Inference in Probabilistic Programming II

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Part of the content is from “An Introduction to Probabilistic Programming” by Jan-Willem van de Meent, Brooks Paige, Hongseok Yang, and Frank Wood
And
“An Introduction to Sequential Monte Carlo Methods” by Arnaud Doucet, Nando De Freitas, and Neil Gordon
Recap of Last Lecture

• Graph-based inference
  • Static
  • Cannot deal with programs with unbounded loops
Graph Translation: Example

\[
\begin{align*}
    x &= \text{bernoulli}(0.2) \\
    \text{if}(x) \{ & \quad y_1 = \text{uniform}(0, 2) \\
    \} & \quad \text{else} \\
    & \quad y_2 = \text{gaussian}(0, 5) \\
    y_3 &= \text{phi}(x, y_1, y_2) \\
    z &= \text{gaussian}(y_3, 1) \\
    \text{condition}(z > 10)
\end{align*}
\]
Inference on Translated Graphs

• Loopy belief propagation

• Sampling
  • Gibbs
  • Hamiltonian Monte Carlo
Gibbs Sampling

- Proposal distribution
  - Change one assignment at a time
  - $p(x \mid Y, X\setminus\{x\})$, where $Y$ are observed variables

- When we cannot evaluate $p(x \mid Y, X\setminus\{x\})$, we can turn to Metropolis-Hasting while using $q(x \mid Y, X\setminus\{x\})$ as the proposal distribution
Hamiltonian Monte Carlo (HMC)

• An more scalable MCMC algorithm

\[ H(z, r) = E(z) + K(r) \]

Potential energy, \( z \) are the random variables to sample from

Kinetic energy, \( r \) are auxiliary variables, provides momentum
Intuition Behind HMC

• https://arogozhnikov.github.io/2016/12/19/markov_chain_monte_carlo.html
Put Things Together: HMC

• Augment distribution $p(z)$ with $p(z, r)$

• Proposal distribution:
  • Update $z, r$ using Hamiltonian dynamics (in practice, a discretized approximation called leapfrog integration)
  • Judge whether to accept $z, r$ (see below)
  • Update $r$ stochastically

• Acceptance probability (After applying Hamiltonian dynamics):
  $$\min (1, \exp\{H(z, r) - H(z^*, r^*)\})$$

Account for approximation
The Leapfrog Approximation

\[
\hat{r}_i(\tau + \epsilon/2) = \hat{r}_i(\tau) - \frac{\epsilon}{2} \frac{\partial E}{\partial z_i}(\hat{z}(\tau))
\]
\[
\hat{z}_i(\tau + \epsilon) = \hat{z}_i(\tau) + \epsilon \hat{r}_i(\tau + \epsilon/2)
\]
\[
\hat{r}_i(\tau + \epsilon) = \hat{r}_i(\tau + \epsilon/2) - \frac{\epsilon}{2} \frac{\partial E}{\partial z_i}(\hat{z}(\tau + \epsilon)).
\]

To remove biases introduced by numerical errors, the steps are sampled from $\epsilon$ and $-\epsilon$. 
Question 1: Is the statement right?

• For any given probabilistic program with loops, it cannot be converted into a graphical model
Question 2: Is the statement right?

• The graph obtained by translating a probabilistic program is always a tree
Question 3: Translate the program into a graph

\[ x = \text{gaussian}(0, 1) \]
\[ y = \text{uniform}(0, x) \]
\[ \text{if } (x > 10) \{ \]
\[ \quad z = x \]
\[ \quad \text{condition}(y > 1.5) \]
\[ \} \]
\[ \text{else} \{ \]
\[ \quad \text{condition}(y < 0.5) \]
\[ \quad z = y \]
\[ \} \]
\[ w = \text{gaussian}(z, 0) \]
Question 4: Is the statement right?

• Gibbs sampling can be applied to sample any distribution
Question 5: Is the statement right?

• In HMC, the gradient is the gradient of the density function of the target distribution
Question 6: Is the statement right?

