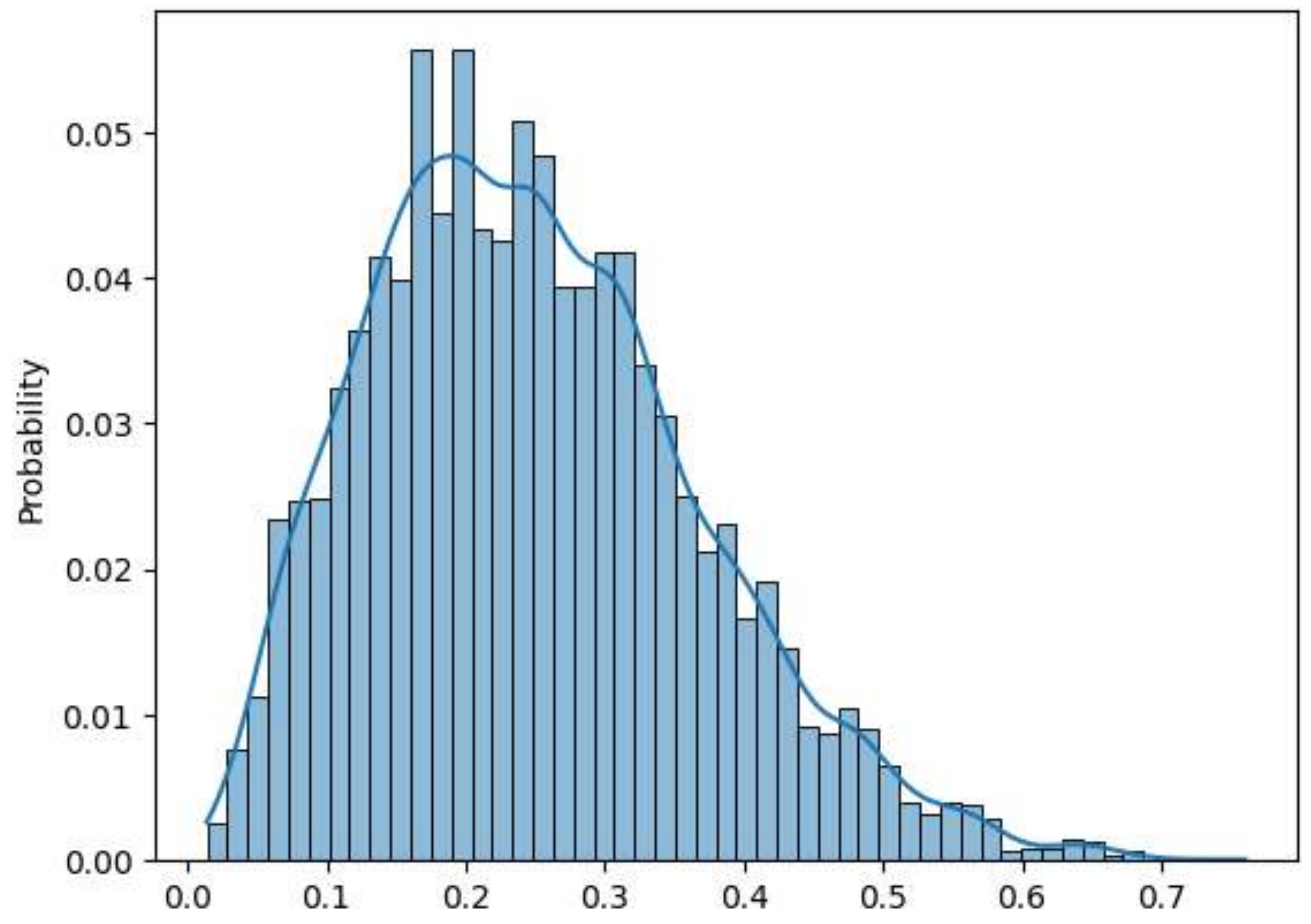
with MetropolisHastings(num_particles=10000):
  dist = infer(coin, [0, 0, 0, 0, 0, 0, 0, 0, 1, 1])
  viz(dist)
```



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Metropolis Hastings

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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)

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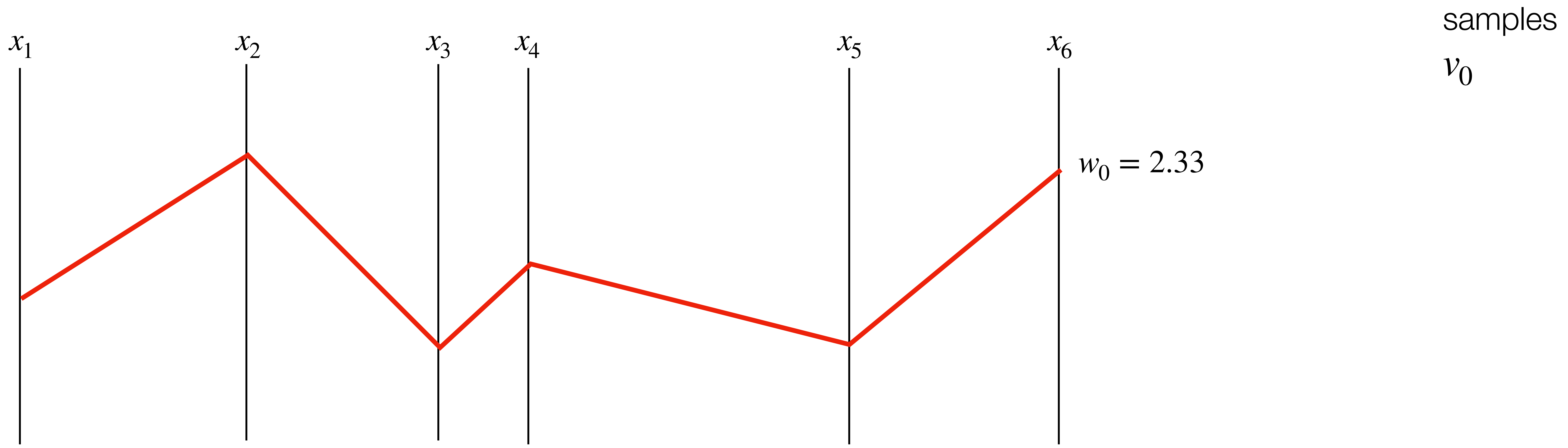
Metropolis-Hastings algorithm

- Initialization: draw X_0 at random to get a pair (v_0, W_0).
- At each step:
  1. Draw a *candidate* $X' \sim Q(X' \mid X_i)$ to get (v', W')
  2. Acceptance rate: $\alpha = \dfrac{P(X')\, W'\, Q(X_i \mid X')}{P(X_i)\, W_i\, Q(X' \mid X_i)}$.
  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*) $\begin{cases} X_{i+1} & = & X_i \\ v_{i+1} & = & v_i \\ W_{i+1} & = & W_i \end{cases}$

Single-site Metropolis Hastings

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

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



