# 13 QUANTIFYING UNCERTAINTY

In which we see how an agent can tame uncertainty with degrees of belief.

# 13.1 ACTING UNDER UNCERTAINTY

UNCERTAINTY

Agents may need to handle **uncertainty**, whether due to partial observability, nondeterminism, or a combination of the two. An agent may never know for certain what state it's in or where it will end up after a sequence of actions.

We have seen problem-solving agents (Chapter 4) and logical agents (Chapters 7 and 11) designed to handle uncertainty by keeping track of a **belief state**—a representation of the set of all possible world states that it might be in—and generating a contingency plan that handles every possible eventuality that its sensors may report during execution. Despite its many virtues, however, this approach has significant drawbacks when taken literally as a recipe for creating agent programs:

- When interpreting partial sensor information, a logical agent must consider *every logically possible* explanation for the observations, no matter how unlikely. This leads to impossible large and complex belief-state representations.
- A correct contingent plan that handles every eventuality can grow arbitrarily large and must consider arbitrarily unlikely contingencies.
- Sometimes there is no plan that is guaranteed to achieve the goal—yet the agent must act. It must have some way to compare the merits of plans that are not guaranteed.

Suppose, for example, that an automated taxi!automated has the goal of delivering a passenger to the airport on time. The agent forms a plan,  $A_{90}$ , that involves leaving home 90 minutes before the flight departs and driving at a reasonable speed. Even though the airport is only about 5 miles away, a logical taxi agent will not be able to conclude with certainty that "Plan  $A_{90}$  will get us to the airport in time." Instead, it reaches the weaker conclusion "Plan  $A_{90}$  will get us to the airport in time, as long as the car doesn't break down or run out of gas, and I don't get into an accident, and there are no accidents on the bridge, and the plane doesn't leave early, and no meteorite hits the car, and . . . ." None of these conditions can be

deduced for sure, so the plan's success cannot be inferred. This is the qualification problem (page 268), for which we so far have seen no real solution.

Nonetheless, in some sense  $A_{90}$  is in fact the right thing to do. What do we mean by this? As we discussed in Chapter 2, we mean that out of all the plans that could be executed,  $A_{90}$  is expected to maximize the agent's performance measure (where the expectation is relative to the agent's knowledge about the environment). The performance measure includes getting to the airport in time for the flight, avoiding a long, unproductive wait at the airport, and avoiding speeding tickets along the way. The agent's knowledge cannot guarantee any of these outcomes for  $A_{90}$ , but it can provide some degree of belief that they will be achieved. Other plans, such as  $A_{180}$ , might increase the agent's belief that it will get to the airport on time, but also increase the likelihood of a long wait. The right thing to do—the rational decision—therefore depends on both the relative importance of various goals and the likelihood that, and degree to which, they will be achieved. The remainder of this section hones these ideas, in preparation for the development of the general theories of uncertain reasoning and rational decisions that we present in this and subsequent chapters.

13.1.1

Let's consider an example of uncertain reasoning: diagnosing a dental patient's toothache. Diagnosis—whether for medicine, automobile repair, or whatever—almost always involves uncertainty. Let us try to write rules for dental diagnosis using propositional logic, so that we can see how the logical approach breaks down. Consider the following simple rule:

 $Toothache \Rightarrow Cavity$ .

**Summarizing uncertainty** 

The problem is that this rule is wrong. Not all patients with toothaches have cavities; some of them have gum disease, an abscess, or one of several other problems:

 $Toothache \Rightarrow Cavity \lor GumProblem \lor Abscess...$ 

Unfortunately, in order to make the rule true, we have to add an almost unlimited list of possible problems. We could try turning the rule into a causal rule:

 $Cavity \Rightarrow Toothache$ .

But this rule is not right either; not all cavities cause pain. The only way to fix the rule is to make it logically exhaustive: to augment the left-hand side with all the qualifications required for a cavity to cause a toothache. Trying to use logic to cope with a domain like medical diagnosis thus fails for three main reasons:

- Laziness: It is too much work to list the complete set of antecedents or consequents needed to ensure an exceptionless rule and too hard to use such rules.
- Theoretical ignorance: Medical science has no complete theory for the domain.
- Practical ignorance: Even if we know all the rules, we might be uncertain about a particular patient because not all the necessary tests have been or can be run.

The connection between toothaches and cavities is just not a logical consequence in either direction. This is typical of the medical domain, as well as most other judgmental domains: law, business, design, automobile repair, gardening, dating, and so on. The agent's knowledge



LAZINESS

**IGNORANCE** PRACTICAL IGNORANCE DEGREE OF BELIEF
PROBABILITY
THEORY



can at best provide only a **degree of belief** in the relevant sentences. Our main tool for dealing with degrees of belief is **probability theory**. In the terminology of Section 8.1, the **ontological commitments** of logic and probability theory are the same—that the world is composed of facts that do or do not hold in any particular case—but the **epistemological commitments** are different: a logical agent believes each sentence to be true or false or has no opinion, whereas a probabilistic agent may have a numerical degree of belief between 0 (for sentences that are certainly false) and 1 (certainly true).

Probability provides a way of summarizing the uncertainty that comes from our laziness and ignorance, thereby solving the qualification problem. We might not know for sure what afflicts a particular patient, but we believe that there is, say, an 80% chance—that is, a probability of 0.8—that the patient who has a toothache has a cavity. That is, we expect that out of all the situations that are indistinguishable from the current situation as far as our knowledge goes, the patient will have a cavity in 80% of them. This belief could be derived from statistical data—80% of the toothache patients seen so far have had cavities—or from some general dental knowledge, or from a combination of evidence sources.

One confusing point is that at the time of our diagnosis, there is no uncertainty in the actual world: the patient either has a cavity or doesn't. So what does it mean to say the probability of a cavity is 0.8? Shouldn't it be either 0 or 1? The answer is that probability statements are made with respect to a knowledge state, not with respect to the real world. We say "The probability that the patient has a cavity, given that she has a toothache, is 0.8." If we later learn that the patient has a history of gum disease, we can make a different statement: "The probability that the patient has a cavity, given that she has a toothache and a history of gum disease, is 0.4." If we gather further conclusive evidence against a cavity, we can say "The probability that the patient has a cavity, given all we now know, is almost 0." Note that these statements do not contradict each other; each is a separate assertion about a different knowledge state.

# 13.1.2 Uncertainty and rational decisions

Consider again the  $A_{90}$  plan for getting to the airport. Suppose it gives us a 97% chance of catching our flight. Does this mean it is a rational choice? Not necessarily: there might be other plans, such as  $A_{180}$ , with higher probabilities. If it is vital not to miss the flight, then it is worth risking the longer wait at the airport. What about  $A_{1440}$ , a plan that involves leaving home 24 hours in advance? In most circumstances, this is not a good choice, because although it almost guarantees getting there on time, it involves an intolerable wait—not to mention a possibly unpleasant diet of airport food.

PREFERENCE OUTCOME

UTILITY THEORY

To make such choices, an agent must first have **preferences** between the different possible **outcomes** of the various plans. An outcome is a completely specified state, including such factors as whether the agent arrives on time and the length of the wait at the airport. We use **utility theory** to represent and reason with preferences. (The term **utility** is used here in the sense of "the quality of being useful," not in the sense of the electric company or water works.) Utility theory says that every state has a degree of usefulness, or utility, to an agent and that the agent will prefer states with higher utility.

The utility of a state is relative to an agent. For example, the utility of a state in which White has checkmated Black in a game of chess is obviously high for the agent playing White, but low for the agent playing Black. But we can't go strictly by the scores of 1, 1/2, and 0 that are dictated by the rules of tournament chess—some players (including the authors) might be thrilled with a draw against the world champion, whereas other players (including the former world champion) might not. There is no accounting for taste or preferences: you might think that an agent who prefers jalapeño bubble-gum ice cream to chocolate chocolate chip is odd or even misguided, but you could not say the agent is irrational. A utility function can account for any set of preferences—quirky or typical, noble or perverse. Note that utilities can account for altruism, simply by including the welfare of others as one of the factors.

DECISION THEORY

Preferences, as expressed by utilities, are combined with probabilities in the general theory of rational decisions called **decision theory**:

#### Decision theory = probability theory + utility theory.



The fundamental idea of decision theory is that an agent is rational if and only if it chooses the action that yields the highest expected utility, averaged over all the possible outcomes of the action. This is called the principle of **maximum expected utility** (MEU). Note that "expected" might seem like a vague, hypothetical term, but as it is used here it has a precise meaning: it means the "average," or "statistical mean" of the outcomes, weighted by the probability of the outcome. We saw this principle in action in Chapter 5 when we touched briefly on optimal decisions in backgammon; it is in fact a completely general principle.

Figure 13.1 sketches the structure of an agent that uses decision theory to select actions. The agent is identical, at an abstract level, to the agents described in Chapters 4 and 7 that maintain a belief state reflecting the history of percepts to date. The primary difference is that the decision-theoretic agent's belief state represents not just the *possibilities* for world states but also their *probabilities*. Given the belief state, the agent can make probabilistic predictions of action outcomes and hence select the action with highest expected utility. This chapter and the next concentrate on the task of representing and computing with probabilistic information in general. Chapter 15 deals with methods for the specific tasks of representing and updating the belief state over time and predicting the environment. Chapter 16 covers utility theory in more depth, and Chapter 17 develops algorithms for planning sequences of actions in uncertain environments.

# 13.2 Basic Probability Notation

For our agent to represent and use probabilistic information, we need a formal language. The language of probability theory has traditionally been informal, written by human mathematicians to other human mathematicians. Appendix A includes a standard introduction to elementary probability theory; here, we take an approach more suited to the needs of AI and more consistent with the concepts of formal logic.

**function** DT-AGENT(percept) **returns** an action

**persistent**: belief\_state, probabilistic beliefs about the current state of the world action, the agent's action

update belief\_state based on action and percept calculate outcome probabilities for actions, given action descriptions and current belief\_state select action with highest expected utility given probabilities of outcomes and utility information return action

**Figure 13.1** A decision-theoretic agent that selects rational actions.

# 13.2.1 What probabilities are about

Like logical assertions, probabilistic assertions are about possible worlds. Whereas logical assertions say which possible worlds are strictly ruled out (all those in which the assertion is false), probabilistic assertions talk about how probable the various worlds are. In probability theory, the set of all possible worlds is called the **sample space**. The possible worlds are *mutually exclusive* and *exhaustive*—two possible worlds cannot both be the case, and one possible world must be the case. For example, if we are about to roll two (distinguishable) dice, there are 36 possible worlds to consider:  $(1,1), (1,2), \ldots, (6,6)$ . The Greek letter  $\Omega$  (uppercase omega) is used to refer to the sample space, and  $\omega$  (lowercase omega) refers to elements of the space, that is, particular possible worlds.

SAMPLE SPACE

PROBABILITY MODEL

**EVENT** 

A fully specified **probability model** associates a numerical probability  $P(\omega)$  with each possible world. The basic axioms of probability theory say that every possible world has a probability between 0 and 1 and that the total probability of the set of possible worlds is 1:

$$0 \le P(\omega) \le 1$$
 for every  $\omega$  and  $\sum_{\omega \in \Omega} P(\omega) = 1$ . (13.1)

For example, if we assume that each die is fair and the rolls don't interfere with each other, then each of the possible worlds (1,1), (1,2), ..., (6,6) has probability 1/36. On the other hand, if the dice conspire to produce the same number, then the worlds (1,1), (2,2), (3,3), etc., might have higher probabilities, leaving the others with lower probabilities.

Probabilistic assertions and queries are not usually about particular possible worlds, but about sets of them. For example, we might be interested in the cases where the two dice add up to 11, the cases where doubles are rolled, and so on. In probability theory, these sets are called **events**—a term already used extensively in Chapter 12 for a different concept. In AI, the sets are always described by **propositions** in a formal language. (One such language is described in Section 13.2.2.) For each proposition, the corresponding set contains just those possible worlds in which the proposition holds. The probability associated with a proposition

<sup>&</sup>lt;sup>1</sup> For now, we assume a discrete, countable set of worlds. The proper treatment of the continuous case brings in certain complications that are less relevant for most purposes in AI.

is defined to be the sum of the probabilities of the worlds in which it holds:

For any proposition 
$$\phi$$
,  $P(\phi) = \sum_{\omega \in \phi} P(\omega)$ . (13.2)

For example, when rolling fair dice, we have P(Total = 11) = P((5,6)) + P((6,5)) = 1/36 + 1/36 = 1/18. Note that probability theory does not require complete knowledge of the probabilities of each possible world. For example, if we believe the dice conspire to produce the same number, we might *assert* that P(doubles) = 1/4 without knowing whether the dice prefer double 6 to double 2. Just as with logical assertions, this assertion *constrains* the underlying probability model without fully determining it.

UNCONDITIONAL PROBABILITY PRIOR PROBABILITY

**EVIDENCE** 

CONDITIONAL PROBABILITY POSTERIOR PROBABILITY Probabilities such as P(Total = 11) and P(doubles) are called **unconditional** or **prior probabilities** (and sometimes just "priors" for short); they refer to degrees of belief in propositions in the absence of any other information. Most of the time, however, we have some information, usually called **evidence**, that has already been revealed. For example, the first die may already be showing a 5 and we are waiting with bated breath for the other one to stop spinning. In that case, we are interested not in the unconditional probability of rolling doubles, but the **conditional** or **posterior** probability (or just "posterior" for short) of rolling doubles given that the first die is a 5. This probability is written  $P(doubles \mid Die_1 = 5)$ , where the " $\mid$ " is pronounced "given." Similarly, if I am going to the dentist for a regular checkup, the probability P(cavity) = 0.2 might be of interest; but if I go to the dentist because I have a toothache, it's  $P(cavity \mid toothache) = 0.6$  that matters. Note that the precedence of " $\mid$ " is such that any expression of the form  $P(\ldots)$  always means  $P((\ldots)|(\ldots))$ .

It is important to understand that P(cavity) = 0.2 is still valid after toothache is observed; it just isn't especially useful. When making decisions, an agent needs to condition on all the evidence it has observed. It is also important to understand the difference between conditioning and logical implication. The assertion that  $P(cavity \mid toothache) = 0.6$  does not mean "Whenever toothache is true, conclude that cavity is true with probability 0.6" rather it means "Whenever toothache is true and we have no further information, conclude that cavity is true with probability 0.6." The extra condition is important; for example, if we had the further information that the dentist found no cavities, we definitely would not want to conclude that cavity is true with probability 0.6; instead we need to use  $P(cavity \mid toothache \land \neg cavity) = 0$ .

Mathematically speaking, conditional probabilities are defined in terms of unconditional probabilities as follows: for any propositions a and b, we have

$$P(a \mid b) = \frac{P(a \land b)}{P(b)}, \tag{13.3}$$

which holds whenever P(b) > 0. For example,

$$P(doubles \mid Die_1 = 5) = \frac{P(doubles \land Die_1 = 5)}{P(Die_1 = 5)}$$

The definition makes sense if you remember that observing b rules out all those possible worlds where b is false, leaving a set whose total probability is just P(b). Within that set, the a-worlds satisfy  $a \wedge b$  and constitute a fraction  $P(a \wedge b)/P(b)$ .

PRODUCT RULE

The definition of conditional probability, Equation (13.3), can be written in a different form called the **product rule**:

$$P(a \wedge b) = P(a \mid b)P(b) ,$$

The product rule is perhaps easier to remember: it comes from the fact that, for a and b to be true, we need b to be true, and we also need a to be true given b.

#### 13.2.2 The language of propositions in probability assertions

In this chapter and the next, propositions describing sets of possible worlds are written in a notation that combines elements of propositional logic and constraint satisfaction notation. In the terminology of Section 2.4.7, it is a **factored representation**, in which a possible world is represented by a set of variable/value pairs.

RANDOM VARIABLE

DOMAIN

Variables in probability theory are called **random variables** and their names begin with an uppercase letter. Thus, in the dice example, Total and  $Die_1$  are random variables. Every random variable has a **domain**—the set of possible values it can take on. The domain of Total for two dice is the set  $\{2, \ldots, 12\}$  and the domain of  $Die_1$  is  $\{1, \ldots, 6\}$ . A Boolean random variable has the domain  $\{true, false\}$  (notice that values are always lowercase); for example, the proposition that doubles are rolled can be written as Doubles = true. By convention, propositions of the form A = true are abbreviated simply as a, while A = false is abbreviated as  $\neg a$ . (The uses of doubles, cavity, and toothache in the preceding section are abbreviations of this kind.) As in CSPs, domains can be sets of arbitrary tokens; we might choose the domain of Age to be  $\{juvenile, teen, adult\}$  and the domain of Weather might be  $\{sunny, rain, cloudy, snow\}$ . When no ambiguity is possible, it is common to use a value by itself to stand for the proposition that a particular variable has that value; thus, sunny can stand for Weather = sunny.

The preceding examples all have finite domains. Variables can have infinite domains, too—either discrete (like the integers) or continuous (like the reals). For any variable with an ordered domain, inequalities are also allowed, such as  $NumberOfAtomsInUniverse > 10^{70}$ .

Finally, we can combine these sorts of elementary propositions (including the abbreviated forms for Boolean variables) by using the connectives of propositional logic. For example, we can express "The probability that the patient has a cavity, given that she is a teenager with no toothache, is 0.1" as follows:

$$P(cavity | \neg toothache \land teen) = 0.1$$
.

Sometimes we will want to talk about the probabilities of *all* the possible values of a random variable. We could write:

$$P(Weather = sunny) = 0.6$$
  
 $P(Weather = rain) = 0.1$   
 $P(Weather = cloudy) = 0.29$   
 $P(Weather = snow) = 0.01$ ,

but as an abbreviation we will allow

$$\mathbf{P}(Weather) = \langle 0.6, 0.1, 0.29, 0.01 \rangle$$
,

PROBABILITY DISTRIBUTION where the bold **P** indicates that the result is a vector of numbers, and where we assume a predefined ordering  $\langle sunny, rain, cloudy, snow \rangle$  on the domain of *Weather*. We say that the **P** statement defines a **probability distribution** for the random variable *Weather*. The **P** notation is also used for conditional distributions:  $\mathbf{P}(X \mid Y)$  gives the values of  $P(X = x_i \mid Y = y_j)$  for each possible i, j pair.

For continuous variables, it is not possible to write out the entire distribution as a vector, because there are infinitely many values. Instead, we can define the probability that a random variable takes on some value x as a parameterized function of x. For example, the sentence

$$P(NoonTemp = x) = Uniform_{[18C,26C]}(x)$$

PROBABILITY DENSITY FUNCTION expresses the belief that the temperature at noon is distributed uniformly between 18 and 26 degrees Celsius. We call this a **probability density function**.

