Probabilistic Programming Languages

Build Your Owl PPL

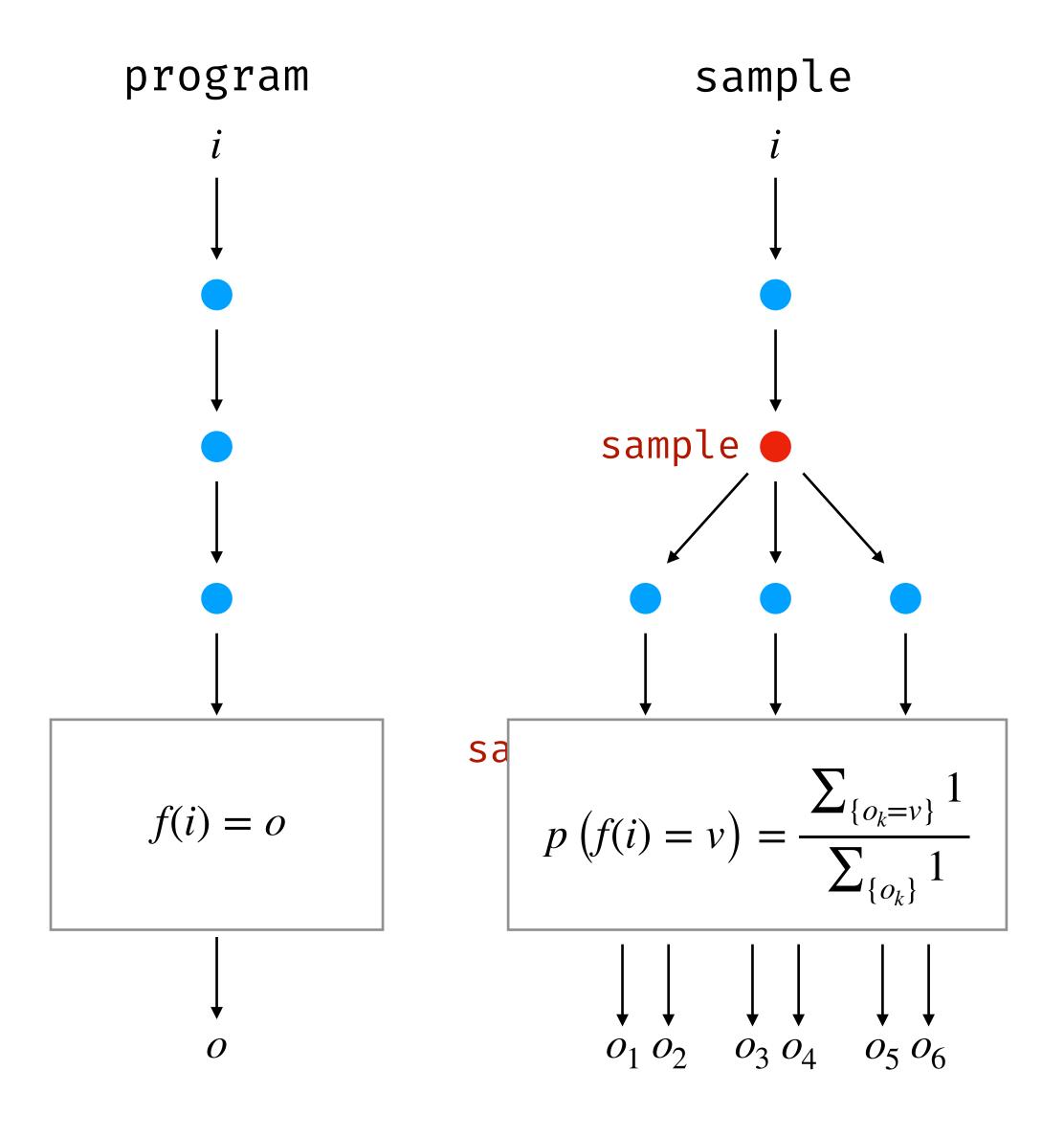
Guillaume Baudart

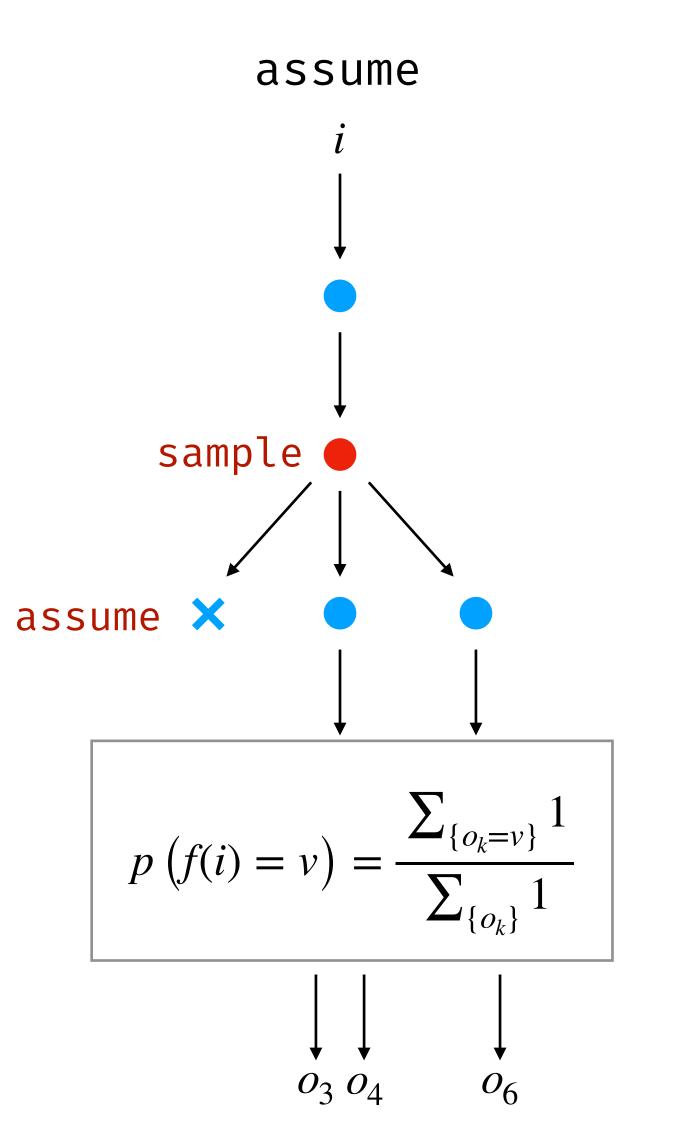
MPRI 2023-2024

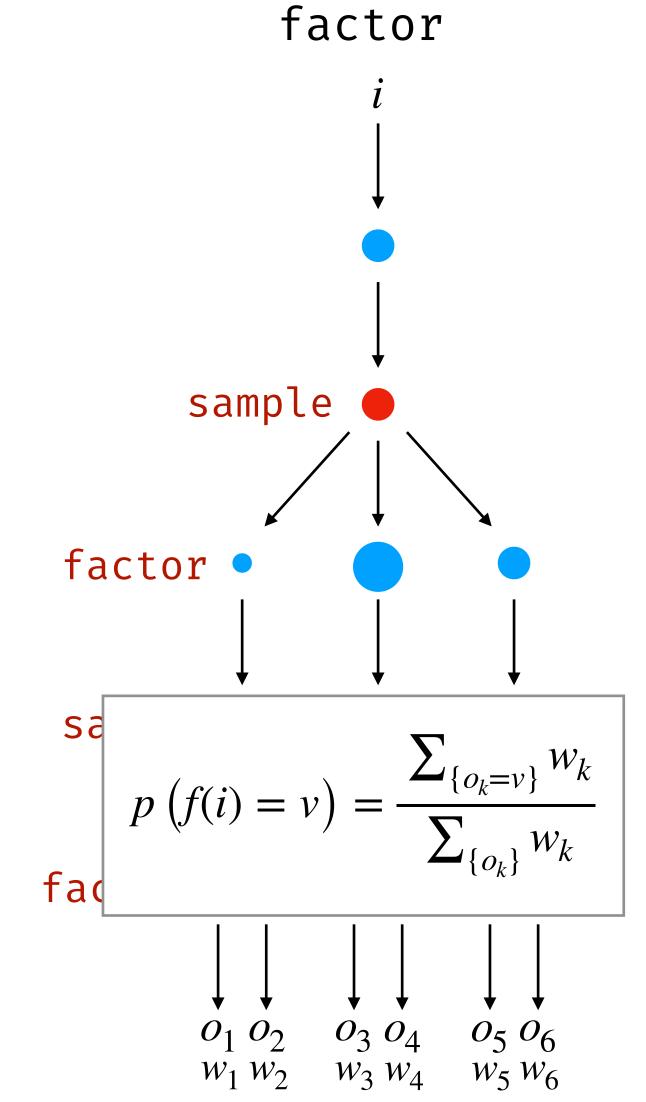
Reminders

BYO-PPL

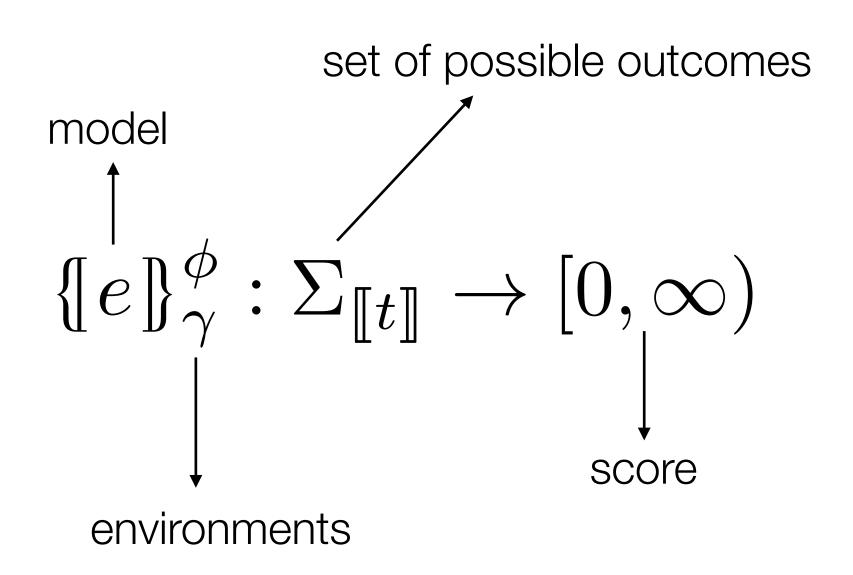
infer : $(\alpha \rightarrow \beta) \rightarrow \alpha \rightarrow \beta$ dist







