

PAI. Approximate Inference

Anastasia Makarova

ETH Zürich

2.11.2018

Tree-structured:

- Variable elimination
- Belief propagation

Loopy networks:

- Loopy belief propagation
- Variational inference
- Gibbs sampling (Monte Carlo Sampling)

Stochastic Approximate Inference

- Algorithms that “randomize” to compute marginals as expectations
- In contrast to the deterministic methods, guaranteed to converge to right answer (if wait looong enough..)
- More exact, but slower than deterministic variants
- Also work for continuous distributions

Monte Carlo

Monte Carlo methods aim to find the expectation of some function $f(x)$ with respect to a probability distribution $p(x)$:

- Draw samples x_1, \dots, x_N
- Compute $\hat{f} = \frac{1}{N} \sum_{i=1}^N f(x_i)$

For i.i.d from $p(x)$: \hat{f} is unbiased with variance $\frac{1}{N} \mathbb{E}[(f - \mathbb{E}(f))^2]$

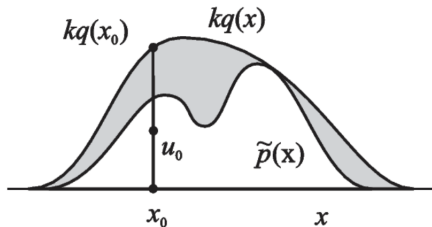
Basic samplings:

- Uniform Sampling
- Rejection Sampling
- Importance Sampling

Problem: can be very ineffective, particularly in high dimensions

Problem with Rejection sampling

If proposal distribution $q(x)$ poorly matches our target distribution $p(x)$ – almost always rejects



Example: d -dimensional target $p(x) = N(x; \mu, \sigma_p^{2/d})$ and the proposal $q(x) = N(x; \mu, \sigma_q^{2/d})$. Optimal acceptance rate can be accomplished with $k = \frac{\sigma_q}{\sigma_p}$. With $d = 1000$ and $\sigma_q = 1.01\sigma_p$ $k = 1/20000$ resulting in a large waste in samples.

Markov chains: random variables $\{x_1, \dots, x_N\}$ $n \in \{1, \dots, N - 1\}$:

$$p(x^{n+1}|x^1, \dots, x^n) = p(x^{n+1}|x^n)$$

Transitional kernel: $T(x^n, x^{n+1}) = p(x^{n+1}|x^n)$

Stationary distribution π^∞ : $\pi^\infty T = \pi^\infty$

A given Markov chain may have many stationary distributions.

Example: $T(x', x) = \mathbb{I}(x' = x)$: any distribution is invariant.

Detailed balance: sufficient condition for ensuring π^∞ is stationary: choose T such that

$$\pi^\infty(x) T(x, x') = \pi^\infty(x') T(x', x)$$

MCMC: Metropolis-Hastings

- Aim to sample from $p(x)$ (possibly unnormalized)
- Use easier distribution $q(x^*|x)$ (opposed to $q(x)$ and given as a stochastic matrix) and acceptance test to sample
 - 1 Initialize x^0
 - 2 Burn-in: for $t \in \{1, \dots, t_0\}$:
 - $x = x^t$
 - $t = t + 1$
 - sample $u \sim Unif(0, 1)$
 - sample $x^* \sim q(x^*|x)$:
 - if $u \leq A(x^*|x) = \min\{1, \frac{p(x^*)q(x|x^*)}{p(x)q(x^*|x)}\}$: $x^t = x^*$ (transition)
 - else: $x^t = x$ (stay in current state)
 - 3 Draw samples
- This induces a transition matrix $T(x^*|x) = q(x^*|x)A(x^*|x)$ that satisfies detailed balance \rightarrow after t_0 sampling will lead to sampling from stationary $p(x)$

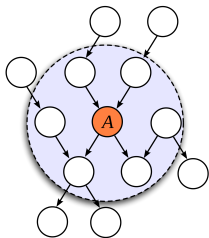
Gibbs sampling: acceptance probability is 1

- 1 Initializing starting values for x_1, \dots, x_n
- 2 Do until convergence:
 - randomly pick x_j
 - $x \sim P(x_j | x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n)$
 - $x_j = x$

Note: given Markov Blanket of x_j :

$$bl(x_j) = pa(j) \cup ch(j) \cup_{v \in ch(i)} pa(v)$$

$$P(x_j | x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n) = P(x_j | bl(x_j))$$



Computing Expectations via GS

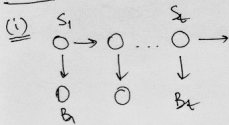
One of the MCMC goals - compute the mean of $f(x)$ with respect to $p(x)$:

- 1 Use Gibbs Sampling to obtain T samples: $\{X^t\}_{t=1}^{t=T}$
- 2 Note: t_0 samples for burn-in
- 3

$$\mathbb{E}[f(x)|x_B] \approx \frac{1}{T - t_0} \sum_{t=t_0+1}^T f(X^t)$$

Exam 2016. HMM

HMM



S_t	T	F
	0,95	0,05

S_{t+1}	T	F
T	0,9	0,1
F	0,6	0,4

S_t	T	F
T	0,8	0,2
F	0,1	0,9

(iii) estimate $b_i = T$

we have N samples $j = 1 \dots N: \{x_j\}_1^N$

$$u^{(j)} = \sum_{i=1}^{30} \mathbb{I}(b_i = T)$$

estimation: $u = \frac{1}{N} \sum_{j=1}^N u^{(j)}$

(ii) single sample:

$$\left(\{T, F\}^6 \right)^{30}, \left(T^5, F^{25} \right)$$

pseudo code:

$$S_1 \sim P(S_1)$$

$$b_1 \sim P(b_1 | S_1 = s_1)$$

for $t = 2 \dots 30$:

$$S_t \sim P(S_t | S_{t-1} = s_{t-1})$$

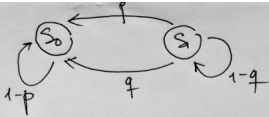
$$b_t \sim P(b_t | S_t = s_t)$$

return $(S_1 \dots S_{30}); (b_1 \dots b_{30})$

↳ x_j - single sample

Exam 2016. Sampling

Sampling



$$(i) \quad T_{(x,y)} = \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix}$$

(ii) stationary distribution $\pi(S_0) = r$ $\pi(S_1) = 1-r$

$$(r \quad 1-r) \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} = (r \quad 1-r) \quad \text{or} \quad rp = (1-r)q$$

(ii) solve linear alg. eq: $\begin{pmatrix} 1/3 \\ 2/3 \end{pmatrix}^T \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} = \begin{pmatrix} 1/3 \\ 2/3 \end{pmatrix}^T$

$$\rightarrow p = 2q$$

$$(p, q) = (2k, k) \quad 0 \leq k \leq 0,5$$

Questions

Extra: why MH works

When we draw a sample x' given $Q(x'|x)$, the transition kernel is $T(x'|x) = Q(x'|x)A(x'|x)$. In Metropolis-Hastings Algorithm, we compute the ratio of importance weight where $A(x'|x) = \min(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)})$. Suppose $A(x'|x) < 1$ and $A(x|x') = 1$, we have:

$$\begin{aligned}A(x'|x) &= \frac{P(x')Q(x|x')}{P(x)Q(x'|x)} \\P(x)Q(x'|x)A(x'|x) &= P(x')Q(x|x') \\P(x)Q(x'|x)A(x'|x) &= P(x')Q(x|x')A(x|x') \\P(x)T(x'|x) &= P(x')T(x|x'),\end{aligned}$$