Introduction to probabilistic programming

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Objectives For Today

Get you to

- Understand what probabilistic programming is
- Think generatively
- Understand inference
 - Importance sampling
 - SMC
 - MCMC
- Understand something about how modern, performant higher-order probabilistic programming systems are implemented at a very high level

Probabilistic Programming



Intuition Inference $p(\mathbf{x}|\mathbf{y})$ **Parameters** Parameters $p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$ Program Program **Observations** Output У

CS Probabilistic Programming Statistics

Probabilistic Programs

"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."

Key Ideas

Models



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

Programming Language Abstraction Layer



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

Evaluators that automate Bayesian inference

Long History

Hakaru R2 Gamble Figaro Figaro Figaro Hakaru Probabilistic-ML,Haskell,Scheme, WebPPL,Haskell,Scheme, Probabilistic-C Venture Anglican STAN	
Figaro Probabilistic-M_,Haskell,Scheme, WebPPL,Haskell,Scheme, Probabilistic-C LibBi Venture Anglican STAN	
2010 HANSAI	
ProbLog Ao Factorie JAGS	
Blog	
2000 IBAL	
Prism KMP WinBUGS	
1990 BUGS	

Existing Languages

Graphical Models

Factor Graphs







Factorie



Infer.NET

Infinite Dimensional Parameter Space Models



Unsupervised Deep Learning





PYRO

ProbTorch

BUGS

```
model
{
    x ~ dnorm(1, 1/5)
    for(i in 1:N) {
        y[i] ~ dnorm(x, 1/2)
    }
}
"N" <- 2
"y" <- c(9, 8)</pre>
```



- Language restrictions
 - Bounded loops
 - No branching

- Model class
 - Finite graphical models
- Inference sampling
 - Gibbs

STAN : Finite Dimensional Differentiable Distributions

```
parameters {
    real xs[T];
}
model {
    xs[1] ~ normal(0.0, 1.0);
    for (t in 2:T)
        xs[t] ~ normal(a * xs[t - 1], q);
    for (t in 1:T)
        ys[t] ~ normal(xs[t], 1.0);
}
```

- Language restrictions
 - Bounded loops
 - No discrete random variables*
- Model class
 - Finite dimensional differentiable distributions
- Inference
 - Hamiltonian Monte Carlo
 - Reverse-mode automatic differentiation
 - Black box variational inference, etc.



STAN Development Team "Stan: A C++ Library for Probability and Sampling." 2014.

Modeling language desiderata

- Unrestricted language (C++, Python, Lisp, etc.)
 - "Open-universe" / infinite dim. parameter spaces
 - Mixed variable types
- Pros
 - Unfettered access to existing libraries
 - Easily extensible
- Cons
 - Inference is going to be harder
 - More ways to shoot yourself in the foot



Deterministic Simulation and Other Libraries

```
(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)]

```
{:balls balls
:num-balls-in-box num-balls-in-box
:bumper-positions bumper-positions}))
```



goal: "world" that puts ~20% of balls in box...

Open Universe Models and Nonparametrics







(**defquery** arrange-bumpers []

> ;; 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)]

{:balls balls
:num-balls-in-box num-balls-in-box
:bumper-positions bumper-positions}))



Conditional (Stochastic) Simulation