Probability density functions (sometimes called **pdfs**) differ in meaning from discrete distributions. Saying that the probability density is uniform from 18C to 26C means that there is a 100% chance that the temperature will fall somewhere in that 8C-wide region and a 50% chance that it will fall in any 4C-wide region, and so on. We write the probability density for a continuous random variable X at value x as P(X=x) or just P(x); the intuitive definition of P(x) is the probability that X falls within an arbitrarily small region beginning at x, divided by the width of the region:

$$P(x) = \lim_{dx \to 0} P(x \le X \le x + dx)/dx.$$

For NoonTemp we have

$$P(\textit{NoonTemp} = x) = \textit{Uniform}_{[18C, 26C]}(x) = \left\{ \begin{array}{l} \frac{1}{8C} \text{ if } 18C \leq x \leq 26C \\ 0 \text{ otherwise} \end{array} \right.,$$

where C stands for centigrade (not for a constant). In  $P(NoonTemp = 20.18C) = \frac{1}{8C}$ , note that  $\frac{1}{8C}$  is not a probability, it is a probability density. The probability that NoonTemp is exactly 20.18C is zero, because 20.18C is a region of width 0. Some authors use different symbols for discrete distributions and density functions; we use P in both cases, since confusion seldom arises and the equations are usually identical. Note that probabilities are unitless numbers, whereas density functions are measured with a unit, in this case reciprocal degrees.

In addition to distributions on single variables, we need notation for distributions on multiple variables. Commas are used for this. For example, P(Weather, Cavity) denotes the probabilities of all combinations of the values of Weather and Cavity. This is a  $4 \times 2$  table of probabilities called the **joint probability distribution** of Weather and Cavity. We can also mix variables with and without values; P(sunny, Cavity) would be a two-element vector giving the probabilities of a sunny day with a cavity and a sunny day with no cavity. The P notation makes certain expressions much more concise than they might otherwise be. For example, the product rules for all possible values of Weather and Cavity can be written as a single equation:

$$\mathbf{P}(Weather, Cavity) = \mathbf{P}(Weather \mid Cavity)\mathbf{P}(Cavity)$$
,

JOINT PROBABILITY DISTRIBUTION

instead of as these  $4 \times 2 = 8$  equations (using abbreviations W and C):

$$\begin{split} &P(W=sunny \land C=true) = P(W=sunny | C=true) \ P(C=true) \\ &P(W=rain \land C=true) = P(W=rain | C=true) \ P(C=true) \\ &P(W=cloudy \land C=true) = P(W=cloudy | C=true) \ P(C=true) \\ &P(W=snow \land C=true) = P(W=snow | C=true) \ P(C=true) \\ &P(W=sunny \land C=false) = P(W=sunny | C=false) \ P(C=false) \\ &P(W=rain \land C=false) = P(W=rain | C=false) \ P(C=false) \\ &P(W=cloudy \land C=false) = P(W=cloudy | C=false) \ P(C=false) \\ &P(W=snow \land C=false) = P(W=snow | C=false) \ P(C=false) \ . \end{split}$$

As a degenerate case, P(sunny, cavity) has no variables and thus is a one-element vector that is the probability of a sunny day with a cavity, which could also be written as P(sunny, cavity) or  $P(sunny \land cavity)$ . We will sometimes use P notation to derive results about individual P values, and when we say "P(sunny) = 0.6" it is really an abbreviation for "P(sunny) is the one-element vector (0.6), which means that P(sunny) = 0.6."

Now we have defined a syntax for propositions and probability assertions and we have given part of the semantics: Equation (13.2) defines the probability of a proposition as the sum of the probabilities of worlds in which it holds. To complete the semantics, we need to say what the worlds are and how to determine whether a proposition holds in a world. We borrow this part directly from the semantics of propositional logic, as follows. A possible world is defined to be an assignment of values to all of the random variables under consideration. It is easy to see that this definition satisfies the basic requirement that possible worlds be mutually exclusive and exhaustive (Exercise 13.5). For example, if the random variables are Cavity, Toothache, and Weather, then there are  $2 \times 2 \times 4 = 16$  possible worlds. Furthermore, the truth of any given proposition, no matter how complex, can be determined easily in such worlds using the same recursive definition of truth as for formulas in propositional logic.

From the preceding definition of possible worlds, it follows that a probability model is completely determined by the joint distribution for all of the random variables—the so-called **full joint probability distribution**. For example, if the variables are Cavity, Toothache, and Weather, then the full joint distribution is given by P(Cavity, Toothache, Weather). This joint distribution can be represented as a  $2 \times 2 \times 4$  table with 16 entries. Because every proposition's probability is a sum over possible worlds, a full joint distribution suffices, in principle, for calculating the probability of any proposition.

# 13.2.3 Probability axioms and their reasonableness

The basic axioms of probability (Equations (13.1) and (13.2)) imply certain relationships among the degrees of belief that can be accorded to logically related propositions. For example, we can derive the familiar relationship between the probability of a proposition and the probability of its negation:

$$\begin{array}{ll} P(\neg a) &=& \sum_{\omega \in \neg a} P(\omega) & \text{by Equation (13.2)} \\ &=& \sum_{\omega \in \neg a} P(\omega) + \sum_{\omega \in a} P(\omega) - \sum_{\omega \in a} P(\omega) & \text{grouping the first two terms} \\ &=& \sum_{\omega \in \Omega} P(\omega) - \sum_{\omega \in a} P(\omega) & \text{by (13.1) and (13.2)}. \end{array}$$



FULL JOINT PROBABILITY DISTRIBUTION INCLUSION-EXCLUSION PRINCIPLE We can also derive the well-known formula for the probability of a disjunction, sometimes called the **inclusion–exclusion principle**:

$$P(a \lor b) = P(a) + P(b) - P(a \land b). \tag{13.4}$$

This rule is easily remembered by noting that the cases where a holds, together with the cases where b holds, certainly cover all the cases where  $a \lor b$  holds; but summing the two sets of cases counts their intersection twice, so we need to subtract  $P(a \land b)$ . The proof is left as an exercise (Exercise 13.6).

KOLMOGOROV'S AXIOMS Equations (13.1) and (13.4) are often called **Kolmogorov's axioms** in honor of the Russian mathematician Andrei Kolmogorov, who showed how to build up the rest of probability theory from this simple foundation and how to handle the difficulties caused by continuous variables.<sup>2</sup> While Equation (13.2) has a definitional flavor, Equation (13.4) reveals that the axioms really do constrain the degrees of belief an agent can have concerning logically related propositions. This is analogous to the fact that a logical agent cannot simultaneously believe A, B, and  $\neg(A \land B)$ , because there is no possible world in which all three are true. With probabilities, however, statements refer not to the world directly, but to the agent's own state of knowledge. Why, then, can an agent not hold the following set of beliefs (even though they violate Kolmogorov's axioms)?

$$P(a) = 0.4$$
  $P(a \land b) = 0.0$   
 $P(b) = 0.3$   $P(a \lor b) = 0.8$ . (13.5)

This kind of question has been the subject of decades of intense debate between those who advocate the use of probabilities as the only legitimate form for degrees of belief and those who advocate alternative approaches.

One argument for the axioms of probability, first stated in 1931 by Bruno de Finetti (and translated into English in de Finetti (1993)), is as follows: If an agent has some degree of belief in a proposition a, then the agent should be able to state odds at which it is indifferent to a bet for or against a.<sup>3</sup> Think of it as a game between two agents: Agent 1 states, "my degree of belief in event a is 0.4." Agent 2 is then free to choose whether to wager for or against a at stakes that are consistent with the stated degree of belief. That is, Agent 2 could choose to accept Agent 1's bet that a will occur, offering \$6 against Agent 1's \$4. Or Agent 2 could accept Agent 1's bet that  $\neg a$  will occur, offering \$4 against Agent 1's \$6. Then we observe the outcome of a, and whoever is right collects the money. If an agent's degrees of belief do not accurately reflect the world, then you would expect that it would tend to lose money over the long run to an opposing agent whose beliefs more accurately reflect the state of the world.



But de Finetti proved something much stronger: If Agent 1 expresses a set of degrees of belief that violate the axioms of probability theory then there is a combination of bets by Agent 2 that guarantees that Agent 1 will lose money every time. For example, suppose that Agent 1 has the set of degrees of belief from Equation (13.5). Figure 13.2 shows that if Agent

 $<sup>^2</sup>$  The difficulties include the **Vitali set**, a well-defined subset of the interval [0,1] with no well-defined size.

<sup>&</sup>lt;sup>3</sup> One might argue that the agent's preferences for different bank balances are such that the possibility of losing \$1 is not counterbalanced by an equal possibility of winning \$1. One possible response is to make the bet amounts small enough to avoid this problem. Savage's analysis (1954) circumvents the issue altogether.

2 chooses to bet \$4 on a, \$3 on b, and \$2 on  $\neg(a \lor b)$ , then Agent 1 always loses money, regardless of the outcomes for a and b. De Finetti's theorem implies that no rational agent can have beliefs that violate the axioms of probability.

Agent 1		Agent 2		Outcomes and payoffs to Agent 1			
Proposition	Belief	Bet	Stakes	a, b	$a, \neg b$	$\neg a, b$	$\neg a, \neg b$
a	0.4	a	4 to 6	-6	-6	4	4
b	0.3	b	3 to 7	<b>–</b> 7	3	<b>-</b> 7	3
$a \vee b$	0.8	$\neg(a \lor b)$	2 to 8	2	2	2	-8
				-11	-1	-1	-1

**Figure 13.2** Because Agent 1 has inconsistent beliefs, Agent 2 is able to devise a set of bets that guarantees a loss for Agent 1, no matter what the outcome of a and b.

One common objection to de Finetti's theorem is that this betting game is rather contrived. For example, what if one refuses to bet? Does that end the argument? The answer is that the betting game is an abstract model for the decision-making situation in which every agent is *unavoidably* involved at every moment. Every action (including inaction) is a kind of bet, and every outcome can be seen as a payoff of the bet. Refusing to bet is like refusing to allow time to pass.

Other strong philosophical arguments have been put forward for the use of probabilities, most notably those of Cox (1946), Carnap (1950), and Jaynes (2003). They each construct a set of axioms for reasoning with degrees of beliefs: no contradictions, correspondence with ordinary logic (for example, if belief in A goes up, then belief in  $\neg A$  must go down), and so on. The only controversial axiom is that degrees of belief must be numbers, or at least act like numbers in that they must be transitive (if belief in A is greater than belief in B, which is greater than belief in C, then belief in A must be greater than C) and comparable (the belief in A must be one of equal to, greater than, or less than belief in B). It can then be proved that probability is the only approach that satisfies these axioms.

The world being the way it is, however, practical demonstrations sometimes speak louder than proofs. The success of reasoning systems based on probability theory has been much more effective in making converts. We now look at how the axioms can be deployed to make inferences.

## 13.3 Inference Using Full Joint Distributions

PROBABILISTIC INFERENCE

In this section we describe a simple method for **probabilistic inference**—that is, the computation of posterior probabilities for query propositions given observed evidence. We use the full joint distribution as the "knowledge base" from which answers to all questions may be derived. Along the way we also introduce several useful techniques for manipulating equations involving probabilities.

#### WHERE DO PROBABILITIES COME FROM?

There has been endless debate over the source and status of probability numbers. The **frequentist** position is that the numbers can come only from *experiments*: if we test 100 people and find that 10 of them have a cavity, then we can say that the probability of a cavity is approximately 0.1. In this view, the assertion "the probability of a cavity is 0.1" means that 0.1 is the fraction that would be observed in the limit of infinitely many samples. From any finite sample, we can estimate the true fraction and also calculate how accurate our estimate is likely to be.

The **objectivist** view is that probabilities are real aspects of the universe—propensities of objects to behave in certain ways—rather than being just descriptions of an observer's degree of belief. For example, the fact that a fair coin comes up heads with probability 0.5 is a propensity of the coin itself. In this view, frequentist measurements are attempts to observe these propensities. Most physicists agree that quantum phenomena are objectively probabilistic, but uncertainty at the macroscopic scale—e.g., in coin tossing—usually arises from ignorance of initial conditions and does not seem consistent with the propensity view.

The **subjectivist** view describes probabilities as a way of characterizing an agent's beliefs, rather than as having any external physical significance. The subjective **Bayesian** view allows any self-consistent ascription of prior probabilities to propositions, but then insists on proper Bayesian updating as evidence arrives.

In the end, even a strict frequentist position involves subjective analysis because of the **reference class** problem: in trying to determine the outcome probability of a *particular* experiment, the frequentist has to place it in a reference class of "similar" experiments with known outcome frequencies. I. J. Good (1983, p. 27) wrote, "every event in life is unique, and every real-life probability that we estimate in practice is that of an event that has never occurred before." For example, given a particular patient, a frequentist who wants to estimate the probability of a cavity will consider a reference class of other patients who are similar in important ways—age, symptoms, diet—and see what proportion of them had a cavity. If the dentist considers everything that is known about the patient—weight to the nearest gram, hair color, mother's maiden name—then the reference class becomes empty. This has been a vexing problem in the philosophy of science.

The **principle of indifference** attributed to Laplace (1816) states that propositions that are syntactically "symmetric" with respect to the evidence should be accorded equal probability. Various refinements have been proposed, culminating in the attempt by Carnap and others to develop a rigorous **inductive logic**, capable of computing the correct probability for any proposition from any collection of observations. Currently, it is believed that no unique inductive logic exists; rather, any such logic rests on a subjective prior probability distribution whose effect is diminished as more observations are collected.

	toot	hache	$\neg toothache$		
	catch	$\neg catch$	catch	$\neg catch$	
cavity	0.108	0.012	0.072	0.008	
$\neg cavity$	0.016	0.064	0.144	0.576	

**Figure 13.3** A full joint distribution for the *Toothache*, *Cavity*, *Catch* world.

We begin with a simple example: a domain consisting of just the three Boolean variables Toothache, Cavity, and Catch (the dentist's nasty steel probe catches in my tooth). The full joint distribution is a  $2 \times 2 \times 2$  table as shown in Figure 13.3.

Notice that the probabilities in the joint distribution sum to 1, as required by the axioms of probability. Notice also that Equation (13.2) gives us a direct way to calculate the probability of any proposition, simple or complex: simply identify those possible worlds in which the proposition is true and add up their probabilities. For example, there are six possible worlds in which  $cavity \lor toothache$  holds:

$$P(cavity \lor toothache) = 0.108 + 0.012 + 0.072 + 0.008 + 0.016 + 0.064 = 0.28$$
.

One particularly common task is to extract the distribution over some subset of variables or a single variable. For example, adding the entries in the first row gives the unconditional or **marginal probability**<sup>4</sup> of *cavity*:

$$P(cavity) = 0.108 + 0.012 + 0.072 + 0.008 = 0.2$$
.

MARGINALIZATION

MARGINAL

PROBABILITY

This process is called **marginalization**, or **summing out**—because we sum up the probabilities for each possible value of the other variables, thereby taking them out of the equation. We can write the following general marginalization rule for any sets of variables **Y** and **Z**:

$$\mathbf{P}(\mathbf{Y}) = \sum_{\mathbf{z} \in \mathbf{Z}_{\mathbf{z}}} \mathbf{P}(\mathbf{Y}, \mathbf{z}) , \qquad (13.6)$$

where  $\sum_{z \in Z}$  means to sum over all the possible combinations of values of the set of variables Z. We sometimes abbreviate this as  $\sum_z$ , leaving Z implicit. We just used the rule as

$$\mathbf{P}(Cavity) = \sum_{\mathbf{z} \in \{Catch, Toothache\}} \mathbf{P}(Cavity, \mathbf{z}).$$
(13.7)

A variant of this rule involves conditional probabilities instead of joint probabilities, using the product rule:

$$\mathbf{P}(\mathbf{Y}) = \sum_{\mathbf{z}} \mathbf{P}(\mathbf{Y} \mid \mathbf{z}) P(\mathbf{z}) . \tag{13.8}$$

CONDITIONING

This rule is called **conditioning**. Marginalization and conditioning turn out to be useful rules for all kinds of derivations involving probability expressions.

In most cases, we are interested in computing *conditional* probabilities of some variables, given evidence about others. Conditional probabilities can be found by first using

<sup>&</sup>lt;sup>4</sup> So called because of a common practice among actuaries of writing the sums of observed frequencies in the margins of insurance tables.

Equation (13.3) to obtain an expression in terms of unconditional probabilities and then evaluating the expression from the full joint distribution. For example, we can compute the probability of a cavity, given evidence of a toothache, as follows:

$$P(cavity \mid toothache) = \frac{P(cavity \land toothache)}{P(toothache)}$$
  
=  $\frac{0.108 + 0.012}{0.108 + 0.012 + 0.016 + 0.064} = 0.6$ .

Just to check, we can also compute the probability that there is no cavity, given a toothache:

$$\begin{split} P(\neg cavity \,|\, toothache) \; &= \; \frac{P(\neg cavity \wedge toothache)}{P(toothache)} \\ &= \; \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4 \; . \end{split}$$

The two values sum to 1.0, as they should. Notice that in these two calculations the term 1/P(toothache) remains constant, no matter which value of Cavity we calculate. In fact, it can be viewed as a **normalization** constant for the distribution  $P(Cavity \mid toothache)$ , ensuring that it adds up to 1. Throughout the chapters dealing with probability, we use  $\alpha$  to denote such constants. With this notation, we can write the two preceding equations in one:

$$\begin{aligned} \mathbf{P}(\textit{Cavity} \mid \textit{toothache}) &= \alpha \, \mathbf{P}(\textit{Cavity}, \textit{toothache}) \\ &= \alpha \, [\mathbf{P}(\textit{Cavity}, \textit{toothache}, \textit{catch}) + \mathbf{P}(\textit{Cavity}, \textit{toothache}, \neg \textit{catch})] \\ &= \alpha \, [\langle 0.108, 0.016 \rangle + \langle 0.012, 0.064 \rangle] = \alpha \, \langle 0.12, 0.08 \rangle = \langle 0.6, 0.4 \rangle \; . \end{aligned}$$

In other words, we can calculate  $P(Cavity \mid toothache)$  even if we don't know the value of P(toothache)! We temporarily forget about the factor 1/P(toothache) and add up the values for cavity and  $\neg cavity$ , getting 0.12 and 0.08. Those are the correct relative proportions, but they don't sum to 1, so we normalize them by dividing each one by 0.12 + 0.08, getting the true probabilities of 0.6 and 0.4. Normalization turns out to be a useful shortcut in many probability calculations, both to make the computation easier and to allow us to proceed when some probability assessment (such as P(toothache)) is not available.

From the example, we can extract a general inference procedure. We begin with the case in which the query involves a single variable, X (Cavity in the example). Let  $\mathbf{E}$  be the list of evidence variables (just Toothache in the example), let  $\mathbf{e}$  be the list of observed values for them, and let  $\mathbf{Y}$  be the remaining unobserved variables (just Catch in the example). The query is  $\mathbf{P}(X \mid \mathbf{e})$  and can be evaluated as

$$\mathbf{P}(X \mid \mathbf{e}) = \alpha \, \mathbf{P}(X, \mathbf{e}) = \alpha \sum_{\mathbf{y}} \mathbf{P}(X, \mathbf{e}, \mathbf{y}) , \qquad (13.9)$$

where the summation is over all possible ys (i.e., all possible combinations of values of the unobserved variables Y). Notice that together the variables X, E, and Y constitute the complete set of variables for the domain, so P(X, e, y) is simply a subset of probabilities from the full joint distribution.