• HMC cannot be applied to any probabilistic programs with branches
This Lecture

• Evaluation-based inference

• More sampling algorithms
Motivation

• The number of random variables is unknown at compile time
  • Introduce an upper bound on the number of variables

• Implement inference methods that dynamically instantiate variables
Likelihood Weighting

- A form of importance sampling where the proposal is the prior

\[
\mathbb{E}_{q(X)} \left[ \frac{p(X|Y)}{q(X)} r(X) \right] = \frac{1}{p(Y)} \mathbb{E}_{q(X)} \left[ \frac{p(Y, X)}{q(X)} r(X) \right]
\]

\[
\approx \frac{1}{p(Y)} \frac{1}{L} \sum_{l=1}^{L} W^l r(X^l),
\]

\[
W^l = \frac{p(Y, X^l)}{q(X^l)} = \frac{p(Y|X^l)p(X^l)}{p(X^l)} = p(Y|X^l)
\]

If we use \( p(X^l) \) as the proposal distribution

Y are observed/conditioned variables
Likelihood Weighting

• But wait, every run of the program only evaluates a subset of all variables!

• It is OK: \( r(X) \) is the return value projection of all variables \( X \)
Likelihood Weighting

• What happens if there are no factor statements but only condition statements in the program?

• How to implement it in a graph-based inference?
Likelihood Weighting: Evaluation-based Implementation

• Run the program to draw samples

• Update the weight $W$ while running the program
  • Initially, $\log W = 0$

  • Whenever encounter an expression $condition(b)$, update $\log W \leftarrow \log W + \log p_B(\text{true})$
Metropolis-Hasting

• Similar problem: each execution only evaluates a subset of variables

• Naïve method: use the prior distribution $p(X)$ as the proposal distribution:

$$
\alpha = \frac{P(X'|Y)q(X|X')} {P(X'|Y)q(X|X')} = \frac{P(X',Y)q(X|X')} {P(X,Y)q(X'|X)} = \frac{P(Y|X')} {P(Y|X)}
$$
Metropolis-Hasting: Single-Site Proposals

- Most commonly used evaluation-based proposal

- Try to only change the value of a one variable at a time
  - Not always possible due to dependencies
Metropolis-Hasting: Single-Site Proposals

• Map $\sigma(X)$, such that $X(x)$ refers to the value of $x$ (only variables in the current execution)

• Map $\sigma(\log P)$, where $\log P(v)$ evaluates the density for each variable
  • When sampling from a distribution $d$, we have
    $$\sigma(\log P(x)) = \text{LOG} - \text{PROB}(d, X(x))$$
  
  • When encounter $\text{condition}(b)$, we have
    $$\sigma(\log P(y)) = \text{LOG} - \text{PROB}(b, \text{true})$$
Metropolis-Hasting: Single-Site Proposals

• Pick a variable $x_0 \in \text{dom}(X)$ at a random from the current sample

• Construct a proposal $X', P'$ by re-running the program
  • For an expression $d$ that sample from a variable $x$
    • If $x == x_0$, or $x \notin \text{dom}(X)$, then samples from the expression. Otherwise, reuse the value $X'(x) \leftarrow X(x)$
    • Calculate the probability $P'(x) \leftarrow \text{PROB}(d, X'(x))$
  • For expression $\text{condition}(b)$ with variable $y$:
    • Calculate the probability $P'(y) \leftarrow \text{PROB}(b, y) = 1_{b==y}$
  • For expression $\text{observe}(e, v)$ with variable $y$:
    • Calculate the probability $P'(y) \leftarrow \text{PROB}(e, v)$
Metropolis-Hasting: Single-Site Proposals

\[ \alpha = \frac{p(Y, X') q(X | X')}{p(Y, X) q(X' | X)} = \frac{p(Y, X') q(X | X', x_0)}{q(X' | X, x_0)} \frac{q(x_0 | X')}{p(Y, X) q(x_0 | X)}. \]
Metropolis-Hasting: Single-Site Proposals

\[
\frac{p(Y, X')}{q(X'|X, x_0)} \cdot \frac{q(X'|X', x_0)}{p(Y, X)} \cdot \frac{q(x_0|X')}{q(x_0|X)}
\]

\[
\frac{q(x_0|X')}{q(x_0|X)} = \frac{|X|}{|X'|}.
\]

\[
p(Y, X') = p(Y|X')p(X') = \prod_{y \in Y'} \mathcal{P}'(y) \prod_{x \in X'} \mathcal{P}'(x)
\]

\[
q(X'|X, x_0) = \prod_{x \in X'} \mathcal{P}'(x). \quad \frac{p(Y, X')}{q(X'|X, x_0)} = \prod_{y \in Y'} \mathcal{P}'(y) \prod_{x \in X'} \mathcal{P}'(x)
\]