Semantics: (un)normalized measures



Exercises

Prove the following properties

```
sample mu (* where mu is defined on [a, b] *)
  \equiv
  let x = sample (uniform (a, b)) in
  let () = observe (mu, x) in
  X
observe (mu, x) (* where mu is a discrete distribution *)
  \equiv
  let y = sample mu in
  assume x = y
sample (bernoulli (0.5))
  \equiv
  let x = sample (gaussian (0., 1.)) in
```

Build Your Owl PPL

BYO-PPL

Outline

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

- I Problem with basic inference
- Curse of dimensionality
- Resampling and checkpoints
- II Continuation Passing Style (CPS) models
- III Revisiting inference with CPS programming
- Sample generation
- Importance sampling
- Particle filter
- IV Inference formalization
- Weighted samplers
- Big-step semantics with checkpoints

HMM: Hidden Markov Model

Track the position of an agent from noisy observations

- The current position should not be too far from the previous position
- The observations should not be too far from the current position

Probabilistic model: $\forall t \in \mathbb{N}$

- $x_t \sim \mathcal{N}(x_{t-1}, \text{speed})$
- $y_t \sim \mathcal{N}(x_t, \textit{noise})$

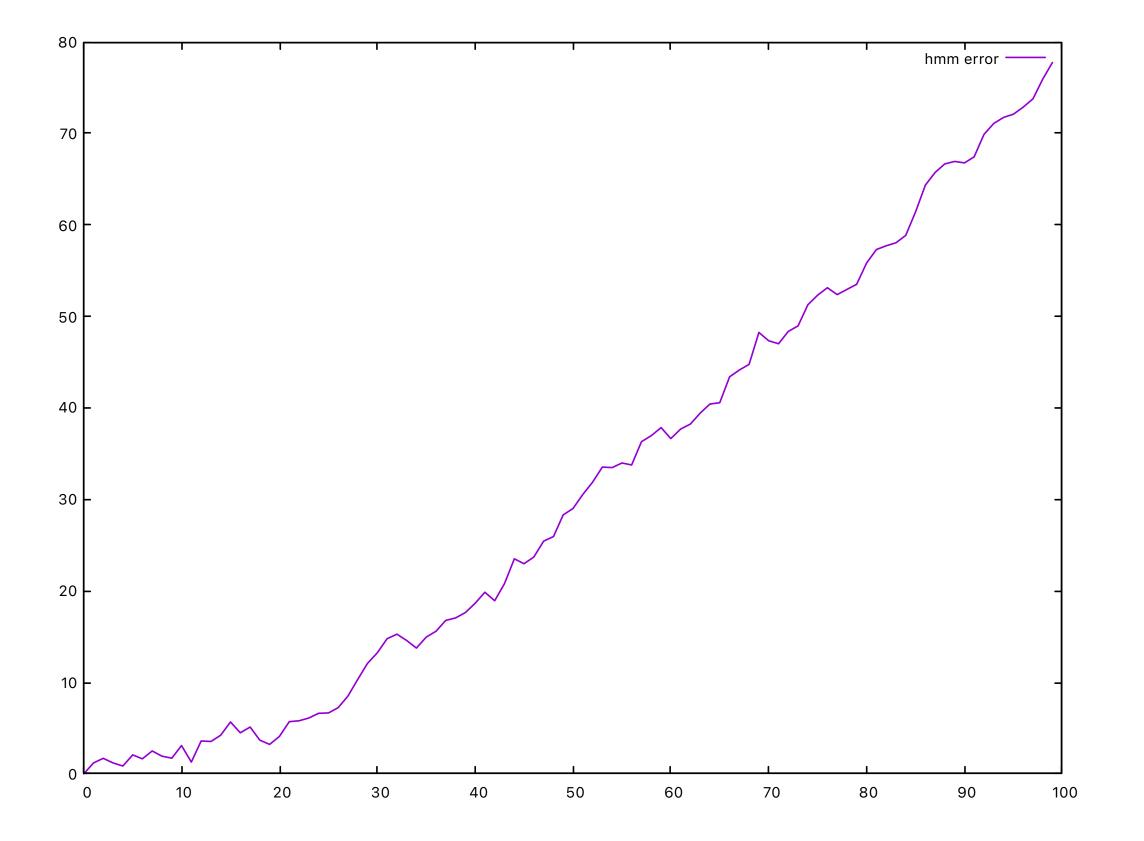
HMM: Hidden Markov Model

```
open Basic.Importance_sampling
let hmm prob data =
  let rec gen states data =
    match (states, data) with
    [], y :: data \rightarrow gen [y] data
    \mid states, [] \rightarrow states
      pre_x :: _, y :: data \rightarrow
        let x = sample prob (gaussian ~mu:pre_x ~sigma:1.0) in
        let () = observe prob (gaussian ~mu:x ~sigma:1.0) y in
        gen (x :: states) data
  in
  gen [] data
let =
  let data = Owl.Arr.linspace 0. 20. 20 > Owl.Arr.to_array > Array.to_list in
  let dist = Distribution.split_list (infer hmm data) in
  let m_x = List.rev (List.map Distribution.mean dist) in
  List.iter2 (Format.printf "%f >> %f@.") data m_x
```

HMM: Hidden Markov Model

> dune exec ./examples/hmm.exe

```
0.000000 >> 0.000000
1.052632 >> 0.278989
2.105263 >> 2.923428
3.157895 >> 2.812035
4.210526 >> 2.328341
5.263158 >> 1.742109
6.315789 >> 2.518105
7.368421 >> 3.958375
8.421053 >> 5.946233
9.473684 >> 7.329554
10.526316 >> 9.293653
11.578947 >> 10.181831
12.631579 >> 8.549409
13.684211 >> 9.323073
14.736842 >> 9.280692
15.789474 >> 9.352218
```

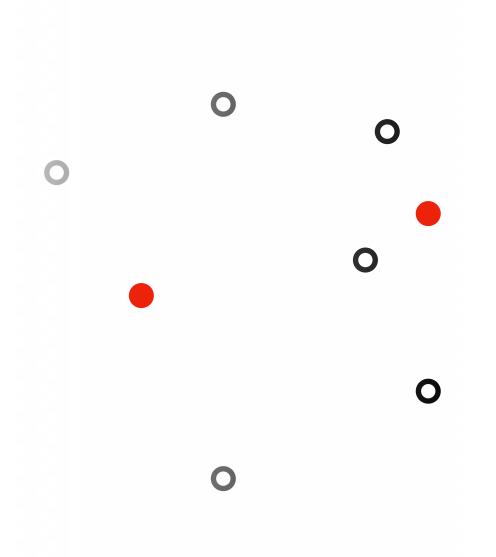


Problem:

- Each particle does a random walk and compute a score
- No re-calibration based on observations
- Score decreases at each factor statement

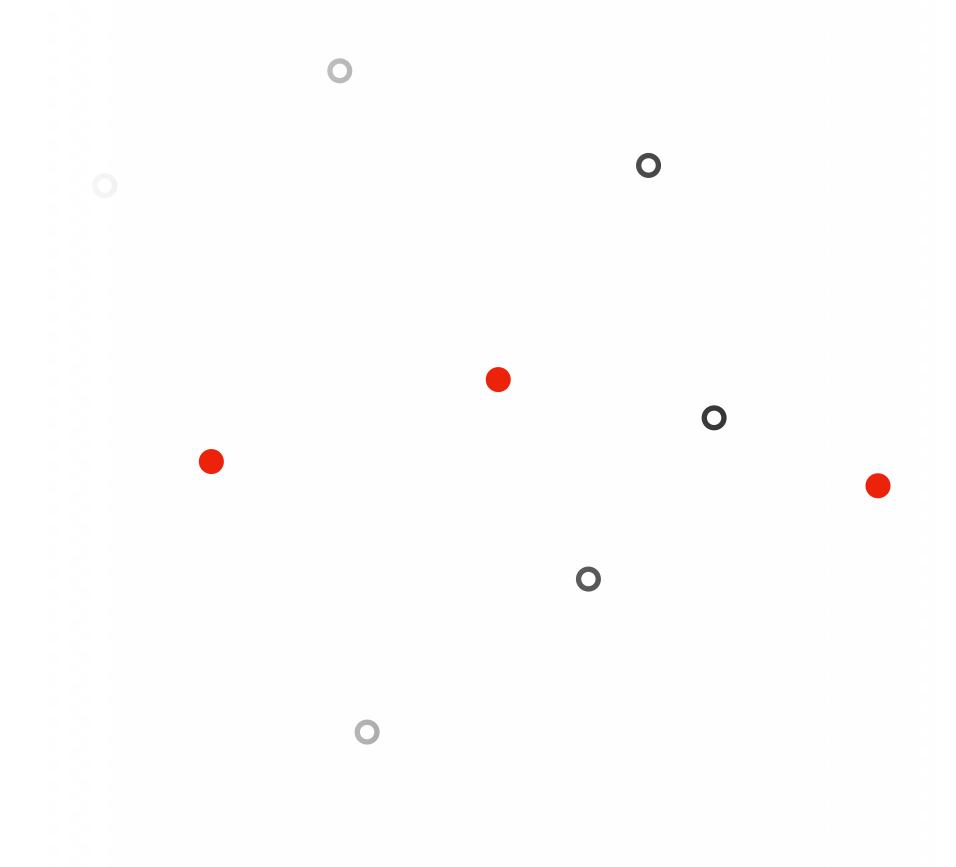
Problem:

- Each particle does a random walk and compute a score
- No re-calibration based on observations
- Score decreases at each factor statement



Problem:

- Each particle does a random walk and compute a score
- No re-calibration based on observations
- Score decreases at each factor statement