Given the full joint distribution to work with, Equation (13.9) can answer probabilistic queries for discrete variables. It does not scale well, however: for a domain described by n Boolean variables, it requires an input table of size  $O(2^n)$  and takes  $O(2^n)$  time to process the

NORMALIZATION

Section 13.3.

table. In a realistic problem we could easily have n > 100, making  $O(2^n)$  impractical. The full joint distribution in tabular form is just not a practical tool for building reasoning systems. Instead, it should be viewed as the theoretical foundation on which more effective approaches may be built, just as truth tables formed a theoretical foundation for more practical algorithms like DPLL. The remainder of this chapter introduces some of the basic ideas required in preparation for the development of realistic systems in Chapter 14.

#### 13.4 INDEPENDENCE

Let us expand the full joint distribution in Figure 13.3 by adding a fourth variable, Weather. The full joint distribution then becomes P(Toothache, Catch, Cavity, Weather), which has  $2 \times 2 \times 2 \times 4 = 32$  entries. It contains four "editions" of the table shown in Figure 13.3, one for each kind of weather. What relationship do these editions have to each other and to the original three-variable table? For example, how are P(toothache, catch, cavity, cloudy) and P(toothache, catch, cavity) related? We can use the product rule:

P(toothache, catch, cavity, cloudy)

 $= P(cloudy \mid toothache, catch, cavity)P(toothache, catch, cavity)$ .

Now, unless one is in the deity business, one should not imagine that one's dental problems influence the weather. And for indoor dentistry, at least, it seems safe to say that the weather does not influence the dental variables. Therefore, the following assertion seems reasonable:

$$P(cloudy \mid toothache, catch, cavity) = P(cloudy)$$
. (13.10)

From this, we can deduce

 $P(toothache, catch, cavity, cloudy) = P(cloudy)P(toothache, catch, cavity) \; .$ 

A similar equation exists for *every entry* in  $\mathbf{P}(Toothache, Catch, Cavity, Weather)$ . In fact, we can write the general equation

$$\mathbf{P}(\textit{Toothache}, \textit{Catch}, \textit{Cavity}, \textit{Weather}) = \mathbf{P}(\textit{Toothache}, \textit{Catch}, \textit{Cavity})\mathbf{P}(\textit{Weather})$$
.

Thus, the 32-element table for four variables can be constructed from one 8-element table and one 4-element table. This decomposition is illustrated schematically in Figure 13.4(a).

The property we used in Equation (13.10) is called **independence** (also **marginal independence** and **absolute independence**). In particular, the weather is independent of one's dental problems. Independence between propositions a and b can be written as

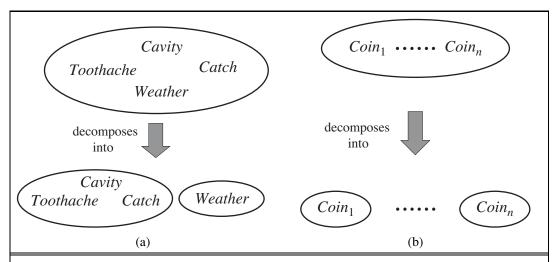
$$P(a \mid b) = P(a)$$
 or  $P(b \mid a) = P(b)$  or  $P(a \land b) = P(a)P(b)$ . (13.11)

All these forms are equivalent (Exercise 13.12). Independence between variables X and Y can be written as follows (again, these are all equivalent):

$$\mathbf{P}(X \mid Y) = \mathbf{P}(X)$$
 or  $\mathbf{P}(Y \mid X) = \mathbf{P}(Y)$  or  $\mathbf{P}(X, Y) = \mathbf{P}(X)\mathbf{P}(Y)$ .

Independence assertions are usually based on knowledge of the domain. As the toothache—weather example illustrates, they can dramatically reduce the amount of information necessary to specify the full joint distribution. If the complete set of variables can be divided

INDEPENDENCE



**Figure 13.4** Two examples of factoring a large joint distribution into smaller distributions, using absolute independence. (a) Weather and dental problems are independent. (b) Coin flips are independent.

into independent subsets, then the full joint distribution can be *factored* into separate joint distributions on those subsets. For example, the full joint distribution on the outcome of n independent coin flips,  $\mathbf{P}(C_1, \dots, C_n)$ , has  $2^n$  entries, but it can be represented as the product of n single-variable distributions  $\mathbf{P}(C_i)$ . In a more practical vein, the independence of dentistry and meteorology is a good thing, because otherwise the practice of dentistry might require intimate knowledge of meteorology, and vice versa.

When they are available, then, independence assertions can help in reducing the size of the domain representation and the complexity of the inference problem. Unfortunately, clean separation of entire sets of variables by independence is quite rare. Whenever a connection, however indirect, exists between two variables, independence will fail to hold. Moreover, even independent subsets can be quite large—for example, dentistry might involve dozens of diseases and hundreds of symptoms, all of which are interrelated. To handle such problems, we need more subtle methods than the straightforward concept of independence.

### 13.5 BAYES' RULE AND ITS USE

On page 486, we defined the **product rule**. It can actually be written in two forms:

$$P(a \wedge b) = P(a \mid b)P(b)$$
 and  $P(a \wedge b) = P(b \mid a)P(a)$ .

Equating the two right-hand sides and dividing by P(a), we get

$$P(b \mid a) = \frac{P(a \mid b)P(b)}{P(a)}.$$
(13.12)

This equation is known as **Bayes' rule** (also Bayes' law or Bayes' theorem). This simple equation underlies most modern AI systems for probabilistic inference.

The more general case of Bayes' rule for multivalued variables can be written in the **P** notation as follows:

$$\mathbf{P}(Y \mid X) = \frac{\mathbf{P}(X \mid Y)\mathbf{P}(Y)}{\mathbf{P}(X)},$$

As before, this is to be taken as representing a set of equations, each dealing with specific values of the variables. We will also have occasion to use a more general version conditionalized on some background evidence **e**:

$$\mathbf{P}(Y \mid X, \mathbf{e}) = \frac{\mathbf{P}(X \mid Y, \mathbf{e})\mathbf{P}(Y \mid \mathbf{e})}{\mathbf{P}(X \mid \mathbf{e})}.$$
 (13.13)

#### 13.5.1 Applying Bayes' rule: The simple case

On the surface, Bayes' rule does not seem very useful. It allows us to compute the single term  $P(b \mid a)$  in terms of three terms:  $P(a \mid b)$ , P(b), and P(a). That seems like two steps backwards, but Bayes' rule is useful in practice because there are many cases where we do have good probability estimates for these three numbers and need to compute the fourth. Often, we perceive as evidence the *effect* of some unknown *cause* and we would like to determine that cause. In that case, Bayes' rule becomes

$$P(cause \mid effect) = \frac{P(effect \mid cause)P(cause)}{P(effect)}$$
.

CAUSAL DIAGNOSTIC The conditional probability  $P(effect \mid cause)$  quantifies the relationship in the **causal** direction, whereas  $P(cause \mid effect)$  describes the **diagnostic** direction. In a task such as medical diagnosis, we often have conditional probabilities on causal relationships (that is, the doctor knows  $P(symptoms \mid disease)$ ) and want to derive a diagnosis,  $P(disease \mid symptoms)$ . For example, a doctor knows that the disease meningitis causes the patient to have a stiff neck, say, 70% of the time. The doctor also knows some unconditional facts: the prior probability that a patient has meningitis is 1/50,000, and the prior probability that any patient has a stiff neck is 1%. Letting s be the proposition that the patient has a stiff neck and m be the proposition that the patient has meningitis, we have

$$P(s \mid m) = 0.7$$

$$P(m) = 1/50000$$

$$P(s) = 0.01$$

$$P(m \mid s) = \frac{P(s \mid m)P(m)}{P(s)} = \frac{0.7 \times 1/50000}{0.01} = 0.0014.$$
(13.14)

That is, we expect less than 1 in 700 patients with a stiff neck to have meningitis. Notice that even though a stiff neck is quite strongly indicated by meningitis (with probability 0.7), the probability of meningitis in the patient remains small. This is because the prior probability of stiff necks is much higher than that of meningitis.

Section 13.3 illustrated a process by which one can avoid assessing the prior probability of the evidence (here, P(s)) by instead computing a posterior probability for each value of

the query variable (here, m and  $\neg m$ ) and then normalizing the results. The same process can be applied when using Bayes' rule. We have

$$\mathbf{P}(M \mid s) = \alpha \langle P(s \mid m)P(m), P(s \mid \neg m)P(\neg m) \rangle.$$

Thus, to use this approach we need to estimate  $P(s \mid \neg m)$  instead of P(s). There is no free lunch—sometimes this is easier, sometimes it is harder. The general form of Bayes' rule with normalization is

$$\mathbf{P}(Y \mid X) = \alpha \mathbf{P}(X \mid Y)\mathbf{P}(Y) , \qquad (13.15)$$

where  $\alpha$  is the normalization constant needed to make the entries in  $\mathbf{P}(Y \mid X)$  sum to 1.

One obvious question to ask about Bayes' rule is why one might have available the conditional probability in one direction, but not the other. In the meningitis domain, perhaps the doctor knows that a stiff neck implies meningitis in 1 out of 5000 cases; that is, the doctor has quantitative information in the **diagnostic** direction from symptoms to causes. Such a doctor has no need to use Bayes' rule. Unfortunately, *diagnostic knowledge is often more fragile than causal knowledge*. If there is a sudden epidemic of meningitis, the unconditional probability of meningitis, P(m), will go up. The doctor who derived the diagnostic probability  $P(m \mid s)$  directly from statistical observation of patients before the epidemic will have no idea how to update the value, but the doctor who computes  $P(m \mid s)$  from the other three values will see that  $P(m \mid s)$  should go up proportionately with P(m). Most important, the causal information  $P(s \mid m)$  is *unaffected* by the epidemic, because it simply reflects the way meningitis works. The use of this kind of direct causal or model-based knowledge provides the crucial robustness needed to make probabilistic systems feasible in the real world.

# 13.5.2 Using Bayes' rule: Combining evidence

We have seen that Bayes' rule can be useful for answering probabilistic queries conditioned on one piece of evidence—for example, the stiff neck. In particular, we have argued that probabilistic information is often available in the form  $P(effect \mid cause)$ . What happens when we have two or more pieces of evidence? For example, what can a dentist conclude if her nasty steel probe catches in the aching tooth of a patient? If we know the full joint distribution (Figure 13.3), we can read off the answer:

$$\mathbf{P}(Cavity \mid toothache \land catch) = \alpha \langle 0.108, 0.016 \rangle \approx \langle 0.871, 0.129 \rangle$$
.

We know, however, that such an approach does not scale up to larger numbers of variables. We can try using Bayes' rule to reformulate the problem:

$$\mathbf{P}(Cavity \mid toothache \land catch)$$

$$= \alpha \mathbf{P}(toothache \land catch \mid Cavity) \mathbf{P}(Cavity) . \tag{13.16}$$

For this reformulation to work, we need to know the conditional probabilities of the conjunction  $toothache \wedge catch$  for each value of Cavity. That might be feasible for just two evidence variables, but again it does not scale up. If there are n possible evidence variables (X rays, diet, oral hygiene, etc.), then there are  $2^n$  possible combinations of observed values for which we would need to know conditional probabilities. We might as well go back to using the full joint distribution. This is what first led researchers away from probability theory toward



approximate methods for evidence combination that, while giving incorrect answers, require fewer numbers to give any answer at all.

Rather than taking this route, we need to find some additional assertions about the domain that will enable us to simplify the expressions. The notion of **independence** in Section 13.4 provides a clue, but needs refining. It would be nice if *Toothache* and *Catch* were independent, but they are not: if the probe catches in the tooth, then it is likely that the tooth has a cavity and that the cavity causes a toothache. These variables *are* independent, however, *given the presence or the absence of a cavity*. Each is directly caused by the cavity, but neither has a direct effect on the other: toothache depends on the state of the nerves in the tooth, whereas the probe's accuracy depends on the dentist's skill, to which the toothache is irrelevant. Mathematically, this property is written as

$$P(\textit{toothache} \land \textit{catch} \mid \textit{Cavity}) = P(\textit{toothache} \mid \textit{Cavity})P(\textit{catch} \mid \textit{Cavity}) \; . \quad (13.17)$$

This equation expresses the **conditional independence** of *toothache* and *catch* given *Cavity*. We can plug it into Equation (13.16) to obtain the probability of a cavity:

$$\mathbf{P}(Cavity \mid toothache \land catch) 
= \alpha \mathbf{P}(toothache \mid Cavity) \mathbf{P}(catch \mid Cavity) \mathbf{P}(Cavity) .$$
(13.18)

Now the information requirements are the same as for inference, using each piece of evidence separately: the prior probability P(Cavity) for the query variable and the conditional probability of each effect, given its cause.

The general definition of **conditional independence** of two variables X and Y, given a third variable Z, is

$$\mathbf{P}(X,Y \mid Z) = \mathbf{P}(X \mid Z)\mathbf{P}(Y \mid Z) .$$

In the dentist domain, for example, it seems reasonable to assert conditional independence of the variables *Toothache* and *Catch*, given *Cavity*:

$$\mathbf{P}(Toothache, Catch \mid Cavity) = \mathbf{P}(Toothache \mid Cavity)\mathbf{P}(Catch \mid Cavity)$$
. (13.19)

Notice that this assertion is somewhat stronger than Equation (13.17), which asserts independence only for specific values of *Toothache* and *Catch*. As with absolute independence in Equation (13.11), the equivalent forms

$$\mathbf{P}(X \mid Y, Z) = \mathbf{P}(X \mid Z)$$
 and  $\mathbf{P}(Y \mid X, Z) = \mathbf{P}(Y \mid Z)$ 

can also be used (see Exercise 13.17). Section 13.4 showed that absolute independence assertions allow a decomposition of the full joint distribution into much smaller pieces. It turns out that the same is true for conditional independence assertions. For example, given the assertion in Equation (13.19), we can derive a decomposition as follows:

 $P(\mathit{Toothache}, \mathit{Catch}, \mathit{Cavity})$ 

- $= \mathbf{P}(Toothache, Catch \mid Cavity)\mathbf{P}(Cavity)$  (product rule)
- $= \mathbf{P}(\textit{Toothache} \mid \textit{Cavity}) \mathbf{P}(\textit{Catch} \mid \textit{Cavity}) \mathbf{P}(\textit{Cavity}) \quad \text{(using 13.19)}.$

(The reader can easily check that this equation does in fact hold in Figure 13.3.) In this way, the original large table is decomposed into three smaller tables. The original table has seven

CONDITIONAL INDEPENDENCE

<sup>&</sup>lt;sup>5</sup> We assume that the patient and dentist are distinct individuals.



independent numbers ( $2^3 = 8$  entries in the table, but they must sum to 1, so 7 are independent). The smaller tables contain five independent numbers (for a conditional probability distributions such as  $\mathbf{P}(T|C)$  there are two rows of two numbers, and each row sums to 1, so that's two independent numbers; for a prior distribution like  $\mathbf{P}(C)$  there is only one independent number). Going from seven to five might not seem like a major triumph, but the point is that, for n symptoms that are all conditionally independent given Cavity, the size of the representation grows as O(n) instead of  $O(2^n)$ . That means that conditional independence assertions can allow probabilistic systems to scale up; moreover, they are much more commonly available than absolute independence assertions. Conceptually, Cavity separates Toothache and Catch because it is a direct cause of both of them. The decomposition of large probabilistic domains into weakly connected subsets through conditional independence is one of the most important developments in the recent history of AI.

The dentistry example illustrates a commonly occurring pattern in which a single cause directly influences a number of effects, all of which are conditionally independent, given the cause. The full joint distribution can be written as

$$\mathbf{P}(\mathit{Cause}, \mathit{Effect}_1, \dots, \mathit{Effect}_n) = \mathbf{P}(\mathit{Cause}) \prod_i \mathbf{P}(\mathit{Effect}_i \mid \mathit{Cause})$$
.

NAIVE BAYES

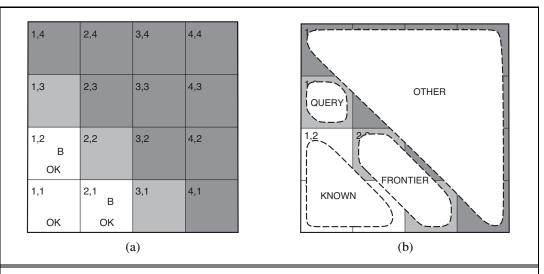
Such a probability distribution is called a **naive Bayes** model—"naive" because it is often used (as a simplifying assumption) in cases where the "effect" variables are *not* actually conditionally independent given the cause variable. (The naive Bayes model is sometimes called a **Bayesian classifier**, a somewhat careless usage that has prompted true Bayesians to call it the **idiot Bayes** model.) In practice, naive Bayes systems can work surprisingly well, even when the conditional independence assumption is not true. Chapter 20 describes methods for learning naive Bayes distributions from observations.

# 13.6 THE WUMPUS WORLD REVISITED

We can combine of the ideas in this chapter to solve probabilistic reasoning problems in the wumpus world. (See Chapter 7 for a complete description of the wumpus world.) Uncertainty arises in the wumpus world because the agent's sensors give only partial information about the world. For example, Figure 13.5 shows a situation in which each of the three reachable squares—[1,3], [2,2], and [3,1]—might contain a pit. Pure logical inference can conclude nothing about which square is most likely to be safe, so a logical agent might have to choose randomly. We will see that a probabilistic agent can do much better than the logical agent.

Our aim is to calculate the probability that each of the three squares contains a pit. (For this example we ignore the wumpus and the gold.) The relevant properties of the wumpus world are that (1) a pit causes breezes in all neighboring squares, and (2) each square other than [1,1] contains a pit with probability 0.2. The first step is to identify the set of random variables we need:

• As in the propositional logic case, we want one Boolean variable  $P_{ij}$  for each square, which is true iff square [i, j] actually contains a pit.



**Figure 13.5** (a) After finding a breeze in both [1,2] and [2,1], the agent is stuck—there is no safe place to explore. (b) Division of the squares into *Known*, *Frontier*, and *Other*, for a query about [1,3].

• We also have Boolean variables  $B_{ij}$  that are true iff square [i, j] is breezy; we include these variables only for the observed squares—in this case, [1,1], [1,2], and [2,1].

The next step is to specify the full joint distribution,  $\mathbf{P}(P_{1,1}, \dots, P_{4,4}, B_{1,1}, B_{1,2}, B_{2,1})$ . Applying the product rule, we have

$$\mathbf{P}(P_{1,1},\ldots,P_{4,4},B_{1,1},B_{1,2},B_{2,1}) = \mathbf{P}(B_{1,1},B_{1,2},B_{2,1} \mid P_{1,1},\ldots,P_{4,4})\mathbf{P}(P_{1,1},\ldots,P_{4,4}).$$

This decomposition makes it easy to see what the joint probability values should be. The first term is the conditional probability distribution of a breeze configuration, given a pit configuration; its values are 1 if the breezes are adjacent to the pits and 0 otherwise. The second term is the prior probability of a pit configuration. Each square contains a pit with probability 0.2, independently of the other squares; hence,

$$\mathbf{P}(P_{1,1},\ldots,P_{4,4}) = \prod_{i,j=1,1}^{4,4} \mathbf{P}(P_{i,j}).$$
(13.20)

For a particular configuration with exactly n pits,  $P(P_{1,1}, \dots, P_{4,4}) = 0.2^n \times 0.8^{16-n}$ .

