Lecture: Inference in Graphical Models

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Exact Inference
Variable Elimination and Belief Propagation
Inference

Inference corresponds to using the distribution to answers questions about the environment.

examples

- What is the probability \( p(x = 4|y = 1, z = 2) \)?
- What is the most likely joint state of the distribution \( p(x, y) \)?
- What is the entropy of the distribution \( p(x, y, z) \)?
- What is the probability that this example is in class 1?
- What is the probability the stock market will do down tomorrow?

Computational Efficiency

- Inference can be computationally very expensive and we wish to characterise situations in which inferences can be computed efficiently.
- For singly-connected graphical models, and certain inference questions, there exist efficient algorithms based on the concept of message passing.
- In general, the case of multiply-connected models is computationally inefficient.
Sum-Product Algorithm

\[ p(a, b, c, d) \propto f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \quad a, b, c, d \text{ binary variables} \]

\[ p(a) = \sum_{b,c,d} p(a, b, c, d) \]

\[ \propto \sum_{b,c,d} f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \Rightarrow 2^3 \text{ sums} \]
Sum-Product Algorithm

\[ p(a, b, c, d) \propto f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \quad a, b, c, d \text{ binary variables} \]

\[ p(a) = \sum_{b,c,d} p(a, b, c, d) \]

\[ \propto \sum_{b,c,d} f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \Rightarrow 2^3 \text{ sums} \]

\[ = \sum_b f_1(a, b) \sum_c f_2(b, c) \sum_d f_3(c, d) f_4(d) \Rightarrow 2 \times 3 \text{ sums} \]
Sum-Product Algorithm

\[ p(a, b, c, d) \propto f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \quad a, b, c, d \text{ binary variables} \]

\[ p(a) = \sum_{b, c, d} p(a, b, c, d) \]

\[ \propto \sum_{b, c, d} f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \]

\[ = \sum_{b} f_1(a, b) \sum_{c} f_2(b, c) \sum_{d} f_3(c, d) f_4(d) \]

\[ = \mu_{d \rightarrow c}(c) \quad \mu_{c \rightarrow b}(b) \quad \mu_{b \rightarrow a}(a) \]
Sum-Product Algorithm

\[ p(a, b, c, d) \propto f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \quad a, b, c, d \text{ binary variables} \]

\[ \mu_{b\rightarrow a}(a) \quad \mu_{c\rightarrow b}(b) \quad \mu_{d\rightarrow c}(c) \]

\[ a \rightarrow f_1 \rightarrow b \rightarrow f_2 \rightarrow c \rightarrow f_3 \rightarrow d \rightarrow f_4 \]

Passing variable-to-variable messages from \( d \) up to \( a \)

\[ p(a) = \sum_{b,c,d} p(a, b, c, d) \]

\[ \propto \sum_{b,c,d} f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \]

\[ = \sum_{b} f_1(a, b) \sum_{c} f_2(b, c) \sum_{d} f_3(c, d) f_4(d) \]

\[ \mu_{d\rightarrow c}(c) \quad \mu_{c\rightarrow b}(b) \quad \mu_{b\rightarrow a}(a) \]
Sum-Product Algorithm

For $p(c)$ need to send messages in both directions

$$p(c) \propto \sum_{a,b,d} f_1(a,b) f_2(b,c) f_3(c,d) f_4(d)$$

$$= \sum_{b} \sum_{a} f_1(a,b) f_2(b,c) \left( \sum_{d} f_3(c,d) f_4(d) \right)$$

$$\underbrace{\mu_{a \rightarrow b}(b)}_{\mu_{b \rightarrow c}(c)} \underbrace{\mu_{d \rightarrow c}(c)}_{\mu_{a \rightarrow b}(b)}$$
Sum-Product Algorithm

\[ p(a, b, c, d, e) \propto f_1(a, b) f_2(b, c, d) f_3(c) f_4(d, e) f_5(d) \]

Need to define factor-to-variable messages and variable-to-factor messages

\[ p(a) \propto f_1(a, b) \sum_{c,d} f_2(b, c, d) \]

\[ f_3(c) \quad f_5(d) \quad \sum_{e} f_4(d, e) \]

\[ \mu_{c \rightarrow f_2(c)} = \mu_{f_3 \rightarrow c(c)} \quad \mu_{f_5 \rightarrow d(d)} \]

\[ \mu_{d \rightarrow f_2(d)} \]

\[ \mu_{b \rightarrow f_1(b)} = \mu_{f_2 \rightarrow b(b)} \]

\[ \mu_{f_1 \rightarrow a(a)} \]

