Programs as probabilistic models

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Generative models?

aG8?PY



Can you write a program to do this?

Forward models are "easy"

2	1	4	7	3	9	6	5	8
6	8	5	1	4	2	9	3	7
9	7	З	8	5	6	2	4	1
4	9	8	6	1	З	5	7	2
5	2	7	9	8	4	3	1	6
З	6	1	2	7	5	4	8	9
8	5	6	4	2	7	1	9	3
7	4	2	3	9	1	8	6	5
1	3	9	5	6	8	7	2	4

Can you write a program to solve Sudoku problems?

Can you write a program to generate Sudoku problems?

Model relationships between many variables



Lauritzen & Spiegelhalter, 1988





Quantification of uncertainty



Motivation: models in machine learning

Data (input)







Generative Model (assumptions)





 $\mu_k, \Sigma_k \sim \text{NormalWishart}(\psi)$ $z_n \sim \text{Discrete}(\pi)$ $\mathbf{y}_n \sim \operatorname{Normal}(\boldsymbol{\mu}_{z_n}, \boldsymbol{\Sigma}_{z_n})$







Motivation: models in machine learning

Data (input)









Generative Model (assumptions)

Inference (output)



Machine Learning Software





Motivation: models in machine learning

Data (input) **Generative Model** (assumptions)







Inference (output)

Probabilistic Programming System





2.0



Programming

Probabilistic Programming

Statistics



A probabilistic program

"Probabilistic programs are usual functional or imperative programs with two added constructs:

(1) the ability to draw values at random from distributions, and

(2) the ability to condition values of variables in a program via observations."

> Gordon, Henzinger, Nori, and Rajamani "Probabilistic programming." In Proceedings of On The Future of Software Engineering (2014).



Languages and systems





Why would we do this?

Question: Why are you writing a probabilistic programming language?

Answer 1: I'm really tired of writing the same inference code again and again for each new model!

Answer 2: How esperopability ticppodel I can simulate from, but I have no idea how to condition it on data!

 $x \sim \mathcal{N}(a, b^{-1})$ $y_i \sim \mathcal{N}(x, c^{-1}), \ i = 1, \dots, N$

model { $x \sim dnorm(a, 1/b)$ for (i in 1:N) { y[i] \sim dnorm(x, 1/c)

An example BUGS program





Language restrictions? Model class? Inference?

Spiegelhalter et al. "BUGS: Bayesian inference using Gibbs sampling"





Loop iterations are **deterministic**!

No if statement (no branching)

data N = 10)# inits list(a = 1, b = 1)# model for (i in 1 : N) { $y[i] \sim dpois(l[i])$ } ~ dexp(1) $b \sim dgamma(0.1, 1.0)$ }

An example BUGS program

list(t = c(94.3, 15.7, 62.9, 126, 5.24,31.4, 1.05, 1.05, 2.1, 10.5), y = c(5, 1, 5, 14, 3, 19, 1, 1, 4, 22),

```
theta[i] ~ dgamma(a, b)
l[i] <- theta[i] * t[i]
```

Program 2.7: The Pumps example model from BUGS (OpenBugs, 2009).

"Inference first" approach to PPLs

"I never want to write this inference code again!"



ModelsFinitegraphical models

Continuous latent variables

Factor graphs

Language

Bounded loops; no branching

Bounded loops; no discrete r.v.s

Finite composition of factors

Pros: these languages work.

Cons?

Example: "Anglican"

Anglican is a Turing-complete probabilistic programming language embedded in Clojure.

(Disclaimer: I helped work on developing it back when I was at Oxford)

Other similar (and probably more current) projects:

turing.jl (Cambridge), gen (MIT), Birch, PyProb (UBC), webPPL, ...