In the situation in Figure 13.5(a), the evidence consists of the observed breeze (or its absence) in each square that is visited, combined with the fact that each such square contains no pit. We abbreviate these facts as  $b = \neg b_{1,1} \land b_{1,2} \land b_{2,1}$  and  $known = \neg p_{1,1} \land \neg p_{1,2} \land \neg p_{2,1}$ . We are interested in answering queries such as  $\mathbf{P}(P_{1,3} \mid known, b)$ : how likely is it that [1,3] contains a pit, given the observations so far?

To answer this query, we can follow the standard approach of Equation (13.9), namely, summing over entries from the full joint distribution. Let Unknown be the set of  $P_{i,j}$  vari-

ables for squares other than the Known squares and the query square [1,3]. Then, by Equation (13.9), we have

$$\mathbf{P}(P_{1,3} \mid known, b) = \alpha \sum_{unknown} \mathbf{P}(P_{1,3}, unknown, known, b) .$$

The full joint probabilities have already been specified, so we are done—that is, unless we care about computation. There are 12 unknown squares; hence the summation contains  $2^{12} = 4096$  terms. In general, the summation grows exponentially with the number of squares.

Surely, one might ask, aren't the other squares irrelevant? How could [4,4] affect whether [1,3] has a pit? Indeed, this intuition is correct. Let *Frontier* be the pit variables (other than the query variable) that are adjacent to visited squares, in this case just [2,2] and [3,1]. Also, let *Other* be the pit variables for the other unknown squares; in this case, there are 10 other squares, as shown in Figure 13.5(b). The key insight is that the observed breezes are *conditionally independent* of the other variables, given the known, frontier, and query variables. To use the insight, we manipulate the query formula into a form in which the breezes are conditioned on all the other variables, and then we apply conditional independence:

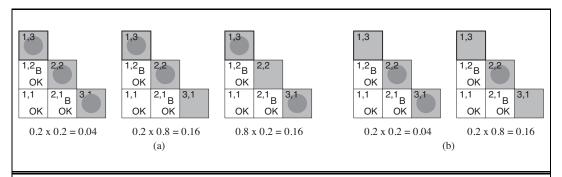
$$\begin{split} \mathbf{P}(P_{1,3} \mid known, b) \\ &= \alpha \sum_{unknown} \mathbf{P}(P_{1,3}, known, b, unknown) \quad \text{(by Equation (13.9))} \\ &= \alpha \sum_{unknown} \mathbf{P}(b \mid P_{1,3}, known, unknown) \mathbf{P}(P_{1,3}, known, unknown) \\ &= \alpha \sum_{frontier} \sum_{other} \mathbf{P}(b \mid known, P_{1,3}, frontier, other) \mathbf{P}(P_{1,3}, known, frontier, other) \\ &= \alpha \sum_{frontier} \sum_{other} \mathbf{P}(b \mid known, P_{1,3}, frontier) \mathbf{P}(P_{1,3}, known, frontier, other) \\ &= \alpha \sum_{frontier} \sum_{other} \mathbf{P}(b \mid known, P_{1,3}, frontier) \mathbf{P}(P_{1,3}, known, frontier, other) \\ \end{split}$$

where the final step uses conditional independence: b is independent of *other* given *known*,  $P_{1,3}$ , and *frontier*. Now, the first term in this expression does not depend on the *Other* variables, so we can move the summation inward:

$$\begin{aligned} \mathbf{P}(P_{1,3} \mid known, b) \\ &= \alpha \sum_{frontier} \mathbf{P}(b \mid known, P_{1,3}, frontier) \sum_{other} \mathbf{P}(P_{1,3}, known, frontier, other) \; . \end{aligned}$$

By independence, as in Equation (13.20), the prior term can be factored, and then the terms can be reordered:

$$\begin{split} &\mathbf{P}(P_{1,3} \mid known, b) \\ &= \alpha \sum_{frontier} \mathbf{P}(b \mid known, P_{1,3}, frontier) \sum_{other} \mathbf{P}(P_{1,3}) P(known) P(frontier) P(other) \\ &= \alpha P(known) \mathbf{P}(P_{1,3}) \sum_{frontier} \mathbf{P}(b \mid known, P_{1,3}, frontier) P(frontier) \sum_{other} P(other) \\ &= \alpha' \mathbf{P}(P_{1,3}) \sum_{frontier} \mathbf{P}(b \mid known, P_{1,3}, frontier) P(frontier) \;, \end{split}$$



**Figure 13.6** Consistent models for the frontier variables  $P_{2,2}$  and  $P_{3,1}$ , showing P(frontier) for each model: (a) three models with  $P_{1,3} = true$  showing two or three pits, and (b) two models with  $P_{1,3} = false$  showing one or two pits.

where the last step folds P(known) into the normalizing constant and uses the fact that  $\sum_{other} P(other)$  equals 1.

Now, there are just four terms in the summation over the frontier variables  $P_{2,2}$  and  $P_{3,1}$ . The use of independence and conditional independence has completely eliminated the other squares from consideration.

Notice that the expression  $P(b \mid known, P_{1,3}, frontier)$  is 1 when the frontier is consistent with the breeze observations, and 0 otherwise. Thus, for each value of  $P_{1,3}$ , we sum over the *logical models* for the frontier variables that are consistent with the known facts. (Compare with the enumeration over models in Figure 7.5 on page 241.) The models and their associated prior probabilities—P(frontier)—are shown in Figure 13.6. We have

$$\mathbf{P}(P_{1,3} \mid known, b) = \alpha' \langle 0.2(0.04 + 0.16 + 0.16), 0.8(0.04 + 0.16) \rangle \approx \langle 0.31, 0.69 \rangle$$
.

That is, [1,3] (and [3,1] by symmetry) contains a pit with roughly 31% probability. A similar calculation, which the reader might wish to perform, shows that [2,2] contains a pit with roughly 86% probability. The wumpus agent should definitely avoid [2,2]! Note that our logical agent from Chapter 7 did not know that [2,2] was worse than the other squares. Logic can tell us that it is unknown whether there is a pit in [2, 2], but we need probability to tell us how likely it is.

What this section has shown is that even seemingly complicated problems can be formulated precisely in probability theory and solved with simple algorithms. To get *efficient* solutions, independence and conditional independence relationships can be used to simplify the summations required. These relationships often correspond to our natural understanding of how the problem should be decomposed. In the next chapter, we develop formal representations for such relationships as well as algorithms that operate on those representations to perform probabilistic inference efficiently.

Section 13.7. Summary 503

# 13.7 SUMMARY

This chapter has suggested probability theory as a suitable foundation for uncertain reasoning and provided a gentle introduction to its use.

- Uncertainty arises because of both laziness and ignorance. It is inescapable in complex, nondeterministic, or partially observable environments.
- Probabilities express the agent's inability to reach a definite decision regarding the truth of a sentence. Probabilities summarize the agent's beliefs relative to the evidence.
- Decision theory combines the agent's beliefs and desires, defining the best action as the one that maximizes expected utility.
- Basic probability statements include prior probabilities and conditional probabilities over simple and complex propositions.
- The axioms of probability constrain the possible assignments of probabilities to propositions. An agent that violates the axioms must behave irrationally in some cases.
- The **full joint probability distribution** specifies the probability of each complete assignment of values to random variables. It is usually too large to create or use in its explicit form, but when it is available it can be used to answer queries simply by adding up entries for the possible worlds corresponding to the query propositions.
- **Absolute independence** between subsets of random variables allows the full joint distribution to be factored into smaller joint distributions, greatly reducing its complexity. Absolute independence seldom occurs in practice.
- Bayes' rule allows unknown probabilities to be computed from known conditional probabilities, usually in the causal direction. Applying Bayes' rule with many pieces of evidence runs into the same scaling problems as does the full joint distribution.
- Conditional independence brought about by direct causal relationships in the domain might allow the full joint distribution to be factored into smaller, conditional distributions. The **naive Bayes** model assumes the conditional independence of all effect variables, given a single cause variable, and grows linearly with the number of effects.
- A wumpus-world agent can calculate probabilities for unobserved aspects of the world, thereby improving on the decisions of a purely logical agent. Conditional independence makes these calculations tractable.

#### BIBLIOGRAPHICAL AND HISTORICAL NOTES

Probability theory was invented as a way of analyzing games of chance. In about 850 A.D. the Indian mathematician Mahaviracarya described how to arrange a set of bets that can't lose (what we now call a Dutch book). In Europe, the first significant systematic analyses were produced by Girolamo Cardano around 1565, although publication was posthumous (1663). By that time, probability had been established as a mathematical discipline due to a series of

results established in a famous correspondence between Blaise Pascal and Pierre de Fermat in 1654. As with probability itself, the results were initially motivated by gambling problems (see Exercise 13.9). The first published textbook on probability was *De Ratiociniis in Ludo Aleae* (Huygens, 1657). The "laziness and ignorance" view of uncertainty was described by John Arbuthnot in the preface of his translation of Huygens (Arbuthnot, 1692): "It is impossible for a Die, with such determin'd force and direction, not to fall on such determin'd side, only I don't know the force and direction which makes it fall on such determin'd side, and therefore I call it Chance, which is nothing but the want of art..."

Laplace (1816) gave an exceptionally accurate and modern overview of probability; he was the first to use the example "take two urns, A and B, the first containing four white and two black balls, ..." The Rev. Thomas Bayes (1702–1761) introduced the rule for reasoning about conditional probabilities that was named after him (Bayes, 1763). Bayes only considered the case of uniform priors; it was Laplace who independently developed the general case. Kolmogorov (1950, first published in German in 1933) presented probability theory in a rigorously axiomatic framework for the first time. Rényi (1970) later gave an axiomatic presentation that took conditional probability, rather than absolute probability, as primitive.

Pascal used probability in ways that required both the objective interpretation, as a property of the world based on symmetry or relative frequency, and the subjective interpretation, based on degree of belief—the former in his analyses of probabilities in games of chance, the latter in the famous "Pascal's wager" argument about the possible existence of God. However, Pascal did not clearly realize the distinction between these two interpretations. The distinction was first drawn clearly by James Bernoulli (1654–1705).

Leibniz introduced the "classical" notion of probability as a proportion of enumerated, equally probable cases, which was also used by Bernoulli, although it was brought to prominence by Laplace (1749–1827). This notion is ambiguous between the frequency interpretation and the subjective interpretation. The cases can be thought to be equally probable either because of a natural, physical symmetry between them, or simply because we do not have any knowledge that would lead us to consider one more probable than another. The use of this latter, subjective consideration to justify assigning equal probabilities is known as the **principle of indifference**. The principle is often attributed to Laplace, but he never isolated the principle explicitly. George Boole and John Venn both referred to it as the **principle of insufficient reason**; the modern name is due to Keynes (1921).

The debate between objectivists and subjectivists became sharper in the 20th century. Kolmogorov (1963), R. A. Fisher (1922), and Richard von Mises (1928) were advocates of the relative frequency interpretation. Karl Popper's (1959, first published in German in 1934) "propensity" interpretation traces relative frequencies to an underlying physical symmetry. Frank Ramsey (1931), Bruno de Finetti (1937), R. T. Cox (1946), Leonard Savage (1954), Richard Jeffrey (1983), and E. T. Jaynes (2003) interpreted probabilities as the degrees of belief of specific individuals. Their analyses of degree of belief were closely tied to utilities and to behavior—specifically, to the willingness to place bets. Rudolf Carnap, following Leibniz and Laplace, offered a different kind of subjective interpretation of probability—not as any actual individual's degree of belief, but as the degree of belief that an idealized individual *should* have in a particular proposition a, given a particular body of evidence e.

PRINCIPLE OF INDIFFERENCE

PRINCIPLE OF INSUFFICIENT REASON

CONFIRMATION INDUCTIVE LOGIC

Carnap attempted to go further than Leibniz or Laplace by making this notion of degree of **confirmation** mathematically precise, as a logical relation between a and e. The study of this relation was intended to constitute a mathematical discipline called **inductive logic**, analogous to ordinary deductive logic (Carnap, 1948, 1950). Carnap was not able to extend his inductive logic much beyond the propositional case, and Putnam (1963) showed by adversarial arguments that some fundamental difficulties would prevent a strict extension to languages capable of expressing arithmetic.

Cox's theorem (1946) shows that any system for uncertain reasoning that meets his set of assumptions is equivalent to probability theory. This gave renewed confidence to those who already favored probability, but others were not convinced, pointing to the assumptions (primarily that belief must be represented by a single number, and thus the belief in  $\neg p$  must be a function of the belief in p). Halpern (1999) describes the assumptions and shows some gaps in Cox's original formulation. Horn (2003) shows how to patch up the difficulties. Jaynes (2003) has a similar argument that is easier to read.

The question of reference classes is closely tied to the attempt to find an inductive logic. The approach of choosing the "most specific" reference class of sufficient size was formally proposed by Reichenbach (1949). Various attempts have been made, notably by Henry Kyburg (1977, 1983), to formulate more sophisticated policies in order to avoid some obvious fallacies that arise with Reichenbach's rule, but such approaches remain somewhat *ad hoc*. More recent work by Bacchus, Grove, Halpern, and Koller (1992) extends Carnap's methods to first-order theories, thereby avoiding many of the difficulties associated with the straightforward reference-class method. Kyburg and Teng (2006) contrast probabilistic inference with nonmonotonic logic.

Bayesian probabilistic reasoning has been used in AI since the 1960s, especially in medical diagnosis. It was used not only to make a diagnosis from available evidence, but also to select further questions and tests by using the theory of information value (Section 16.6) when available evidence was inconclusive (Gorry, 1968; Gorry *et al.*, 1973). One system outperformed human experts in the diagnosis of acute abdominal illnesses (de Dombal *et al.*, 1974). Lucas *et al.* (2004) gives an overview. These early Bayesian systems suffered from a number of problems, however. Because they lacked any theoretical model of the conditions they were diagnosing, they were vulnerable to unrepresentative data occurring in situations for which only a small sample was available (de Dombal *et al.*, 1981). Even more fundamentally, because they lacked a concise formalism (such as the one to be described in Chapter 14) for representing and using conditional independence information, they depended on the acquisition, storage, and processing of enormous tables of probabilistic data. Because of these difficulties, probabilistic methods for coping with uncertainty fell out of favor in AI from the 1970s to the mid-1980s. Developments since the late 1980s are described in the next chapter.

The naive Bayes model for joint distributions has been studied extensively in the pattern recognition literature since the 1950s (Duda and Hart, 1973). It has also been used, often unwittingly, in information retrieval, beginning with the work of Maron (1961). The probabilistic foundations of this technique, described further in Exercise 13.22, were elucidated by Robertson and Sparck Jones (1976). Domingos and Pazzani (1997) provide an explanation

for the surprising success of naive Bayesian reasoning even in domains where the independence assumptions are clearly violated.

There are many good introductory textbooks on probability theory, including those by Bertsekas and Tsitsiklis (2008) and Grinstead and Snell (1997). DeGroot and Schervish (2001) offer a combined introduction to probability and statistics from a Bayesian standpoint. Richard Hamming's (1991) textbook gives a mathematically sophisticated introduction to probability theory from the standpoint of a propensity interpretation based on physical symmetry. Hacking (1975) and Hald (1990) cover the early history of the concept of probability. Bernstein (1996) gives an entertaining popular account of the story of risk.

#### **EXERCISES**

- **13.1** Show from first principles that  $P(a \mid b \land a) = 1$ .
- **13.2** Using the axioms of probability, prove that any probability distribution on a discrete random variable must sum to 1.
- **13.3** For each of the following statements, either prove it is true or give a counterexample.
  - **a.** If P(a | b, c) = P(b | a, c), then P(a | c) = P(b | c)
  - **b.** If P(a | b, c) = P(a), then P(b | c) = P(b)
  - **c.** If  $P(a \mid b) = P(a)$ , then  $P(a \mid b, c) = P(a \mid c)$
- **13.4** Would it be rational for an agent to hold the three beliefs P(A) = 0.4, P(B) = 0.3, and  $P(A \lor B) = 0.5$ ? If so, what range of probabilities would be rational for the agent to hold for  $A \land B$ ? Make up a table like the one in Figure 13.2, and show how it supports your argument about rationality. Then draw another version of the table where  $P(A \lor B) = 0.7$ . Explain why it is rational to have this probability, even though the table shows one case that is a loss and three that just break even. (*Hint:* what is Agent 1 committed to about the probability of each of the four cases, especially the case that is a loss?)
- 13.5 This question deals with the properties of possible worlds, defined on page 488 as assignments to all random variables. We will work with propositions that correspond to exactly one possible world because they pin down the assignments of all the variables. In probability theory, such propositions are called **atomic events**. For example, with Boolean variables  $X_1, X_2, X_3$ , the proposition  $x_1 \wedge \neg x_2 \wedge \neg x_3$  fixes the assignment of the variables; in the language of propositional logic, we would say it has exactly one model.
  - **a.** Prove, for the case of n Boolean variables, that any two distinct atomic events are mutually exclusive; that is, their conjunction is equivalent to false.
  - **b**. Prove that the disjunction of all possible atomic events is logically equivalent to true.
  - **c**. Prove that any proposition is logically equivalent to the disjunction of the atomic events that entail its truth.

ATOMIC EVENT

Exercises 507

- **13.6** Prove Equation (13.4) from Equations (13.1) and (13.2).
- **13.7** Consider the set of all possible five-card poker hands dealt fairly from a standard deck of fifty-two cards.
  - **a**. How many atomic events are there in the joint probability distribution (i.e., how many five-card hands are there)?
  - **b**. What is the probability of each atomic event?
  - c. What is the probability of being dealt a royal straight flush? Four of a kind?
- **13.8** Given the full joint distribution shown in Figure 13.3, calculate the following:
  - **a. P**(toothache).
  - **b**. P(Cavity).
  - **c**. **P**( $Toothache \mid cavity$ ).
  - **d**.  $P(Cavity \mid toothache \lor catch)$ .
- 13.9 In his letter of August 24, 1654, Pascal was trying to show how a pot of money should be allocated when a gambling game must end prematurely. Imagine a game where each turn consists of the roll of a die, player E gets a point when the die is even, and player O gets a point when the die is odd. The first player to get 7 points wins the pot. Suppose the game is interrupted with E leading 4–2. How should the money be fairly split in this case? What is the general formula? (Fermat and Pascal made several errors before solving the problem, but you should be able to get it right the first time.)
- **13.10** Deciding to put probability theory to good use, we encounter a slot machine with three independent wheels, each producing one of the four symbols BAR, BELL, LEMON, or CHERRY with equal probability. The slot machine has the following payout scheme for a bet of 1 coin (where "?" denotes that we don't care what comes up for that wheel):

```
BAR/BAR/BAR pays 20 coins
BELL/BELL pays 15 coins
LEMON/LEMON/LEMON pays 5 coins
CHERRY/CHERRY/CHERRY pays 3 coins
CHERRY/CHERRY/? pays 2 coins
CHERRY/?/? pays 1 coin
```

- **a**. Compute the expected "payback" percentage of the machine. In other words, for each coin played, what is the expected coin return?
- **b**. Compute the probability that playing the slot machine once will result in a win.
- c. Estimate the mean and median number of plays you can expect to make until you go broke, if you start with 10 coins. You can run a simulation to estimate this, rather than trying to compute an exact answer.
- 13.11 We wish to transmit an n-bit message to a receiving agent. The bits in the message are independently corrupted (flipped) during transmission with  $\epsilon$  probability each. With an extra parity bit sent along with the original information, a message can be corrected by the receiver

if at most one bit in the entire message (including the parity bit) has been corrupted. Suppose we want to ensure that the correct message is received with probability at least  $1 - \delta$ . What is the maximum feasible value of n? Calculate this value for the case  $\epsilon = 0.001$ ,  $\delta = 0.01$ .