⇒ Marginal inference for a singly-connected structure is easy.
Sum-Product Algorithm for Factor Graphs

**Variable to factor message**

\[ \mu_{v \rightarrow f} (v) = \prod_{f_i \sim v \setminus f} \mu_{f_i \rightarrow v} (v) \]

Messages from extremal variables are set to 1

**Factor to variable message**

\[ \mu_{f \rightarrow v} (v) = \sum_{\{v_i\}} f(v, \{v_i\}) \prod_{v_i \sim f \setminus v} \mu_{v_i \rightarrow f} (v_i) \]

Messages from extremal factors are set to the factor

**Marginal**

\[ p(v) \propto \prod_{f_i \sim v} \mu_{f_i \rightarrow v} (v) \]
Max Product Algorithm

\[ p(a, b, c, d) \propto f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \quad a, b, c, d \text{ binary variables} \]

\[
\max_{a,b,c,d} p(a, b, c, d) = \max_{a,b,c,d} f_1(a, b) f_2(b, c) f_3(c, d) f_4(d) \\
= \max_a \max_b f_1(a, b) \max_c f_2(b, c) \max_d f_3(c, d) f_4(d)
\]

\[
\begin{align*}
\mu_{d \rightarrow c}(c) \\
\mu_{c \rightarrow b}(b) \\
\mu_{b \rightarrow a}(a)
\end{align*}
\]
Max Product Algorithm

Variable to factor message
\[
\mu_{v \rightarrow f}(v) = \prod_{f_i \sim v \setminus f} \mu_{f_i \rightarrow v}(v)
\]

Factor to variable message
\[
\mu_{f \rightarrow v}(v) = \max_{\{v_i\}} f(v, \{v_i\}) \prod_{v_i \sim f \setminus v} \mu_{v_i \rightarrow f}(v_i)
\]

Marginal
\[
v^* = \arg\max_v \prod_{f_i \sim v} \mu_{f_i \rightarrow v}(v)
\]
Message Passing

- Also known as **belief propagation** or **dynamic programming**
- Note that for non-branching graphs (they look like lines), only variable to variable messages are required.
- For message passing to work we need to be able to distribute the operator over the factors (which means that the operator algebra is a semiring) and that the graph is singly-connected.
- Provided the above conditions hold, marginal inference scales linearly with the number of nodes in the graph.
Approximate Inference
Sampling Methods
Inference for Graphical Models

Before we looked into **Exact Inference**:
- Can be slow in many cases!

**Approximate Inference**: **Sampling Methods** represent desired distribution with a set of samples \(\rightarrow\) as more samples are used, obtain more accurate representation.
Sampling

Fundamental problem we address:

- How to obtain samples from a probability distribution \( p(z) \)
- This could be a conditional distribution \( p(z|e) \)

We wish to evaluate expectations such as

\[
\mathbb{E}[f] = \int f(z)p(z)dz
\]  
(1)

- e.g mean when \( f(z) = z \)

For complicated \( p(z) \), this is difficult to do exactly, so approximate as

\[
\hat{f} = \frac{1}{Z} \sum_{l=1}^{L} f(z^{(l)})
\]  
(2)

where \( \{z^{(l)}|l = 1, ...L\} \) are independent samples from \( p(z) \)
Sampling

- Approximate

\[ \hat{f} = \frac{1}{L} \sum_{l=1}^{L} f(z^{(l)}) \]

where \( \{z^{(l)}|l = 1, \ldots, L\} \) are independent samples from \( p(z) \)
Simple Monte Carlo

Statistical sampling can be applied to any expectation:

In general:

\[ \int f(x)P(x) \, dx \approx \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x) \]

Example: making predictions

\[ p(x|D) = \int P(x|\theta, D) P(\theta|D) \, d\theta \]

\[ \approx \frac{1}{S} \sum_{s=1}^{S} P(x|\theta^{(s)}, D), \quad \theta^{(s)} \sim P(\theta|D) \]
Properties of Monte Carlo

Estimator: \[\int f(x)P(x) \, dx \approx \hat{f} \equiv \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)\]

Estimator is unbiased:

\[\mathbb{E}_{P(\{x^{(s)}\})}[\hat{f}] = \frac{1}{S} \sum_{s=1}^{S} \mathbb{E}_{P(x)}[f(x)] = \mathbb{E}_{P(x)}[f(x)]\]

