Probabilistic Foundations of Artificial Intelligence Solutions to Problem Set 4

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1. Bayesian networks and Markov chains

Consider the query P(R|S = t, W = t) in the following Bayesian network, and how Gibbs



Figure 1: Bayesian Network

sampling can answer it.

- (i) How many states does the Markov chain have?
- (ii) Calculate the transition matrix T containing $P(X_{t+1} = y \mid X_t = x)$ for all x, y.
- (iii) What does T^2 , the square of the transition matrix, represent?
- (iv) What about T^n as $n \to \infty$?
- (v) Explain how to do probabilistic inference in Bayesian networks, assuming that T^n is available. Is this a practical way to do inference?

Solution

- (i) There are two uninstantiated Boolean variables (*Cloudy* and *Rain*) and therefore four possible states.
- (ii) First, we compute the sampling distribution for each variable, conditioned on its Markov blanket.

$$\begin{split} P(C|r,s) &= \frac{1}{Z} P(C) P(s|C) P(r|C) \\ &= \frac{1}{Z} \langle 0.5, 0.5 \rangle \langle 0.1, 0.5 \rangle \langle 0.8, 0.2 \rangle = \frac{1}{Z} \langle 0.04, 0.05 \rangle = \langle 4/9, 5/9 \rangle \\ P(C|\neg r,s) &= \frac{1}{Z} P(C) P(s|C) P(\neg r|C) \\ &= \frac{1}{Z} \langle 0.5, 0.5 \rangle \langle 0.1, 0.5 \rangle \langle 0.2, 0.8 \rangle = \frac{1}{Z} \langle 0.01, 0.2 \rangle = \langle 1/21, 20/21 \rangle \\ P(R|c,s,w) &= \frac{1}{Z} P(R|c) P(w|s,R) \\ &= \frac{1}{Z} \langle 0.8, 0.2 \rangle \langle 0.99, 0.9 \rangle = \frac{1}{Z} \langle 0.792, 0.18 \rangle = \langle 22/27, 5/27 \rangle \\ P(R|\neg c,s,w) &= \frac{1}{Z} P(R|\neg c) P(w|s,R) \\ &= \frac{1}{Z} \langle 0.2, 0.8 \rangle \langle 0.99, 0.9 \rangle = \frac{1}{Z} \langle 0.198, 0.72 \rangle = \langle 11/51, 40/51 \rangle \end{split}$$

Strictly speaking, the transition matrix is only well-defined for the variant of MCMC in which the variable to be sampled is chosen randomly¹. (In the variant where the variables are chosen in a fixed order, the transition probabilities depend on where we are in the ordering.) Now consider the transition matrix.

• Entries on the diagonal correspond to self-loops. Such transitions can occur by sampling *either* variable. For example, for the self-loop on (c, r), we obtain:

$$t((c,r) \rightarrow (c,r)) = 0.5P(c|r,s) + 0.5P(r|c,s,w) = 17/27,$$

where the two factors of 0.5 are corresponding to the probability that the variables to be sampled are C and R, respectively.

• Entries where one variable is changed must sample that variable. For example,

$$t((c,r) \to (c,\neg r)) = 0.5P(\neg r|c,s,w) = 5/54$$

• Entries where both variables change cannot occur. For example,

$$t((c,r) \to (\neg c, \neg r)) = 0$$

This gives us the following transition matrix T, where the transition is from the state given by the row label to the state given by the column label:

 $^{^1}Slide\ 14\ of\ https://las.inf.ethz.ch/courses/pai-f17/slides/pai-07-bayesian-networks-mcmc.pdf$

	(c,r)	$(c, \neg r)$	$(\neg c, r)$	$(\neg c, \neg r)$
(c,r)	(17/27)	5/54	5/18	$0 \rightarrow$
$(c, \neg r)$	11/27	22/189	0	10/21
$(\neg c, r)$	2/9	0	59/153	20/51
$(\neg c, \neg r)$	$\begin{pmatrix} 0 \end{pmatrix}$	1/42	11/102	310/357 /

- (iii) T^2 represents the probability of going from each state to each state in two steps.
- (iv) T^n (as $n \to \infty$) represents the long-term probability of being in each state starting in each state; for ergodic T these probabilities are independent of the starting state, so every row of T is the same and represents the posterior distribution over states given the evidence.
- (v) We can produce very large powers of T with very few matrix multiplications. For example, we can get T^2 with one multiplication, T^4 with two, and T^{2^k} with k. Unfortunately, in a network with n non-event Boolean variables, the matrix is of size $2^n \times 2^n$, so each multiplication takes $O(2^{3n})$ operations.

2. Markov chains and detailed balance

Assume that you are given a Markov chain with state space Ω and transition matrix T, which is defined for all $x, y \in \Omega$ and $t \ge 0$ as $T(x, y) := P(X_{t+1} = y \mid X_t = x)$. Furthermore, let π be the stationary distribution of the chain.

(i) Show that, if for some t the current state X_t is distributed according to the stationary distribution and additionally the chain satisfies the detailed balance equations

$$\pi(x)T(x,y) = \pi(y)T(y,x), \text{ for all } x, y \in \Omega,$$

then the following holds for all $k \ge 0$ and $x_0, \ldots, x_k \in \Omega$:

$$P(X_t = x_0, \dots, X_{t+k} = x_k) = P(X_t = x_k, \dots, X_{t+k} = x_0).$$

(This is why a chain that satisfies detailed balance is called *reversible*.)

(ii) Show that, if T is a symmetric matrix, then the chain satisfies detailed balance, and the uniform distribution on Ω is stationary for that chain.

Solution

(i) We use the chain rule, as well as the detailed balance condition:

$$\begin{split} P(X_t = x_0, \dots, X_{t+k} = x_k) \\ &= P(X_t = x_0) P(X_{t+1} = x_1 \mid X_t = x_0) \dots P(X_{t+k} = x_k \mid X_{t+k-1} = x_{k-1}) \text{ ch. rule} \\ &= \pi(x_0) T(x_0, x_1) \dots T(x_{k-1}, x_k) \\ &= T(x_1, x_0) \pi(x_1) \dots T(x_{k-1}, x_k) \\ &= \dots \\ &= \dots \\ &= T(x_1, x_0) \dots T(x_k, x_{k-1}) \pi(x_k) \\ &= \pi(x_k) T(x_k, x_{k-1}) \dots T(x_1, x_0) \\ &= P(X_t = x_k) P(X_{t+1} = x_{k-1} \mid X_t = x_k) \dots P(X_{t+k} = x_0 \mid X_{t+k-1} = x_1) \quad X_t \sim \pi \\ &= P(X_t = x_k, \dots, X_{t+k} = x_0). \end{split}$$

(ii) By definition of a symmetric matrix, we have that $\pi(x)T(x,y) = \pi(x)T(y,x)$, for all $x, y \in \Omega$. Therefore, if $\pi(x) = \frac{1}{|\Omega|}$, for all $x \in \Omega$, then $\pi(x)T(x,y) = \pi(y)T(y,x)$, which means that detailed balance holds for the chain and the uniform distribution is stationary.