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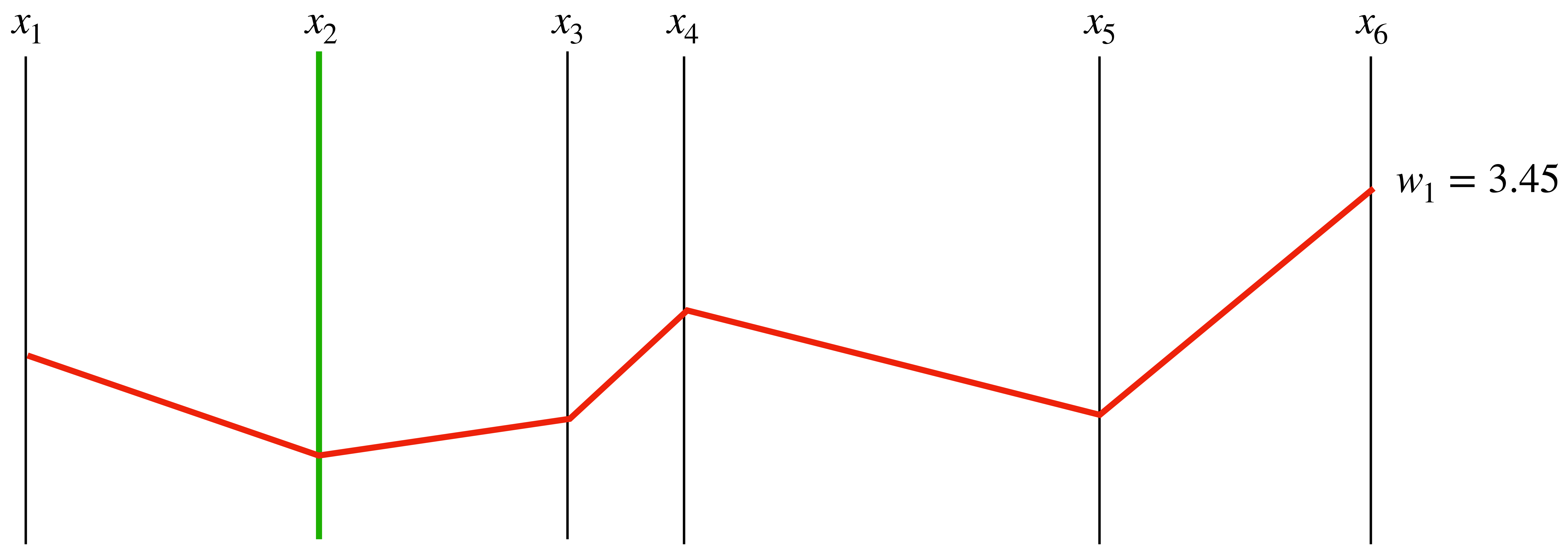

samples

v_0

v_1

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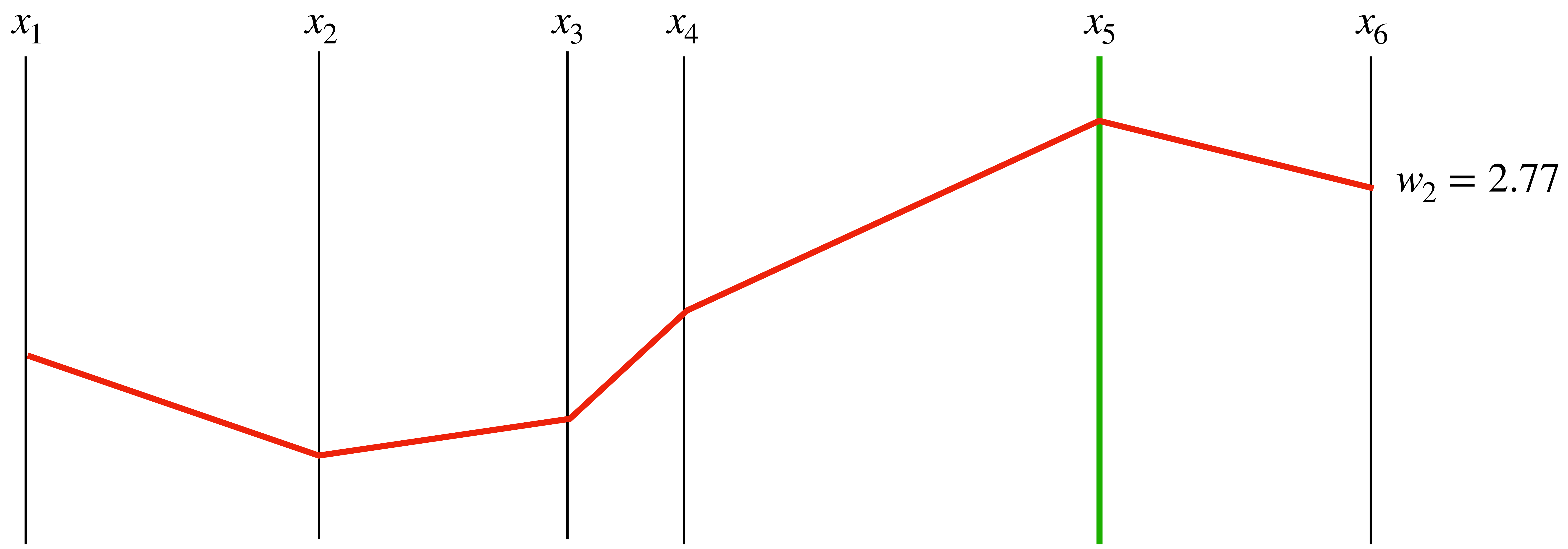

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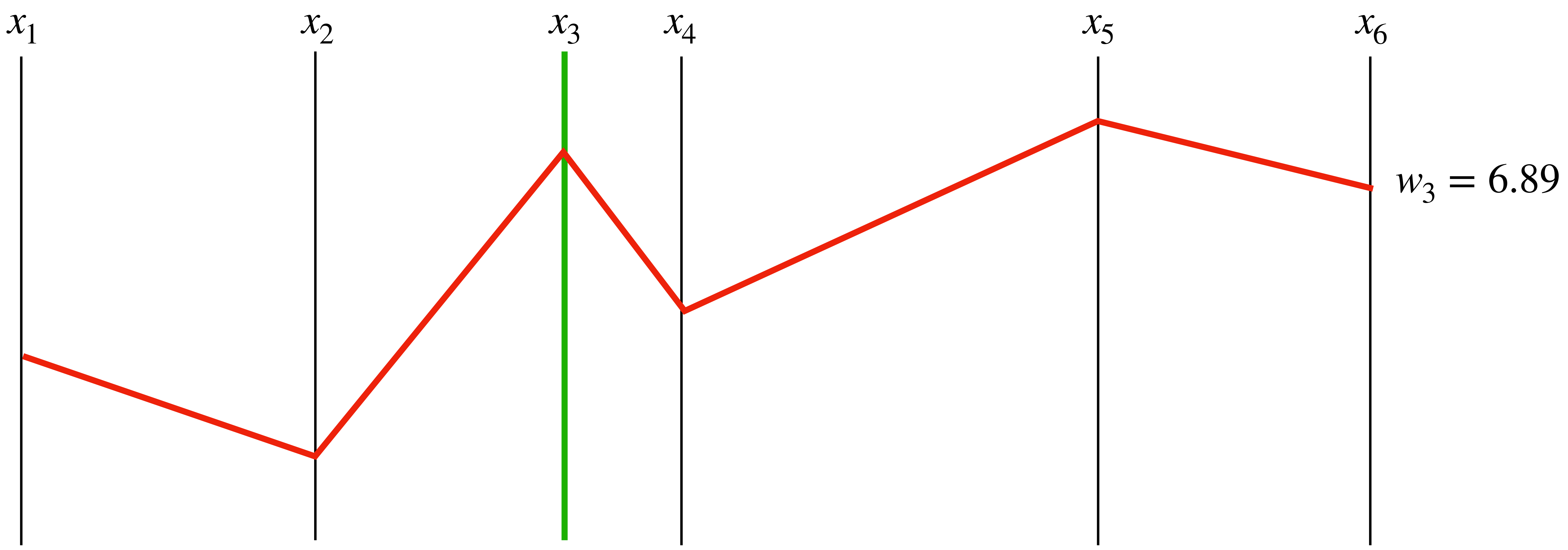

samples

v_0

v_1

v_1

v_3

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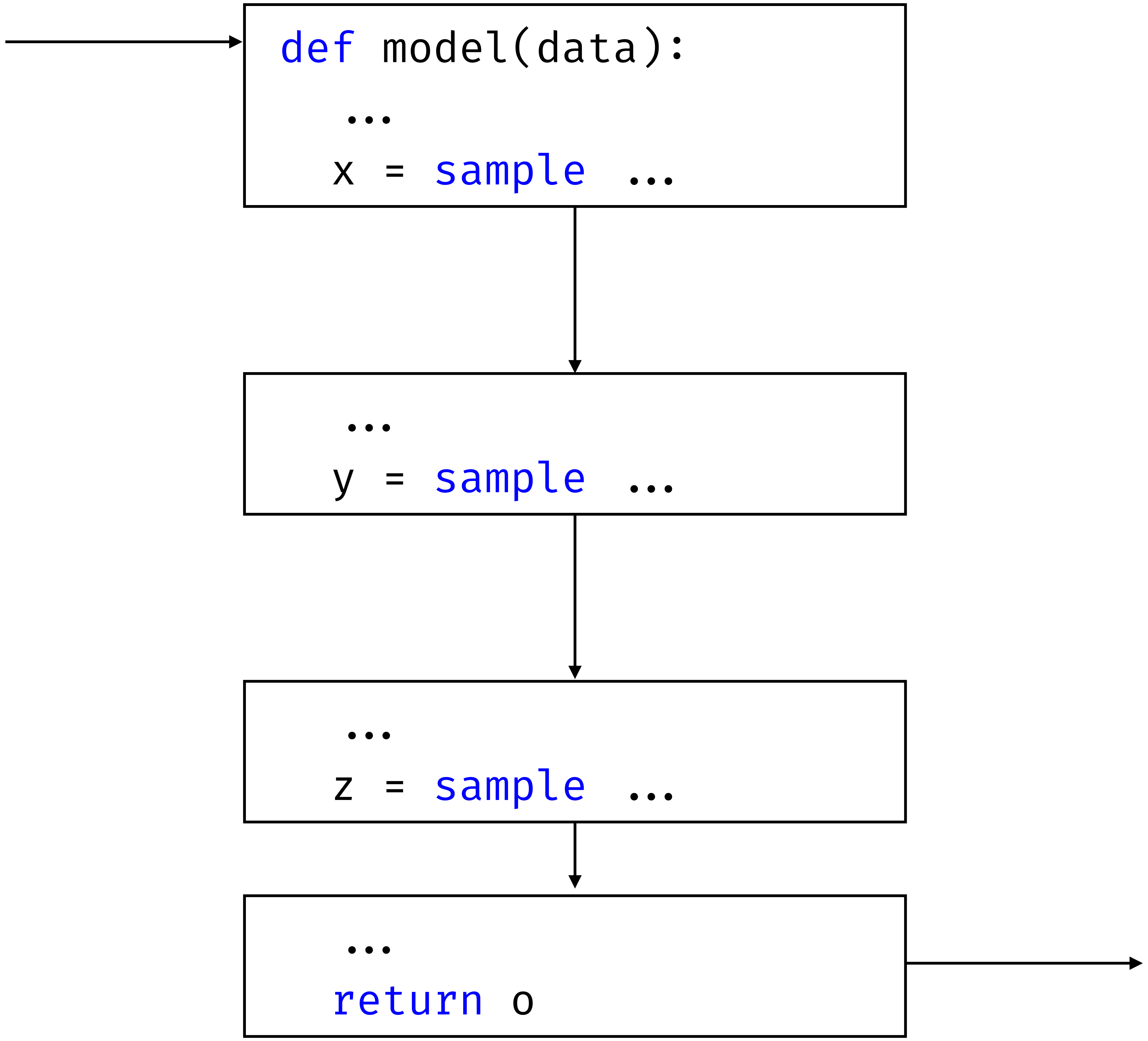

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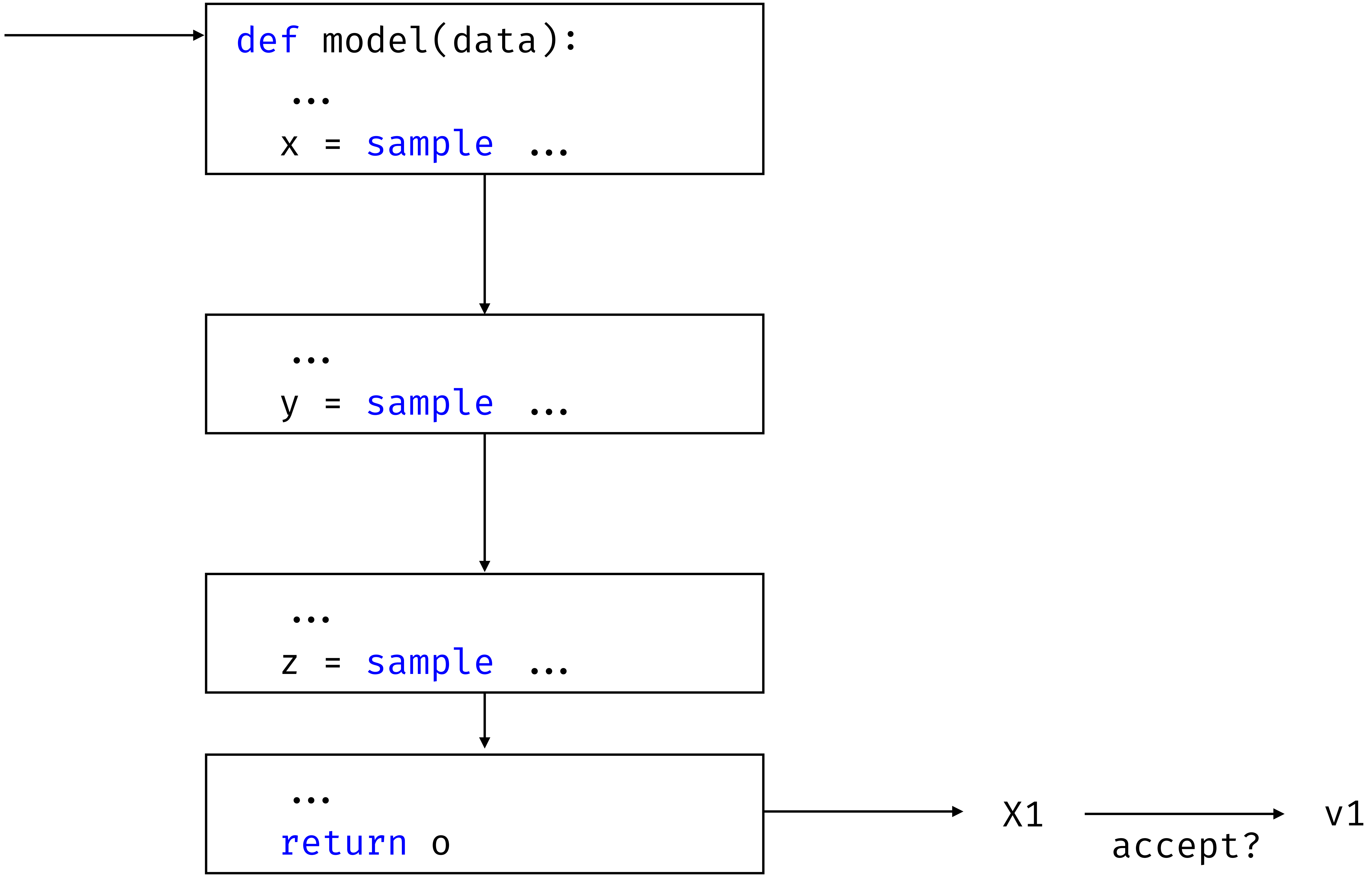

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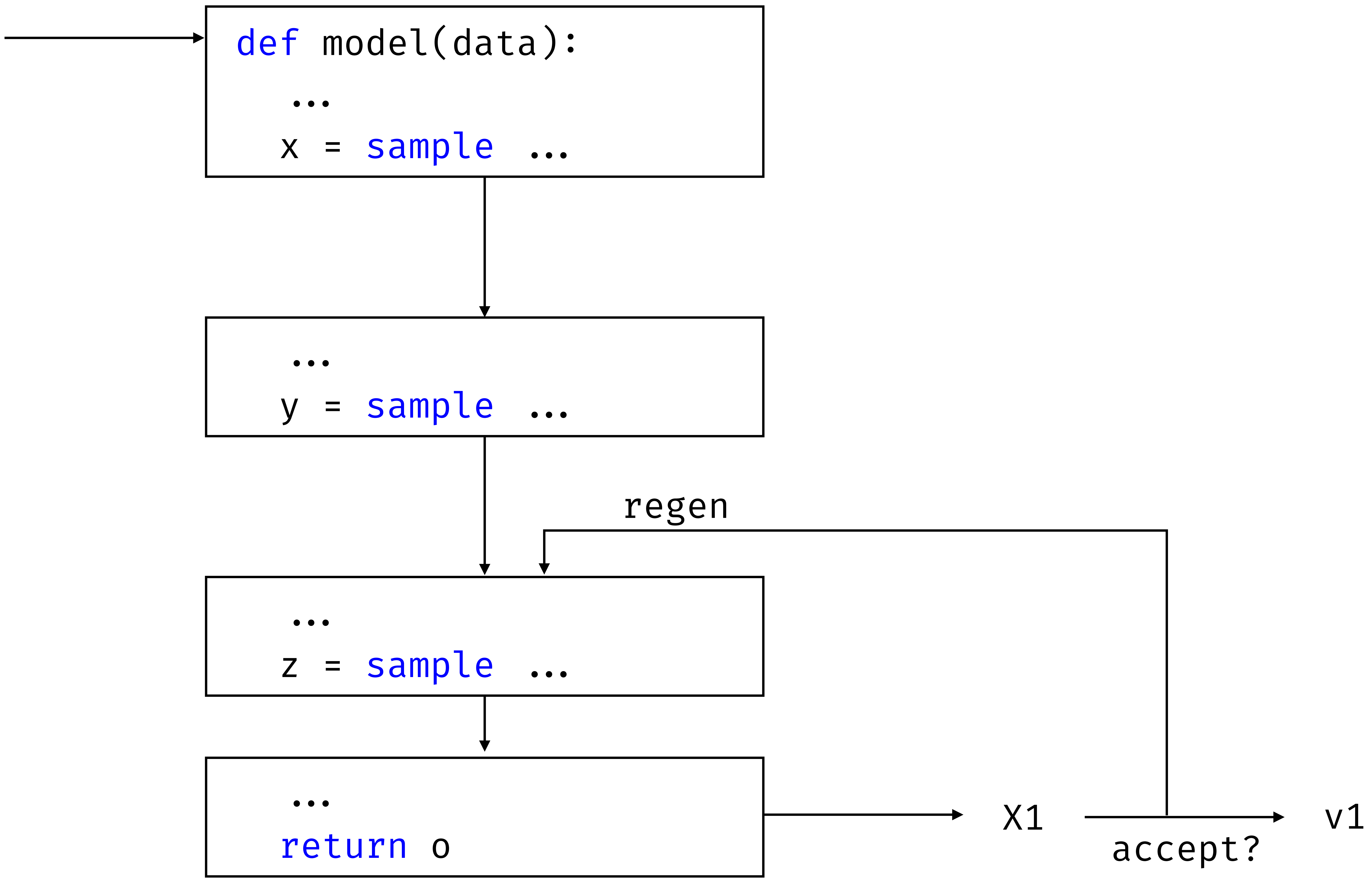

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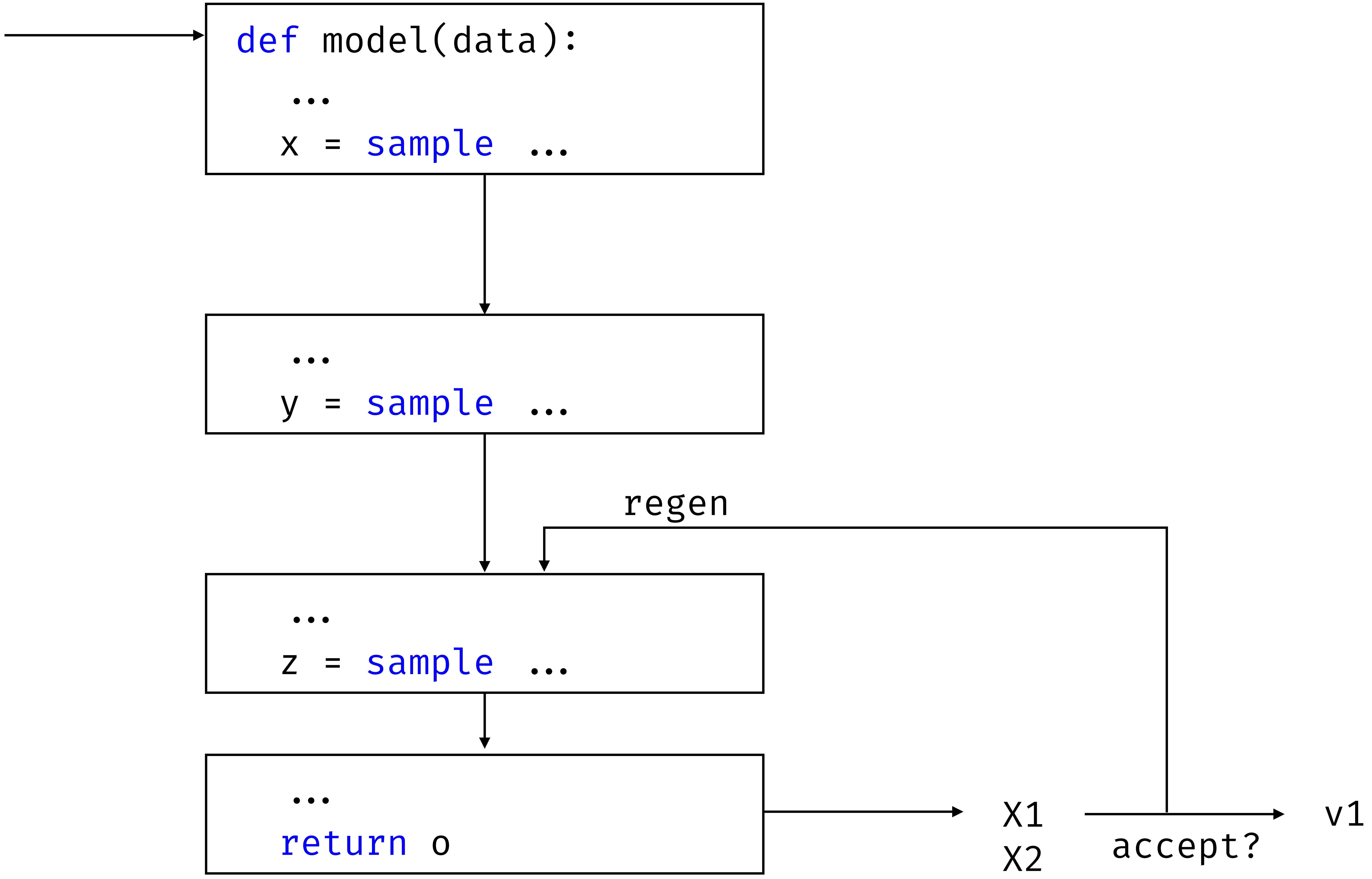

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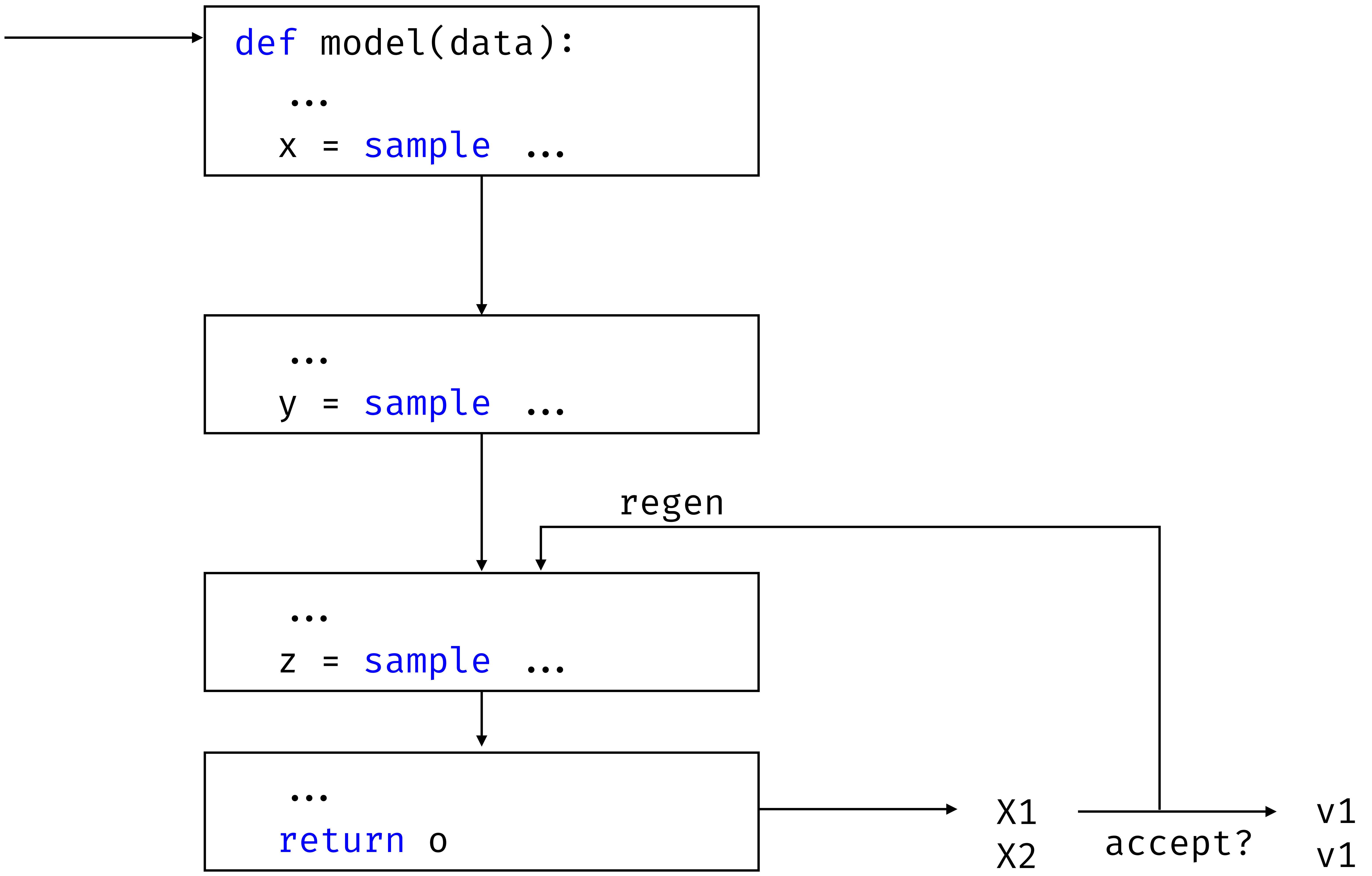

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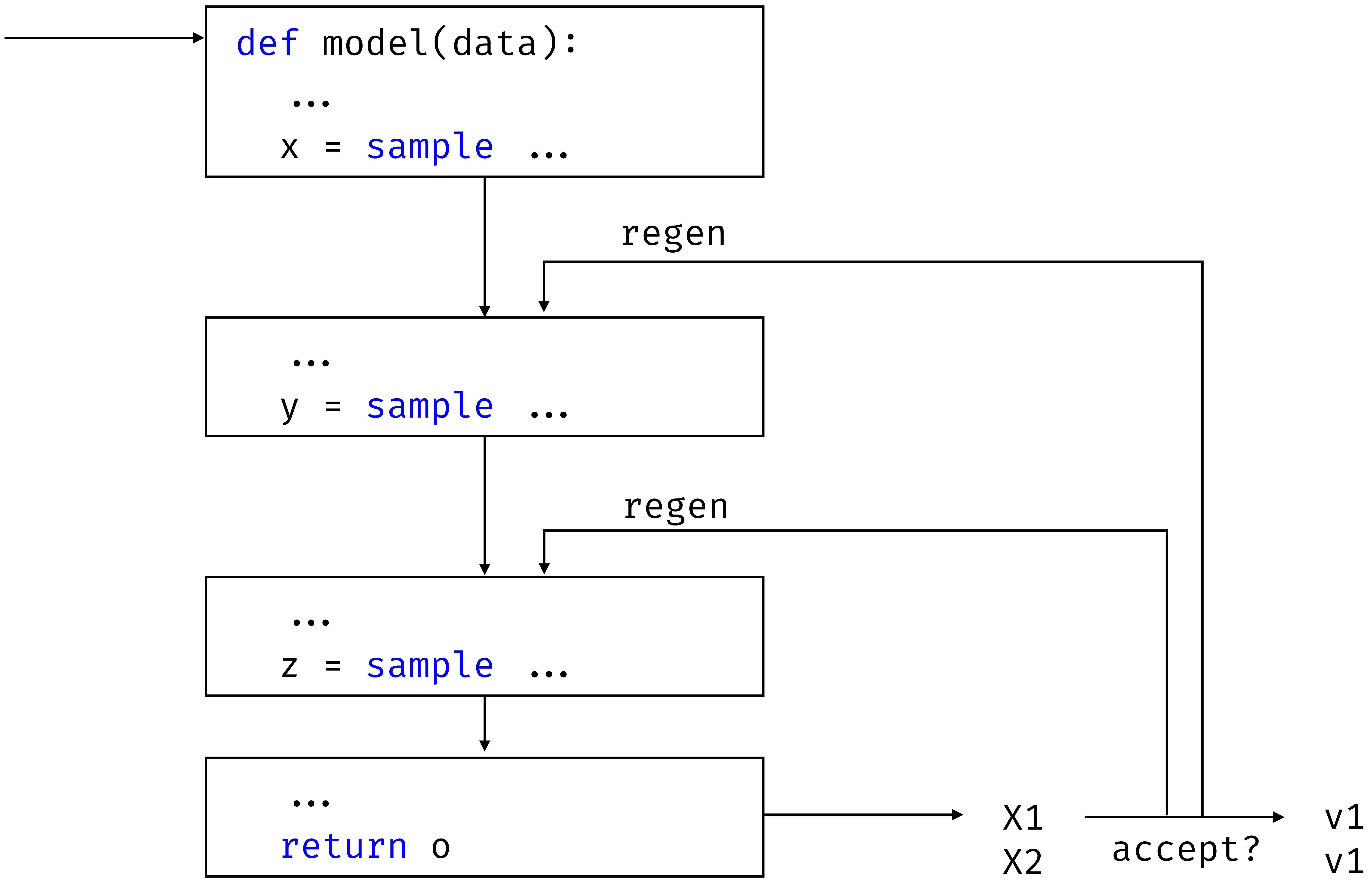
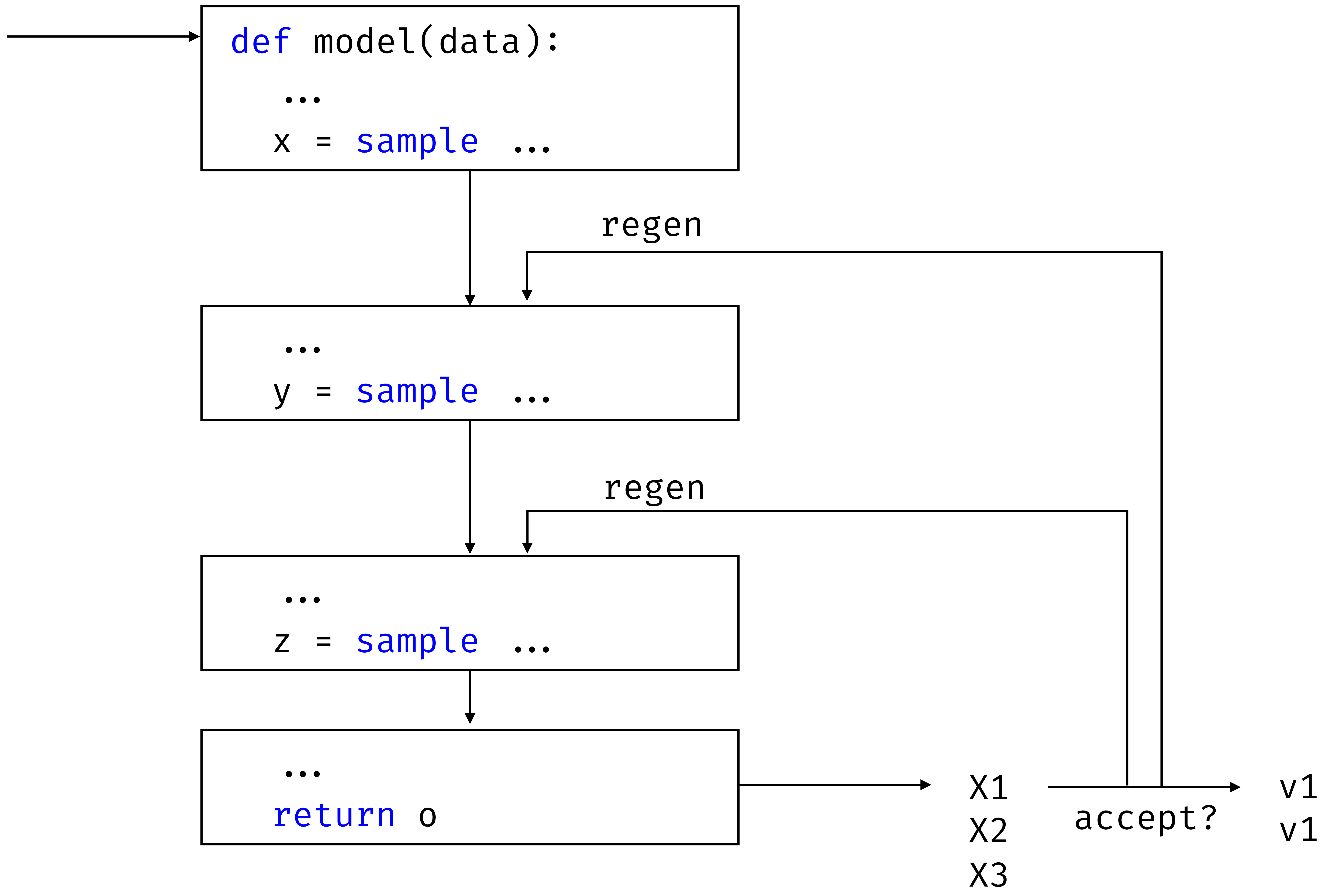


Single-site Metropolis Hastings