```
;; 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)
```

```
{:balls balls
:num-balls-in-box num-balls-in-box
:bumper-positions bumper-positions}))
```









New Kinds of Models

X	У
program source code	program return value
scene description	image
policy and world	rewards
cognitive process	observed behavior
simulation	simulator output

Thinking Generatively

CAPTCHA breaking

SMKBDF Can you write a program to do this?





Mansinghka, Kulkarni, Perov, and Tenenbaum

"Approximate Bayesian image interpretation using generative probabilistic graphics programs." NIPS (2013).

Captcha Generative Model





(defm sample-char []
{:symbol (sample (uniform ascii))
:x-pos (sample (uniform-cont 0.0 1.0))
:y-pos (sample (uniform-cont 0.0 1.0))
:size (sample (beta 1 2))
:style (sample (uniform-dis styles))
...})

(defm sample-captcha [] (let [n-chars (sample (poisson 4)) chars (repeatedly n-chars sample-char) noise (sample salt-pepper) ...] gen-image))

Conditioning



(defquery captcha [true-image] (let [gen-image (sample-captcha)] (observe (similarity-kernel gen-image) true-image) gen-image))



Generative Model

(doquery :ipmcmc captcha true-image)

Inference

Perception / Inverse Graphics





Mansinghka, Kulkarni, Perov, and Tenenbaum. "Approximate Bayesian image interpretation using generative probabilistic graphics programs." NIPS (2013). Kulkarni, Kohli, Tenenbaum, Mansinghka "Picture: a probabilistic programming language for scene perception." CVPR (2015). 20

Directed Procedural Graphics

Stable Static Structures

Procedural Graphics







Ritchie, Lin, Goodman, & Hanrahan. Generating Design Suggestions under Tight Constraints with Gradient-based Probabilistic Programming. In Computer Graphics Forum, (2015) Ritchie, Mildenhall, Goodman, & Hanrahan. "Controlling Procedural Modeling Programs with Stochastically-Ordered Sequential Monte Carlo."₂₁ SIGGRAPH (2015)

Program Induction



(lambda (stack-id) (safe-uc (* (if (< 0.0 (* (* (* -1.0 (begin (define G_1147 (safe-uc 1.0 1.0)) 0.0)) (* 0.0 (+ 0.0 (safe-uc (* (* (dec -2 .0) (safe-sqrt (begin (define G_1148 3.14159) (safe-log -1.0)))) 2.0) 0.0)))) 1.0)) (+ (safe-div (begin (define G_1149 (* (+ 3.14159 -1.0) 1.0)) 1.0) 0.0) (safe-log 1.0)) (safe-log -1.0)) (begin (define G 11 . . .

 $\mathbf{x} \sim p(\mathbf{x})$



Perov and Wood.

"Automatic Sampler Discovery via Probabilistic Programming and Approximate Bayesian Computation" AGI (2016).

22

Thinking Generatively about Discriminative Tasks



(doquery :ipmcmc lin-reg data options)

([0.58 -0.05] [0.49 0.1] [0.55 0.05] [0.53 0.04]

(Re-?) Introduction to Bayesian Inference

A simple continuous example

- Measure the temperature of some water using an inexact thermometer
- The actual water temperature *x* is somewhere near room temperature of 22°; we record an estimate *y*.

 $x \sim \text{Normal}(22, 10)$ $y | x \sim \text{Normal}(x, 1)$

Easy question: what is p(y | x = 25)?

Hard question: what is p(x | y = 25)?

General problem:



- Our *data* is given by *y*
- Our generative model specifies the prior and likelihood
- We are interested in answering questions about the *posterior* distribution of $p(x \mid y)$

General problem:



- Typically we are not trying to compute a probability density function for $p(x \mid y)$ as our end goal
- Instead, we want to compute *expected values* of some function *f(x)* under the posterior distribution

Expectation

• Discrete and continuous:

$$\mathbb{E}[f] = \sum_{x} p(x) f(x)$$
$$\mathbb{E}[f] = \int p(x) f(x) \, \mathrm{d}x.$$

• Conditional on another random variable:

$$\mathbb{E}_x[f|y] = \sum_x p(x|y)f(x)$$

Key Monte Carlo identity

• We can approximate expectations using *samples* drawn from a distribution *p*. If we want to compute

$$\mathbb{E}[f] = \int p(x)f(x) \,\mathrm{d}x.$$

we can approximate it with a finite set of points sampled from p(x) using

$$\mathbb{E}[f] \simeq \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

which becomes exact as N approaches infinity.

How do we draw samples?

- Simple, well-known distributions: samplers exist (for the moment take as given)
- We will look at:
 - 1. Build samplers for complicated distributions out of samplers for simple distributions compositionally
 - 2. Rejection sampling
 - 3. Likelihood weighting
 - 4. Markov chain Monte Carlo

Ancestral sampling from a model

 In our example with estimating the water temperature, suppose we already know how to sample from a normal distribution.

 $x \sim \text{Normal}(22, 10)$

 $y|x \sim Normal(x, 1)$