We divide a sample into sampled part and reused part

\[
\frac{p(Y, X)}{q(X|X, x_0)} = \prod_{y \in Y} \mathcal{P}(y) \prod_{x \in X'} \mathcal{P}(x).
\]
Metropolis-Hasting: Single-Site Proposals

$$\alpha = \frac{|\text{dom}(\mathcal{X})|}{|\text{dom}(\mathcal{X}')|} \frac{\prod_{y \in \mathcal{Y}} \mathcal{P}'(y) \prod_{x \in X' \text{reused}} \mathcal{P}'(x)}{\prod_{y \in \mathcal{Y}} \mathcal{P}(y) \prod_{x \in X \text{reused}} \mathcal{P}(x)}$$
Example

x = 0

while(bernoulli(0.5) {
    x += uniform(0,1)
}

condition(x >= 10)
Sequential Monte Carlo

• Problem with likelihood weighting algorithm:
  • Essentially a “guess-and-check”
  • Doesn’t work well with models where there are a lot of random variables

• Sequential Monte Carlo
  • In probabilistic programming, sample a high-dimensional distribution by sampling a sequence of lower dimensional distributions
  • Also called particle filters
  • Used in signal processing and probabilistic inference
Informal Example

• See the example by Andreas Svensson
  • https://www.bilibili.com/video/BV1XE41177D1?share_source=copy_web
  • https://www.youtube.com/watch?v=aUkBa1zMKV4
Given
\[ p(x_0) \text{ and } \]
\[ p(x_t|x_{t-1}) \text{ and } \]
\[ p(y_t|x_t) \text{ and } \]
Observations \( y_{1:t} \)

Estimate
\[ p(x_{0:t}|y_{1:t}) \text{ or } \]
\[ p(x_t|y_{1:t}) \text{ or } \]
\[ I(f_t) = E_{p(x_{0:t}|y_{1:t})}[f_t(x_{0:t})] = \int f_t(x_{0:t})p(x_{0:t}|y_{1:t})dx_{0:t} \]
SMC: Problem Analysis

Can you compute these expressions?

\[
p(x_{0:t} \mid y_{1:t}) = \frac{p(y_{1:t} \mid x_{0:t}) p(x_{0:t})}{\int p(y_{1:t} \mid x_{0:t}) p(x_{0:t}) \, dx_{0:t}}.
\]

\[
p(x_{0:t+1} \mid y_{1:t+1}) = p(x_{0:t} \mid y_{1:t}) \frac{p(y_{t+1} \mid x_{t+1}) p(x_{t+1} \mid x_t)}{p(y_{t+1} \mid y_{1:t})}.
\]

**Prediction:** \( p(x_t \mid y_{1:t-1}) = \int p(x_t \mid x_{t-1}) p(x_{t-1} \mid y_{1:t-1}) \, dx_{t-1}; \)

**Updating:** \( p(x_t \mid y_{1:t}) = \frac{p(y_t \mid x_t) p(x_t \mid y_{1:t-1})}{\int p(y_t \mid x_t) p(x_t \mid y_{1:t-1}) \, dx_t}. \)
SMC: Problem Analysis

• Evaluation of complex high-dimensional integrals is hard

• People turn to approximate methods such as sampling
SMC: Approach

• Use samples to deal with integrations

• Effective method that leverages importance sampling
SMC: Naïve Importance Sampling

Let the proposal distribution be $\pi(x_{0:t} | y_{1:t})$, then we have

$$I(f_t) = \frac{\int f_t(x_{0:t}) w(x_{0:t}) \pi(x_{0:t} | y_{1:t}) \, dx_{0:t}}{\int w(x_{0:t}) \pi(x_{0:t} | y_{1:t}) \, dx_{0:t}}$$

$$w(x_{0:t}) = \frac{p(x_{0:t} | y_{1:t})}{\pi(x_{0:t} | y_{1:t})}.$$

$$\hat{I}_N(f_t) = \frac{1}{N} \sum_{i=1}^{N} f_t(x_{0:t}^{(i)}) w(x_{0:t}^{(i)}) = \sum_{i=1}^{N} f_t(x_{0:t}^{(i)}) \tilde{w}_t^{(i)}, \quad \tilde{w}_t^{(i)} = \frac{w(x_{0:t}^{(i)})}{\sum_{j=1}^{N} w(x_{0:t}^{(j)})}.$$
SMC: Naïve Importance Sampling