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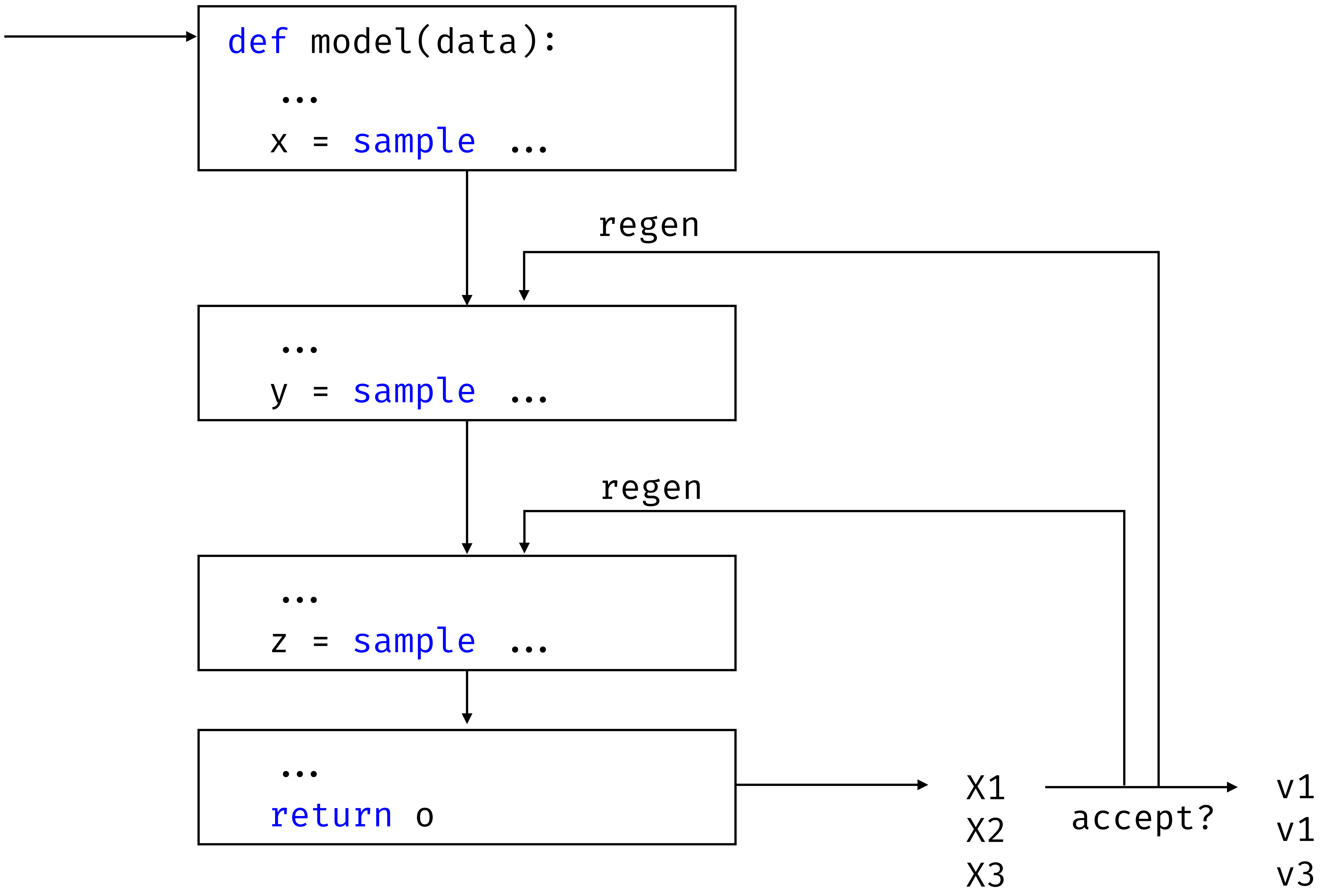

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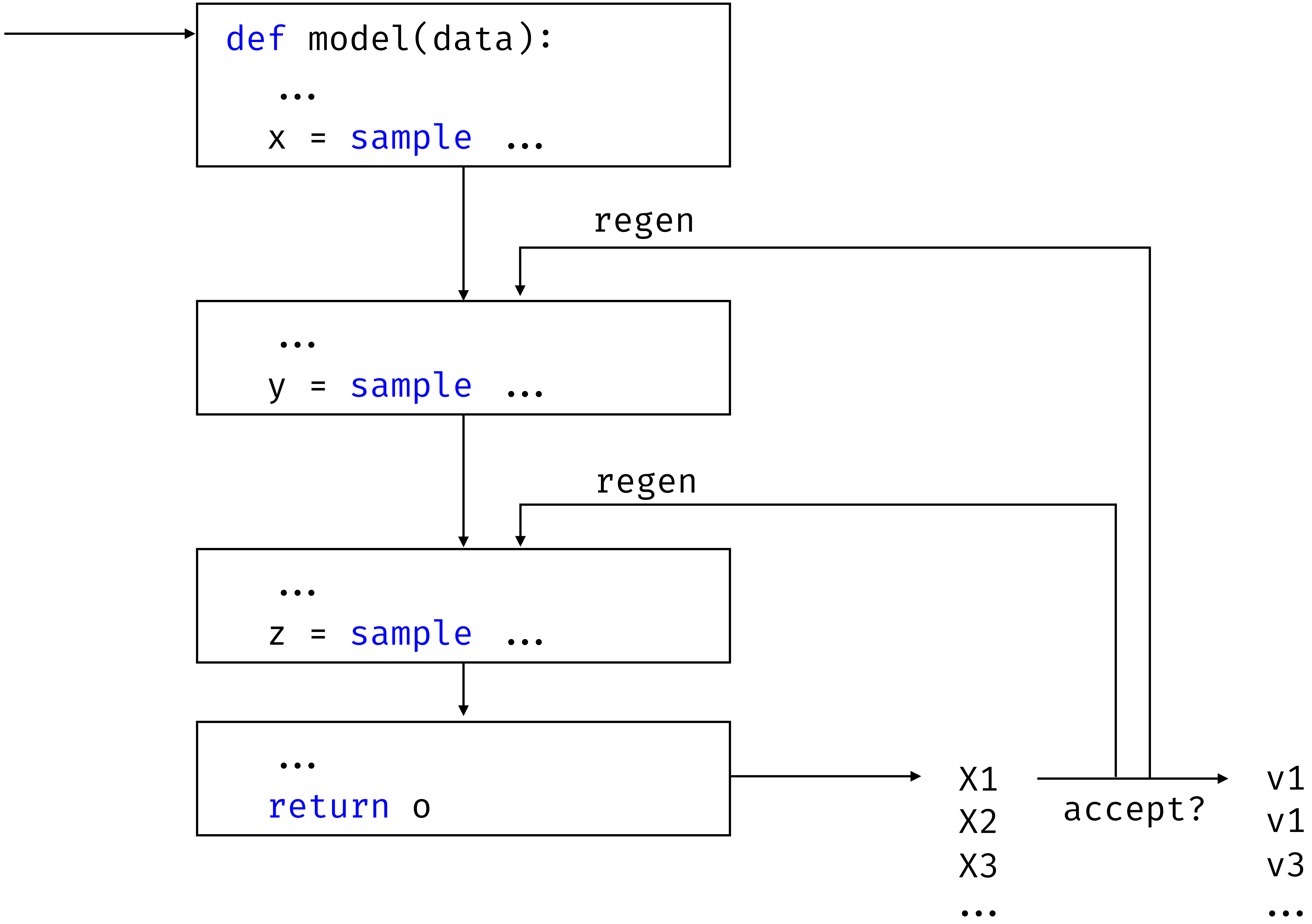

Single-site Metropolis Hastings: acceptation

Single-site Metropolis Hastings: acceptation

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'

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

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

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

Single-site Metropolis Hastings: acceptation

Notations

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

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

Reused variables are treated as observations

Single-site Metropolis Hastings

Rerun (part of) a trace

- Assign a unique name to each random variable `sample` (can be added by a compiler)
- `cache` : *name* $\to V$, reused samples
- `x_samples` : *name* $\to V$, samples for each random variable
- `x_scores` : *name* $\to \mathbb{R}^+$, corresponding score $w(x)$