- **13.12** Show that the three forms of independence in Equation (13.11) are equivalent.
- 13.13 Consider two medical tests, A and B, for a virus. Test A is 95% effective at recognizing the virus when it is present, but has a 10% false positive rate (indicating that the virus is present, when it is not). Test B is 90% effective at recognizing the virus, but has a 5% false positive rate. The two tests use independent methods of identifying the virus. The virus is carried by 1% of all people. Say that a person is tested for the virus using only one of the tests, and that test comes back positive for carrying the virus. Which test returning positive is more indicative of someone really carrying the virus? Justify your answer mathematically.
- 13.14 Suppose you are given a coin that lands *heads* with probability x and tails with probability 1-x. Are the outcomes of successive flips of the coin independent of each other given that you know the value of x? Are the outcomes of successive flips of the coin independent of each other if you do *not* know the value of x? Justify your answer.
- 13.15 After your yearly checkup, the doctor has bad news and good news. The bad news is that you tested positive for a serious disease and that the test is 99% accurate (i.e., the probability of testing positive when you do have the disease is 0.99, as is the probability of testing negative when you don't have the disease). The good news is that this is a rare disease, striking only 1 in 10,000 people of your age. Why is it good news that the disease is rare? What are the chances that you actually have the disease?
- **13.16** It is quite often useful to consider the effect of some specific propositions in the context of some general background evidence that remains fixed, rather than in the complete absence of information. The following questions ask you to prove more general versions of the product rule and Bayes' rule, with respect to some background evidence **e**:
  - a. Prove the conditionalized version of the general product rule:

$$\mathbf{P}(X, Y \mid \mathbf{e}) = \mathbf{P}(X \mid Y, \mathbf{e})\mathbf{P}(Y \mid \mathbf{e})$$
.

- **b**. Prove the conditionalized version of Bayes' rule in Equation (13.13).
- **13.17** Show that the statement of conditional independence

$$\mathbf{P}(X,Y \mid Z) = \mathbf{P}(X \mid Z)\mathbf{P}(Y \mid Z)$$

is equivalent to each of the statements

$$\mathbf{P}(X \mid Y, Z) = \mathbf{P}(X \mid Z)$$
 and  $\mathbf{P}(B \mid X, Z) = \mathbf{P}(Y \mid Z)$ .

- 13.18 Suppose you are given a bag containing n unbiased coins. You are told that n-1 of these coins are normal, with heads on one side and tails on the other, whereas one coin is a fake, with heads on both sides.
  - **a.** Suppose you reach into the bag, pick out a coin at random, flip it, and get a head. What is the (conditional) probability that the coin you chose is the fake coin?

Exercises 509

**b.** Suppose you continue flipping the coin for a total of k times after picking it and see k heads. Now what is the conditional probability that you picked the fake coin?

- **c.** Suppose you wanted to decide whether the chosen coin was fake by flipping it *k* times. The decision procedure returns *fake* if all *k* flips come up heads; otherwise it returns *normal*. What is the (unconditional) probability that this procedure makes an error?
- **13.19** In this exercise, you will complete the normalization calculation for the meningitis example. First, make up a suitable value for  $P(s \mid \neg m)$ , and use it to calculate unnormalized values for  $P(m \mid s)$  and  $P(\neg m \mid s)$  (i.e., ignoring the P(s) term in the Bayes' rule expression, Equation (13.14)). Now normalize these values so that they add to 1.
- **13.20** Let X, Y, Z be Boolean random variables. Label the eight entries in the joint distribution P(X, Y, Z) as a through h. Express the statement that X and Y are conditionally independent given Z, as a set of equations relating a through h. How many *nonredundant* equations are there?
- **13.21** (Adapted from Pearl (1988).) Suppose you are a witness to a nighttime hit-and-run accident involving a taxi in Athens. All taxis in Athens are blue or green. You swear, under oath, that the taxi was blue. Extensive testing shows that, under the dim lighting conditions, discrimination between blue and green is 75% reliable.
  - **a.** Is it possible to calculate the most likely color for the taxi? (*Hint:* distinguish carefully between the proposition that the taxi *is* blue and the proposition that it *appears* blue.)
  - **b**. What if you know that 9 out of 10 Athenian taxis are green?
- 13.22 Text categorization is the task of assigning a given document to one of a fixed set of categories on the basis of the text it contains. Naive Bayes models are often used for this task. In these models, the query variable is the document category, and the "effect" variables are the presence or absence of each word in the language; the assumption is that words occur independently in documents, with frequencies determined by the document category.
  - **a.** Explain precisely how such a model can be constructed, given as "training data" a set of documents that have been assigned to categories.
  - **b**. Explain precisely how to categorize a new document.
  - **c.** Is the conditional independence assumption reasonable? Discuss.
- 13.23 In our analysis of the wumpus world, we used the fact that each square contains a pit with probability 0.2, independently of the contents of the other squares. Suppose instead that exactly N/5 pits are scattered at random among the N squares other than [1,1]. Are the variables  $P_{i,j}$  and  $P_{k,l}$  still independent? What is the joint distribution  $\mathbf{P}(P_{1,1},\ldots,P_{4,4})$  now? Redo the calculation for the probabilities of pits in [1,3] and [2,2].
- **13.24** Redo the probability calculation for pits in [1,3] and [2,2], assuming that each square contains a pit with probability 0.01, independent of the other squares. What can you say about the relative performance of a logical versus a probabilistic agent in this case?
- 13.25
- **13.25** Implement a hybrid probabilistic agent for the wumpus world, based on the hybrid agent in Figure 7.20 and the probabilistic inference procedure outlined in this chapter.

# 14 PROBABILISTIC REASONING

In which we explain how to build network models to reason under uncertainty according to the laws of probability theory.

Chapter 13 introduced the basic elements of probability theory and noted the importance of independence and conditional independence relationships in simplifying probabilistic representations of the world. This chapter introduces a systematic way to represent such relationships explicitly in the form of **Bayesian networks**. We define the syntax and semantics of these networks and show how they can be used to capture uncertain knowledge in a natural and efficient way. We then show how probabilistic inference, although computationally intractable in the worst case, can be done efficiently in many practical situations. We also describe a variety of approximate inference algorithms that are often applicable when exact inference is infeasible. We explore ways in which probability theory can be applied to worlds with objects and relations—that is, to *first-order*, as opposed to *propositional*, representations. Finally, we survey alternative approaches to uncertain reasoning.

# 14.1 REPRESENTING KNOWLEDGE IN AN UNCERTAIN DOMAIN

In Chapter 13, we saw that the full joint probability distribution can answer any question about the domain, but can become intractably large as the number of variables grows. Furthermore, specifying probabilities for possible worlds one by one is unnatural and tedious.

BAYESIAN NETWORK

We also saw that independence and conditional independence relationships among variables can greatly reduce the number of probabilities that need to be specified in order to define the full joint distribution. This section introduces a data structure called a **Bayesian network**<sup>1</sup> to represent the dependencies among variables. Bayesian networks can represent essentially *any* full joint probability distribution and in many cases can do so very concisely.

<sup>&</sup>lt;sup>1</sup> This is the most common name, but there are many synonyms, including **belief network**, **probabilistic network**, **causal network**, and **knowledge map**. In statistics, the term **graphical model** refers to a somewhat broader class that includes Bayesian networks. An extension of Bayesian networks called a **decision network** or **influence diagram** is covered in Chapter 16.

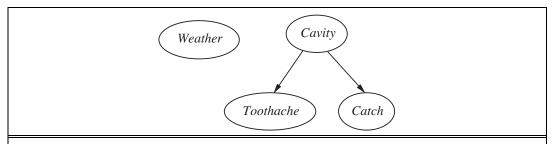
A Bayesian network is a directed graph in which each node is annotated with quantitative probability information. The full specification is as follows:

- 1. Each node corresponds to a random variable, which may be discrete or continuous.
- 2. A set of directed links or arrows connects pairs of nodes. If there is an arrow from node X to node Y, X is said to be a *parent* of Y. The graph has no directed cycles (and hence is a directed cyclic graph, or DAG.
- 3. Each node  $X_i$  has a conditional probability distribution  $\mathbf{P}(X_i \mid Parents(X_i))$  that quantifies the effect of the parents on the node.

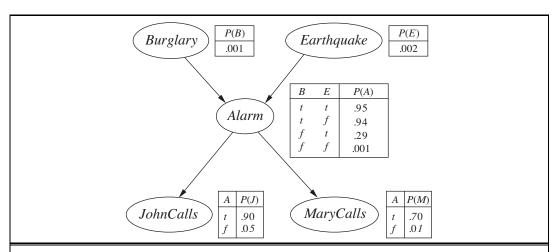
The topology of the network—the set of nodes and links—specifies the conditional independence relationships that hold in the domain, in a way that will be made precise shortly. The *intuitive* meaning of an arrow is typically that X has a *direct influence* on Y, which suggests that causes should be parents of effects. It is usually easy for a domain expert to decide what direct influences exist in the domain—much easier, in fact, than actually specifying the probabilities themselves. Once the topology of the Bayesian network is laid out, we need only specify a conditional probability distribution for each variable, given its parents. We will see that the combination of the topology and the conditional distributions suffices to specify (implicitly) the full joint distribution for all the variables.

Recall the simple world described in Chapter 13, consisting of the variables *Toothache*, *Cavity*, *Catch*, and *Weather*. We argued that *Weather* is independent of the other variables; furthermore, we argued that *Toothache* and *Catch* are conditionally independent, given *Cavity*. These relationships are represented by the Bayesian network structure shown in Figure 14.1. Formally, the conditional independence of *Toothache* and *Catch*, given *Cavity*, is indicated by the *absence* of a link between *Toothache* and *Catch*. Intuitively, the network represents the fact that *Cavity* is a direct cause of *Toothache* and *Catch*, whereas no direct causal relationship exists between *Toothache* and *Catch*.

Now consider the following example, which is just a little more complex. You have a new burglar alarm installed at home. It is fairly reliable at detecting a burglary, but also responds on occasion to minor earthquakes. (This example is due to Judea Pearl, a resident of Los Angeles—hence the acute interest in earthquakes.) You also have two neighbors, John and Mary, who have promised to call you at work when they hear the alarm. John nearly always calls when he hears the alarm, but sometimes confuses the telephone ringing with



**Figure 14.1** A simple Bayesian network in which *Weather* is independent of the other three variables and *Toothache* and *Catch* are conditionally independent, given *Cavity*.



**Figure 14.2** A typical Bayesian network, showing both the topology and the conditional probability tables (CPTs). In the CPTs, the letters B, E, A, J, and M stand for Burglary, Earthquake, Alarm, JohnCalls, and MaryCalls, respectively.

the alarm and calls then, too. Mary, on the other hand, likes rather loud music and often misses the alarm altogether. Given the evidence of who has or has not called, we would like to estimate the probability of a burglary.

A Bayesian network for this domain appears in Figure 14.2. The network structure shows that burglary and earthquakes directly affect the probability of the alarm's going off, but whether John and Mary call depends only on the alarm. The network thus represents our assumptions that they do not perceive burglaries directly, they do not notice minor earthquakes, and they do not confer before calling.

The conditional distributions in Figure 14.2 are shown as a **conditional probability table**, or CPT. (This form of table can be used for discrete variables; other representations, including those suitable for continuous variables, are described in Section 14.2.) Each row in a CPT contains the conditional probability of each node value for a **conditioning case**. A conditioning case is just a possible combination of values for the parent nodes—a miniature possible world, if you like. Each row must sum to 1, because the entries represent an exhaustive set of cases for the variable. For Boolean variables, once you know that the probability of a true value is p, the probability of false must be 1-p, so we often omit the second number, as in Figure 14.2. In general, a table for a Boolean variable with k Boolean parents contains  $2^k$  independently specifiable probabilities. A node with no parents has only one row, representing the prior probabilities of each possible value of the variable.

Notice that the network does not have nodes corresponding to Mary's currently listening to loud music or to the telephone ringing and confusing John. These factors are summarized in the uncertainty associated with the links from *Alarm* to *JohnCalls* and *MaryCalls*. This shows both laziness and ignorance in operation: it would be a lot of work to find out why those factors would be more or less likely in any particular case, and we have no reasonable way to obtain the relevant information anyway. The probabilities actually summarize a *potentially* 

CONDITIONAL PROBABILITY TABLE

CONDITIONING CASE

infinite set of circumstances in which the alarm might fail to go off (high humidity, power failure, dead battery, cut wires, a dead mouse stuck inside the bell, etc.) or John or Mary might fail to call and report it (out to lunch, on vacation, temporarily deaf, passing helicopter, etc.). In this way, a small agent can cope with a very large world, at least approximately. The degree of approximation can be improved if we introduce additional relevant information.

#### 14.2 THE SEMANTICS OF BAYESIAN NETWORKS

The previous section described what a network is, but not what it means. There are two ways in which one can understand the semantics of Bayesian networks. The first is to see the network as a representation of the joint probability distribution. The second is to view it as an encoding of a collection of conditional independence statements. The two views are equivalent, but the first turns out to be helpful in understanding how to *construct* networks, whereas the second is helpful in designing inference procedures.

#### 14.2.1 Representing the full joint distribution

Viewed as a piece of "syntax," a Bayesian network is a directed acyclic graph with some numeric parameters attached to each node. One way to define what the network means—its semantics—is to define the way in which it represents a specific joint distribution over all the variables. To do this, we first need to retract (temporarily) what we said earlier about the parameters associated with each node. We said that those parameters correspond to conditional probabilities  $P(X_i | Parents(X_i))$ ; this is a true statement, but until we assign semantics to the network as a whole, we should think of them just as numbers  $\theta(X_i | Parents(X_i))$ .

A generic entry in the joint distribution is the probability of a conjunction of particular assignments to each variable, such as  $P(X_1 = x_1 \land \ldots \land X_n = x_n)$ . We use the notation  $P(x_1, \ldots, x_n)$  as an abbreviation for this. The value of this entry is given by the formula

$$P(x_1, \dots, x_n) = \prod_{i=1}^n \theta(x_i \mid parents(X_i)), \qquad (14.1)$$

where  $parents(X_i)$  denotes the values of  $Parents(X_i)$  that appear in  $x_1, \ldots, x_n$ . Thus, each entry in the joint distribution is represented by the product of the appropriate elements of the conditional probability tables (CPTs) in the Bayesian network.

From this definition, it is easy to prove that the parameters  $\theta(X_i | Parents(X_i))$  are exactly the conditional probabilities  $\mathbf{P}(X_i | Parents(X_i))$  implied by the joint distribution (see Exercise 14.2). Hence, we can rewrite Equation (14.1) as

$$P(x_1, ..., x_n) = \prod_{i=1}^{n} P(x_i | parents(X_i)).$$
 (14.2)

In other words, the tables we have been calling conditional probability tables really *are* conditional probability tables according to the semantics defined in Equation (14.1).

To illustrate this, we can calculate the probability that the alarm has sounded, but neither a burglary nor an earthquake has occurred, and both John and Mary call. We multiply entries from the joint distribution (using single-letter names for the variables):

$$P(j, m, a, \neg b, \neg e) = P(j \mid a)P(m \mid a)P(a \mid \neg b \land \neg e)P(\neg b)P(\neg e)$$
  
= 0.90 × 0.70 × 0.001 × 0.999 × 0.998 = 0.000628 .

Section 13.3 explained that the full joint distribution can be used to answer any query about the domain. If a Bayesian network is a representation of the joint distribution, then it too can be used to answer any query, by summing all the relevant joint entries. Section 14.4 explains how to do this, but also describes methods that are much more efficient.

### A method for constructing Bayesian networks

Equation (14.2) defines what a given Bayesian network means. The next step is to explain how to *construct* a Bayesian network in such a way that the resulting joint distribution is a good representation of a given domain. We will now show that Equation (14.2) implies certain conditional independence relationships that can be used to guide the knowledge engineer in constructing the topology of the network. First, we rewrite the entries in the joint distribution in terms of conditional probability, using the product rule (see page 486):

$$P(x_1,\ldots,x_n) = P(x_n | x_{n-1},\ldots,x_1) P(x_{n-1},\ldots,x_1)$$
.

Then we repeat the process, reducing each conjunctive probability to a conditional probability and a smaller conjunction. We end up with one big product:

$$P(x_1, \dots, x_n) = P(x_n | x_{n-1}, \dots, x_1) P(x_{n-1} | x_{n-2}, \dots, x_1) \cdots P(x_2 | x_1) P(x_1)$$
$$= \prod_{i=1}^n P(x_i | x_{i-1}, \dots, x_1) .$$

CHAIN RULE

This identity is called the **chain rule**. It holds for any set of random variables. Comparing it with Equation (14.2), we see that the specification of the joint distribution is equivalent to the general assertion that, for every variable  $X_i$  in the network,

$$\mathbf{P}(X_i \mid X_{i-1}, \dots, X_1) = \mathbf{P}(X_i \mid Parents(X_i)), \qquad (14.3)$$

provided that  $Parents(X_i) \subseteq \{X_{i-1}, \dots, X_1\}$ . This last condition is satisfied by numbering the nodes in a way that is consistent with the partial order implicit in the graph structure.

What Equation (14.3) says is that the Bayesian network is a correct representation of the domain only if each node is conditionally independent of its other predecessors in the node ordering, given its parents. We can satisfy this condition with this methodology:

- 1. *Nodes:* First determine the set of variables that are required to model the domain. Now order them,  $\{X_1, \ldots, X_n\}$ . Any order will work, but the resulting network will be more compact if the variables are ordered such that causes precede effects.
- 2. *Links*: For i = 1 to n do:
  - Choose, from  $X_1, \ldots, X_{i-1}$ , a minimal set of parents for  $X_i$ , such that Equation (14.3) is satisfied.
  - For each parent insert a link from the parent to  $X_i$ .
  - CPTs: Write down the conditional probability table,  $P(X_i|Parents(X_i))$ .