• Problem
  • Cannot be used for recursive estimation
  • One needs to get all $y_{1:t}$ before estimating $p(x_{0:t}|y_{1:t})$
  • Need to re-evaluate whenever there is a new $y$
  • Does not scale
SMC: Sequential Importance Sampling

- If we want to do recursive evaluation, the proposal distribution needs to satisfy
  \[
  \pi \left( x_{0:t} \mid y_{1:t} \right) = \pi \left( x_{0:t-1} \mid y_{1:t-1} \right) \pi \left( x_t \mid x_{0:t-1}, y_{1:t} \right).
  \]

- Which indicates
  \[
  \pi \left( x_{0:t} \mid y_{1:t} \right) = \pi \left( x_0 \right) \prod_{k=1}^{t} \pi \left( x_k \mid x_{0:k-1}, y_{1:k} \right).
  \]
SMC: Sequential Importance Sampling

• Then we have

\[
\tilde{w}_t^{(i)} \propto \tilde{w}_{t-1}^{(i)} \frac{p(y_t | x_t^{(i)}) p(x_t^{(i)} | x_{t-1}^{(i)})}{\pi(x_t^{(i)} | x_{0:t-1}^{(i)}, y_{1:t})}.
\]

• Important case

\[
\pi(x_{0:t} | y_{1:t}) = p(x_{0:t}) = p(x_0) \prod_{k=1}^{t} p(x_k | x_{k-1}).
\]
How to Derive the Formula

\[
\tilde{w}_t^{(i)} \propto \tilde{w}_t^{(i)} \frac{p(y_t | x_t^{(i)}) p(x_t^{(i)} | x_{t-1}^{(i)})}{\pi(x_t^{(i)} | x_{0:t-1}, y_{1:t})}.
\]

Given

\[
\tilde{w}_t^{(i)} = \frac{w(x_{0:t}^{(i)})}{\sum_{j=1}^{N} w(x_{0:t}^{(j)})}.
\]

\[
w(x_{0:t}) = \frac{p(x_{0:t} | y_{1:t})}{\pi(x_{0:t} | y_{1:t})} \cdot \pi(x_{0:t} | y_{1:t}) = \frac{p(x_{0:t-1} | y_{1:t-1}) \pi(x_t | x_{0:t-1}, y_{1:t})}{\pi(x_{0:t-1} | y_{1:t-1}) \pi(x_t | x_{0:t-1}, y_{1:t})}.
\]

\[
p(x_{0:t+1} | y_{1:t+1}) = p(x_{0:t} | y_{1:t}) \frac{p(y_{t+1} | x_{t+1}) p(x_{t+1} | x_t)}{p(y_{t+1} | y_{1:t})}.
\]

We have

\[
\omega(x_{0:t}) = \frac{p(x_{0:t} | y_{1:t})}{\pi(x_{0:t} | y_{1:t})} = \frac{p(x_{0:t-1}, y_{1:t-1}) * p(y_t | x_t) * p(x_t | x_{t-1}) / p(y_t | y_{1:t-1})}{\pi(x_{0:t-1} | y_{1:t-1}) \pi(x_t | y_{1:t-1}, y_{1:t})}
\]

\[
= \omega(x_{0:t-1}) * \frac{p(y_t | x_t) * p(x_t | x_{t-1})}{\pi(x_t | y_{1:t-1}, y_{1:t})} * \frac{1}{p(y_{t+1} | y_{1:t})}
\]

\[
= \omega(x_{0:t-1}) * \frac{p(y_t | x_t) * p(x_t | x_{t-1})}{\pi(x_t | y_{1:t-1}, y_{1:t})} * \frac{1}{p(y_{t+1} | y_{1:t})}
\]

\[
= \omega(x_{0:t-1}) * \frac{p(y_t | x_t) * p(x_t | x_{t-1})}{\pi(x_t | y_{1:t-1}, y_{1:t})} * \frac{1}{p(y_{t+1} | y_{1:t})}
\]

\[
= \omega(x_{0:t-1}) * \frac{p(y_t | x_t) * p(x_t | x_{t-1})}{\pi(x_t | y_{1:t-1}, y_{1:t})} * \frac{1}{p(y_{t+1} | y_{1:t})}
\]
SMC: Sequential Importance Sampling