```
def coin(obs: List[int]) → float:
  p = sample(Uniform(0, 1), name="p")
  for o in obs:
    observe(Bernoulli(p), o)
  return p
```

Single-site Metropolis Hastings


```
class MetropolisHastings(ImportanceSampling):
  def __init__(self, num_samples: int) → None:
    self.num_samples = num_samples
    self.score: float = 0 # current score
    self.x_samples: Dict[str, Any] = {}   # samples store
    self.x_scores: Dict[str, float] = {}   # X scores
    self.cache: Dict[str, Any] = {}   # sample cache to be reused

  def sample(self, dist: Distribution[T], name: str) → T:
    try:   # reuse if possible
      v = self.cache[name]
    except KeyError:
      v = dist.sample()   # otherwise draw a sample
    self.x_samples[name] = v   # store the sample
    self.x_scores[name] = dist.log_prob(v)   # store the score
    return v
```

Single-site Metropolis Hastings


```
def mh(self, p_state):
  p_score, cache, p_x_scores = p_state
  alpha = np.log(len(p_x_scores)) - np.log(len(self.x_scores))
  alpha += self.score - p_score
  for x in self.cache:
    alpha += self.x_scores[x]
    alpha -= p_x_scores[x]
  return np.exp(alpha)
```

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

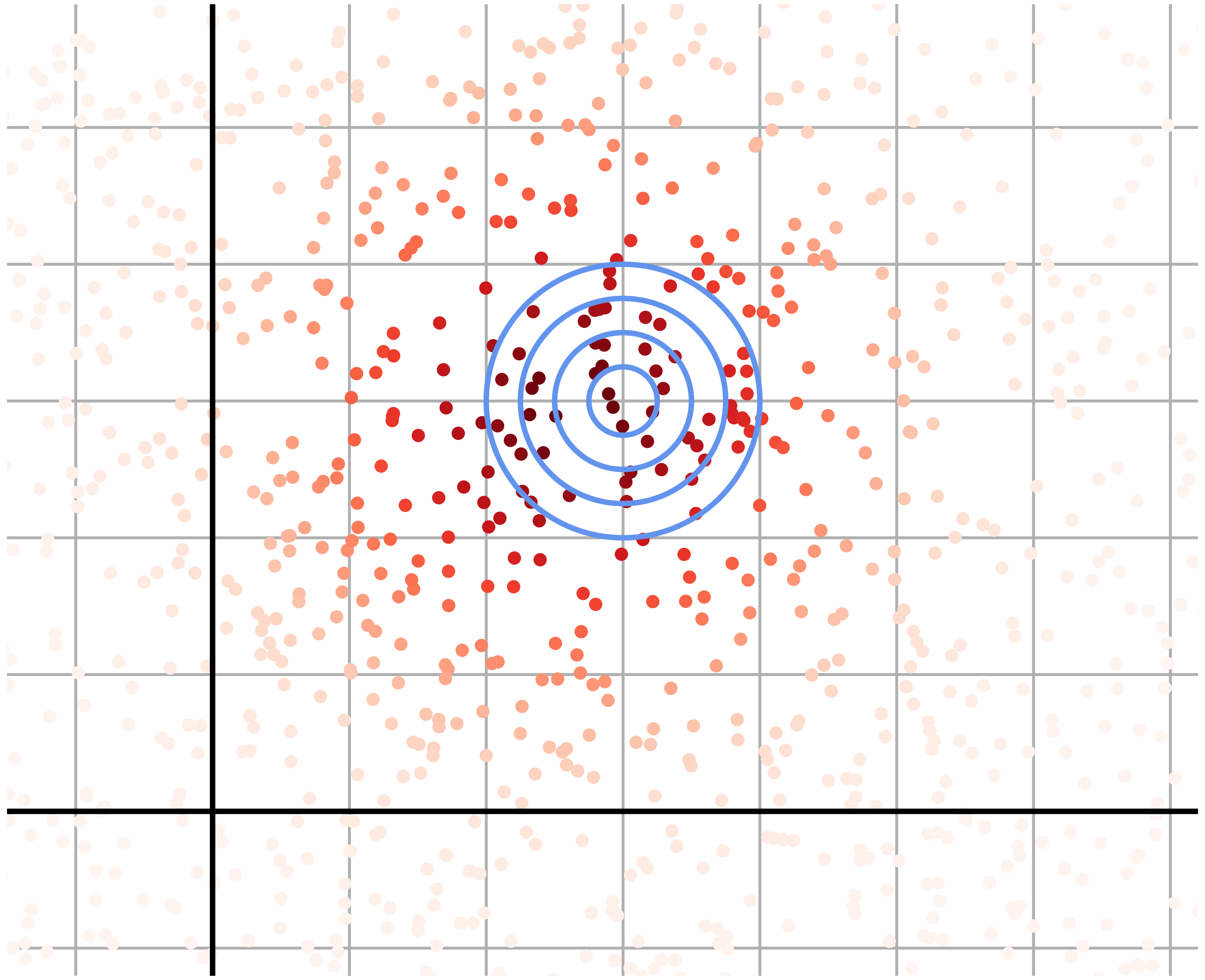
Single-site Metropolis Hastings


```
def infer(self, model: Callable[P, T], data: P) → Empirical[T]:
  samples: List[T] = []
  new_value = model(data)   # generate first trace
  for _ in range(self.num_samples):
    p_state = self.score, self.x_samples, self.x_scores   # store previous state
    p_value = new_value   # store current value
    regen = np.random.choice([n for n in self.x_samples])
    self.cache = deepcopy(self.x_samples)   # use samples as next cache
    del self.cache[regen]   # force regen to be resampled
    self.score, self.x_samples, self.x_scores = 0, {}, {}   # reset the state
    new_value = model(data)   # generate a new trace
    alpha = self.mh(p_state)
    u = np.random.random()
    if not (u < alpha):   # reject
      self.score, self.x_samples, self.scores = p_state   # rollback
      new_value = p_value
    samples.append(new_value)
  return Empirical(samples)
```

Example: Noisy position