Syntax: basically Clojure (similar to LISP)

• Notation: *prefix* vs infix

- ;; Add two numbers
 (+ 1 1)
- ;; Subtract: "10 3" (- 10 3)
- ;; (10 * (2.1 + 4.3) / 2) (/ (* 10 (+ 2.1 4.3)) 2)

• Branching

;; outputs 4 (+ (if (< 4 5) 1 2) 3)

Functions

• Functions are first class

;; evaluates to 32 10 2)

Local bindings

(let [x 10 y 2] (+ (* x 3) y))

((fn [x y] (+ (* x 3) y))

;; let is syntactic "sugar" for the same

Higher-order functions

• map

;; Apply the function f(x,y) = x + 2y to the ;; x values [1 2 3] and the y values [10 9 8] ;; Produces [21 20 19] (map (fn [x y] (+ x (* 2 y))) [1 2 3] ; these are values x1, x2, x3 [10 9 8]); these are values y1, y2, y3

reduce

;; Reduce recursively applies function,

- ;; to result and next element, i.e.
- (reduce + 0 [1 2 3 4])
- ;; does (+ (+ (+ 0 1) 2) ...
- ;; and evaluates to 10

```
y applies function,
t element, i.e.
])
) 2) ...
10
```

The need for higher-order languages

Unfortunately, restrictions can be quite limiting!

Simple example: Bernoulli trials

- (defm sample-geometric [p] (if (sample (flip p)) 0
 - (+ 1 (sample-geometric p))))

sampling from a geometric distribution, by counting number of failures before first success, in independent





Other way around: language first

Unrestricted Languages:

- "Open-universe": unbounded numbers of parameters
- Mixed variable types
- Access to existing software libraries
- Easily extensible

What is the catch?

- Inference is going to be harder
- More ways to shoot yourself in the foot



 $E_{p(\mathbf{x} | \mathbf{y})}[Q(\mathbf{x})]$

 $p(\mathbf{x} | \mathbf{y}) = p(\mathbf{y} | \mathbf{x})p(\mathbf{x})/p(\mathbf{y})$ Likelihood ^L Prior

Estimate predict values, under posterior on sample values, given observe values.



y X



- Observed data (flip outcomes)
- Unknown variable (coin bias)





 $p(\mathbf{y} \mid \mathbf{x})$ $p(\mathbf{x})$

- Likelihood of outcome given bias
- Prior belief about bias
- Posterior belief after seeing data













Example: Biased Coin







Example: Biased Coin



p(x | y).0





Separating models and inference

Modeling Language (Anglican)

(let [bias (sample (uniform 0 1)) likelihood (flip bias)] (observe likelihood true) (observe likelihood true) (observe likelihood true) (predict bias))

Special Forms

1 **sample** *random* value **x** 2 **observe** condition on value **y** 3 return value Q(x)

Inference Back End

Estimate distribution over output values under posterior of sample values, given observe values.

$$p(\mathbf{x} | \mathbf{y}) = p(\mathbf{y} | \mathbf{x})p(\mathbf{x})/p(\mathbf{y})$$

- Implements (inference-algorithm-specifc) sample and observe handlers
- Returns weighted samples



Generative model for Captcha-breaking

Target Image



Model for Characters

(defn sample-char [] {:symbol (sample (uniform ascii)) :x (sample (uniform-cont 0.0 1.0)) :y (sample (uniform-cont 0.0 1.0)) :scale (sample (beta 1 2)) :weight (sample (gamma 2 2)) :blur (sample (gamma 1 1))})



Generative model for Captcha-breaking

Target Image



Samples from Program



Model for Characters

(defquery captcha [image max-chars tol] (let [[w h] (size image) ;; sample random characters num-chars (sample (uniform-discrete 1 (inc max-chars))) chars (repeatedly num-chars sample-char)] ;; compare rendering to true image (map (fn [y z] (observe (normal z tol) y)) (reduce-dim image) (reduce-dim (render chars w h))) ;; output captcha text (map :symbol (sort-by :x chars)))