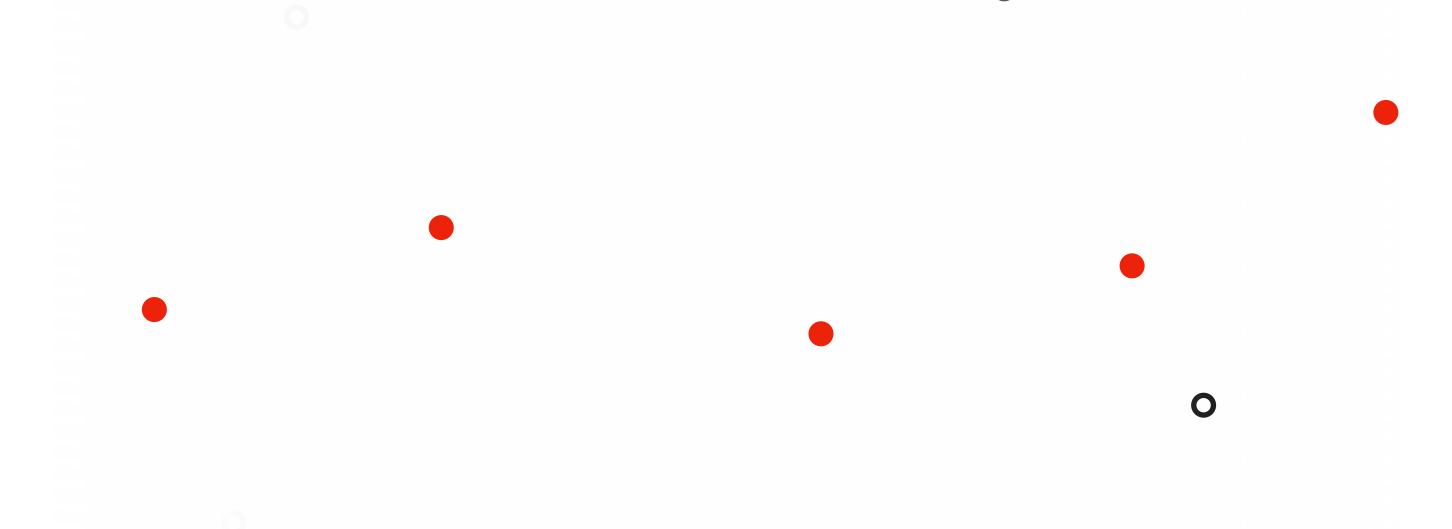
Problem:

- Each particle does a random walk and compute a score
- No re-calibration based on observations
- Score decreases at each factor statement

0

Problem:

- Each particle does a random walk and compute a score
- No re-calibration based on observations
- Score decreases at each factor statement



Bad estimation

The curse of dimensionality

Problem becomes harder as the dimension increases

Basic inference: rejection sampling, importance sampling

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

How to mitigate this problem?

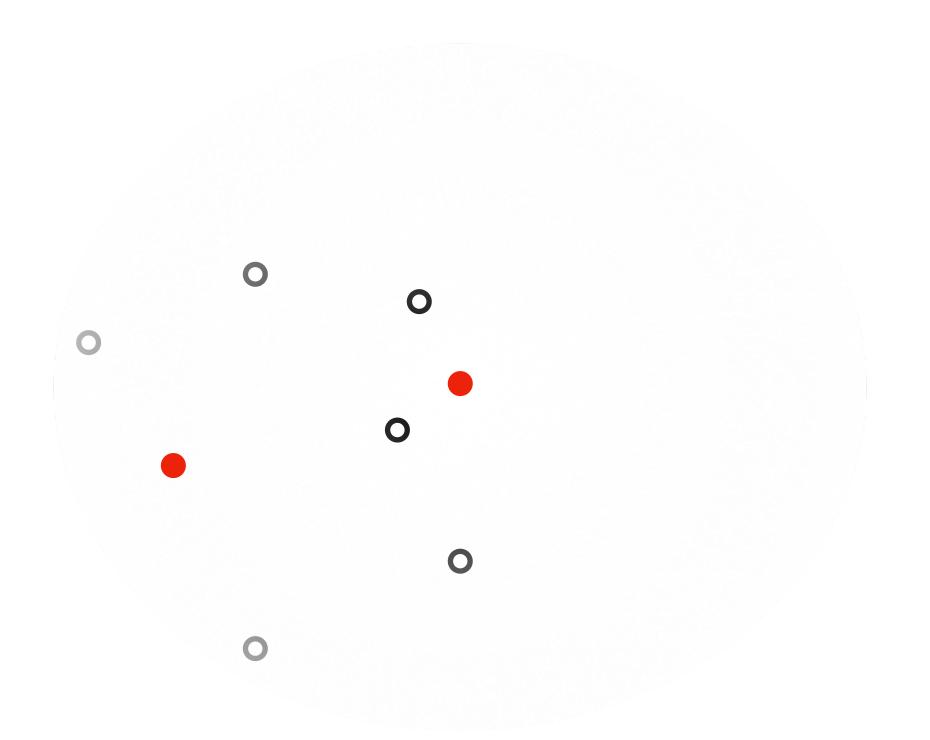
- Make assumptions about the posterior distributions
- Break the problem into simpler, smaller problems



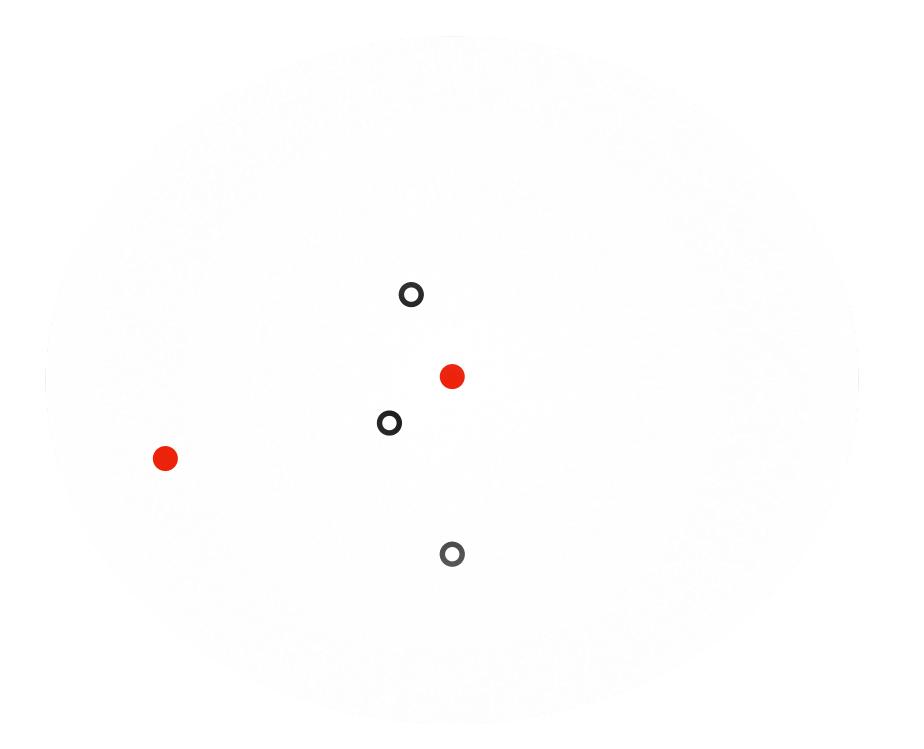
17h45mn

- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution

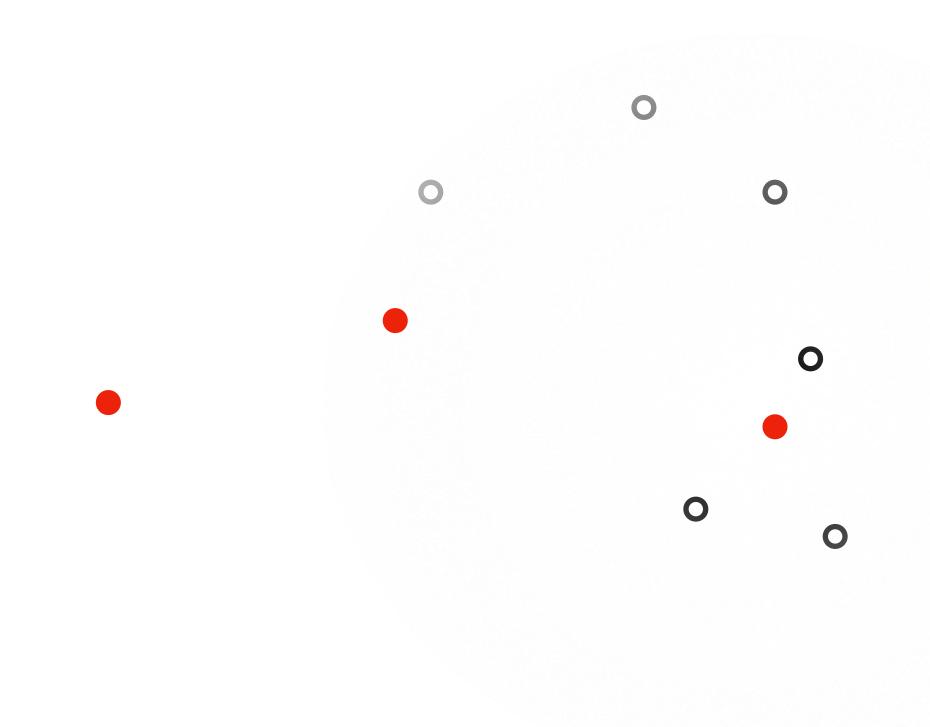
- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution



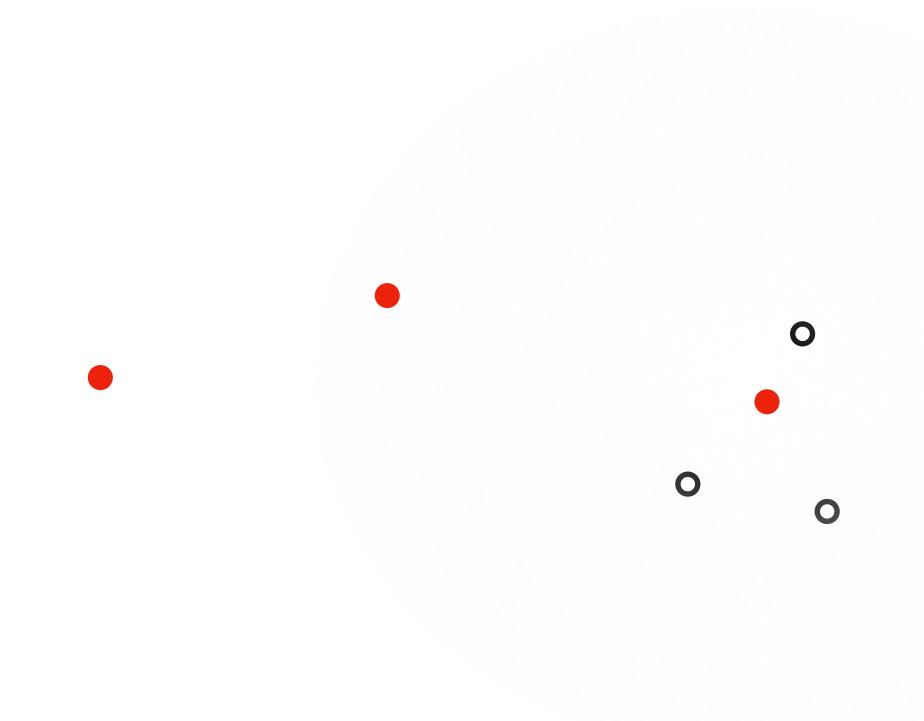
- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution



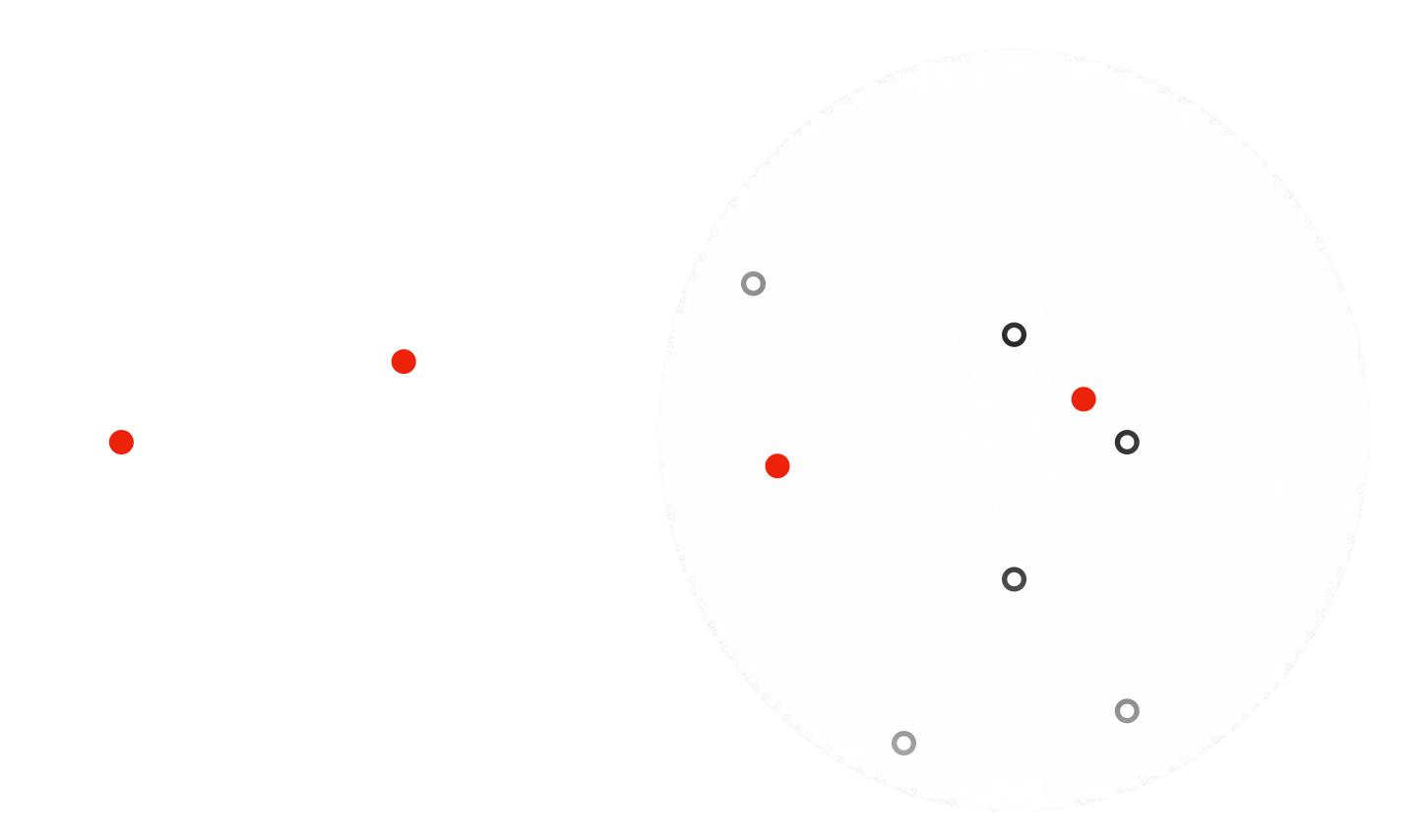
- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution



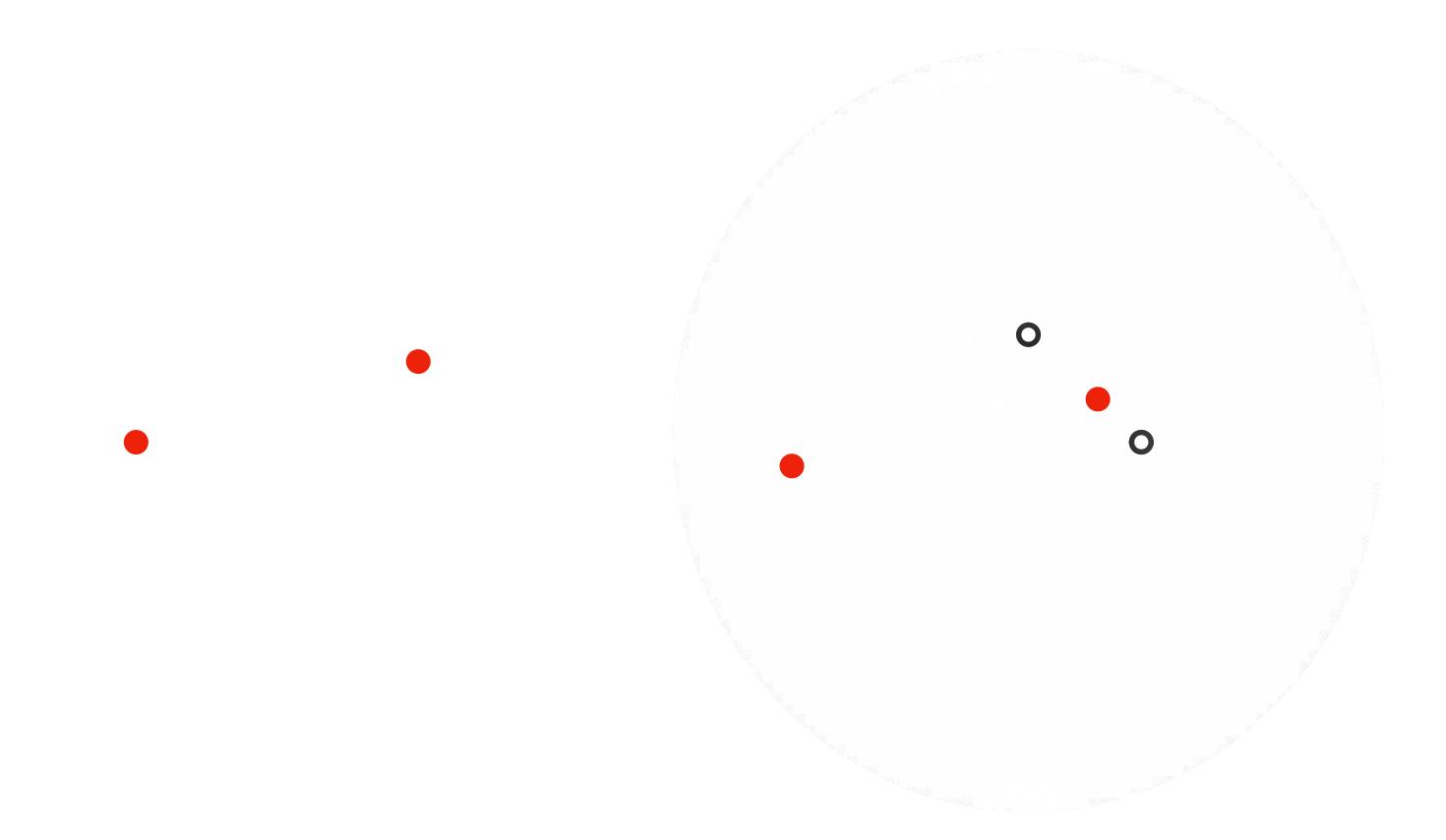
- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution



- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution

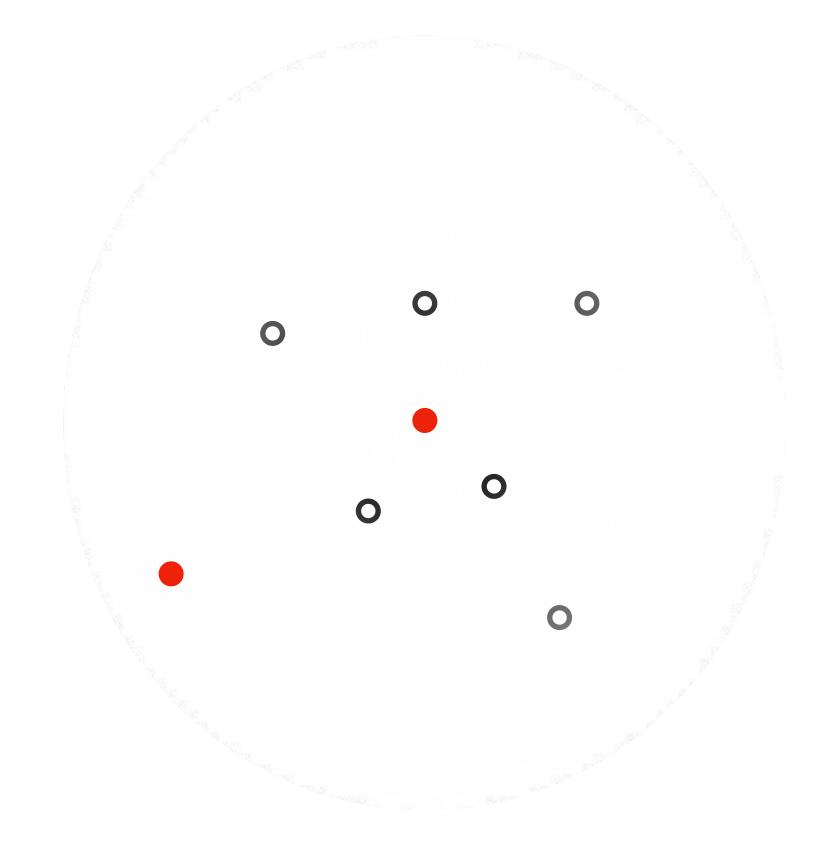


- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution



Add a resampling step

- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution



Better estimation

Problem: Duplications

How can we duplicate a particle during execution?

- Rerun the particle from the start?
- Force reuse sampled values?
- Clone the memory state?

Continuation Passing Style

- Functions take an extra argument k: the continuation
- k implements what should be done with the result of the function
- In our context, we can use continuation to interrupt/restart the execution of a model

Continuation Passing Style (CPS)

BYO-PPL

Reminders: CPS

```
let rec tree_height t =
  match t with
  | Empty → 0
  | Node (_, l, r) → 1 + max (tree_height l) (tree_height r)
```

tree.ml

Reminders: CPS

```
let rec tree_height t =
  match t with
  | Empty → 0
  | Node (_, l, r) → 1 + max (tree_height l) (tree_height r)
```

```
let rec tree_height t =
  match t with
  | Empty → 0
  | Node (_, l, r) →
  let hl = tree_height l in
  let hr = tree_heigh r in
  (1 + max hl hr)
```

1. Add intermediate values

tree.ml

Reminders: CPS

```
let rec tree_height t =
  match t with
  | Empty → 0
  | Node (_, l, r) → 1 + max (tree_height l) (tree_height r)
```

```
let rec tree_height t k =
  match t with
  | Empty → k 0
  | Node (_, l, r) →
   let hl = tree_height l in
  let hr = tree_heigh r in
  k (1 + max hl hr)
```

- 1. Add intermediate values
- 2. Add call to continuation

tree.ml

Reminders: CPS

```
let rec tree_height t =
  match t with
  | Empty → 0
  | Node (_, l, r) → 1 + max (tree_height l) (tree_height r)
```

```
let rec tree_height t k =
  match t with
  | Empty → k 0
  | Node (_, l, r) →
    tree_height l (fun hl →
        tree_heigh r (fun hr →
        k (1 + max hl hr)))
```

- 1. Add intermediate values
- 2. Add call to continuation
- 3. Turn let/in into nested function call

funny_bernoulli.ml

Funny bernoulli CPS

```
let funny_bernoulli () =
  let a = sample (bernoulli ~p:0.5) in
  let b = sample (bernoulli ~p:0.5) in
  let c = sample (bernoulli ~p:0.5) in
  let () = assume (a = 1 || b = 1) in
  a + b + c
```

- 1. Add intermediate values
- 2. Add call to continuation
- 3. Turn let/in into nested function call

Funny bernoulli CPS

```
let funny_bernoulli () =
  let a = sample (bernoulli ~p:0.5) in
  let b = sample (bernoulli ~p:0.5) in
  let c = sample (bernoulli ~p:0.5) in
  let () = assume (a = 1 || b = 1) in
  a + b + c
```

```
let funny_bernoulli () k = sample (bernoulli \sim p:0.5) (fun a \rightarrow sample (bernoulli \sim p:0.5) (fun b \rightarrow sample (bernoulli \sim p:0.5) (fun c \rightarrow assume (a = 1 || b = 1) (fun () \rightarrow k (a + b + c)))
```

- 1. Add intermediate values
- 2. Add call to continuation
- 3. Turn let/in into nested function call

cps_operators.ml

CPS monadic operators

CPS monadic operators

```
let return e k = k e  \text{let (let*) e f k = e (fun x \rightarrow f x k) (* let* x = e in f(x) *) }
```

```
let funny_bernoulli () k = sample (bernoulli \sim p:0.5) (fun a \rightarrow sample (bernoulli \sim p:0.5) (fun b \rightarrow sample (bernoulli \sim p:0.5) (fun c \rightarrow assume (a = 1 || b = 1) (fun () \rightarrow k (a + b + c)))
```

```
let funny_bernoulli () =
  let* a = sample (bernoulli ~p:0.5) in
  let* b = sample (bernoulli ~p:0.5) in
  let* c = sample (bernoulli ~p:0.5) in
  let* () = assume (a = 1 || b = 1) in
  return (a + b + c)
```

Sample generation (CPS)

BYO-PPL

infer.ml

CPS models

```
module Gen : sig
  type 'a prob
  and 'a next = 'a prob → 'a prob
  and ('a, 'b) model = 'a → ('b → 'b next) → 'b next

val sample : 'a Distribution.t → ('a → 'b next) → 'b next
  val factor : float → (unit → 'b next) → 'b next
  val draw: ('a, 'b) model → 'a → 'b
end = struct ... end
```

Type 'a prob

- Store all information required for inference (e.g., particles array)
- Type ('a, 'b) model capture input/output types

Models where probabilistic constructs are CPS functions

- Two arguments: input 'a and a continuation on the return value ('b \rightarrow 'b next).
- The return value is a continuation 'a next that updates a probabilistic state of type 'a prob.

Sample generation

```
let model data =
  let x = sample ... in
  let () = factor ... in
  output
       exit
           0
```

Sample generation

```
module Gen = struct
  type 'a prob = 'a option
  and 'a next = 'a prob \rightarrow 'a prob
  and ('a, 'b) model = 'a \rightarrow ('b \rightarrow 'b next) \rightarrow 'b next
  let exit v _prob = Some v
  let sample d k prob =
    let v = Distribution.draw d in
    k v prob
  let factor _s k prob = k () prob
  let draw m data =
    let v = (m data) exit None in
    Option.get v
end
```

Funny bernoulli

```
open Infer.Gen
let funny_bernoulli () =
  let* a = sample (bernoulli ~p:0.5) in
  let* b = sample (bernoulli ~p:0.5) in
  let* c = sample (bernoulli ~p:0.5) in
  let* () = assume (a = 1 || b = 1) in
  return (a + b + c)
let _ =
  for _ = 1 to 10 do
    let v = draw funny_bernoulli () in
    Format.printf "%d " v
  done
```

```
    dune exec ./examples/funny_bernoulli.exe
1 1 2 2 2 2 1 3 2
```

Importance sampling (CPS)

BYO-PPL

infer.ml

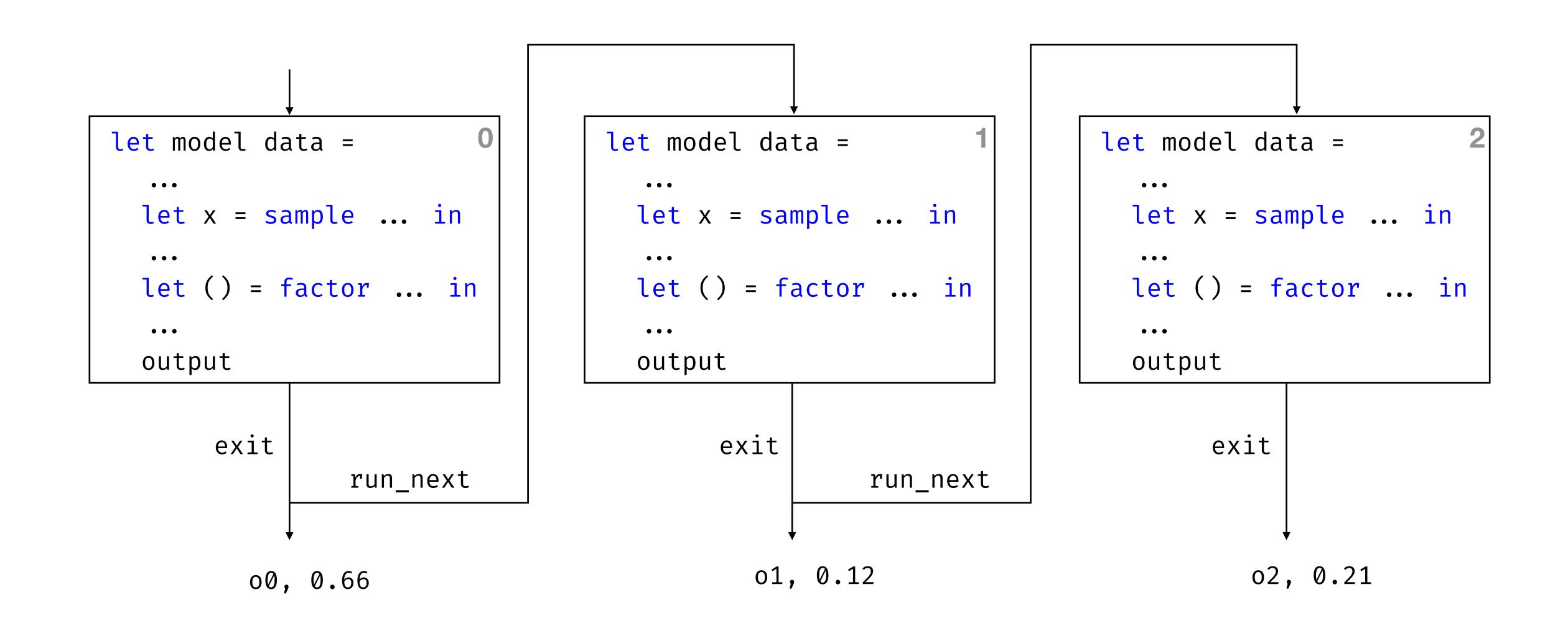
Importance sampling

```
module Importance_sampling : sig
  type 'a prob
  and 'a next = 'a prob → 'a prob
  and ('a, 'b) model = 'a → ('b → 'b next) → 'b next

val sample : 'a Distribution.t → ('a → 'b next) → 'b next
  val factor : float → (unit → 'b next) → 'b next
  val infer : ('a, 'b) model → '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



infer.ml

