# 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 Bayesian network on Slide 9 of https://las.inf.ethz.ch/courses/pai-f16/slides/pai-06-bayesian-networks-sampling-annotated.pdf and how Gibbs 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 randomly<sup>1</sup>. (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:

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

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,

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

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:

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

- (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. Gibbs sampling

See .zip file on course website.

 $<sup>^1</sup>Slide\ 33\ of\ https://las.inf.ethz.ch/courses/pai-f16/slides/pai-06-bayesian-networks-sampling-annotated.pdf$ 

## 3. Markov chains and detailed balance

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

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

then the following holds for all  $k \geq 0$  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  $\Omega$  is stationary for that chain.

Solution

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

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

(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.