We can sample *y* by literally simulating from the generative process: we first sample a "true" temperature *x*, and then we sample the observed *y*.

• This draws a sample from the **joint** distribution p(x, y).

Samples from the joint distribution



Conditioning via rejection

- What if we want to sample from a conditional distribution? The simplest form is via rejection.
- Use the ancestral sampling procedure to simulate from the generative process, draw a sample of x and a sample of y. These are drawn together from the joint distribution p(x, y).
- To estimate the posterior $p(x \mid y = 25)$, we say that x is a sample from the posterior if its corresponding value y = 25.
- **Question:** is this a good idea?

Conditioning via rejection



Black bar shows measurement at y = 25. How many of these samples from the joint have y = 25?

Conditioning via importance sampling

- One option is to sidestep sampling from the posterior p(x | y = 3) entirely, and draw from some proposal distribution q(x) instead.
- Instead of computing an expectation with respect to p(x|y), we compute an expectation with respect to q(x): $\mathbb{E}_{p(x|y)}[f(x)] = \int f(x)p(x|y)dx$

$$\begin{split} f(x)] &= \int f(x)p(x|y)dx \\ &= \int f(x)p(x|y)\frac{q(x)}{q(x)}dx \\ &= \mathbb{E}_{q(x)}\left[f(x)\frac{p(x|y)}{q(x)}\right] \end{split}$$

Conditioning via importance sampling

- Define an "importance weight" $W(x) = \frac{p(x|y)}{a(x)}$
- Then, with $x_i \sim q(x)$

$$\mathbb{E}_{p(x|y)}[f(x)] = \mathbb{E}_{q(x)}\left[f(x)W(x)\right] \approx \frac{1}{N} \sum_{i=1}^{N} f(x_i)W(x_i)$$

 Expectations now computed using *weighted* samples from *q(x)*, instead of unweighted samples from *p(x|y)*
Conditioning via importance sampling

 Typically, can only evaluate W(x) up to a constant (but this is not a problem):

$$W(x_i) = \frac{p(x_i|y)}{q(x_i)} \qquad \qquad w(x_i) = \frac{p(x_i, y)}{q(x_i)}$$

• Approximation:

$$W(x_i) \approx \frac{w(x_i)}{\sum_{j=1}^N w(x_j)}$$

$$\mathbb{E}_{p(x|y)}[f(x)] \approx \sum_{i=1}^{N} \frac{w(x_i)}{\sum_{j=1}^{N} w(x_j)} f(x_i)$$

Conditioning via importance sampling

- We already have very simple proposal distribution we know how to sample from: the prior p(x).
- The algorithm then resembles the rejection sampling algorithm, except instead of sampling both the latent variables and the observed variables, we only sample the latent variables
- Then, instead of a "hard" rejection step, we use the values of the latent variables and the data to assign "soft" weights to the sampled values.



Draw a sample of *x* from the prior



What does p(y|x) look like for this sampled x?



What does p(y|x) look like for this sampled x?



What does p(y|x) look like for this sampled x?



Compute p(y|x) for all of our x drawn from the prior



for a representation of the posterior

Conditioning via MCMC

- Problem: Likelihood weighting degrades poorly as the dimension of the latent variables increases, <u>unless we have a very well-chosen proposal distribution</u> q(x).
- **An alternative**: Markov chain Monte Carlo (MCMC) methods draw samples from a target distribution by performing a biased random walk over the space of the latent variables *x*.
- Idea: create a Markov chain such that the sequence of states x₀, x₁, x₂, ... are samples from p(x | y)



Conditioning via MCMC

- MCMC also uses a proposal distribution, but this proposal distribution makes **local** changes to the latent variables *x*. The proposal *q(x' | x)* defines a conditional distribution over *x'* given a current value *x*.
 - Typical choice: add small amount of Gaussian noise
- We use the proposal and the joint density to define an "acceptance ratio"

$$A(x \to x') = \min\left(1, \frac{p(x', y)q(x|x')}{p(x, y)q(x'|x)}\right)$$

 Metropolis-Hastings: with probability A we "move" state with the new value x', otherwise we stay at x.



MCMC initialization



Initialize arbitrarily (e.g. with a sample from the prior)

First MCMC step



Propose a local move on x from a transition distribution

1 MCMC iteration



10 MCMC iterations



Continue: propose a local move, and accept or reject. At first, this will look like a stochastic search algorithm!

100 MCMC iterations



Once in a high-density region, it will explore the space

200 MCMC iterations



Once in a high-density region, it will explore the space



Helpful diagnostic: a "trace plot" of the path of the sampled values, as the number of MCMC iterations increases



Histogram of trace plot, overlaid on prior probability density

How It Works: PPL Inference

Start With A Program