```
module Importance_sampling = struct
  type 'a prob = ...

let sample d k prob = assert false
  let factor s k prob = assert false

let infer ?(n = 1000) m data = assert false
end
```

infer.ml

```
module Importance_sampling = struct
  type 'a prob = { id : int; particles : 'a particle array }
  and 'a particle = { k : 'a next; value : 'a option; score : float }
  • • •
  let sample d k prob =
    let v = Distribution.draw d in
    k v prob
  let factor s k prob =
    let particle = prob.particles.(prob.id) in
    prob.particles.(prob.id) \leftarrow { particle with score = s +. particle.score };
    k() prob
end
```

```
module Importance_sampling = struct
  type 'a prob = { id : int; particles : 'a particle array }
  and 'a particle = { k : 'a next; value : 'a option; score : float }
  • • •
  let exit v prob =
    let particle = prob.particles.(prob.id) in
    prob.particles.(prob.id) \leftarrow { particle with value = Some v };
    prob
  let infer ?(n = 1000) model data =
    let particles = Array.make n { value = None; score = 0.; k = (model data) exit } in
    Array.iteri (fun i particle \rightarrow ignore (particle.k { id = i; particles })) particles;
    let values = Array.map (fun p \rightarrow Option.get p.value) particles in
    let logits = Array.map (fun p \rightarrow p.score) particles in
    Distribution.support ~values ~logits
end
```

Coin

```
open Infer.Importance_sampling

let coin x =
    let* z = sample (uniform ~a:0. ~b:1.) in
    let* () = Cps_list.iter (observe (bernoulli ~p:z)) x in
    return z

let _ =
    let dist = infer coin [1; 1; 0; 0; 0; 0; 0; 0; 0; 0] in
    let m, s = Distribution.stats dist in
    Format.printf "Coin bias, mean:%f, std:%f@." m s
```

```
} dune exec ./examples/coin.exe

Coin bias, mean:0.247876, std:0.118921

Beta(2+1, 8+1), mean:0.250000, std:0.120096
```

Particle filter (CPS)

BYO-PPL

Particle filter basic.ml

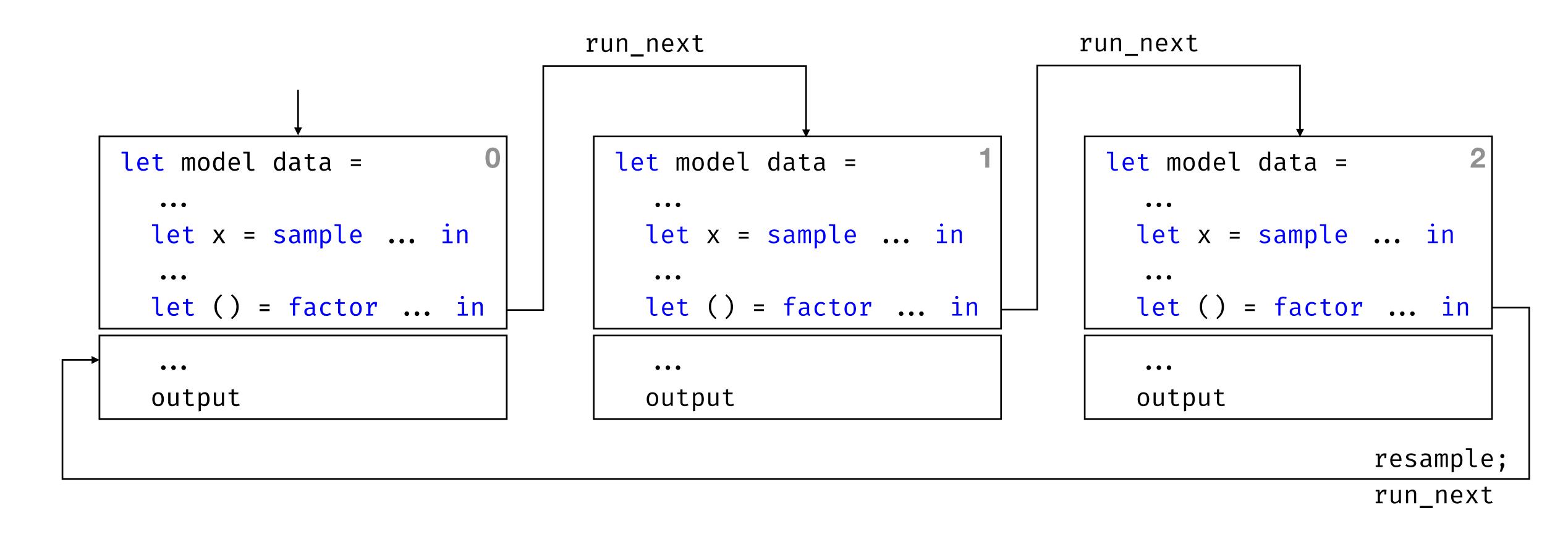
```
module Particle_filter = struct
  include Importance_sampling

let resample particles = assert false
  let factor s k prob = assert false
end
```

Inference algorithm: importance sampling, but...

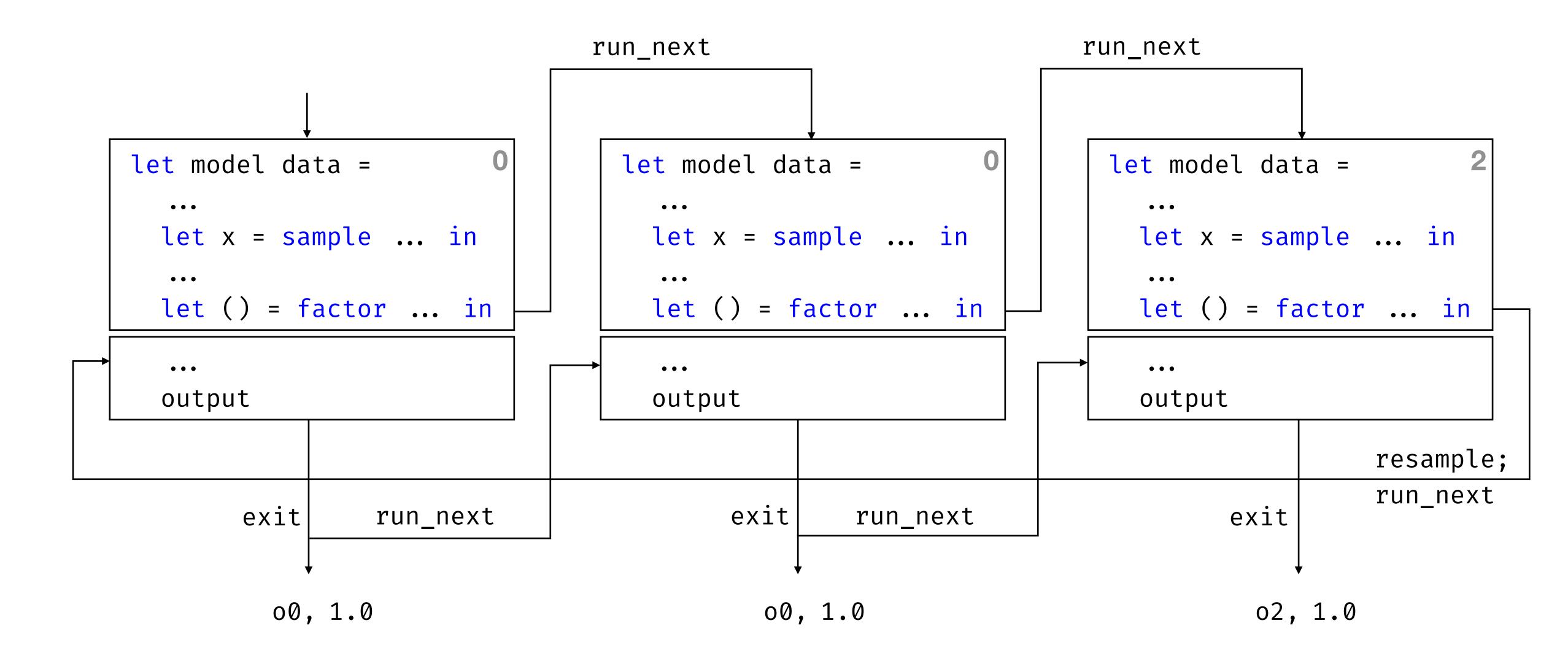
- Add a resampling step at each factor
- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution

Particle filter



0.66 0.12

Particle filter



Particle filter infer.ml

```
module Particle_filter = struct
  include Importance_sampling
  let resample particles =
    let logits = Array.map (fun x \rightarrow x.score) particles in
    let values = Array.map (fun x \rightarrow \{ x \text{ with score} = \emptyset. \}) particles in
    let dist = Distribution.support ~values ~logits in
    Array.iteri (fun i \_\rightarrow particles.(i) \leftarrow Distribution.draw dist) particles
  let factor s k prob =
    let particle = prob.particles.(prob.id) in
    prob.particles.(prob.id) \leftarrow { particle with k = k (); score = s +. particle.score };
    prob
end
```

Particle filter infer.ml