```
def gauss(obs: List[Tuple[float, float]]) → Tuple[float, float]:
  x = sample(Gaussian(0, 10), name="x")
  y = sample(Gaussian(0, 10), name="y")
  for (xo, yo) in obs:
    observe(Gaussian(x, 1), xo)
    observe(Gaussian(y, 1), yo)
  return x, y

with ImportanceSampling(num_particles=10000):
  dist = infer(gauss, data)
```



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  for (xo, yo) in obs:
    observe(Gaussian(x, 1), xo)
    observe(Gaussian(y, 1), yo)
  return x, y

with MetropolisHastings(num_samples=1000):
  dist = infer(gauss, data)
```
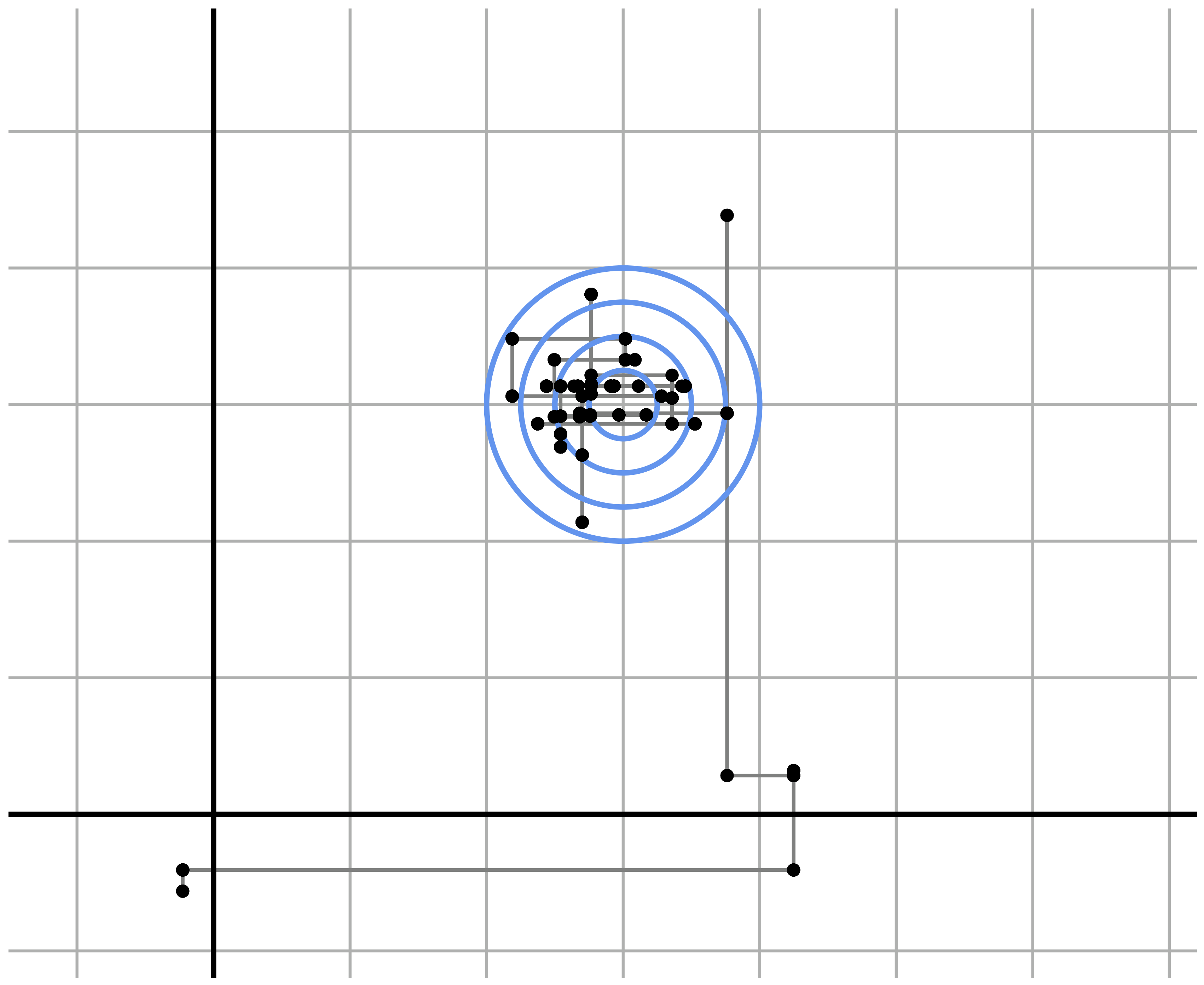



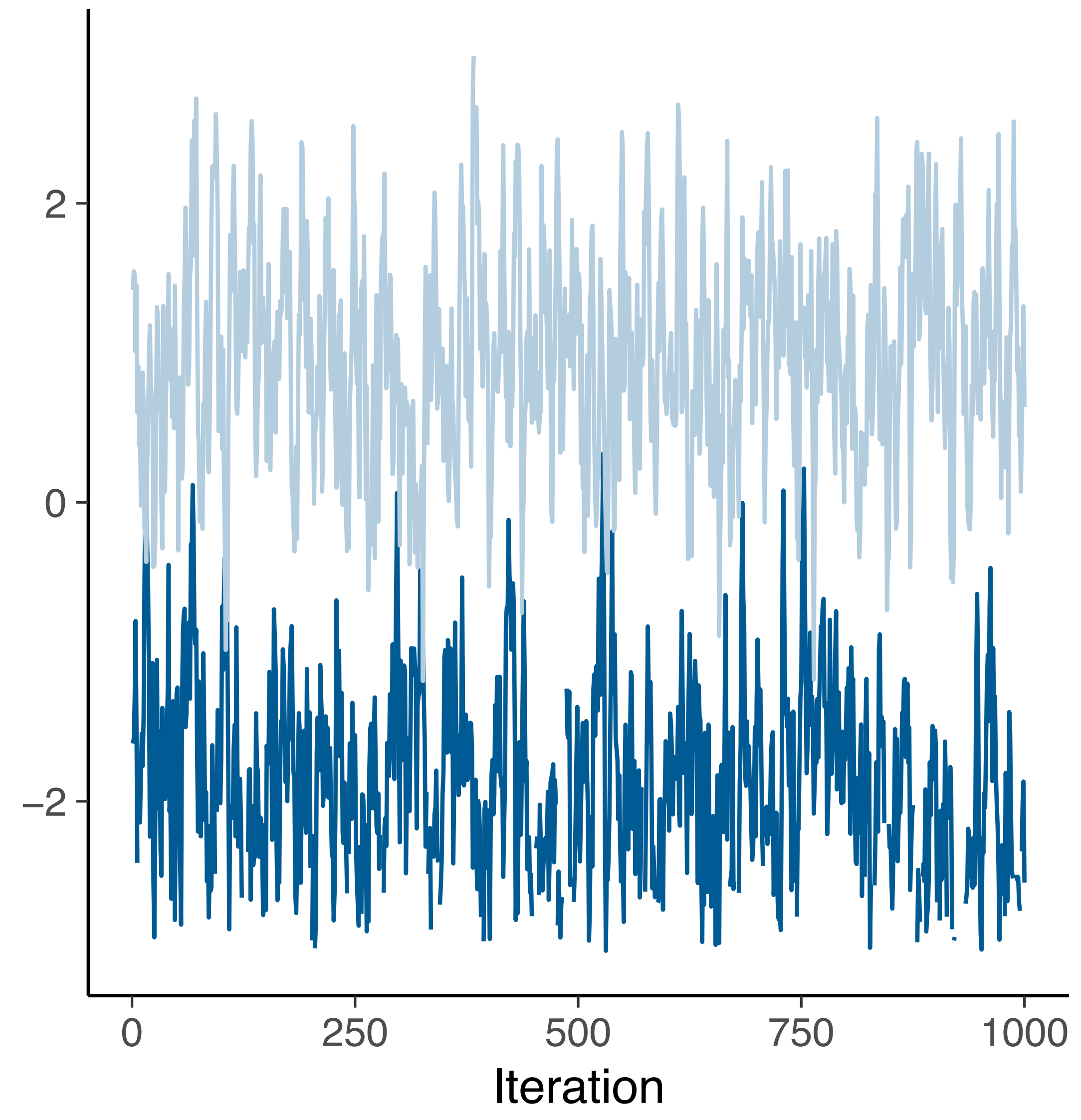
Limitations

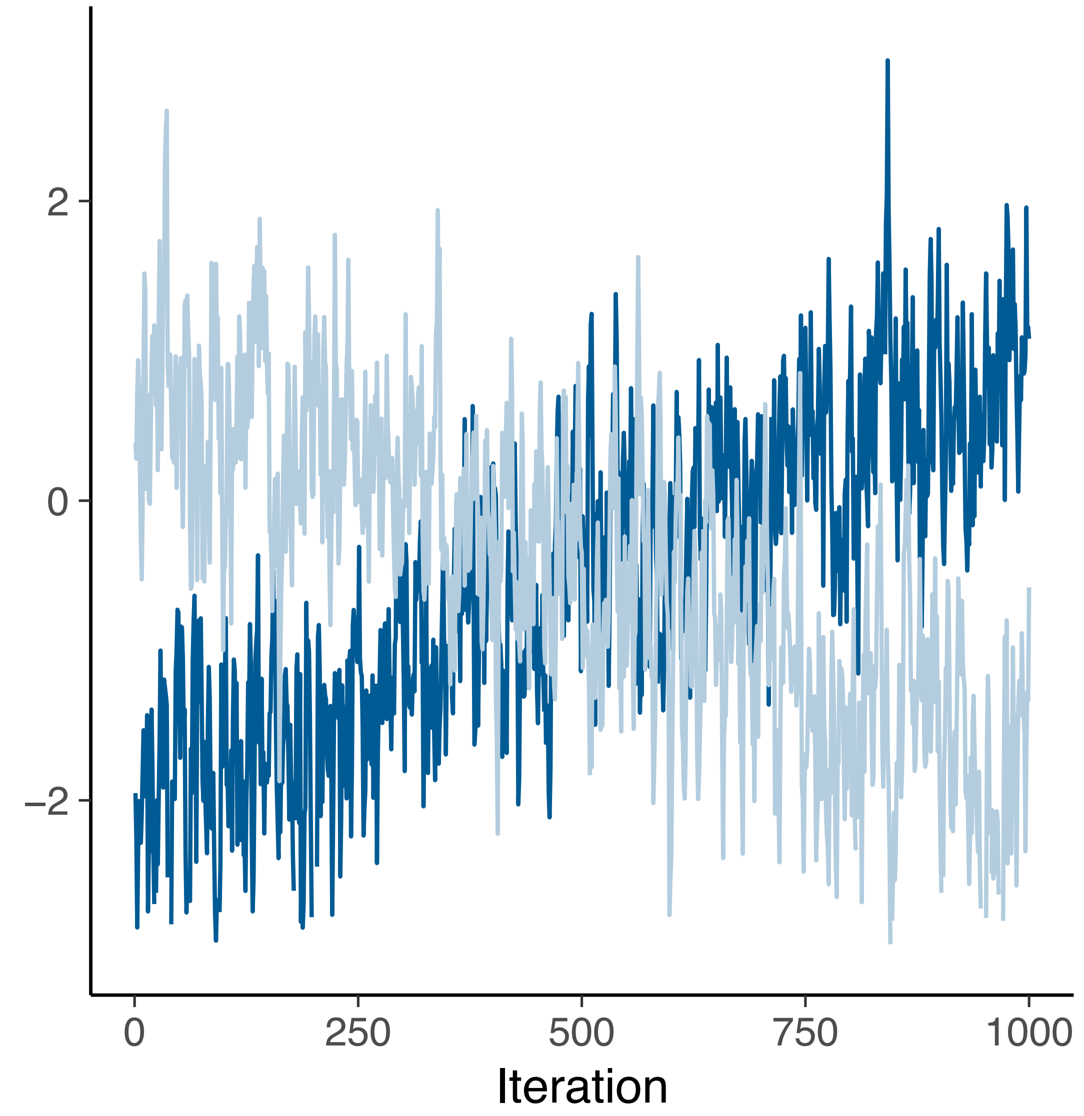
Convergence: theoretical conditions are complex