Generative model for Captcha-breaking

Target Image



Samples from Program



Model for Characters

(defquery captcha [image max-chars tol] (let [[w h] (size image) ;; sample random characters num-chars (sample (uniform-discrete 1 (inc max-chars))) chars (repeatedly num-chars sample-char)] ;; compare rendering to true image (map (fn [y z] (observe (normal z tol) y)) (reduce-dim image) (reduce-dim (render chars w h))) ;; output captcha text (map :symbol (sort-by :x chars)))



Deterministic Simulation

(defquery arrange-bumpers []
 (let [bumper-positions []

;; code to simulate the world world (create-world bumper-positions) end-world (simulate-world world) balls (:balls end-world)

;; how many balls entered the box? num-balls-in-box (balls-in-box end-world)]

(predict :balls balls)
(predict :num-balls-in-box num-balls-in-box)
(predict :bumper-positions bumper-positions)))

What if we want a "world" that puts ~20% of balls in box?



Stochastic Simulation

```
(defquery arrange-bumpers []
    (let [number-of-bumpers (sample (poisson 20))
         bumpydist (uniform-continuous 0 10)
         bumpxdist (uniform-continuous -5 14)
         bumper-positions (repeatedly
                            number-of-bumpers
                            #(vector (sample bumpxdist)
                                     (sample bumpydist)))
          ;; code to simulate the world
         world (create-world bumper-positions)
         end-world (simulate-world world)
         balls (:balls end-world)
```

```
;; how many balls entered the box?
num-balls-in-box (balls-in-box end-world)]
```

```
(predict :balls balls)
(predict :num-balls-in-box num-balls-in-box)
(predict :bumper-positions bumper-positions)))
```








Constrained Stochastic Simulation

```
(defquery arrange-bumpers []
   (let [number-of-bumpers (sample (poisson 20))
          bumpydist (uniform-continuous 0 10)
          bumpxdist (uniform-continuous -5 14)
          bumper-positions (repeatedly
                            number-of-bumpers
                            #(vector (sample bumpxdist)
                                     (sample bumpydist)))
```

```
;; code to simulate the world
world (create-world bumper-positions)
end-world (simulate-world world)
balls (:balls end-world)
```

```
;; how many balls entered the box?
num-balls-in-box (balls-in-box end-world)
```

```
obs-dist (normal 4 0.1)]
```

```
(observe obs-dist num-balls-in-box)
```

```
(predict :balls balls)
(predict :num-balls-in-box num-balls-in-box)
(predict :bumper-positions bumper-positions)))
```







Other sorts of examples

- pub?
 - Alice simulates Bob's decision process
 - ... which simulates Alice's decision process ...
 - ... which simulates Bob's decision process ...

very annoying to write out as an explicit game tree...

• Coordination game: cell phone dead. Do we meet at the cafe, or meet at the

Mutually recursive functions! Easy to write as functional programming code,

How can we perform inference?

• Two special forms are the entire interface between model code and inference code:

(sample ...)

• **Q:** what kinds of inference algorithms can we develop and implement using **just this** as our interface?

(observe ...)

Inference over partial program executions

From the perspective of the inference engine, what happens as a program runs?

- Sequence of *M* sample statements $\{(f_j, \theta_j)\}_{j=1}^M$
- Sequence of Nobserve statements $\{(g_i, \phi_i, y_i)\}_{i=1}^N$ • Sequence of *M* sampled values $\{x_j\}_{j=1}^M$
- Conditioned on these sampled values the entire computation is *deterministic*

$$\gamma(\mathbf{x}) \triangleq p(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^{N} g_i(y_i | \phi_i) \prod_{j=1}^{M} f_j(x_j | \theta_j).$$





Interaction between inference engine and model?

Inference engine (controller)



- Inference engine launches (instances of the) program

- Program yields result to inference engine upon termination





• sample and observe "checkpoints" yield control back to engine Engine updates internal state, and resumes program execution





Implementing "checkpoints": continuations

How do continuations work?