Variance shrinks \(\propto 1/S:\)

\[\text{var}_{P(\{x^{(s)}\})}[\hat{f}] = \frac{1}{S^2} \sum_{s=1}^{S} \text{var}_{P(x)}[f(x)] = \frac{\text{var}_{P(x)}[f(x)]}{S}\]

"Error bars" shrink like \(\sqrt{S}\)
Sampling from a Bayesian Network

**Ancestral pass** for directed graphical models:
- sample each top level variable from its marginal
- sample each other node from its conditional once its parents have been sampled

**Sample:**
- \( A \sim P(A) \)
- \( B \sim P(B) \)
- \( C \sim P(C | A, B) \)
- \( D \sim P(D | B, C) \)
- \( E \sim P(D | C, D) \)

\[
P(A, B, C, D, E) = P(A) P(B) P(C | A, B) P(D | B, C) P(E | C, D)
\]
Sampling from Bayesian Networks

- Sampling from discrete Bayesian networks with no observations is straightforward, using ancestral sampling.
- Bayesian network specifies factorization of joint distribution

\[
P(z_1, \ldots, z_n) = \prod_{i=1}^{n} P(z_i | pa(z_i))
\]

- Sample in-order, sample parents before children
  - Possible because graph is a DAG
- Choose value for \( z_i \) from \( p(z_i | pa(z_i)) \)
Rejection Sampling

Sampling from target distribution $p(z) = \tilde{p}(z)/Z_p$ is difficult. Suppose we have an easy-to-sample proposal distribution $q(z)$, such that $kq(z) \geq \tilde{p}(z)$, $\forall z$.

Sample $z_0$ from $q(z)$.
Sample $u_0$ from Uniform$[0, kq(z_0)]$

The pair $(z_0, u_0)$ has uniform distribution under the curve of $kq(z)$.

If $u_0 > \tilde{p}(z_0)$, the sample is rejected.
Rejection Sampling

Probability that a sample is accepted is:

\[
p(\text{accept}) = \int \frac{\tilde{p}(z)}{kq(z)} q(z) dz
= \frac{1}{k} \int \tilde{p}(z) dz
\]

The fraction of accepted samples depends on the ratio of the area under \( \tilde{p}(z) \) and \( kq(z) \).

Hard to find appropriate \( q(z) \) with optimal \( k \).

Useful technique in one or two dimensions. Typically applied as a subroutine in more advanced algorithms.
Rejection Sampling

Need a proposal density $Q(x)$ [e.g. uniform or Gaussian], and a constant $c$ such that $c(Qx)$ is an upper bound for $P^*(x)$

Example with $Q(x)$ uniform

- **upper bound**
- $cQ(x)$
- $P^*(x)$

- generate uniform random samples in upper bound volume

- accept samples that fall below the $P^*(x)$ curve

- the marginal density of the $x$ coordinates of the points is then proportional to $P^*(x)$

Note the relationship to Monte Carlo integration.
Rejection Sampling

While true:
\[\theta \sim q\]
\[h \sim \text{Uniform}[0, kq(\theta)]\]
\[\text{if } h < \pi^*(\theta): \]
\[\text{return } \theta\]
Importance Sampling

Suppose we have an easy-to-sample proposal distribution $q(z)$, such that $q(z) > 0$ if $p(z) > 0$.

\[
E[f] = \int f(z)p(z)dz = \int f(z)\frac{p(z)}{q(z)}q(z)dz \\
\approx \frac{1}{N} \sum_{n} \frac{p(z^n)}{q(z^n)}f(z^n), \quad z^n \sim q(z)
\]

The quantities $w^n = p(z^n)/q(z^n)$ are known as importance weights. Unlike rejection sampling, all samples are retained. But wait: we cannot compute $p(z)$, only $\hat{p}(z)$. 

Importance Sampling

Let our proposal be of the form \( q(z) = \frac{\tilde{q}(z)}{Z_q} \):

\[
\mathbb{E}[f] = \int f(z)p(z)dz = \int f(z)\frac{p(z)}{q(z)}q(z)dz = \frac{Z_q}{Z_p} \int f(z)\frac{\tilde{p}(z)}{\tilde{q}(z)}q(z)dz \\
\approx \frac{Z_q}{Z_p N} \sum_n \tilde{p}(z^n) f(z^n) = \frac{Z_q}{Z_p N} \sum_n w^n f(z^n), \quad z^n \sim q(z)
\]