• Problem: as $t$ increases, importance weights $\tilde{\omega}_t^{(i)}$ becomes more and more skewed
  • Almost all weights will become 0 except 1

• Solution: the bootstrap filter
SMC: Bootstrap Filter

• Key idea: remove particles with low weights and keep particles with high weights

• Formally replace

\[ \hat{P}_N \left( dx_{0:t} \mid y_{1:t} \right) = \sum_{i=1}^{N} \tilde{w}_t^{(i)} \delta_{x_{0:t}^{(i)}} \left( dx_{0:t} \right) \]

\[ P_N \left( dx_{0:t} \mid y_{1:t} \right) = \frac{1}{N} \sum_{i=1}^{N} N_t^{(i)} \delta_{x_{0:t}^{(i)}} \left( dx_{0:t} \right), \]

\( \delta \) is the Dirac measure
SMC: Bootstrap Filter

\[
P_N \left( dx_{0:t} \mid y_{1:t} \right) = \frac{1}{N} \sum_{i=1}^{N} N_t^{(i)} \delta_{x_{0:t}^{(i)}} \left( dx_{0:t} \right),
\]

\[\sum_{i=1}^{N} N_t^{(i)} = 0, \text{ if } N_t^{(j)} = 0, \text{ then the particle } x_{0:t}^{j} \text{ dies}\]

• How to select \( N_t^{(i)} \)?
  • Many methods
  • The most popular method: sampling \( N \) times from \( \hat{P}_N \left( dx_{0:t} \mid y_{1:t} \right) \)
SMC: Bootstrap Filter

Assume the proposal distribution is \( p(x_{1:t}) \)

1. Initialization. \( T = 0 \)
   - For \( i = 1, \ldots, N \), sample \( x_0^{(i)} \sim p(x_0) \) and set \( t = 1 \)

2. Importance sampling step.
   - For sample \( \tilde{x}_t^{(i)} \sim p(x_t | \tilde{x}_{t-1}^{(i)}) \) and set \( (\tilde{x}_0^{(i)}, \tilde{x}_t^{(i)}) \).
   - For \( i = 1, \ldots, N \), evaluate the importance weights.
   - Normalize the importance weights

3. Selection step
   - Resample with replacement \( N \) particles from the current particles according to importance weights
   - Set \( t \to t + 1 \)
More on Bootstrap Filter

• Compared to sequential importance sampling, it basically
  • Allows more variations under the prefixes with high weights
  • Throws away prefixes with low weights

• Advantages:
  • Easy to implement
  • Efficient
  • Modular
  • Can be parallelized
  • Can be used for complex models
Bootstrap Filter: Example

\[ x_t = \frac{1}{2} x_{t-1} + 25 \frac{x_{t-1}}{1 + x^2_{t-1}} + 8 \cos(1.2t) + v_t \]

\[ y_t = \frac{x_t^2}{20} + w_t, \]

\[ x_1 \sim N(0,10), v_k \sim N(0,10), w_k \sim N(0,1) \]

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SMC in Probabilistic Programming

\[ x_0 \rightarrow x_1 \rightarrow x_2 \rightarrow \ldots \]

\[ y_1 \rightarrow y_2 \]
SMC in Probabilistic Programming

x’s are the program trace excluding conditions

y’s are conditions
SMC in Probabilistic Programming

• We can evaluate intermediate densities using breakpoints

• We can use the prior distribution as the proposal distribution
More on Inference in Probabilistic Programming

• There are other general methods
  • Varational Inference

• No silver bullet
  • The general problem is a counting problem
  • Some researchers are exploring programmable inference frameworks: Gen: a general-purpose probabilistic programming system with programmable inference. Cusumano-Towner, M. F.; Saad, F. A.; Lew, A. K.; and Mansinghka, V. K. In PLDI 2019:
More on Inference in Probabilistic Programming

• Implementation issues
  • How can we avoid re-running programs
    • Fork at sampling statements and conditions
    • Can be Implemented through program transformation

• For a comprehensive understanding, read http://dippl.org/chapters/03-enumeration.html
Next Lecture

• Learning in probabilistic programming