```
module Particle_filter = struct
  include Importance_sampling
   • • •
  let infer ?(n = 1000) model data =
    let particles = Array.make n { value = None; score = 0.; k = (model data) exit } in
    while Array.for_all (fun p \rightarrow Option.is_none p.value) particles do
      Array.iteri (fun i particle \rightarrow ignore (particle.k { id = i; particles })) particles;
      resample particles
    done;
    let values = Array.map (fun p \rightarrow Option.get p.value) particles in
    let logits = Array.map (fun p \rightarrow p.score) particles in
    Distribution.support ~values ~logits
end
```

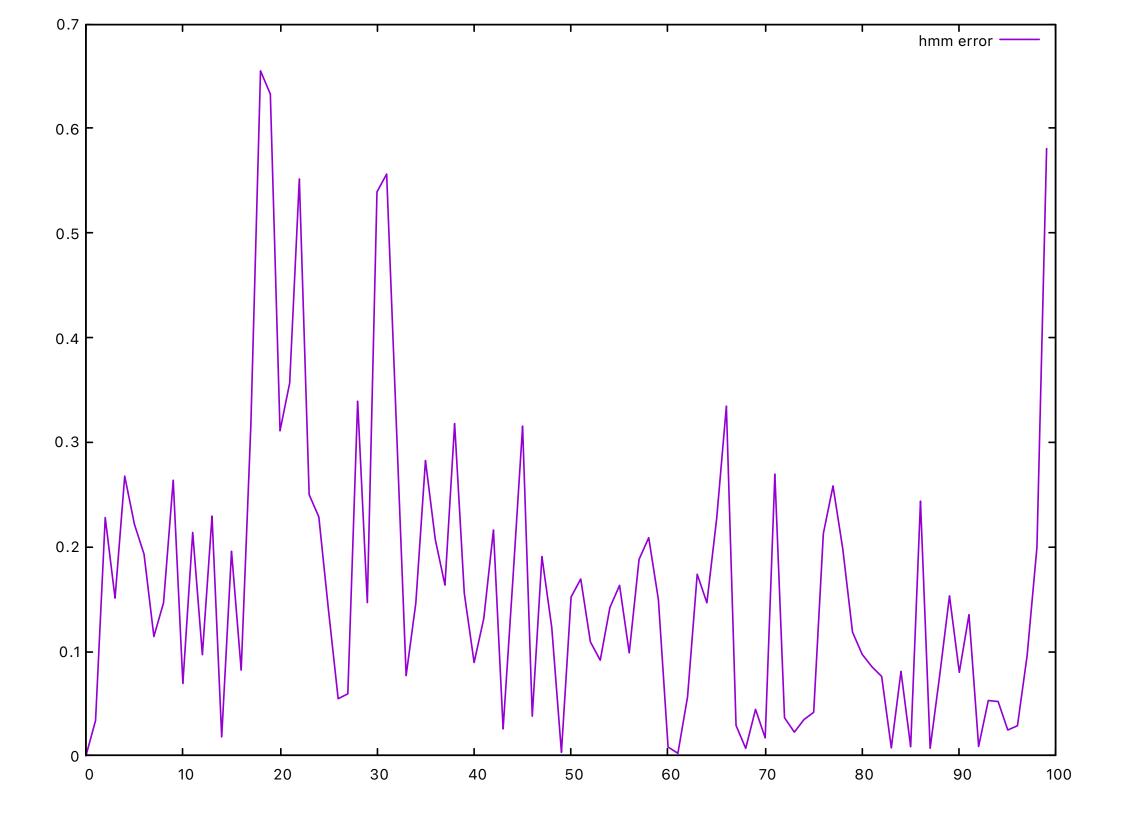
HMM: Hidden Markov Model

```
open Infer.Particle_filter
let hmm prob data =
  let rec gen states data =
    match (states, data) with
    [], y :: data \rightarrow gen [y] data
    | states, [] → return states
     pre_x :: _, y :: data \rightarrow
        let* x = sample prob (gaussian ~mu:pre_x ~sigma:1.0) in
        let* () = observe prob (gaussian ~mu:x ~sigma:1.0) y in
        gen (x :: states) data
  in
  gen [] data
let =
 let data = Owl.Arr.linspace 0. 20. 20 > Owl.Arr.to_array > Array.to_list in
  let dist = Distribution.split_list (infer ~n:100 hmm data) in
  let m_x = List.map Distribution.mean dist in
  List.iter2 (Format.printf "%f >> %f") data m_x
```

HMM: Hidden Markov Model

```
> dune exec ./hmm.exe
```

```
0.000000 >> 0.000000
1.052632 >> 0.997546
2.105263 >> 2.300316
3.157895 >> 3.289649
4.210526 >> 4.857555
5.263158 >> 4.907179
6.315789 >> 6.254198
7.368421 >> 7.208341
8.421053 >> 8.432642
9.473684 >> 8.938143
10.526316 >> 9.555007
11.578947 >> 11.098199
12.631579 >> 12.823460
13.684211 >> 13.701444
14.736842 >> 14.934314
15.789474 >> 16.115058
```



Exercises

What if the particles do not terminate at the same time?

```
let foo () =
  let* c = sample (bernoulli ~p:0.5) in
  if c = 1 then
    let* () = factor 1. in return c
  else
    return c

let _ =
  let dist = infer foo () in
  let { values; probs; _ } = get_support ~shrink:true dist in
  Array.iteri (fun i x → Format.printf "%d %f@." x probs.(i)) values
```

Exercises foo.m/

What if the particles do not terminate at the same time?

```
let foo () =
  let* c = sample (bernoulli ~p:0.5) in
  let* () = if c = 1 then factor 10. else skip in
  return c

let _ =
  let dist = infer foo () in
  let { values; probs; _ } = get_support ~shrink:true dist in
  Array.iteri (fun i x → Format.printf "%d %f@." x probs.(i)) values
```

```
dune exec ./examples/foo.exe
Fatal error: exception Invalid_argument("option is None")
```

Exercise: Enumeration (CPS)

BYO-PPL

Enumeration infer.ml

```
module : sig
  type 'a prob
  and 'a next = 'a prob → 'a prob
  and ('a, 'b) model = 'a → ('b → 'b next) → 'b next

val sample : 'a Distribution.t → ('a → 'b next) → 'b next
  val factor : float → (unit → 'b next) → 'b next
  val infer : ('a, 'b) model → 'a → 'b Distribution.t
end = struct... end
```

Inference algorithm: depth first exploration

- Maintain a continuation queue
- sample: pick one value (and score), push the other in the queue
- **factor**: update the score
- At the end of the model, store the pair (value, score), restart from the top of the queue

Inference comparison

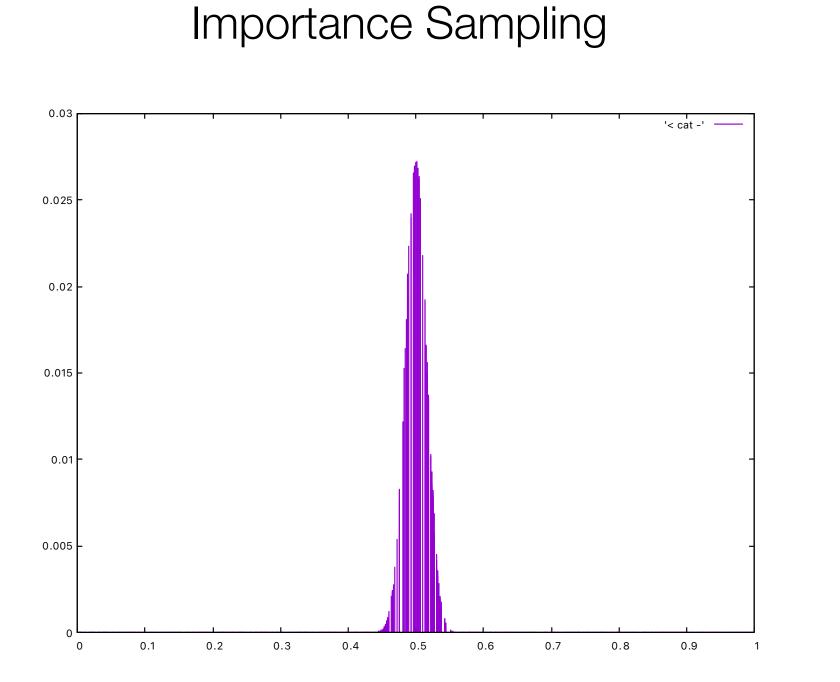
BYO-PPL

Coin

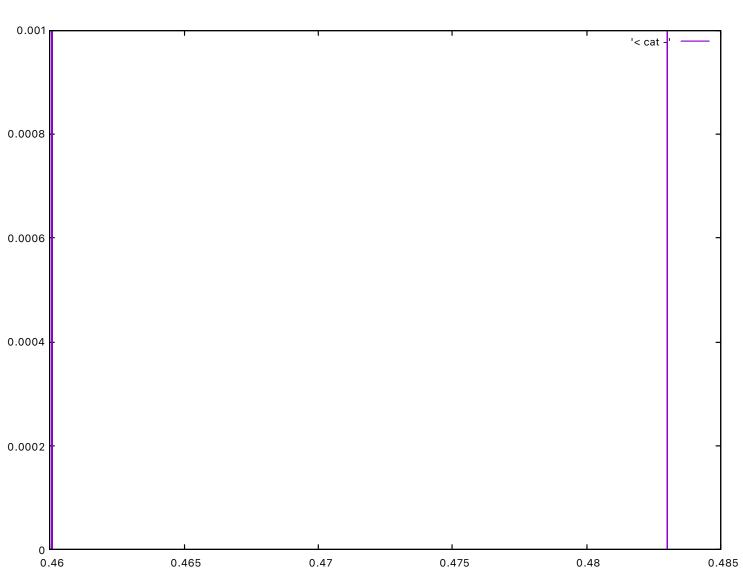
```
let _ =
  let data = List.init 1000 (fun i → i mod 2) in
  let dist = infer coin data in
  plot dist
```

Rejection Sampling

Very (very) slow!







Particle impoverishment

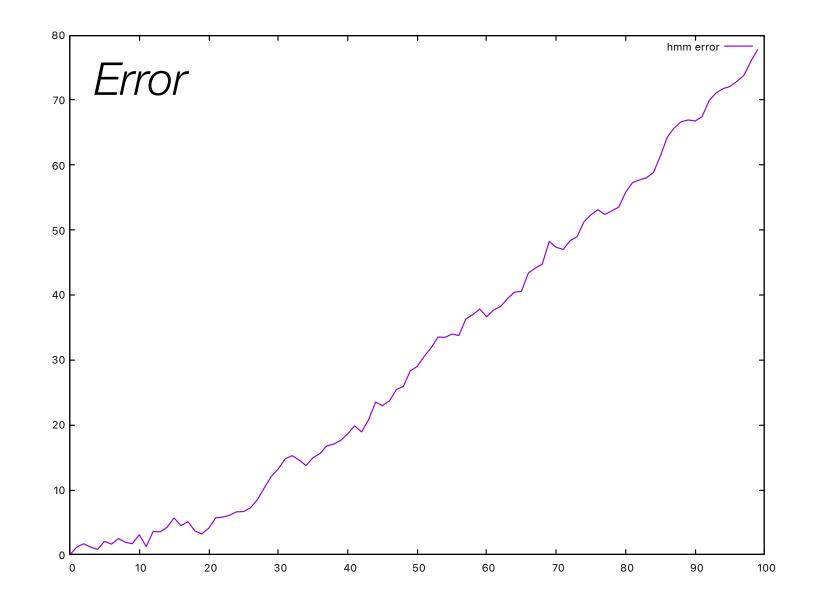
HMM