- 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)





images from Vehtari et al. 2021

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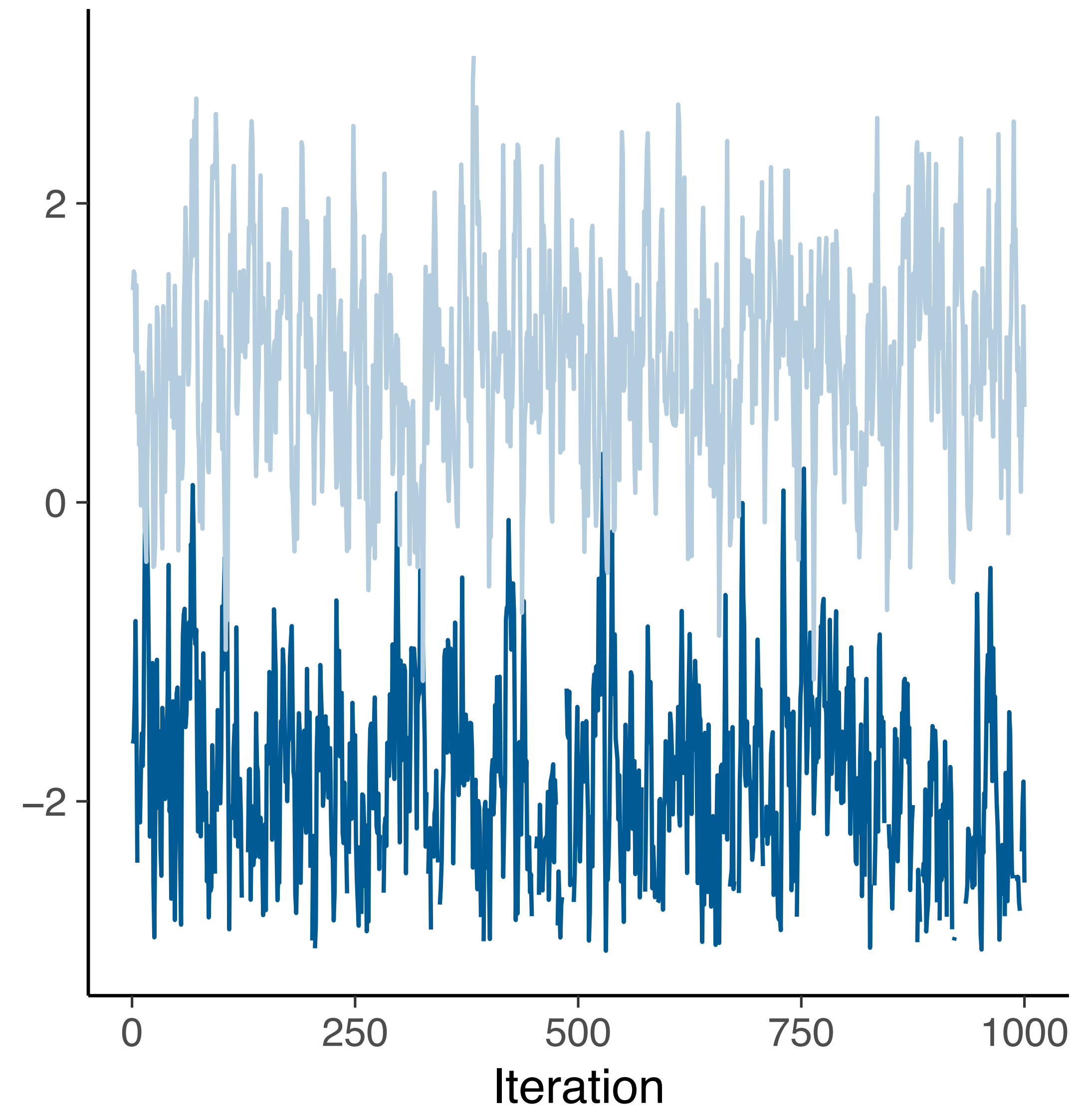
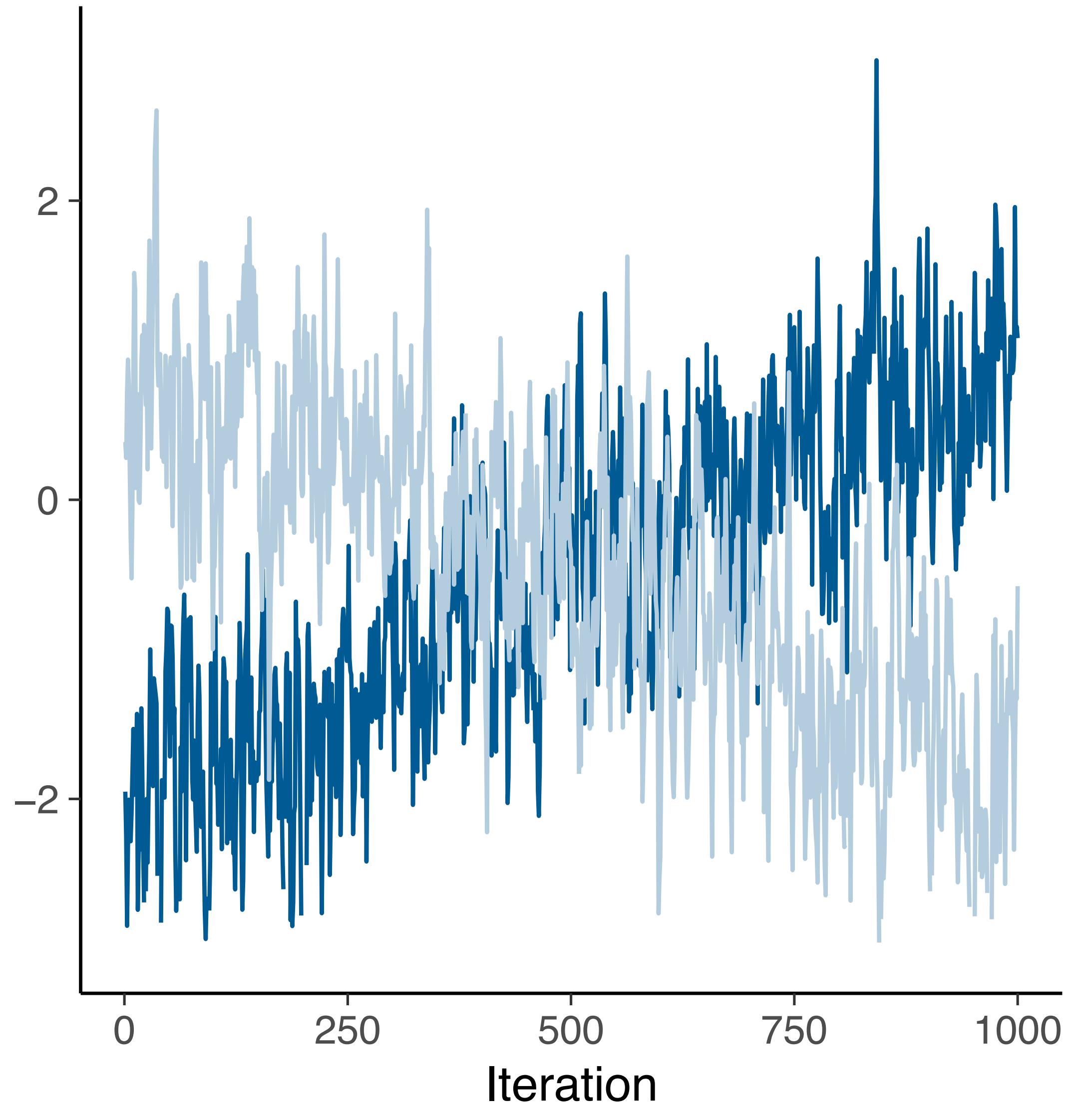
```
import arviz as az

with MetropolisHastings(num_particles=1000, warmups=1000):
  chains = [infer(gauss, obs).samples for _ in range(4)]
  az_data = az.convert_to_inference_data(np.array(chains))
  az.summary(az_data)
```

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





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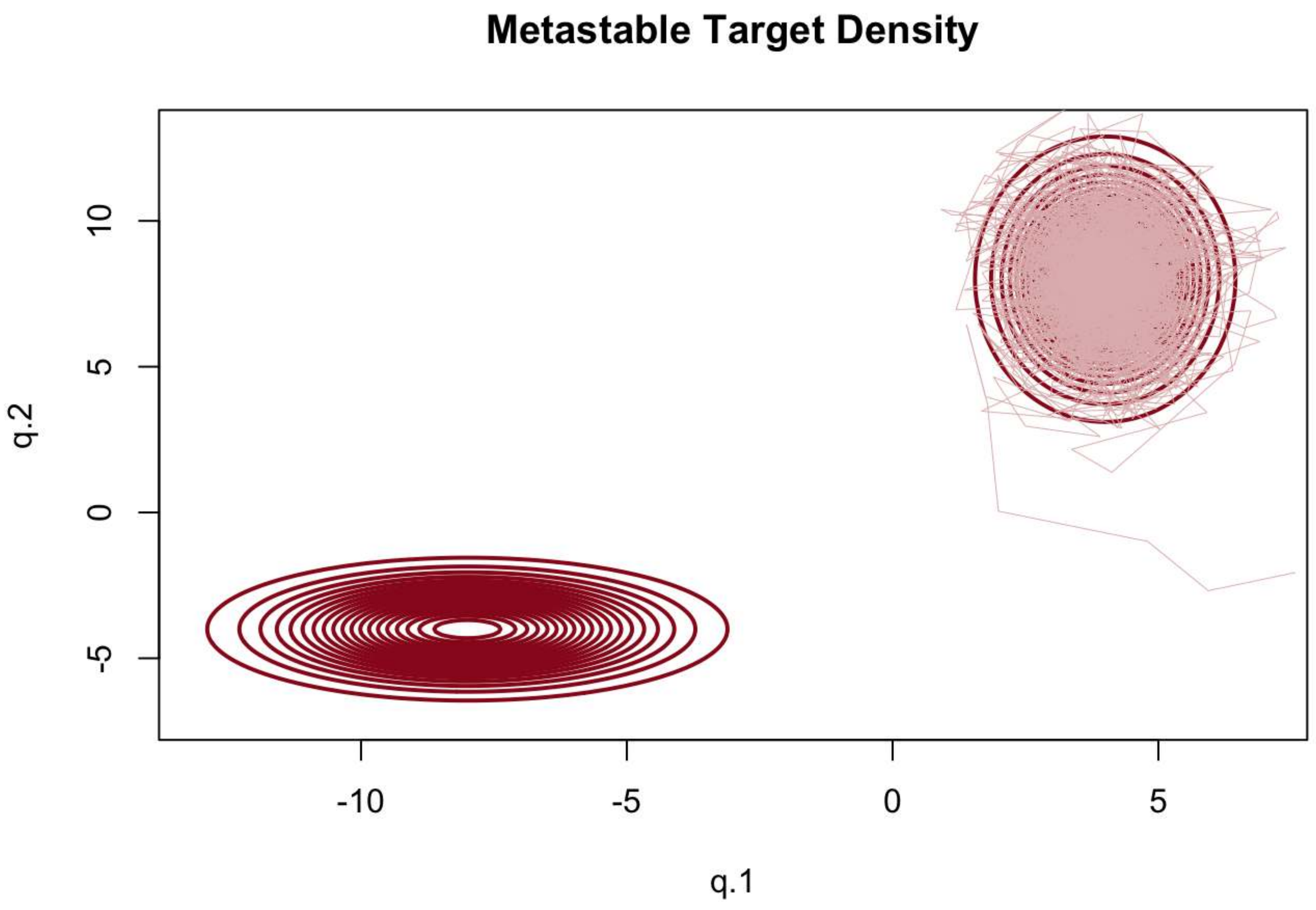
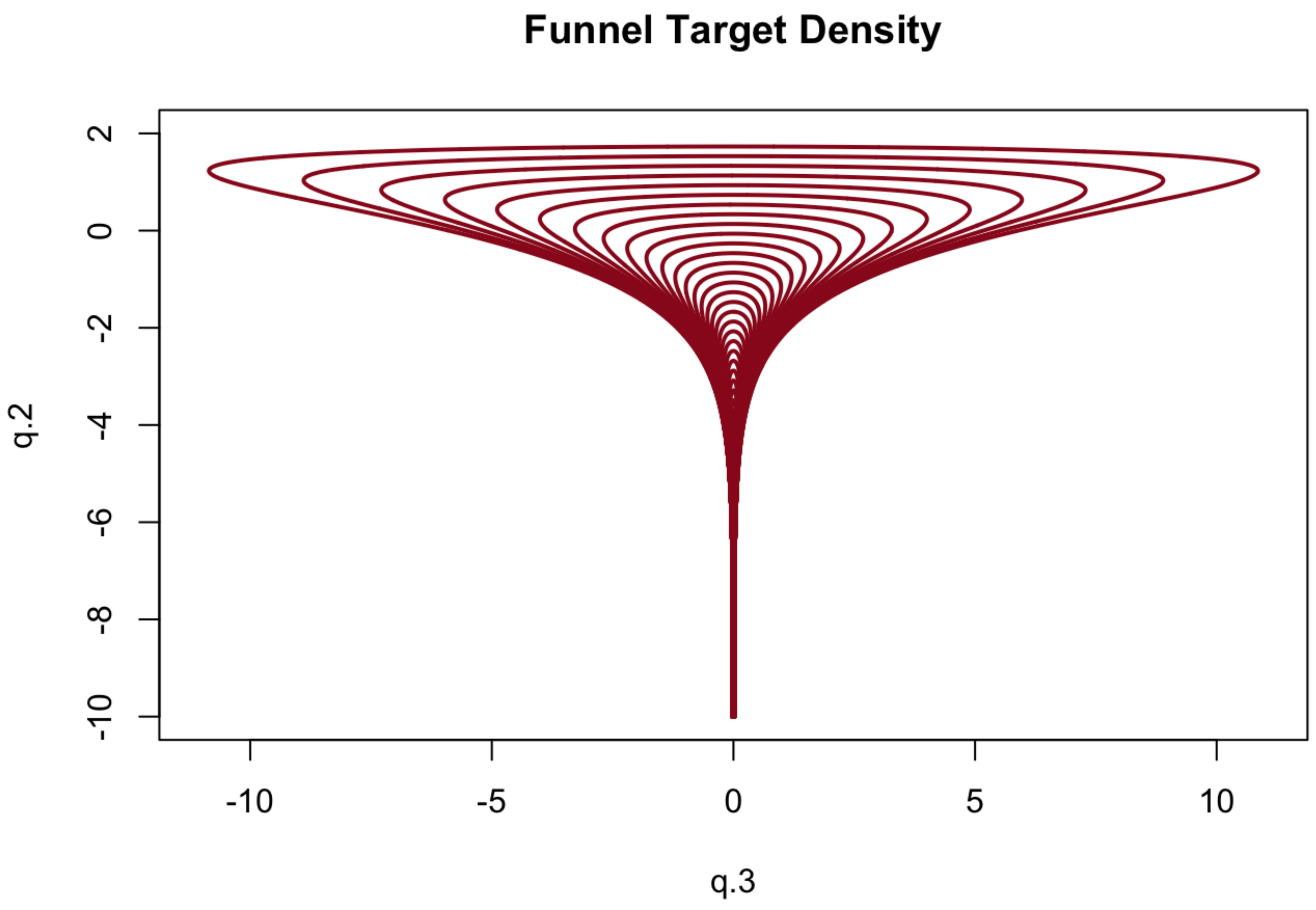
Pathological models