;; Standard Clojure:
(println (+ (* 2 3) 4))

First continuation

;; CPS-transformed "primitives"
(defn +& [a b k] (k (+ a b)))
(defn *& [a b k] (k (* a b)))

How do continuations work?

(defn pythag&
 "compute sqrt(x^2 + y^2)"
 [x y k]
 (square& x
 (fn [xx]
 (square& y
 (fn [



Use in probabilistic program inference

(defquery flip-example [outcome] (let [p (sample (uniform-continuous 0 1))] (observe (flip p) outcome) (predict :p p))

(let [u (uniform-continuous 0 1)

p (sample u)

dist (flip p)]

(observe dist outcome)

(predict :p p))



Use in probabilistic program inference

```
(defn flip-query& [outcome k1]
   (fn [dist1]
    (sample& dist1 
p (sample u)
      (fn [p] ((fn [p k2]
                (fn [dist2]
                   (fn []
             p k1))))))
```

;; CPS-ed distribution constructors (defn uniform-continuous& [a b k] (k (uniform-continuous a b)))

(defn flip& [p k] (k (flip p)))

(flip& p ◀ dist (flip p)] (predict& :p p k2))))) ◀</predict :p p))</predict :p p))



Inference "Backend"

(defn sample& [dist k]
;; [ALGORITHM-SPECIFIC IMPLEMENTATION HERE]
;; Pass the sampled value to the continuation
 (k (sample dist)))

(defn observe& [dist value k]
 (println "log-weight =" (log-prob dist value))
 ;; [ALGORITHM-SPECIFIC IMPLEMENTATION HERE]
 ;; Call continuation with no arguments
 (k))

Pure compiled deterministic computation



Possible inference algorithms

- Importance sampling / likelihood weighting Single-site Metropolis-Hastings ("random DB")
- Sequential Monte Carlo
- Particle MCMC methods (PIMH, CSMC, IPMCMC)
 Easy
- Black-box variational inference

Some inference engines ("backends") we are ready to implement:



Where does machine learning come in?

Trends in probabilistic programming

One-shot

Inference?

Repeated

Probabilistic Programming

> Amortized Inference

> > Yes

Have fully-specified model?



No

Amortized inference





Can we learn this directly?

Inference networks as proposal distributions





A probabilistic model generates data

An inverse model generates latents

Learning an importance sampling proposal for a single dataset

Target density $\pi(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})$, approximating family $q(\mathbf{x}|\lambda)$

Single dataset y. $\operatorname{argmin} D_{KL}(\pi || q_{\lambda})$ λ



Can we learn how to sample from the inverse model?

fit λ to learn an importance sampling proposal



Inference networks as proposal distributions





A probabilistic model generates data

An inverse model generates latents

Idea: amortize inference by learning a map from data to target

Target density $\pi(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})$, approximating family $q(\mathbf{x}|\lambda)$

Averaging over all possible datasets: $\lambda = \varphi(\eta, \mathbf{y})$



Can we learn how to sample from the inverse model?

learn a mapping from arbitrary datasets to λ

 $\operatorname{argmin} \mathbb{E}_{p(\mathbf{y})} \left[D_{KL}(\pi || q_{\varphi(\eta, \mathbf{y})}) \right]$



Training inference network on synthetic data

Averaging over all possible datasets: $\lambda = \varphi(\eta)$

 $\operatorname*{argmin}_{\eta} \mathbb{E}_p$

New objective function, upper-level parameters: $\mathcal{J}(\eta) = \int$

Tractable gradient! Can train entirely offline: $\nabla_{\eta} \mathcal{J}(\eta) =$