But we can use the same importance weights to approximate \( \frac{Z_p}{Z_q} \):

\[
\frac{Z_p}{Z_q} = \frac{1}{Z_q} \int \tilde{p}(z)dz = \int \frac{\tilde{p}(z)}{\tilde{q}(z)}q(z)dz \approx \frac{1}{N} \sum_n \tilde{p}(z^n) = \frac{1}{N} \sum_n w^n
\]

Hence:

\[
\mathbb{E}[f] \approx \frac{1}{N} \sum_n \frac{w^n}{\sum_n w^n} f(z^n) \quad \text{Consistent but biased.}
\]
If our proposal distribution $q(z)$ poorly matches our target distribution $p(z)$ then:

- Rejection Sampling: almost always rejects
- Importance Sampling: has large, possibly infinite, variance (unreliable estimator).

For high-dimensional problems, finding good proposal distributions is very hard. What can we do?

Markov Chain Monte Carlo.
Summary so far

- Sums and integrals, often expectations, occur frequently in statistics.
- **Monte Carlo** approximates expectations with a sample average.
- **Rejection sampling** draws samples from complex distributions.
- **Importance sampling** applies Monte Carlo to ‘any’ sum/integral.
Application to Large Problems

We often can’t decompose $P(X)$ into low-dimensional conditionals.

**Undirected graphical models:** $P(x) = \frac{1}{Z} \prod_i f_i(x)$

**Posterior** of a directed graphical model:

$$P(A, B, C, D | E) = \frac{P(A, B, C, D, E)}{P(E)}$$

We often don’t know $Z$ or $P(E)$.
Gibbs Sampling

For large graphical models, given a multivariate distribution, it is simpler to sample from a conditional distribution than to marginalize by integrating over a joint distribution

- We want samples approximate the joint distribution of all variables
- The marginal distribution of any subset of variables can be approximated by simply considering the samples for that subset of variables (Markov Blanket in Bayes Nets!)
- The expected value of any variable can be approximated by averaging over all the samples
Gibbs Sampling

A method with no rejections:
- Initialize $x$ to some value
- Pick each variable in turn or randomly and resample $P(x_i|x_j \neq i)$

Figure from PRML, Bishop (2006)
Gibbs Sampler

Consider sampling from $p(z_1, \ldots, z_N)$.

Initialize $z_i, i = 1, \ldots, N$

For $t=1,...,T$

Sample $z_1^{t+1} \sim p(z_1|z_2^t, \ldots, z_N^t)$

Sample $z_2^{t+1} \sim p(z_2|z_1^{t+1}, x_3^t, \ldots, z_N^t)$

\[ \ldots \]

Sample $z_N^{t+1} \sim p(z_N|z_1^{t+1}, \ldots, z_{N-1}^{t+1})$

Gibbs sampler is a particular instance of M-H algorithm with proposals $p(z_n|z_{i\neq n}) \rightarrow$ accept with probability 1. Apply a series (component-wise) of these operators.
Gibbs Sampling for Bayes Nets

1. Initialization
   • Set evidence variables $E$, to the observed values $e$
   • Set all other variables to random values (e.g. by forward sampling)
   This gives us a sample $x_1, \ldots, x_n$.

2. Repeat (as much as wanted)
   • Pick a non-evidence variable $X_i$ uniformly randomly
   • Sample $x'_i$ from $P(X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$.
   • Keep all other values: $x'_j = x_j, \forall j \neq i$
   • The new sample is $x'_1, \ldots, x'_n$

3. Alternatively, you can march through the variables in some predefined order
Why Gibbs works in Bayes Nets

- The key step is sampling according to $P(X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$. How do we compute this?
- In Bayes nets, we know that a variable is conditionally independent of all others given its Markov blanket (parents, children, spouses)

$$P(X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) = P(X_i|\text{MarkovBlanket}(X_i))$$

- So we need to sample from $P(X_i|\text{MarkovBlanket}(X_i))$
- Let $Y_j, j = 1, \ldots, k$ be the children of $X_i$. It is easy to show that:

$$P(X_i = x_i|\text{MarkovBlanket}(X_i)) \propto P(X_i = x_i|\text{Parents}(X_i)) \cdot \prod_{j=1}^{k} P(Y_j = y_j|\text{Parents}(Y_j))$$
Summary

Ways of doing inference in graphical models...

**Exact Inference**
- Message Passing algorithms

**Approximate Inference (Sampling Methods)**
- Monte-Carlo Sampling
- Importance Sampling
- Gibbs Sampling in Bayesian Networks

**Note**: We will cover Sampling Methods in more details when we talk about Approximate Inference and Variational Methods (later...