Intuitively, the parents of node  $X_i$  should contain all those nodes in  $X_1, \ldots, X_{i-1}$  that directly influence  $X_i$ . For example, suppose we have completed the network in Figure 14.2 except for the choice of parents for MaryCalls. MaryCalls is certainly influenced by whether there is a Burglary or an Earthquake, but not directly influenced. Intuitively, our knowledge of the domain tells us that these events influence Mary's calling behavior only through their effect on the alarm. Also, given the state of the alarm, whether John calls has no influence on Mary's calling. Formally speaking, we believe that the following conditional independence statement holds:

 $\mathbf{P}(MaryCalls \mid JohnCalls, Alarm, Earthquake, Burglary) = \mathbf{P}(MaryCalls \mid Alarm)$ .

Thus, Alarm will be the only parent node for MaryCalls.

Because each node is connected only to earlier nodes, this construction method guarantees that the network is acyclic. Another important property of Bayesian networks is that they contain no redundant probability values. If there is no redundancy, then there is no chance for inconsistency: it is impossible for the knowledge engineer or domain expert to create a Bayesian network that violates the axioms of probability.

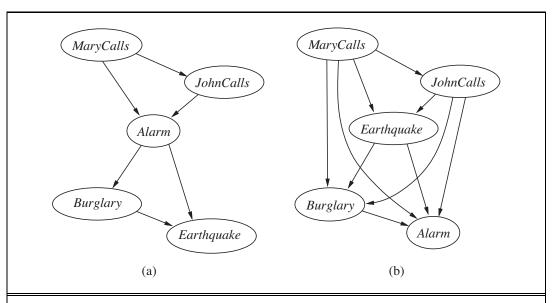
#### Compactness and node ordering

As well as being a complete and nonredundant representation of the domain, a Bayesian network can often be far more *compact* than the full joint distribution. This property is what makes it feasible to handle domains with many variables. The compactness of Bayesian networks is an example of a general property of **locally structured** (also called **sparse**) systems. In a locally structured system, each subcomponent interacts directly with only a bounded number of other components, regardless of the total number of components. Local structure is usually associated with linear rather than exponential growth in complexity. In the case of Bayesian networks, it is reasonable to suppose that in most domains each random variable is directly influenced by at most k others, for some constant k. If we assume n Boolean variables for simplicity, then the amount of information needed to specify each conditional probability table will be at most  $2^k$  numbers, and the complete network can be specified by  $n2^k$  numbers. In contrast, the joint distribution contains  $2^n$  numbers. To make this concrete, suppose we have n=30 nodes, each with five parents (k=5). Then the Bayesian network requires 960 numbers, but the full joint distribution requires over a billion.

There are domains in which each variable can be influenced directly by all the others, so that the network is fully connected. Then specifying the conditional probability tables requires the same amount of information as specifying the joint distribution. In some domains, there will be slight dependencies that should strictly be included by adding a new link. But if these dependencies are tenuous, then it may not be worth the additional complexity in the network for the small gain in accuracy. For example, one might object to our burglary network on the grounds that if there is an earthquake, then John and Mary would not call even if they heard the alarm, because they assume that the earthquake is the cause. Whether to add the link from Earthquake to JohnCalls and MaryCalls (and thus enlarge the tables) depends on comparing the importance of getting more accurate probabilities with the cost of specifying the extra information.



LOCALLY STRUCTURED SPARSE



**Figure 14.3** Network structure depends on order of introduction. In each network, we have introduced nodes in top-to-bottom order.

Even in a locally structured domain, we will get a compact Bayesian network only if we choose the node ordering well. What happens if we happen to choose the wrong order? Consider the burglary example again. Suppose we decide to add the nodes in the order *MaryCalls*, *JohnCalls*, *Alarm*, *Burglary*, *Earthquake*. We then get the somewhat more complicated network shown in Figure 14.3(a). The process goes as follows:

- Adding *MaryCalls*: No parents.
- Adding JohnCalls: If Mary calls, that probably means the alarm has gone off, which of course would make it more likely that John calls. Therefore, JohnCalls needs MaryCalls as a parent.
- Adding *Alarm*: Clearly, if both call, it is more likely that the alarm has gone off than if just one or neither calls, so we need both *MaryCalls* and *JohnCalls* as parents.
- Adding *Burglary*: If we know the alarm state, then the call from John or Mary might give us information about our phone ringing or Mary's music, but not about burglary:

$$\mathbf{P}(Burglary \mid Alarm, JohnCalls, MaryCalls) = \mathbf{P}(Burglary \mid Alarm)$$
.

Hence we need just Alarm as parent.

• Adding *Earthquake*: If the alarm is on, it is more likely that there has been an earthquake. (The alarm is an earthquake detector of sorts.) But if we know that there has been a burglary, then that explains the alarm, and the probability of an earthquake would be only slightly above normal. Hence, we need both *Alarm* and *Burglary* as parents.

The resulting network has two more links than the original network in Figure 14.2 and requires three more probabilities to be specified. What's worse, some of the links represent tenuous relationships that require difficult and unnatural probability judgments, such as as-



sessing the probability of *Earthquake*, given *Burglary* and *Alarm*. This phenomenon is quite general and is related to the distinction between **causal** and **diagnostic** models introduced in Section 13.5.1 (see also Exercise 8.13). If we try to build a diagnostic model with links from symptoms to causes (as from *MaryCalls* to *Alarm* or *Alarm* to *Burglary*), we end up having to specify additional dependencies between otherwise independent causes (and often between separately occurring symptoms as well). *If we stick to a causal model, we end up having to specify fewer numbers, and the numbers will often be easier to come up with. In the domain of medicine, for example, it has been shown by Tversky and Kahneman (1982) that expert physicians prefer to give probability judgments for causal rules rather than for diagnostic ones.* 

Figure 14.3(b) shows a very bad node ordering: MaryCalls, JohnCalls, Earthquake, Burglary, Alarm. This network requires 31 distinct probabilities to be specified—exactly the same number as the full joint distribution. It is important to realize, however, that any of the three networks can represent exactly the same joint distribution. The last two versions simply fail to represent all the conditional independence relationships and hence end up specifying a lot of unnecessary numbers instead.

# 14.2.2 Conditional independence relations in Bayesian networks

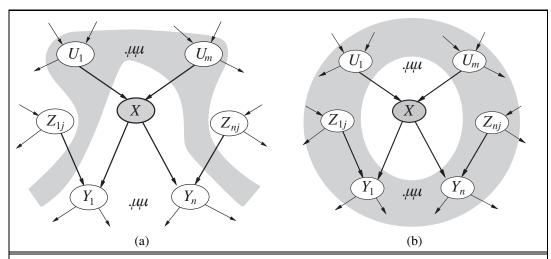
We have provided a "numerical" semantics for Bayesian networks in terms of the representation of the full joint distribution, as in Equation (14.2). Using this semantics to derive a method for constructing Bayesian networks, we were led to the consequence that a node is conditionally independent of its other predecessors, given its parents. It turns out that we can also go in the other direction. We can start from a "topological" semantics that specifies the conditional independence relationships encoded by the graph structure, and from this we can derive the "numerical" semantics. The topological semantics<sup>2</sup> specifies that each variable is conditionally independent of its non-**descendants**, given its parents. For example, in Figure 14.2, JohnCalls is independent of Burglary, Earthquake, and MaryCalls given the value of Alarm. The definition is illustrated in Figure 14.4(a). From these conditional independence assertions and the interpretation of the network parameters  $\theta(X_i \mid Parents(X_i))$  as specifications of conditional probabilities  $\mathbf{P}(X_i \mid Parents(X_i))$ , the full joint distribution given in Equation (14.2) can be reconstructed. In this sense, the "numerical" semantics and the "topological" semantics are equivalent.

Another important independence property is implied by the topological semantics: a node is conditionally independent of all other nodes in the network, given its parents, children, and children's parents—that is, given its **Markov blanket**. (Exercise 14.7 asks you to prove this.) For example, *Burglary* is independent of *JohnCalls* and *MaryCalls*, given *Alarm* and *Earthquake*. This property is illustrated in Figure 14.4(b).

MARKOV BI ANKET

DESCENDANT

 $<sup>^2</sup>$  There is also a general topological criterion called **d-separation** for deciding whether a set of nodes **X** is conditionally independent of another set **Y**, given a third set **Z**. The criterion is rather complicated and is not needed for deriving the algorithms in this chapter, so we omit it. Details may be found in Pearl (1988) or Darwiche (2009). Shachter (1998) gives a more intuitive method of ascertaining d-separation.



Chapter

**Figure 14.4** (a) A node X is conditionally independent of its non-descendants (e.g., the  $Z_{ij}$ s) given its parents (the  $U_i$ s shown in the gray area). (b) A node X is conditionally independent of all other nodes in the network given its Markov blanket (the gray area).

## 14.3 EFFICIENT REPRESENTATION OF CONDITIONAL DISTRIBUTIONS

Even if the maximum number of parents k is smallish, filling in the CPT for a node requires up to  $O(2^k)$  numbers and perhaps a great deal of experience with all the possible conditioning cases. In fact, this is a worst-case scenario in which the relationship between the parents and the child is completely arbitrary. Usually, such relationships are describable by a **canonical distribution** that fits some standard pattern. In such cases, the complete table can be specified by naming the pattern and perhaps supplying a few parameters—much easier than supplying an exponential number of parameters.

DETERMINISTIC NODES

CANONICAL

DISTRIBUTION

The simplest example is provided by **deterministic nodes**. A deterministic node has its value specified exactly by the values of its parents, with no uncertainty. The relationship can be a logical one: for example, the relationship between the parent nodes *Canadian*, *US*, *Mexican* and the child node *NorthAmerican* is simply that the child is the disjunction of the parents. The relationship can also be numerical: for example, if the parent nodes are the prices of a particular model of car at several dealers and the child node is the price that a bargain hunter ends up paying, then the child node is the minimum of the parent values; or if the parent nodes are a lake's inflows (rivers, runoff, precipitation) and outflows (rivers, evaporation, seepage) and the child is the change in the water level of the lake, then the value of the child is the sum of the inflow parents minus the sum of the outflow parents.

Uncertain relationships can often be characterized by so-called **noisy** logical relationships. The standard example is the **noisy-OR** relation, which is a generalization of the logical OR. In propositional logic, we might say that *Fever* is true if and only if *Cold*, *Flu*, or *Malaria* is true. The noisy-OR model allows for uncertainty about the ability of each parent to cause the child to be true—the causal relationship between parent and child may be

NOISY-OR

LEAK NODE

inhibited, and so a patient could have a cold, but not exhibit a fever. The model makes two assumptions. First, it assumes that all the possible causes are listed. (If some are missing, we can always add a so-called **leak node** that covers "miscellaneous causes.") Second, it assumes that inhibition of each parent is independent of inhibition of any other parents: for example, whatever inhibits Malaria from causing a fever is independent of whatever inhibits Flu from causing a fever. Given these assumptions, Fever is false if and only if all its true parents are inhibited, and the probability of this is the product of the inhibition probabilities q for each parent. Let us suppose these individual inhibition probabilities are as follows:

$$\begin{split} q_{\rm cold} &= P(\neg fever \mid cold, \neg flu, \neg malaria) = 0.6 \;, \\ q_{\rm flu} &= P(\neg fever \mid \neg cold, flu, \neg malaria) = 0.2 \;, \\ q_{\rm malaria} &= P(\neg fever \mid \neg cold, \neg flu, malaria) = 0.1 \;. \end{split}$$

Then, from this information and the noisy-OR assumptions, the entire CPT can be built. The general rule is that

$$P(x_i | parents(X_i)) = 1 - \prod_{\{j: X_j = true\}} q_j,$$

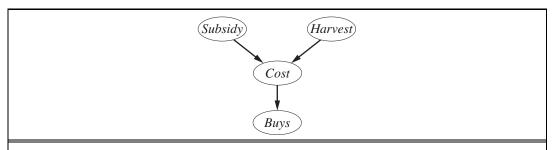
where the product is taken over the parents that are set to true for that row of the CPT. The following table illustrates this calculation:

Cold	Flu	Malaria	P(Fever)	$P(\neg Fever)$
F	F	F	0.0	1.0
F	F	T	0.9	0.1
F	T	F	0.8	0.2
F	T	T	0.98	$0.02 = 0.2 \times 0.1$
T	F	F	0.4	0.6
T	F	T	0.94	$0.06 = 0.6 \times 0.1$
T	T	F	0.88	$0.12 = 0.6 \times 0.2$
T	T	T	0.988	$0.012 = 0.6 \times 0.2 \times 0.1$

In general, noisy logical relationships in which a variable depends on k parents can be described using O(k) parameters instead of  $O(2^k)$  for the full conditional probability table. This makes assessment and learning much easier. For example, the CPCS network (Pradhan *et al.*, 1994) uses noisy-OR and noisy-MAX distributions to model relationships among diseases and symptoms in internal medicine. With 448 nodes and 906 links, it requires only 8,254 values instead of 133,931,430 for a network with full CPTs.

#### **Bayesian nets with continuous variables**

Many real-world problems involve continuous quantities, such as height, mass, temperature, and money; in fact, much of statistics deals with random variables whose domains are continuous. By definition, continuous variables have an infinite number of possible values, so it is impossible to specify conditional probabilities explicitly for each value. One possible way to handle continuous variables is to avoid them by using **discretization**—that is, dividing up the



**Figure 14.5** A simple network with discrete variables (Subsidy and Buys) and continuous variables (Harvest and Cost).

possible values into a fixed set of intervals. For example, temperatures could be divided into ( $<0^{\circ}\text{C}$ ), ( $0^{\circ}\text{C}-100^{\circ}\text{C}$ ), and ( $>100^{\circ}\text{C}$ ). Discretization is sometimes an adequate solution, but often results in a considerable loss of accuracy and very large CPTs. The most common solution is to define standard families of probability density functions (see Appendix A) that are specified by a finite number of **parameters**. For example, a Gaussian (or normal) distribution  $N(\mu, \sigma^2)(x)$  has the mean  $\mu$  and the variance  $\sigma^2$  as parameters. Yet another solution—sometimes called a **nonparametric** representation—is to define the conditional distribution implicitly with a collection of instances, each containing specific values of the parent and child variables. We explore this approach further in Chapter 18.

A network with both discrete and continuous variables is called a **hybrid Bayesian network**. To specify a hybrid network, we have to specify two new kinds of distributions: the conditional distribution for a continuous variable given discrete or continuous parents; and the conditional distribution for a discrete variable given continuous parents. Consider the simple example in Figure 14.5, in which a customer buys some fruit depending on its cost, which depends in turn on the size of the harvest and whether the government's subsidy scheme is operating. The variable *Cost* is continuous and has continuous and discrete parents; the variable *Buys* is discrete and has a continuous parent.

For the Cost variable, we need to specify  $\mathbf{P}(Cost \mid Harvest, Subsidy)$ . The discrete parent is handled by enumeration—that is, by specifying both  $P(Cost \mid Harvest, subsidy)$  and  $P(Cost \mid Harvest, \neg subsidy)$ . To handle Harvest, we specify how the distribution over the cost c depends on the continuous value b of c of c depends on the continuous value c depends on the contin

$$P(c | h, subsidy) = N(a_t h + b_t, \sigma_t^2)(c) = \frac{1}{\sigma_t \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{c - (a_t h + b_t)}{\sigma_t}\right)^2}$$

$$P(c | h, \neg subsidy) = N(a_f h + b_f, \sigma_f^2)(c) = \frac{1}{\sigma_f \sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{c - (a_f h + b_f)}{\sigma_f}\right)^2}$$

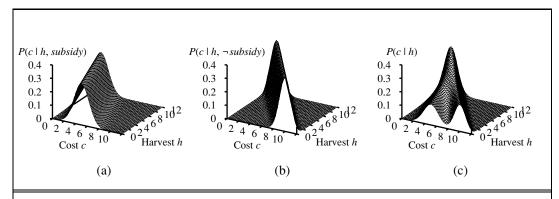
For this example, then, the conditional distribution for Cost is specified by naming the linear Gaussian distribution and providing the parameters  $a_t$ ,  $b_t$ ,  $\sigma_t$ ,  $a_f$ ,  $b_f$ , and  $\sigma_f$ . Figures 14.6(a)

PARAMETER

NONPARAMETRIC

HYBRID BAYESIAN NETWORK

LINEAR GAUSSIAN



**Figure 14.6** The graphs in (a) and (b) show the probability distribution over Cost as a function of Harvest size, with Subsidy true and false, respectively. Graph (c) shows the distribution  $P(Cost \mid Harvest)$ , obtained by summing over the two subsidy cases.

and (b) show these two relationships. Notice that in each case the slope is negative, because cost decreases as supply increases. (Of course, the assumption of linearity implies that the cost becomes negative at some point; the linear model is reasonable only if the harvest size is limited to a narrow range.) Figure 14.6(c) shows the distribution  $P(c \mid h)$ , averaging over the two possible values of Subsidy and assuming that each has prior probability 0.5. This shows that even with very simple models, quite interesting distributions can be represented.

The linear Gaussian conditional distribution has some special properties. A network containing only continuous variables with linear Gaussian distributions has a joint distribution that is a multivariate Gaussian distribution (see Appendix A) over all the variables (Exercise 14.9). Furthermore, the posterior distribution given any evidence also has this property.<sup>3</sup> When discrete variables are added as parents (not as children) of continuous variables, the network defines a **conditional Gaussian**, or CG, distribution: given any assignment to the discrete variables, the distribution over the continuous variables is a multivariate Gaussian.

Now we turn to the distributions for discrete variables with continuous parents. Consider, for example, the Buys node in Figure 14.5. It seems reasonable to assume that the customer will buy if the cost is low and will not buy if it is high and that the probability of buying varies smoothly in some intermediate region. In other words, the conditional distribution is like a "soft" threshold function. One way to make soft thresholds is to use the *integral* of the standard normal distribution:

$$\Phi(x) = \int_{-\infty}^{x} N(0,1)(x) dx .$$

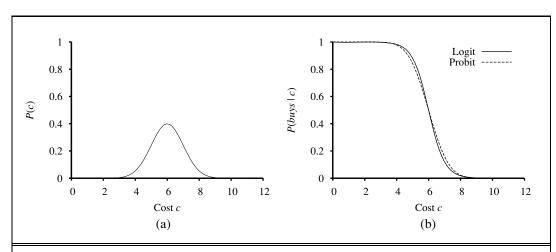
Then the probability of Buys given Cost might be

$$P(\mathit{buys} \mid \mathit{Cost} = c) = \Phi((-c + \mu)/\sigma) \;,$$

which means that the cost threshold occurs around  $\mu$ , the width of the threshold region is proportional to  $\sigma$ , and the probability of buying decreases as cost increases. This **probit distri-**

CONDITIONAL GAUSSIAN

<sup>&</sup>lt;sup>3</sup> It follows that inference in linear Gaussian networks takes only  $O(n^3)$  time in the worst case, regardless of the network topology. In Section 14.4, we see that inference for networks of discrete variables is NP-hard.



Chapter

14.