```
(let [z (sample (bernoulli 0.5))
        mu (if (= z 0) -1.0 1.0)
        d (normal mu 1.0)
        y 0.5]
        (observe d y)
        z)
```

Program

Semantically Agreed Mathematical Object

```
(let [z (sample (bernoulli 0.5))

mu (if (= z 0) -1.0 1.0)

d (normal mu 1.0)

y 0.5]

(observe d y)

z)

V = \{z, y\},

A = \{(z, y)\},

P = [z \mapsto (p_{bern} z 0.5),

y \mapsto (p_{norm} y (if (= z 0) -1.0 1.0) 1.0)]

Y = [y \mapsto 0.5]

E = z
```

Program

Mathematic Object

Rules of Inference

Program

Mathematic Object

$$\begin{array}{ll}\rho, \phi, e_1 \Downarrow G_1, E_1 & \rho, \phi, e_2 \Downarrow G_2, E_2 \\ (V, A, \mathcal{P}, \mathcal{Y}) = G_1 \oplus G_2 & \text{Choose a fresh variable } v \\ F_1 = \text{SCORE}(E_1, v) \neq \bot & F = (\text{if } \phi F_1 1) \\ Z = (\text{FREEVARS}(F_1) \setminus \{v\}) \cap V & \text{FREEVARS}(E_2) \cap V = \emptyset \\ B = \{(z, v) : z \in Z\}\end{array}$$

 $\overline{\rho, \phi, \text{ (observe } e_1 \ e_2)} \Downarrow (V \cup \{v\}, A \cup B, P \oplus [v \mapsto F], \mathcal{Y} \oplus [v \mapsto E_2]), E_2$

Big Step Operational Semantics

Intuitive Evaluation Perspective

(defquery example [y] (let [x (sample (beta 1 1))]; f(x)(observe (bernoulli x) y); g(y|x) } G(y|x)

• Syntactically denotes joint and conditioning

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

• Evaluator characterizes

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

Trace Probability

• Defined as (up to a normalization constant)

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

• Simple notation hides complex dependency structure!



$$\gamma(\mathbf{x}) = p(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^{N} \tilde{g}_i(\mathbf{x}_{n_i}) \left(y_i \Big| \tilde{\phi}_i(\mathbf{x}_{n_i}) \right) \prod_{j=1}^{M} \tilde{f}_j(\mathbf{x}_{j-1}) \left(x_j \Big| \tilde{\theta}_j(\mathbf{x}_{j-1}) \right)$$

Execution (Trace)-Based Inference

• Sequence of *N* **observe**'s

 $\{(g_i, \phi_i, y_i)\}_{i=1}^N$

• Sequence of *M* sample's

 $\{(f_j, \theta_j)\}_{j=1}^M$

• Sequence of *M* sampled values

 $\{x_j\}_{j=1}^M$

• Conditioned on these sampled values the entire trace is *deterministic*

Three Base Algorithms

- Likelihood Weighting
 - Importance sampling with prior as proposal
- Metropolis Hastings
- Sequential Monte Carlo

Likelihood Weighting

• Run *K* independent copies of program simulating from the prior

$$q(\mathbf{x}^k) = \prod_{j=1}^{M^k} f_j(x_j^k | \theta_j^k)$$

• Accumulate unnormalized weights (likelihoods)

$$w(\mathbf{x}^k) = \frac{\gamma(\mathbf{x}^k)}{q(\mathbf{x}^k)} = \prod_{i=1}^{N^k} g_i^k(y_i^k | \phi_i^k)$$

• Use in approximate (Monte Carlo) integration

$$W^{k} = \frac{w(\mathbf{x}^{k})}{\sum_{\ell=1}^{K} w(\mathbf{x}^{\ell})} \qquad \qquad \widehat{\mathbb{E}}_{\pi}[Q(\mathbf{x})] = \sum_{k=1}^{K} W^{k}Q(\mathbf{x}^{k})$$

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 z^K, w^K

•

Metropolis Hastings = "Single Site" MCMC = LMH

Posterior distribution of execution traces is proportional to trace score with observed values plugged in

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

$$\pi(\mathbf{x}) \triangleq p(\mathbf{x}|\mathbf{y}) = \frac{\gamma(\mathbf{x})}{Z}$$

()

Metropolis-Hastings acceptance rule

$$\alpha = \min\left(1, \frac{\pi(\mathbf{x}')q(\mathbf{x}|\mathbf{x}')}{\pi(\mathbf{x})q(\mathbf{x}'|\mathbf{x})}\right)$$

Need proposal

LMH Proposal

Probability of new part of proposed execution trace

$$q(\mathbf{x}'|\mathbf{x}^s) = \frac{1}{M^s} \kappa(x'_{\ell}|x^s_{\ell}) \prod_{j=\ell+1}^{M'} f'_j(x'_j|\theta'_j)$$