Multimodal distribution



Neal's funnel

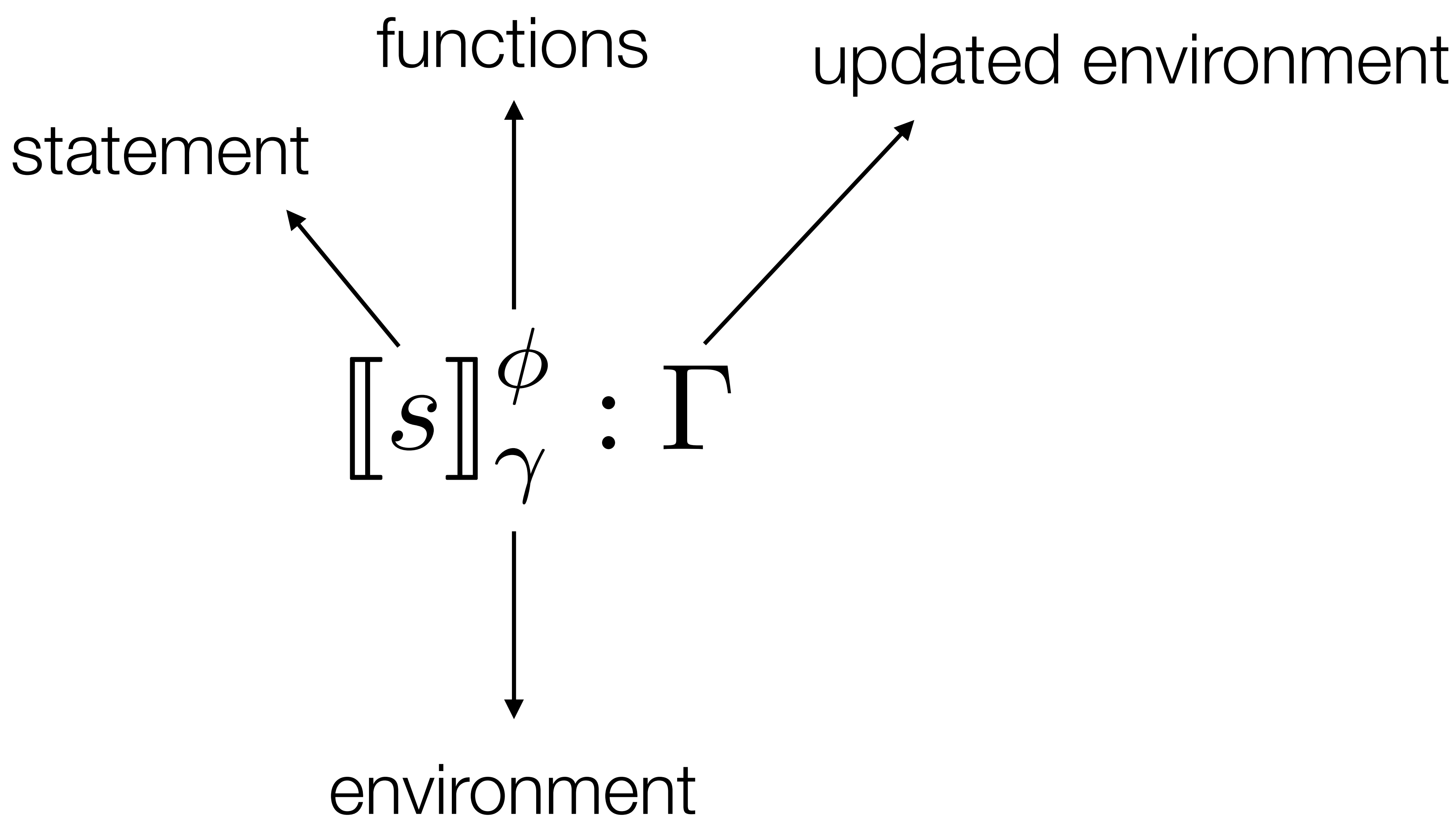
images from Bettancourt 2020

Part II. Sequential Monte Carlo methods

Part III. Density Semantics

Introduction to Probabilistic Programming

Reminders: deterministic semantics



$$[\![s]\!]_{\gamma}^{\phi} : \Gamma$$

Reminders: deterministic semantics

functions

updated environment

statement

$$[\![s]\!]_{\gamma}^{\phi} : \Gamma$$

environment

Example:

$$[\![y \texttt{ = } x + 40]\!]_{[x \leftarrow 2]}^{\emptyset} = [x \leftarrow 2,\ y \leftarrow 42]$$

Reminders: kernel semantics

functions

Measure over updated environments

statement

$$[\![s]\!]^{\phi}_{\gamma} : \mathsf{Meas}(\Gamma)$$

environment

Reminders: kernel semantics

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Example:

$$[\![x = \texttt{sample}(\mathcal{N}(0,1))]\!]_{\emptyset}^{\emptyset}(\{[x \leftarrow v] \mid v > 0\}) = 0.5$$

Reminders: kernel semantics

Unnormalized measure

functions

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$$[\![\texttt{infer}(f, e)]\!]^{\phi}_{\gamma}(U) = \begin{cases} \frac{\mu(U)}{\mu(\top)} & \textit{avec } \mu(U) = \phi(f)([\![e]\!]^{\phi}_{\gamma}) \quad \textit{si } 0 < \mu(\top) < \infty \\ \text{Erreur} & \textit{sinon} \end{cases}$$

Density semantics

Key idea

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

Interpretation close to our weighted samplers for approximate inference

Back to measure

- ρ: uniform distributions on parameters
- We get a measure by integrating f along ρ

$$\mu(U) = \int \rho(dp)W(p)\ \delta_{v(p)}(U)$$

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Problem: Random variables can change between two executions

```
c = sample(Bernoulli(0.5))
if c: x = sample(Gaussian(0, 1))
```

Measure over parameters

Lee et al. 2020

Measure over parameters

Key ideas

- Associate a unique name to each random variable (same as Metropolis-Hastings)
- Map random elements in [0, 1] to samples using inverse transform sampling

Inverse transform sampling

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

Lee et al. 2020

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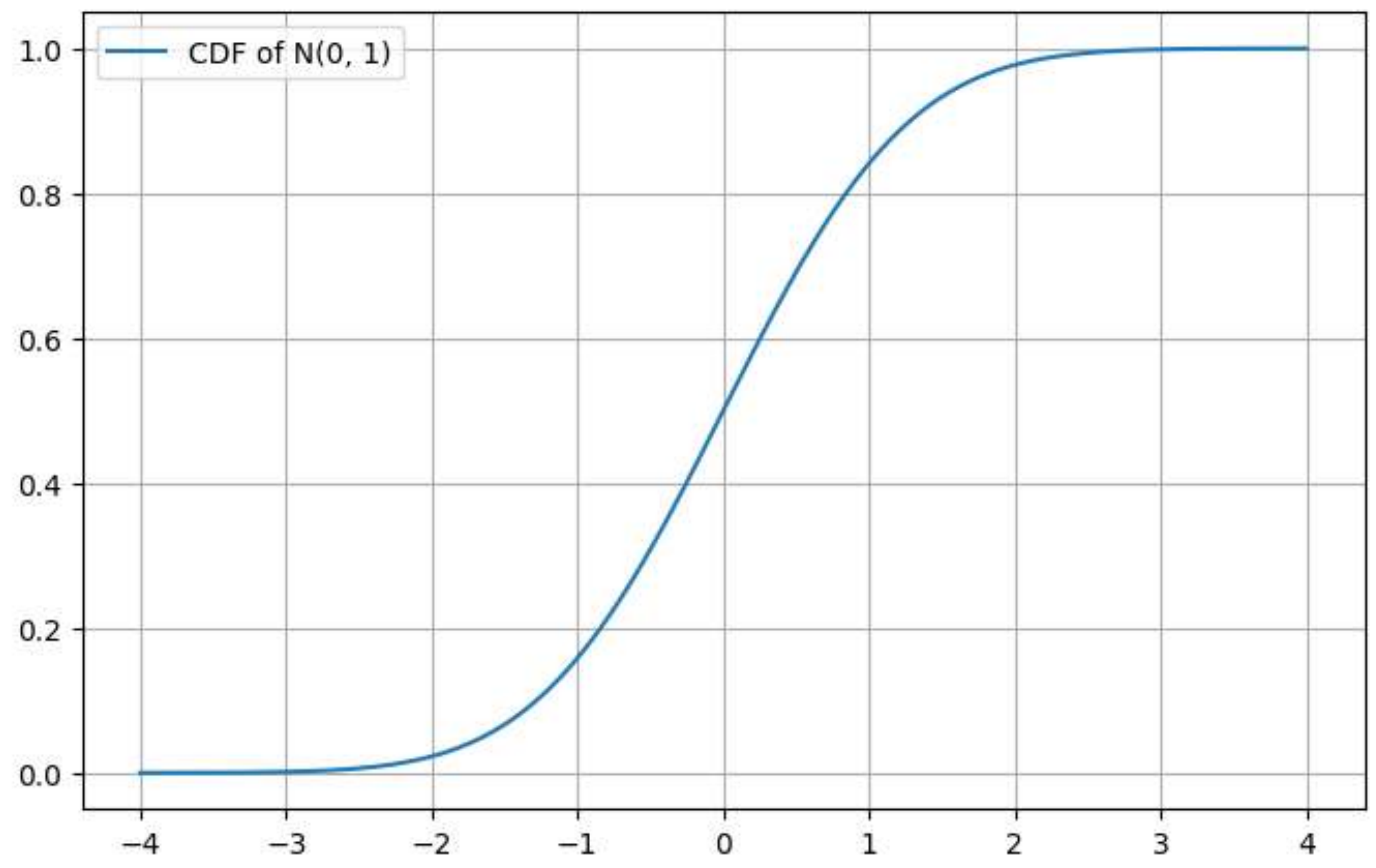

Lee et al. 2020

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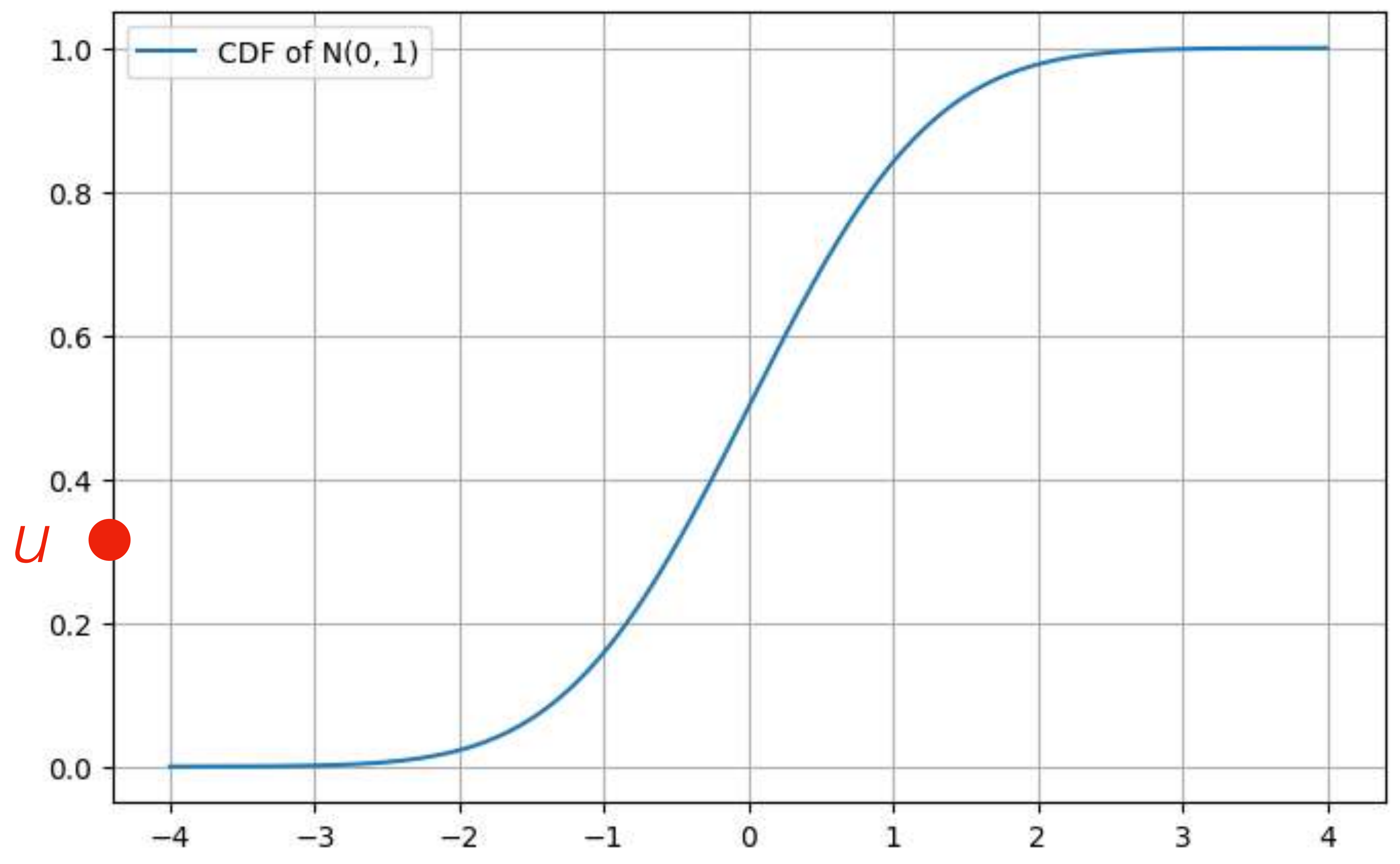