```
let _ =
  let data = Owl.Arr.linspace 0. 100. 100 ▷ Owl.Arr.to_array ▷ Array.to_list in
  let dist = Distribution.split_list (infer hmm data) in
  plot (error (List.rev dist) data)
```

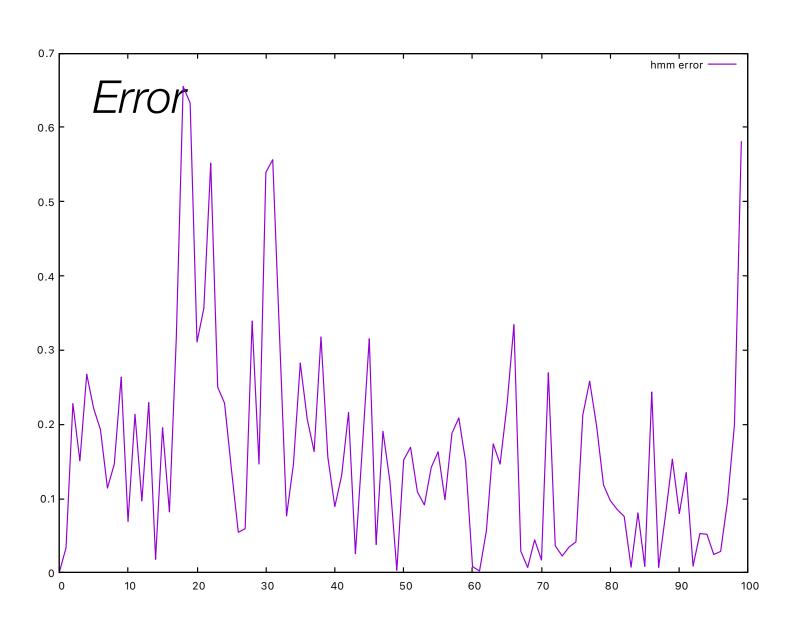
Rejection Sampling

Never terminate!

Importance Sampling



Particle Filter



Inference limitations

Rejection Sampling: Termination

- Only works if valid sample can be generated from the priors
- In practice: simple models with few discrete observations
- E.g., simple discrete models.

Importance Sampling: Weight collapse

- Score strictly decrease at each observation: eventually collapse
- In practice: continuous model to estimate fixed parameters from observations
- E.g., coin, linear regression

Particle Filter: Particle impoverishment

- Duplicate particle without resampling fixed parameter
- In practice: high-dimensional continuous models without fixed parameters
- E.g., hmm, tracker

Inference formalization

BYO-PPL

Sampler

Probabilistic semantics $G \vdash^P e : t$

- Expressions are interpreted as weighted samplers
- Draw random samples and track the execution weight
- Given an environment γ , $\{e\}_{\gamma} = v, w$
- $\blacksquare \quad \{e\}: \Gamma \to V \times [0, \infty)$

Combine weights

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
- Gather output values and score to approximate the posterior distribution

$$\begin{split} & \big[\!\![\text{infer}(e) \big]\!\!]_{\gamma} = \textit{let} \, \big[v_i, w_i = \{\!\!\{e\}\!\!\}_{\gamma} \big]_{1 \leq i \leq N} \, \textit{in} \\ & \textit{let} \, W = \sum_{i=1}^N w_i \, \textit{in} \\ & \lambda U. \, \sum_{i=1}^N \frac{w_i}{W} \times \delta_{v_i}(U) \end{split}$$

Particle filter

Inference algorithm: importance sampling, but...

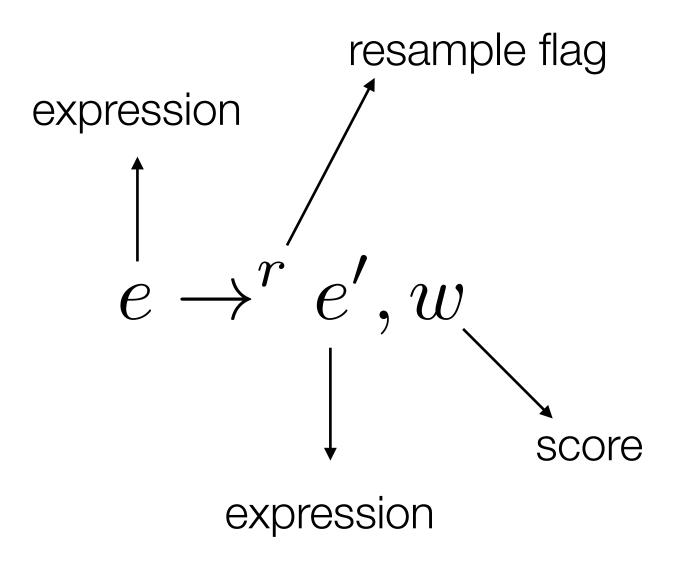
- Add a resampling step at each factor
- Compute the score of the particles to compute a distribution
- Re-sample a new set of particles from this distribution

Resampling

Checkpoints

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Big-step semantics with checkpoints



Reduction rules: stop evaluation when r is true

Big-step semantics with checkpoints

$$\frac{e \rightarrow^{\textit{false}} \textit{true}, 1 \qquad e_1 \rightarrow^r e_1', w_1}{\textit{if } e \textit{ then } e_1 \textit{ else } e_2 \rightarrow^r e_1', w_1} \qquad \qquad \frac{e \rightarrow^{\textit{false}} \textit{ false}, 1 \qquad e_2 \rightarrow^r e_2', w_2}{\textit{if } e \textit{ then } e_1 \textit{ else } e_2 \rightarrow^r e_2', w_2}$$

$$e o false$$
 false, 1 $e_2 o r$ e'_2, w_2 if e then e_1 else $e_2 o r$ e'_2, w_2

$$e_1 \rightarrow^{\textit{true}} e_1', w_1$$

$$e_1 \rightarrow^{\textit{true}} e_1 + w_1$$

$$e_1 \rightarrow^{\textit{true}} e_1 + w_1$$

$$e_2 \rightarrow^{\textit{true}} e_1' + w_1$$

$$\frac{e \rightarrow^{\textit{false}} \mu, 1}{\textit{sample}(e) \rightarrow^{\textit{true}} \textit{draw}(\mu), 1}$$

$$\frac{e_1 \rightarrow^{\textit{false}} v_1, w_1 \qquad e_2 \rightarrow^{r} e_2', w_2}{\text{let } x = e_1 \text{ in } e_2 \rightarrow^{r} e_2', w_1 \times w_2}$$
 Combine weights

$$\frac{e \rightarrow^{\textit{false}} s, 1}{\mathsf{factor}(e) \rightarrow^{\textit{true}} (), s}$$
 Stop!

Particle filter

$$[e_i \to^{r_i} e'_i, w_i]_{1 \le i \le N} \qquad \bigvee_{1 \le i \le N} r_i \qquad \rho = \operatorname{Cat}\left(\{e'_i, w_i\}_{1 \le i \le N}\right) \qquad [\operatorname{draw}(\rho)]_{1 \le i \le N} \Rightarrow \mu$$

 $[e_i]_{1 \le i \le N} \Rightarrow \mu$

Resampling

$$\frac{\left[e_i \to^{\textit{false}} v_i, w_i\right]_{1 \leq i \leq N}}{\left[e_i\right]_{1 \leq i \leq N} \Rightarrow \lambda U. \sum_{i=1}^{N} \frac{w_i}{W} \, \delta_{v_i}}$$
 Gather the results

$$\frac{[e]_{1 \le i \le N} \Rightarrow \mu}{e \Rightarrow^{N} \mu}$$

Launch N particles

References

WebPPL

Noah Goodman and Andreas Stuhlmüller http://webppl.org/

The Design and Implementation of Probabilistic Programming Languages

Noah Goodman and Andreas Stuhlmüller http://dippl.org/

An Introduction to Probabilistic Programming

Jan-Willem van de Meent, Brooks Paige, Hongseok Yang, Frank Wood https://arxiv.org/abs/1809.10756

Embedded probabilistic domain-specific language HANSEI

Oleg Kiselyov, Chung-chieh Shan https://okmij.org/ftp/kakuritu/Hansei.html

BYO-PPL

Build Your Own Probabilistic Language

- Clone the repo: git clone https://github.com/mpri-probprog/byo-ppl-22-23.git
- Install the dependencies: opam install . --deps-only
- Build the project: dune build
- Test an example: dune exec ./examples/funny_bernoulli.exe

Implemented as an OCaml embedded domain specific language (eDSL)

- Distribution: small library of probability distributions and basic statistical functions.
- Basic: basic inference algorithms (rejection sampling inference sampling)
- Infer: inference algorithms for models written in Continuation Passing Style (CPS).
- Cps_operators: syntactic sugar to write CPS style probabilistic models.
- Utils: missing utilities functions used in other modules.