$$\uparrow$$
Number of samples in original trace

LMH Acceptance Ratio

"Single site update" = sample from the prior = run program forward

$$\kappa(x'_m|x_m) = f_m(x'_m|\theta_m), \theta_m = \theta'_m$$

MH acceptance ratio

Number of sample statements
in original traceProbability of original trace continuation
restarting proposal trace at mth sample
$$\alpha = \min \left(1, \frac{\gamma(\mathbf{x}')M\prod_{j=m}^{M} f_j(x_j|\theta_j)}{\gamma(\mathbf{x})M'\prod_{j=m}^{M'} f'_j(x'_j|\theta'_j)} \right)$$
 \wedge Number of sample statements
in new traceProbability of proposal trace continuation
restarting original trace at mth sample



LMH Variants



"C3: Lightweight Incrementalized MCMC for Probabilistic Programs using Continuations and Callsite Caching." D. Ritchie, A. Stuhlmuller, and N. D. Goodman. arXiv:1509.02151 (2015).
2015 : Probabilistic Programming

- Restricted (i.e. STAN, BUGS, infer.NET)
 - Easier inference problems -> fast
 - Impossible for users to denote some models
 - Fixed computation graph
- Unrestricted (i.e. Anglican, WebPPL)
 - Possible for users to denote all models
 - Harder inference problems -> slow
 - Dynamic computation graph
- Fixed, trusted model; one-shot inference

The AI/Repeated-Inference Challenge

"Bayesian inference is computationally expensive. Even approximate, sampling-based algorithms tend to take many iterations before they produce reasonable answers. In contrast, human recognition of words, objects, and scenes is extremely rapid, often taking only a few hundred milliseconds —only enough time for a single pass from perceptual evidence to deeper interpretation. Yet human perception and cognition are often well-described by probabilistic inference in complex models. How can we reconcile the speed of recognition with the expense of coherent probabilistic inference? How can we **build systems**, for applications like robotics and medical diagnosis, that exhibit **similarly rapid performance** at challenging inference tasks?"

Resulting Trend In Probabilistic Programming



Have fully-specified model?

Inference Compilation

Inference Compilation



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.

Example Non-Conjugate Regression



Paige B, Wood F. Inference Networks for Sequential Monte Carlo in Graphical Models. ICML. JMLR W&CP 48: 3040-3049. 2016.

Captcha Breaking

Туре		Baidu (2011)	Baidu (2013)	eBay 8 488 9 9	Yahoo 2805BeG	reCaptcha	Wikipedia nightember	Facebook
Our method	RR BT	99.8% 72 ms	99.9% 67 ms	99.2% 122 ms	98.4% 106 ms	96.4% 78 ms	93.6% 90 ms	91.0% 90 ms
Bursztein et al. [15]	RR BT	38.68% 3.94 s	55.22% 1.9 s	51.39% 2.31 s	5.33% 7.95 s	22.67% 4.59 s	28.29%	
Starostenko et al. [16]	RR BT				91.5%	54.6% < 0.5 s		
Gao et al. [17]	RR	34%			55%	34%		
Gao et al. [18]	RR BT		51% 7.58 s		36% 14.72 s			
Goodfellow et al. [6]	RR					99.8%		
Stark et al. [8]	RR					90%		

Facebook Captcha

Observed		WARGEQ	u V Te B	Mahapa	
images		(W4kgvQ)	(uV7FeWB)	(MqhnpT)	
Inference					
	107	W4kgvQ	uV7EeWB	MqhnpT	
Training traces	10 ⁶	WA4rj∨Q	uV7FeWB	МурррТ	
	10 ⁵	Woxewd9	mTTEMMm	RIrpES	
	104	BK∨u2Q	C9QDsoN	rS5FP2B	



I'm Hiring

- Postdoc(s)
- PhD students

~\$???; '17-'20 New Physics Via ATLAS Simulator Inversion















\$1.8M USD; '17-'21 — Hasty: A Generative Model Compiler



DEFENSE ADVANCED RESEARCH PROJECTS AGENCY ABOUT US / OUR RESEARCH

Defense Advanced Research Projects Agency > Program Information > Data-Driven Discovery of Models

Data-Driven Discovery of Models (D3M) Mr. Wade Shen