**Figure 14.7** (a) A normal (Gaussian) distribution for the cost threshold, centered on  $\mu = 6.0$  with standard deviation  $\sigma = 1.0$ . (b) Logit and probit distributions for the probability of *buys* given *cost*, for the parameters  $\mu = 6.0$  and  $\sigma = 1.0$ .

PROBIT DISTRIBUTION

**bution** (pronounced "pro-bit" and short for "probability unit") is illustrated in Figure 14.7(a). The form can be justified by proposing that the underlying decision process has a hard threshold, but that the precise location of the threshold is subject to random Gaussian noise.

LOGIT DISTRIBUTION
LOGISTIC FUNCTION

An alternative to the probit model is the **logit distribution** (pronounced "low-jit"). It uses the **logistic function**  $1/(1+e^{-x})$  to produce a soft threshold:

$$P(buys \mid Cost = c) = \frac{1}{1 + exp(-2\frac{-c+\mu}{\sigma})}.$$

This is illustrated in Figure 14.7(b). The two distributions look similar, but the logit actually has much longer "tails." The probit is often a better fit to real situations, but the logit is sometimes easier to deal with mathematically. It is used widely in neural networks (Chapter 20). Both probit and logit can be generalized to handle multiple continuous parents by taking a linear combination of the parent values.

# 14.4 EXACT INFERENCE IN BAYESIAN NETWORKS

**EVENT** 

HIDDEN VARIABLE

The basic task for any probabilistic inference system is to compute the posterior probability distribution for a set of **query variables**, given some observed **event**—that is, some assignment of values to a set of **evidence variables**. To simplify the presentation, we will consider only one query variable at a time; the algorithms can easily be extended to queries with multiple variables. We will use the notation from Chapter 13: X denotes the query variable;  $\mathbf{E}$  denotes the set of evidence variables  $E_1, \ldots, E_m$ , and  $\mathbf{e}$  is a particular observed event;  $\mathbf{Y}$  will denotes the nonevidence, nonquery variables  $Y_1, \ldots, Y_l$  (called the **hidden variables**). Thus, the complete set of variables is  $\mathbf{X} = \{X\} \cup \mathbf{E} \cup \mathbf{Y}$ . A typical query asks for the posterior probability distribution  $\mathbf{P}(X \mid \mathbf{e})$ .

In the burglary network, we might observe the event in which JohnCalls = true and MaryCalls = true. We could then ask for, say, the probability that a burglary has occurred:

$$\mathbf{P}(Burglary \mid JohnCalls = true, MaryCalls = true) = \langle 0.284, 0.716 \rangle$$
.

In this section we discuss exact algorithms for computing posterior probabilities and will consider the complexity of this task. It turns out that the general case is intractable, so Section 14.5 covers methods for approximate inference.

## 14.4.1 Inference by enumeration

Chapter 13 explained that any conditional probability can be computed by summing terms from the full joint distribution. More specifically, a query  $P(X \mid e)$  can be answered using Equation (13.9), which we repeat here for convenience:

$$\mathbf{P}(X \,|\, \mathbf{e}) = \alpha \, \mathbf{P}(X, \mathbf{e}) = \alpha \, \sum_{\mathbf{y}} \mathbf{P}(X, \mathbf{e}, \mathbf{y}) \;.$$

Now, a Bayesian network gives a complete representation of the full joint distribution. More specifically, Equation (14.2) on page 513 shows that the terms  $P(x, \mathbf{e}, \mathbf{y})$  in the joint distribution can be written as products of conditional probabilities from the network. Therefore, a query can be answered using a Bayesian network by computing sums of products of conditional probabilities from the network.

Consider the query  $\mathbf{P}(Burglary \mid JohnCalls = true, MaryCalls = true)$ . The hidden variables for this query are Earthquake and Alarm. From Equation (13.9), using initial letters for the variables to shorten the expressions, we have<sup>4</sup>

$$\mathbf{P}(B \mid j, m) = \alpha \, \mathbf{P}(B, j, m) = \alpha \, \sum_{e} \sum_{a} \mathbf{P}(B, j, m, e, a,) \; .$$

The semantics of Bayesian networks (Equation (14.2)) then gives us an expression in terms of CPT entries. For simplicity, we do this just for Burglary = true:

$$P(b \mid j, m) = \alpha \sum_{e} \sum_{a} P(b) P(e) P(a \mid b, e) P(j \mid a) P(m \mid a) .$$

To compute this expression, we have to add four terms, each computed by multiplying five numbers. In the worst case, where we have to sum out almost all the variables, the complexity of the algorithm for a network with n Boolean variables is  $O(n2^n)$ .

An improvement can be obtained from the following simple observations: the P(b) term is a constant and can be moved outside the summations over a and e, and the P(e) term can be moved outside the summation over a. Hence, we have

$$P(b \mid j, m) = \alpha P(b) \sum_{e} P(e) \sum_{a} P(a \mid b, e) P(j \mid a) P(m \mid a) .$$
 (14.4)

This expression can be evaluated by looping through the variables in order, multiplying CPT entries as we go. For each summation, we also need to loop over the variable's possible



Section 14.4.

<sup>&</sup>lt;sup>4</sup> An expression such as  $\sum_e P(a,e)$  means to sum P(A=a,E=e) for all possible values of e. When E is Boolean, there is an ambiguity in that P(e) is used to mean both P(E=true) and P(E=e), but it should be clear from context which is intended; in particular, in the context of a sum the latter is intended.

values. The structure of this computation is shown in Figure 14.8. Using the numbers from Figure 14.2, we obtain  $P(b \mid j, m) = \alpha \times 0.00059224$ . The corresponding computation for  $\neg b$  yields  $\alpha \times 0.0014919$ ; hence,

$$\mathbf{P}(B \mid j, m) = \alpha \langle 0.00059224, 0.0014919 \rangle \approx \langle 0.284, 0.716 \rangle$$
.

That is, the chance of a burglary, given calls from both neighbors, is about 28%.

The evaluation process for the expression in Equation (14.4) is shown as an expression tree in Figure 14.8. The ENUMERATION-ASK algorithm in Figure 14.9 evaluates such trees using depth-first recursion. The algorithm is very similar in structure to the backtracking algorithm for solving CSPs (Figure 6.5) and the DPLL algorithm for satisfiability (Figure 7.17).

The space complexity of ENUMERATION-ASK is only linear in the number of variables: the algorithm sums over the full joint distribution without ever constructing it explicitly. Unfortunately, its time complexity for a network with n Boolean variables is always  $O(2^n)$ —better than the  $O(n \, 2^n)$  for the simple approach described earlier, but still rather grim.

Note that the tree in Figure 14.8 makes explicit the *repeated subexpressions* evaluated by the algorithm. The products  $P(j \mid a)P(m \mid a)$  and  $P(j \mid \neg a)P(m \mid \neg a)$  are computed twice, once for each value of e. The next section describes a general method that avoids such wasted computations.

## 14.4.2 The variable elimination algorithm

The enumeration algorithm can be improved substantially by eliminating repeated calculations of the kind illustrated in Figure 14.8. The idea is simple: do the calculation once and save the results for later use. This is a form of dynamic programming. There are several versions of this approach; we present the **variable elimination** algorithm, which is the simplest. Variable elimination works by evaluating expressions such as Equation (14.4) in *right-to-left* order (that is, *bottom up* in Figure 14.8). Intermediate results are stored, and summations over each variable are done only for those portions of the expression that depend on the variable.

Let us illustrate this process for the burglary network. We evaluate the expression

$$\mathbf{P}(B \mid j, m) = \alpha \underbrace{\mathbf{P}(B)}_{\mathbf{f}_1(B)} \sum_{e} \underbrace{P(e)}_{\mathbf{f}_2(E)} \sum_{a} \underbrace{\mathbf{P}(a \mid B, e)}_{\mathbf{f}_3(A, B, E)} \underbrace{P(j \mid a)}_{\mathbf{f}_4(A)} \underbrace{P(m \mid a)}_{\mathbf{f}_5(A)}.$$

Notice that we have annotated each part of the expression with the name of the corresponding **factor**; each factor is a matrix indexed by the values of its argument variables. For example, the factors  $\mathbf{f}_4(A)$  and  $\mathbf{f}_5(A)$  corresponding to  $P(j \mid a)$  and  $P(m \mid a)$  depend just on A because J and M are fixed by the query. They are therefore two-element vectors:

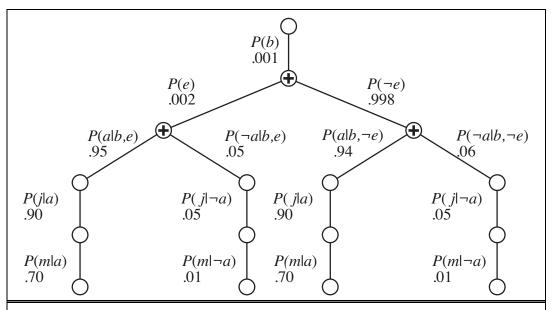
$$\mathbf{f}_4(A) = \begin{pmatrix} P(j \mid a) \\ P(j \mid \neg a) \end{pmatrix} = \begin{pmatrix} 0.90 \\ 0.05 \end{pmatrix} \qquad \mathbf{f}_5(A) = \begin{pmatrix} P(m \mid a) \\ P(m \mid \neg a) \end{pmatrix} = \begin{pmatrix} 0.70 \\ 0.01 \end{pmatrix}.$$

 $\mathbf{f}_3(A,B,E)$  will be a  $2\times 2\times 2$  matrix, which is hard to show on the printed page. (The "first" element is given by  $P(a\,|\,b,e)=0.95$  and the "last" by  $P(\neg a\,|\,\neg b,\neg e)=0.999$ .) In terms of factors, the query expression is written as

$$\mathbf{P}(B \mid j, m) = \alpha \,\mathbf{f}_1(B) \times \sum_{e} \mathbf{f}_2(E) \times \sum_{a} \mathbf{f}_3(A, B, E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A)$$

VARIABLE ELIMINATION

FACTOR



**Figure 14.8** The structure of the expression shown in Equation (14.4). The evaluation proceeds top down, multiplying values along each path and summing at the "+" nodes. Notice the repetition of the paths for j and m.

```
function ENUMERATION-ASK(X, \mathbf{e}, bn) returns a distribution over X
  inputs: X, the query variable
            e, observed values for variables E
            bn, a Bayes net with variables \{X\} \cup \mathbf{E} \cup \mathbf{Y} / \star \mathbf{Y} = hidden \ variables \star /
  \mathbf{Q}(X) \leftarrow a distribution over X, initially empty
  for each value x_i of X do
       \mathbf{Q}(x_i) \leftarrow \text{Enumerate-All}(bn.\text{Vars}, \mathbf{e}_{x_i})
            where \mathbf{e}_{x_i} is \mathbf{e} extended with X = x_i
  return NORMALIZE(\mathbf{Q}(X))
function ENUMERATE-ALL(vars, e) returns a real number
  if Empty?(vars) then return 1.0
   Y \leftarrow \mathsf{FIRST}(vars)
  if Y has value y in e
       then return P(y \mid parents(Y)) \times \text{ENUMERATE-ALL}(\text{REST}(vars), \mathbf{e})
       else return \sum_y \ P(y \mid parents(Y)) \ 	imes \ 	ext{Enumerate-All(Rest($vars$), $\mathbf{e}_y$)}
            where \mathbf{e}_y is \mathbf{e} extended with Y = y
   Figure 14.9
                      The enumeration algorithm for answering queries on Bayesian networks.
```

POINTWISE PRODUCT

where the "×" operator is not ordinary matrix multiplication but instead the **pointwise product** operation, to be described shortly.

The process of evaluation is a process of summing out variables (right to left) from pointwise products of factors to produce new factors, eventually yielding a factor that is the solution, i.e., the posterior distribution over the query variable. The steps are as follows:

• First, we sum out A from the product of  $\mathbf{f}_3$ ,  $\mathbf{f}_4$ , and  $\mathbf{f}_5$ . This gives us a new  $2 \times 2$  factor  $\mathbf{f}_6(B, E)$  whose indices range over just B and E:

$$\mathbf{f}_{6}(B,E) = \sum_{a} \mathbf{f}_{3}(A,B,E) \times \mathbf{f}_{4}(A) \times \mathbf{f}_{5}(A)$$

$$= (\mathbf{f}_{3}(a,B,E) \times \mathbf{f}_{4}(a) \times \mathbf{f}_{5}(a)) + (\mathbf{f}_{3}(\neg a,B,E) \times \mathbf{f}_{4}(\neg a) \times \mathbf{f}_{5}(\neg a)).$$

Now we are left with the expression

$$\mathbf{P}(B \mid j, m) = \alpha \, \mathbf{f}_1(B) \times \sum_{e} \mathbf{f}_2(E) \times \mathbf{f}_6(B, E) .$$

• Next, we sum out E from the product of  $\mathbf{f}_2$  and  $\mathbf{f}_6$ :

$$\mathbf{f}_7(B) = \sum_e \mathbf{f}_2(E) \times \mathbf{f}_6(B, E)$$
$$= \mathbf{f}_2(e) \times \mathbf{f}_6(B, e) + \mathbf{f}_2(\neg e) \times \mathbf{f}_6(B, \neg e) .$$

This leaves the expression

$$\mathbf{P}(B \mid j, m) = \alpha \mathbf{f}_1(B) \times \mathbf{f}_7(B)$$

which can be evaluated by taking the pointwise product and normalizing the result.

Examining this sequence, we see that two basic computational operations are required: pointwise product of a pair of factors, and summing out a variable from a product of factors. The next section describes each of these operations.

#### **Operations on factors**

The pointwise product of two factors  $\mathbf{f}_1$  and  $\mathbf{f}_2$  yields a new factor  $\mathbf{f}$  whose variables are the *union* of the variables in  $\mathbf{f}_1$  and  $\mathbf{f}_2$  and whose elements are given by the product of the corresponding elements in the two factors. Suppose the two factors have variables  $Y_1, \ldots, Y_k$  in common. Then we have

$$\mathbf{f}(X_1 \dots X_j, Y_1 \dots Y_k, Z_1 \dots Z_l) = \mathbf{f}_1(X_1 \dots X_j, Y_1 \dots Y_k) \ \mathbf{f}_2(Y_1 \dots Y_k, Z_1 \dots Z_l).$$

If all the variables are binary, then  $\mathbf{f}_1$  and  $\mathbf{f}_2$  have  $2^{j+k}$  and  $2^{k+l}$  entries, respectively, and the pointwise product has  $2^{j+k+l}$  entries. For example, given two factors  $\mathbf{f}_1(A,B)$  and  $\mathbf{f}_2(B,C)$ , the pointwise product  $\mathbf{f}_1 \times \mathbf{f}_2 = \mathbf{f}_3(A,B,C)$  has  $2^{1+1+1} = 8$  entries, as illustrated in Figure 14.10. Notice that the factor resulting from a pointwise product can contain more variables than any of the factors being multiplied and that the size of a factor is exponential in the number of variables. This is where both space and time complexity arise in the variable elimination algorithm.

Section 14.4.

A	B	$\mathbf{f}_1(A,B)$	B	C	$\mathbf{f}_2(B,C)$	A	В	C	$\mathbf{f}_3(A,B,C)$
Т	T	.3	T	T	.2	T	T	T	$.3 \times .2 = .06$
T	F	.7	Т	F	.8	T	T	F	$.3 \times .8 = .24$
F	T	.9	F	T	.6	T	F	T	$.7 \times .6 = .42$
F	F	.1	F	F	.4	T	F	F	$.7 \times .4 = .28$
						F	T	T	$.9 \times .2 = .18$
						F	T	F	$.9 \times .8 = .72$
						F	F	T	$.1 \times .6 = .06$
						F	F	F	$.1 \times .4 = .04$

**Figure 14.10** Illustrating pointwise multiplication:  $\mathbf{f}_1(A, B) \times \mathbf{f}_2(B, C) = \mathbf{f}_3(A, B, C)$ .

Summing out a variable from a product of factors is done by adding up the submatrices formed by fixing the variable to each of its values in turn. For example, to sum out A from  $\mathbf{f}_3(A, B, C)$ , we write

$$\mathbf{f}(B,C) = \sum_{a} \mathbf{f}_{3}(A,B,C) = \mathbf{f}_{3}(a,B,C) + \mathbf{f}_{3}(\neg a,B,C)$$
$$= \begin{pmatrix} .06 & .24 \\ .42 & .28 \end{pmatrix} + \begin{pmatrix} .18 & .72 \\ .06 & .04 \end{pmatrix} = \begin{pmatrix} .24 & .96 \\ .48 & .32 \end{pmatrix}.$$

The only trick is to notice that any factor that does *not* depend on the variable to be summed out can be moved outside the summation. For example, if we were to sum out E first in the burglary network, the relevant part of the expression would be

$$\sum_{e} \mathbf{f}_2(E) \times \mathbf{f}_3(A,B,E) \times \mathbf{f}_4(A) \times \mathbf{f}_5(A) = \mathbf{f}_4(A) \times \mathbf{f}_5(A) \times \sum_{e} \mathbf{f}_2(E) \times \mathbf{f}_3(A,B,E).$$

Now the pointwise product inside the summation is computed, and the variable is summed out of the resulting matrix.

Notice that matrices are *not* multiplied until we need to sum out a variable from the accumulated product. At that point, we multiply just those matrices that include the variable to be summed out. Given functions for pointwise product and summing out, the variable elimination algorithm itself can be written quite simply, as shown in Figure 14.11.

### Variable ordering and variable relevance

The algorithm in Figure 14.11 includes an unspecified ORDER function to choose an ordering for the variables. Every choice of ordering yields a valid algorithm, but different orderings cause different intermediate factors to be generated during the calculation. For example, in the calculation shown previously, we eliminated A before E; if we do it the other way, the calculation becomes

$$\mathbf{P}(B \mid j,m) = \alpha \, \mathbf{f}_1(B) \times \, \sum_a \mathbf{f}_4(A) \times \mathbf{f}_5(A) \times \, \sum_e \mathbf{f}_2(E) \times \mathbf{f}_3(A,B,E) \; ,$$

during which a new factor  $\mathbf{f}_6(A, B)$  will be generated.

In general, the time and space requirements of variable elimination are dominated by the size of the largest factor constructed during the operation of the algorithm. This in turn

```
function ELIMINATION-ASK(X, \mathbf{e}, bn) returns a distribution over X inputs: X, the query variable \mathbf{e}, observed values for variables \mathbf{E} bn, a Bayesian network specifying joint distribution \mathbf{P}(X_1, \dots, X_n) factors \leftarrow [] for each var in \mathsf{ORDER}(bn.\mathsf{VARS}) do factors \leftarrow [Make-Factor(var, \mathbf{e})|factors] if var is a hidden variable then factors \leftarrow Sum-Out(var, factors) return \mathsf{NORMALIZE}(\mathsf{POINTWISE-PRODUCT}(factors))
```

**Figure 14.11** The variable elimination algorithm for inference in Bayesian networks.

is determined by the order of elimination of variables and by the structure of the network. It turns out to be intractable to determine the optimal ordering, but several good heuristics are available. One fairly effective method is a greedy one: eliminate whichever variable minimizes the size of the next factor to be constructed.