—

$$\begin{split} \varphi(\eta, \mathbf{y}) \\ & \text{in } \mathbb{E}_{p(\mathbf{y})} \left[D_{KL}(\pi || q_{\varphi(\eta, \mathbf{y})}) \right] \\ & \text{ expectation over any data} \\ & \text{ we might observe} \\ & = \int D_{KL}(\pi || q_{\lambda}) p(\mathbf{y}) \mathrm{d} \mathbf{y} \\ & = \int p(\mathbf{y}) \int p(\mathbf{x} | \mathbf{y}) \log \left[\frac{p(\mathbf{x} | \mathbf{y})}{q(\mathbf{x} | \varphi(\eta, \mathbf{y}))} \right] \mathrm{d} \mathbf{x} \mathrm{d} \mathbf{y} \\ & = \mathbb{E}_{p(\mathbf{x}, \mathbf{y})} \left[-\log q(\mathbf{x} | \varphi(\eta, \mathbf{y})) \right] + const. \\ & \text{ approximate with samples} \\ & from the joint distribution} \\ & T(\eta) = \mathbb{E}_{p(\mathbf{x}, \mathbf{y})} \left[-\nabla_{\eta} \log q(\mathbf{x} | \varphi(\eta, \mathbf{y})) \right] \end{split}$$





Samples from prior



Samples from prior



Metropolis-Hastings



Samples from proposal



Metropolis-Hastings



After importance weighting



Metropolis-Hastings



Inference networks for probabilistic programs



Input: an inference problem denoted in a probabilistic programming language **Output**: a trained inference network (deep neural network "compilation artifact")

Le TA, Baydin AG, Wood F. Inference Compilation and Universal Probabilistic Programming. AISTATS. 2017.



Amortized inference in higher-order languages?

- Manually programmed "guide" program?
 - Intersperse model code and inference
 - Requires support over the same set of "addresses" of random choices on every execution
- Automatic?
 - Use a generic regression model to conditionally generate sequences of random choices



Generic structured proposal architecture



 $x^{(n)}, y^{(n)} \sim p(x, y)$

synthetic data





previous sample embedding:

address:

instance:





letters = [] num_letters = sample(Poisson(6)) // i = 0 for i in range(num_letters): letters.append(sample(Uniform("a",...,"z","A",...,"Z")))

observe(render(letters), observed_captcha) return letters





letters = [] num_letters = sample(Poisson(6)) // i = 1 for i in range(num_letters): letters.append(sample(Uniform("a",...,"z","A",...,"Z")))

observe(render(letters), observed_captcha) return letters





letters = [] num_letters = sample(Poisson(6)) // i = 2 for i in range(num_letters): letters.append(sample(Uniform("a",...,"z","A",...,"Z")))

observe(render(letters), observed_captcha) return letters





Solving Sudoku with diffusion models

6	3	1	7	1	9	5	1	6
6	9	1	7	8	5	5	1	З
6	3	1	5	8	6	6	1	4
9	1	4	1	5	7	З	6	8
7	1	5	3	6	8	9	4	2
3	8	6	9	2	7	7	5	1
8	6	9	2	7	1	1	3	5
1	2	7	8	3	5	4	9	6
2	5	3	1	9	4	1	7	6

3	3	5	7	1	9	6	2	4
9	6	5	7	4	2	9	3	8
2	7	4	8	5	6	9	9	1
4	9	8	6	7	1	5	8	2
5	3	7	9	8	4	3	1	6
6	6	1	2	7	5	4	7	9
8	5	6	4	2	7	3	5	5
1	4	2	1	9	3	7	6	4
7	4	9	5	6	8	7	9	4

https://plai.cs.ubc.ca/2022/11/16/graphically-structured-diffusion-models/



Writing a good generative model is **hard**



Pyro http://pyro.ai



What kind of a language is Pyro?