Lee et al. 2020

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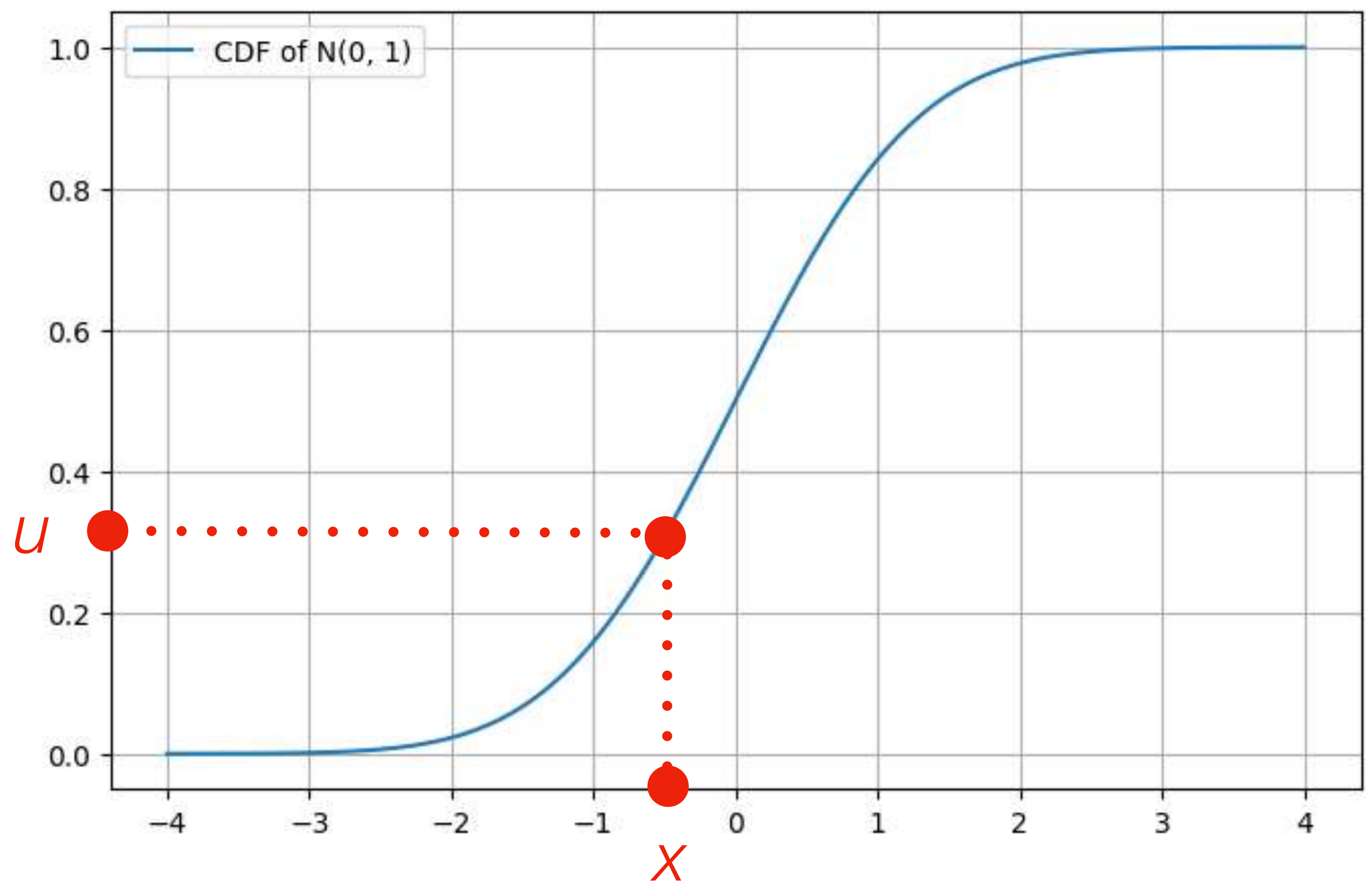

Lee et al. 2020

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Inverse transform sampling

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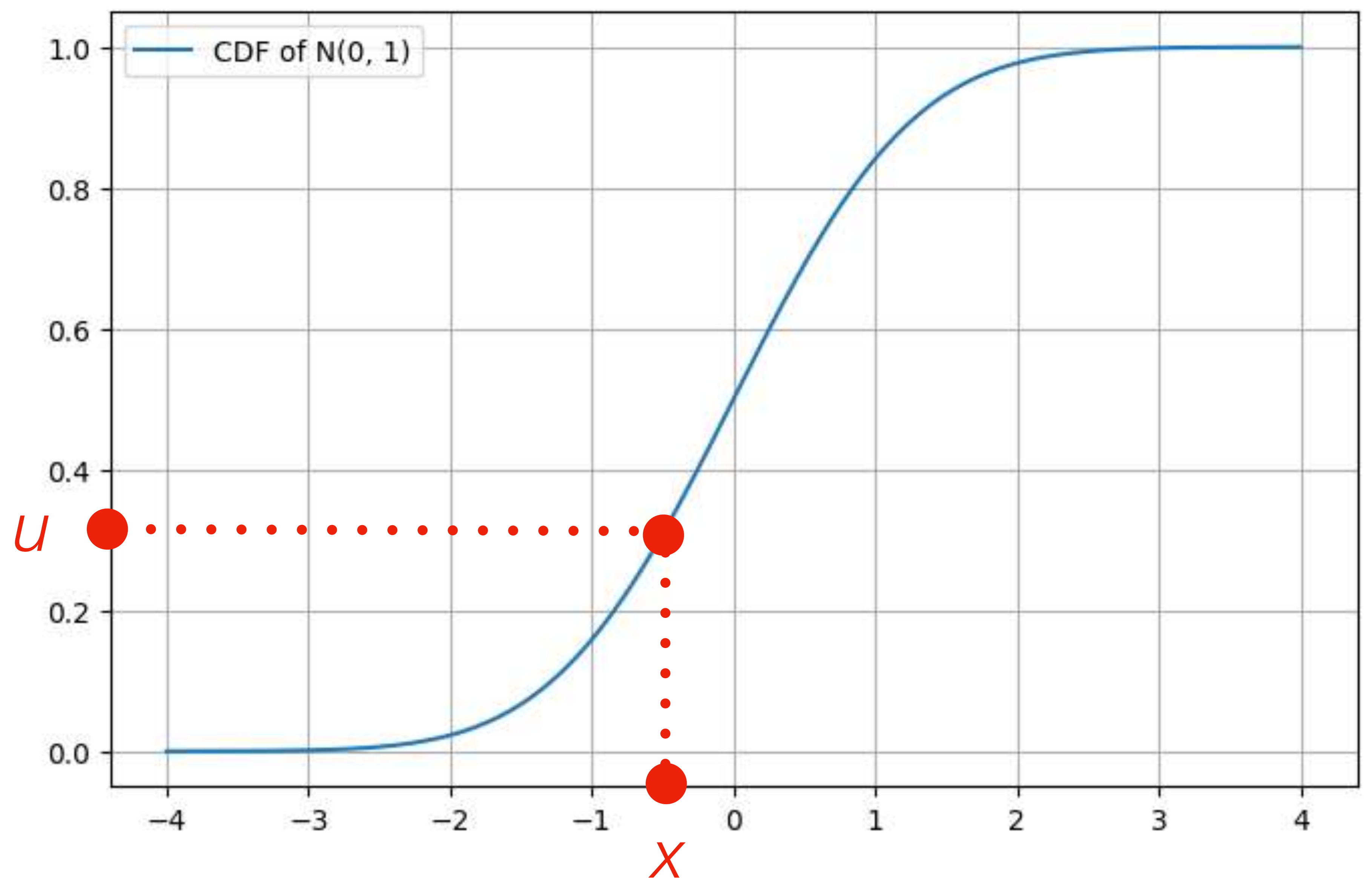
Uniform measure over parameters

- Group set of parameters with same domain names
- Compute the sizes with the Lesbegue measure λ over $[0, 1]$
- Sum all the results

$$\rho(r) = \left(\sum_{K \subset \textit{Str}} \bigotimes_{\alpha \in K} \lambda \right)(r)$$



Lee et al. 2020

Density semantics

functions

statement

random element

score

$$(\!| s |\!)_{\gamma}^{\phi}\,(r) : \Gamma \times \mathbb{R}^{+}$$

updated environment

environment

Density semantics

$$(\!|s|\!)_{\gamma}^{\phi}(r) : \Gamma \times \mathbb{R}^{+}$$

- statement: s
- functions: ϕ
- random element: r
- score: $\mathbb{R}^{+}$
- environment: γ
- updated environment: Γ

Example:

$$[\![x = \texttt{sample}(\mathcal{N}(0,1), \texttt{x})]\!]_{\emptyset}^{\emptyset}(r) = [x \leftarrow \textit{icdf}(r(\texttt{x}))], 1$$

Density semantics

functions

statement — random element — score

$$(\!|s|\!)_\gamma^\phi\,(r) : \Gamma \times \mathbb{R}^+$$

environment — updated environment

Example:

$$[\![x\ \texttt{=}\ \texttt{sample}(\mathcal{N}(0,1), \texttt{x})]\!]_\emptyset^\emptyset\,(r) = [x \leftarrow \textit{icdf}(r(\texttt{x}))], 1$$

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Density semantics

$$
\begin{aligned}
(\!|c|\!)_\gamma^\phi &= c \\
(\!|x|\!)_\gamma^\phi &= \gamma(x) \\
(\!|\mathit{op}(e)|\!)_\gamma^\phi &= \mathit{op}((\!|e|\!)_\gamma^\phi) \\
(\!|(e_1, e_2)|\!)_\gamma^\phi &= \left((\!|e_1|\!)_\gamma^\phi, (\!|e_2|\!)_\gamma^\phi\right)
\end{aligned}
$$

$$
\begin{aligned}
(\!|\texttt{pass}|\!)_\gamma^\phi(r) &= (\gamma, 1) \\
(\!|\texttt{if}\ e\texttt{:}\ s_1\ \texttt{else:}\ s_2|\!)_\gamma^\phi(r) &= (\!|s_1|\!)_\gamma^\phi(r)\ \textit{si}\ (\!|e|\!)_\gamma^\phi\ \textit{sinon}\ (\!|s_2|\!)_\gamma^\phi(r) \\
(\!|s_1\texttt{;}\ s_2|\!)_\gamma^\phi(r) &= (\gamma_2, W_1 \cdot W_2)\ \textit{avec}\ (\gamma_1, W_1) = (\!|s_1|\!)_\gamma^\phi(r) \\
&\qquad \textit{et}\ (\gamma_2, W_2) = (\!|s_2|\!)_{\gamma_1}^\phi(r)
\end{aligned}
$$

$$
\begin{aligned}
(\!|x\ \texttt{=}\ e|\!)_\gamma^\phi(r) &= \left(\gamma + \left[x \leftarrow (\!|e|\!)_\gamma^\phi\right], 1\right) \\
(\!|x\ \texttt{=}\ \texttt{sample}(e, \mathit{name})|\!)_\gamma^\phi(r) &= \left(\gamma + \left[x \leftarrow \mathit{icdf}\left((\!|e|\!)_\gamma^\phi, r(\mathit{name})\right)\right], 1\right) \\
(\!|x\ \texttt{=}\ f(e)|\!)_\gamma^\phi(r) &= (\gamma + [x \leftarrow v], W) \quad \textit{avec}\ v, W = \phi(f)((\!|e|\!)_\gamma^\phi)(r)
\end{aligned}
$$

$$
(\!|\texttt{factor}(e)|\!)_\gamma^\phi(r) = \left(\gamma, (\!|e|\!)_\gamma^\phi\right)
$$

Example: my Gaussian

```
def my_gaussian(mu: float, sigma: float) → float:
    x = sample(Gaussian(mu, sigma))
    return x
```

$$\phi(\texttt{my\_gaussian})(\mu, \sigma)(r) = \mathit{icdf}(\mathcal{N}(\mu, \sigma), r(\texttt{x})), 1$$

$$\begin{aligned}\mu(U) &= \int_0^1 1\ \delta_{\mathit{icdf}(\mathcal{N}(\mu,\sigma),r_x)}(U)\ dr_x \\ &= \int \mathcal{N}(\mu, \sigma)(dv)\ \delta_v(U) \qquad \text{avec } v = \mathit{icdf}(\mathcal{N}(\mu, \sigma), r_x) \\ &= \mathcal{N}(\mu, \sigma)(U)\end{aligned}$$

Semantics equivalence

Theorem. *For a statement* s*, the density semantics of* s *is the density of the measure defined by the kernel semantics.*

$$[\![\mathsf{s}]\!]^{\phi}_{\gamma}(U) = \int \rho(dr) W_{\mathsf{s}}(r) \delta_{\gamma_{\mathsf{s}}(r)}(U) \qquad \textit{où } \gamma_{\mathsf{s}}(r), W_{\mathsf{s}}(r) = (\!| \mathsf{s} |\!)^{\phi}_{\gamma}(r)$$

Proof. By induction... (see notes) □

Semantics equivalence

Theorem. *For a statement* s*, the density semantics of* s *is the density of the measure defined by the kernel semantics.*

$$[\![\mathsf{s}]\!]^{\phi}_{\gamma}(U) = \int \rho(dr) W_{\mathsf{s}}(r) \delta_{\gamma_{\mathsf{s}}(r)}(U) \qquad \text{où } \gamma_{\mathsf{s}}(r), W_{\mathsf{s}}(r) = (\!|\mathsf{s}|\!)^{\phi}_{\gamma}(r)$$

Proof. By induction... (see notes) □

The kernel and density semantics define the same object

Takeaway

For a given inference algorithm, how to implement `sample`, `assume`, `factor`, `observe`, and `infer`?

I - Approximate inference

- Importance sampling: weighted sampler returns pairs (value, score)
- Metropolis-Hastings: generate samples using a Markov chain over executions

II - Labs: Introduction to Sequential Monte Carlo methods

- State-space models for modeling time series
- Particle filtering with resampling

III - Density semantics

- Weighted samplers: operational semantics for approximate inference
- Measures on oracles: uniform measure and inverse transform sampling

References

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