- Built on top of Pytorch: based on *differentiable programming*, and takes advantage of the existing Python and Pytorch ecosystem
- **Idea:** define a generative model as a program, and a "inference model" as a second program
- Assign a "name" to every latent random variable, and make sure that they line up (be careful if support is unbounded...!)
- Variational Bayes: Optimize the parameters of the "inference model" so that it approximates the posterior (i.e. by minimizing a KL divergence)

ropose an alternative approach. We extend the model with an auxiliary v $\rho(\tilde{\mathbf{y}} \mid \mathbf{y}) = \delta_{\tilde{\mathbf{y}}}(\mathbf{y})$ to define densities

- nargi $= \mathbf{y}$

$$p(\tilde{\mathbf{y}}, \mathbf{y}, \mathbf{z}, \mathbf{x}) = p(\tilde{\mathbf{y}} \mid \mathbf{y}) p_{\theta}(\mathbf{x} \mid \mathbf{y}, \mathbf{z}) p(\mathbf{y}, \mathbf{z})$$

$$q(\tilde{\mathbf{y}}, \mathbf{y}, \mathbf{z} \mid \mathbf{x}) = p(\tilde{\mathbf{y}} \mid \mathbf{y}) q(\mathbf{y}, \mathbf{z} \mid \mathbf{x}).$$

$$\phi_{\phi_{i}} \mathbf{z}^{n} + \theta$$
inalize the ELBO for this model over $\tilde{\mathbf{y}}$, we recover the express
 i as observed results in the supervised objective

$$\mathcal{L}(\theta, \phi; \mathbf{x}^{i})|_{\tilde{\mathbf{y}}=\mathbf{y}^{i}} = \mathbb{E}_{q_{\phi}(\mathbf{z}, \mathbf{y} \mid \mathbf{x}^{i})} \left[\delta_{\mathbf{y}^{i}}(\mathbf{y}) \log \frac{p_{\theta}(\mathbf{x}^{i} \mid \mathbf{y}) p(\mathbf{z}, \mathbf{y})}{q_{\phi}(\mathbf{z}, \mathbf{y})} \right] \mathbf{x}^{i} \mathbf{y} \mathbf{x}^{i}$$

over an observed y is then replaced with evaluation of the ELBO and the te Carlo estimator of Equation (4) can be constructed automatically for an mpling latent variables z and weighting the resulting ELBO estimate by


Learning deep generative models **Generative model** Inference (encoder, guide) (decoder)





 $q_{\phi}(\mathbf{z}_n | \mathbf{x}_n)$

 $p_{\theta}(\mathbf{x}_n | \mathbf{z}_n)$ $p(\mathbf{z}_n)$

Incomprehensible Latent Variable

Kingma & Welling 2014; Rezende et al. 2014



Unexplained variation ("nuisance")

Disentangled representations

"Interpretable" (digit)

?	3	3	3	5	?	3	3	3	3
4	4	4	4	ï	4	¥	4	4	Ч
5	5	6	5	5	5	5	5	5	ŝ
6	6	6	6	6	6	6	6	6	6
1	7	Ĵ	7	7	7	2	7	1	~
8	8	Ø	8	8	8	8	8	2	00
9	9	q	9	q	9	9	9	4	9





representations

Generative model: predict pixels x foabi Bisablecaler Representation $p_{\theta}(\boldsymbol{x} | \boldsymbol{y}, \boldsymbol{z})$

Inference: predict label y from pixels x, and then predictbablingin Enandry



Sépáláte i files pretable y frontromusance variables z

when the label v is observing of being sampled from a_{\pm} . When the label v is observing with deep generative models, NIPS 2014





From one digit to many digits



Generative model



Inference model (recurrent neural network)



How do we build models?

Generative model





Inference: counting and locating

Inference model (recurrent neural network)



Transformation

Count





Real-world examples: molecule generation





Recap!

- Probabilistic programming languages can make writing probabilistic models, and doing inference, faster and more efficient
- Big challenge: Bayesian inference is, in general, pretty hard. But:
 - ... restricting the probabilistic programming language can help keep inference more tractable
 - ... even in unrestricted models, it's possible to define algorithms which will still work (though computational / statistical efficiency is not guaranteed...)
- Deep learning can be useful for amortized inference and for model learning
- An Introduction to Probabilistic Programming https://arxiv.org/abs/1809.10756
- Frank Wood's graduate course: <u>https://www.cs.ubc.ca/~fwood/CS532W-539W/</u>











Thanks!