Let us consider one more query:  $P(JohnCalls \mid Burglary = true)$ . As usual, the first step is to write out the nested summation:

$$\mathbf{P}(J \,|\, b) = \alpha \, P(b) \sum_{e} P(e) \sum_{a} P(a \,|\, b, e) \mathbf{P}(J \,|\, a) \sum_{m} P(m \,|\, a) \;.$$

Evaluating this expression from right to left, we notice something interesting:  $\sum_m P(m \mid a)$  is equal to 1 by definition! Hence, there was no need to include it in the first place; the variable M is irrelevant to this query. Another way of saying this is that the result of the query  $P(JohnCalls \mid Burglary = true)$  is unchanged if we remove MaryCalls from the network altogether. In general, we can remove any leaf node that is not a query variable or an evidence variable. After its removal, there may be some more leaf nodes, and these too may be irrelevant. Continuing this process, we eventually find that every variable that is not an ancestor of a query variable or evidence variable is irrelevant to the query. A variable elimination algorithm can therefore remove all these variables before evaluating the query.

# 14.4.3 The complexity of exact inference

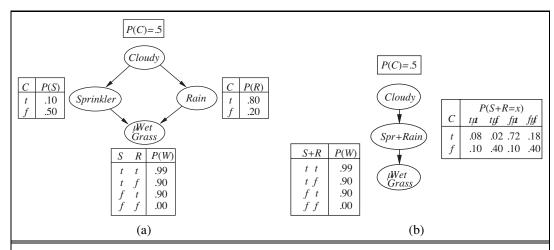
The complexity of exact inference in Bayesian networks depends strongly on the structure of the network. The burglary network of Figure 14.2 belongs to the family of networks in which there is at most one undirected path between any two nodes in the network. These are called **singly connected** networks or **polytrees**, and they have a particularly nice property: *The time and space complexity of exact inference in polytrees is linear in the size of the network*. Here, the size is defined as the number of CPT entries; if the number of parents of each node is bounded by a constant, then the complexity will also be linear in the number of nodes.

For **multiply connected** networks, such as that of Figure 14.12(a), variable elimination can have exponential time and space complexity in the worst case, even when the number of parents per node is bounded. This is not surprising when one considers that *because it* 



SINGLY CONNECTED
POLYTREE

MULTIPLY



**Figure 14.12** (a) A multiply connected network with conditional probability tables. (b) A clustered equivalent of the multiply connected network.

includes inference in propositional logic as a special case, inference in Bayesian networks is NP-hard. In fact, it can be shown (Exercise 14.16) that the problem is as hard as that of computing the *number* of satisfying assignments for a propositional logic formula. This means that it is #P-hard ("number-P hard")—that is, strictly harder than NP-complete problems.

There is a close connection between the complexity of Bayesian network inference and the complexity of constraint satisfaction problems (CSPs). As we discussed in Chapter 6, the difficulty of solving a discrete CSP is related to how "treelike" its constraint graph is. Measures such as **tree width**, which bound the complexity of solving a CSP, can also be applied directly to Bayesian networks. Moreover, the variable elimination algorithm can be generalized to solve CSPs as well as Bayesian networks.

# 14.4.4 Clustering algorithms

The variable elimination algorithm is simple and efficient for answering individual queries. If we want to compute posterior probabilities for all the variables in a network, however, it can be less efficient. For example, in a polytree network, one would need to issue O(n) queries costing O(n) each, for a total of  $O(n^2)$  time. Using **clustering** algorithms (also known as **join tree** algorithms), the time can be reduced to O(n). For this reason, these algorithms are widely used in commercial Bayesian network tools.

The basic idea of clustering is to join individual nodes of the network to form cluster nodes in such a way that the resulting network is a polytree. For example, the multiply connected network shown in Figure 14.12(a) can be converted into a polytree by combining the Sprinkler and Rain node into a cluster node called Sprinkler + Rain, as shown in Figure 14.12(b). The two Boolean nodes are replaced by a "meganode" that takes on four possible values: tt, tf, ft, and ff. The meganode has only one parent, the Boolean variable Cloudy, so there are two conditioning cases. Although this example doesn't show it, the process of clustering often produces meganodes that share some variables.

CLUSTERING JOIN TREE Once the network is in polytree form, a special-purpose inference algorithm is required, because ordinary inference methods cannot handle meganodes that share variables with each other. Essentially, the algorithm is a form of constraint propagation (see Chapter 6) where the constraints ensure that neighboring meganodes agree on the posterior probability of any variables that they have in common. With careful bookkeeping, this algorithm is able to compute posterior probabilities for all the nonevidence nodes in the network in time *linear* in the size of the clustered network. However, the NP-hardness of the problem has not disappeared: if a network requires exponential time and space with variable elimination, then the CPTs in the clustered network will necessarily be exponentially large.

# 14.5 APPROXIMATE INFERENCE IN BAYESIAN NETWORKS

MONTE CARLO

Given the intractability of exact inference in large, multiply connected networks, it is essential to consider approximate inference methods. This section describes randomized sampling algorithms, also called **Monte Carlo** algorithms, that provide approximate answers whose accuracy depends on the number of samples generated. Monte Carlo algorithms, of which simulated annealing (page 126) is an example, are used in many branches of science to estimate quantities that are difficult to calculate exactly. In this section, we are interested in sampling applied to the computation of posterior probabilities. We describe two families of algorithms: direct sampling and Markov chain sampling. Two other approaches—variational methods and loopy propagation—are mentioned in the notes at the end of the chapter.

# **14.5.1** Direct sampling methods

The primitive element in any sampling algorithm is the generation of samples from a known probability distribution. For example, an unbiased coin can be thought of as a random variable Coin with values  $\langle heads, tails \rangle$  and a prior distribution  $\mathbf{P}(Coin) = \langle 0.5, 0.5 \rangle$ . Sampling from this distribution is exactly like flipping the coin: with probability 0.5 it will return heads, and with probability 0.5 it will return tails. Given a source of random numbers uniformly distributed in the range [0,1], it is a simple matter to sample any distribution on a single variable, whether discrete or continuous. (See Exercise 14.17.)

The simplest kind of random sampling process for Bayesian networks generates events from a network that has no evidence associated with it. The idea is to sample each variable in turn, in topological order. The probability distribution from which the value is sampled is conditioned on the values already assigned to the variable's parents. This algorithm is shown in Figure 14.13. We can illustrate its operation on the network in Figure 14.12(a), assuming an ordering [Cloudy, Sprinkler, Rain, WetGrass]:

- 1. Sample from  $P(Cloudy) = \langle 0.5, 0.5 \rangle$ , value is true.
- 2. Sample from  $P(Sprinkler \mid Cloudy = true) = \langle 0.1, 0.9 \rangle$ , value is false.
- 3. Sample from  $\mathbf{P}(Rain \mid Cloudy = true) = \langle 0.8, 0.2 \rangle$ , value is true.
- 4. Sample from  $P(WetGrass \mid Sprinkler = false, Rain = true) = (0.9, 0.1)$ , value is true.

In this case, PRIOR-SAMPLE returns the event [true, false, true, true].

**function** PRIOR-SAMPLE(bn) **returns** an event sampled from the prior specified by bn **inputs**: bn, a Bayesian network specifying joint distribution  $\mathbf{P}(X_1, \dots, X_n)$ 

 $\mathbf{x} \leftarrow$  an event with n elements foreach variable  $X_i$  in  $X_1, \dots, X_n$  do  $\mathbf{x}[i] \leftarrow$  a random sample from  $\mathbf{P}(X_i \mid parents(X_i))$  return  $\mathbf{x}$ 

**Figure 14.13** A sampling algorithm that generates events from a Bayesian network. Each variable is sampled according to the conditional distribution given the values already sampled for the variable's parents.

It is easy to see that PRIOR-SAMPLE generates samples from the prior joint distribution specified by the network. First, let  $S_{PS}(x_1, \ldots, x_n)$  be the probability that a specific event is generated by the PRIOR-SAMPLE algorithm. Just looking at the sampling process, we have

$$S_{PS}(x_1 \dots x_n) = \prod_{i=1}^n P(x_i | parents(X_i))$$

because each sampling step depends only on the parent values. This expression should look familiar, because it is also the probability of the event according to the Bayesian net's representation of the joint distribution, as stated in Equation (14.2). That is, we have

$$S_{PS}(x_1 \dots x_n) = P(x_1 \dots x_n)$$
.

This simple fact makes it easy to answer questions by using samples.

In any sampling algorithm, the answers are computed by counting the actual samples generated. Suppose there are N total samples, and let  $N_{PS}(x_1,\ldots,x_n)$  be the number of times the specific event  $x_1,\ldots,x_n$  occurs in the set of samples. We expect this number, as a fraction of the total, to converge in the limit to its expected value according to the sampling probability:

$$\lim_{N \to \infty} \frac{N_{PS}(x_1, \dots, x_n)}{N} = S_{PS}(x_1, \dots, x_n) = P(x_1, \dots, x_n).$$
 (14.5)

For example, consider the event produced earlier: [true, false, true, true]. The sampling probability for this event is

$$S_{PS}(true, false, true, true) = 0.5 \times 0.9 \times 0.8 \times 0.9 = 0.324$$
.

Hence, in the limit of large N, we expect 32.4% of the samples to be of this event.

Whenever we use an approximate equality (" $\approx$ ") in what follows, we mean it in exactly this sense—that the estimated probability becomes exact in the large-sample limit. Such an estimate is called **consistent**. For example, one can produce a consistent estimate of the probability of any partially specified event  $x_1, \ldots, x_m$ , where  $m \le n$ , as follows:

$$P(x_1, \dots, x_m) \approx N_{PS}(x_1, \dots, x_m)/N.$$
(14.6)

That is, the probability of the event can be estimated as the fraction of all complete events generated by the sampling process that match the partially specified event. For example, if

CONSISTENT

we generate 1000 samples from the sprinkler network, and 511 of them have Rain = true, then the estimated probability of rain, written as  $\hat{P}(Rain = true)$ , is 0.511.

### Rejection sampling in Bayesian networks

REJECTION SAMPLING **Rejection sampling** is a general method for producing samples from a hard-to-sample distribution given an easy-to-sample distribution. In its simplest form, it can be used to compute conditional probabilities—that is, to determine  $P(X \mid \mathbf{e})$ . The REJECTION-SAMPLING algorithm is shown in Figure 14.14. First, it generates samples from the prior distribution specified by the network. Then, it rejects all those that do not match the evidence. Finally, the estimate  $\hat{P}(X = x \mid \mathbf{e})$  is obtained by counting how often X = x occurs in the remaining samples.

Let  $\hat{\mathbf{P}}(X \mid \mathbf{e})$  be the estimated distribution that the algorithm returns. From the definition of the algorithm, we have

$$\hat{\mathbf{P}}(X \mid \mathbf{e}) = \alpha \, \mathbf{N}_{PS}(X, \mathbf{e}) = \frac{\mathbf{N}_{PS}(X, \mathbf{e})}{N_{PS}(\mathbf{e})}$$
.

From Equation (14.6), this becomes

$$\hat{\mathbf{P}}(X \mid \mathbf{e}) \approx \frac{\mathbf{P}(X, \mathbf{e})}{P(\mathbf{e})} = \mathbf{P}(X \mid \mathbf{e}) .$$

That is, rejection sampling produces a consistent estimate of the true probability.

Continuing with our example from Figure 14.12(a), let us assume that we wish to estimate  $\mathbf{P}(Rain \mid Sprinkler = true)$ , using 100 samples. Of the 100 that we generate, suppose that 73 have Sprinkler = false and are rejected, while 27 have Sprinkler = true; of the 27, 8 have Rain = true and 19 have Rain = false. Hence,

$$\mathbf{P}(Rain \mid Sprinkler = true) \approx \mathbf{NORMALIZE}(\langle 8, 19 \rangle) = \langle 0.296, 0.704 \rangle$$
.

The true answer is  $\langle 0.3, 0.7 \rangle$ . As more samples are collected, the estimate will converge to the true answer. The standard deviation of the error in each probability will be proportional to  $1/\sqrt{n}$ , where n is the number of samples used in the estimate.

The biggest problem with rejection sampling is that it rejects so many samples! The fraction of samples consistent with the evidence **e** drops exponentially as the number of evidence variables grows, so the procedure is simply unusable for complex problems.

Notice that rejection sampling is very similar to the estimation of conditional probabilities directly from the real world. For example, to estimate  $P(Rain \mid RedSkyAtNight = true)$ , one can simply count how often it rains after a red sky is observed the previous evening—ignoring those evenings when the sky is not red. (Here, the world itself plays the role of the sample-generation algorithm.) Obviously, this could take a long time if the sky is very seldom red, and that is the weakness of rejection sampling.

#### Likelihood weighting

LIKELIHOOD WEIGHTING

**Likelihood weighting** avoids the inefficiency of rejection sampling by generating only events that are consistent with the evidence **e**. It is a particular instance of the general statistical technique of **importance sampling**, tailored for inference in Bayesian networks. We begin by

IMPORTANCE SAMPLING

```
function REJECTION-SAMPLING(X, \mathbf{e}, bn, N) returns an estimate of \mathbf{P}(X|\mathbf{e}) inputs: X, the query variable

\mathbf{e}, observed values for variables \mathbf{E}
bn, a Bayesian network
N, the total number of samples to be generated local variables: \mathbf{N}, a vector of counts for each value of X, initially zero

for j=1 to N do

\mathbf{x} \leftarrow \text{PRIOR-SAMPLE}(bn)
if \mathbf{x} is consistent with \mathbf{e} then

\mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1 where x is the value of X in \mathbf{x} return \text{NORMALIZE}(\mathbf{N})
```

**Figure 14.14** The rejection-sampling algorithm for answering queries given evidence in a Bayesian network.

describing how the algorithm works; then we show that it works correctly—that is, generates consistent probability estimates.

LIKELIHOOD-WEIGHTING (see Figure 14.15) fixes the values for the evidence variables **E** and samples only the nonevidence variables. This guarantees that each event generated is consistent with the evidence. Not all events are equal, however. Before tallying the counts in the distribution for the query variable, each event is weighted by the *likelihood* that the event accords to the evidence, as measured by the product of the conditional probabilities for each evidence variable, given its parents. Intuitively, events in which the actual evidence appears unlikely should be given less weight.

Let us apply the algorithm to the network shown in Figure 14.12(a), with the query  $\mathbf{P}(Rain \mid Cloudy = true, WetGrass = true)$  and the ordering Cloudy, Sprinkler, Rain, WetGrass. (Any topological ordering will do.) The process goes as follows: First, the weight w is set to 1.0. Then an event is generated:

1. Cloudy is an evidence variable with value true. Therefore, we set

$$w \leftarrow w \times P(Cloudy = true) = 0.5$$
.

- 2. Sprinkler is not an evidence variable, so sample from  $\mathbf{P}(Sprinkler \mid Cloudy = true) = \langle 0.1, 0.9 \rangle$ ; suppose this returns false.
- 3. Similarly, sample from  $\mathbf{P}(Rain \mid Cloudy = true) = \langle 0.8, 0.2 \rangle$ ; suppose this returns true.
- 4. WetGrass is an evidence variable with value true. Therefore, we set

$$w \leftarrow w \times P(WetGrass = true \mid Sprinkler = false, Rain = true) = 0.45$$
.

Here WEIGHTED-SAMPLE returns the event [true, false, true, true] with weight 0.45, and this is tallied under Rain = true.

To understand why likelihood weighting works, we start by examining the sampling probability  $S_{WS}$  for WEIGHTED-SAMPLE. Remember that the evidence variables **E** are fixed

```
function Likelihood-Weighting(X, \mathbf{e}, bn, N) returns an estimate of \mathbf{P}(X|\mathbf{e}) inputs: X, the query variable \mathbf{e}, observed values for variables \mathbf{E} bn, a Bayesian network specifying joint distribution \mathbf{P}(X_1,\ldots,X_n) N, the total number of samples to be generated local variables: \mathbf{W}, a vector of weighted counts for each value of X, initially zero for j=1 to N do \mathbf{x}, w \leftarrow \text{WEIGHTED-SAMPLE}(bn,\mathbf{e}) \mathbf{W}[x] \leftarrow \mathbf{W}[x] + w where x is the value of X in \mathbf{x} return Normalize(\mathbf{W})

function Weighted-Sample(bn, \mathbf{e}) returns an event and a weight w \leftarrow 1; \mathbf{x} \leftarrow an event with n elements initialized from \mathbf{e} foreach variable X_i in X_1, \ldots, X_n do if X_i is an evidence variable with value x_i in \mathbf{e}
```

then  $w \leftarrow w \times P(X_i = x_i \mid parents(X_i))$ 

return x, w

else  $\mathbf{x}[i] \leftarrow$  a random sample from  $\mathbf{P}(X_i \mid parents(X_i))$ 

**Figure 14.15** The likelihood-weighting algorithm for inference in Bayesian networks. In WEIGHTED-SAMPLE, each nonevidence variable is sampled according to the conditional distribution given the values already sampled for the variable's parents, while a weight is accumulated based on the likelihood for each evidence variable.

with values  $\mathbf{e}$ . We call the nonevidence variables  $\mathbf{Z}$  (including the query variable X). The algorithm samples each variable in  $\mathbf{Z}$  given its parent values:

$$S_{WS}(\mathbf{z}, \mathbf{e}) = \prod_{i=1}^{l} P(z_i \mid parents(Z_i)).$$
(14.7)

Notice that  $Parents(Z_i)$  can include both nonevidence variables and evidence variables. Unlike the prior distribution  $P(\mathbf{z})$ , the distribution  $S_{WS}$  pays some attention to the evidence: the sampled values for each  $Z_i$  will be influenced by evidence among  $Z_i$ 's ancestors. For example, when sampling Sprinkler the algorithm pays attention to the evidence Cloudy = true in its parent variable. On the other hand,  $S_{WS}$  pays less attention to the evidence than does the true posterior distribution  $P(\mathbf{z} \mid \mathbf{e})$ , because the sampled values for each  $Z_i$  ignore evidence among  $Z_i$ 's non-ancestors. For example, when sampling Sprinkler and Sprink

Ideally, we would like to use a sampling distribution equal to the true posterior  $P(\mathbf{z} \mid \mathbf{e})$ , to take all the evidence into account. This cannot be done efficiently, however. If it could, then we could approximate the desired probability to arbitrary accuracy with a polynomial number of samples. It can be shown that no such polynomial-time approximation scheme can exist.

The likelihood weight w makes up for the difference between the actual and desired sampling distributions. The weight for a given sample x, composed from z and e, is the product of the likelihoods for each evidence variable given its parents (some or all of which may be among the  $Z_i$ s):

$$w(\mathbf{z}, \mathbf{e}) = \prod_{i=1}^{m} P(e_i \mid parents(E_i)).$$
(14.8)

Multiplying Equations (14.7) and (14.8), we see that the *weighted* probability of a sample has the particularly convenient form

$$S_{WS}(\mathbf{z}, \mathbf{e})w(\mathbf{z}, \mathbf{e}) = \prod_{i=1}^{l} P(z_i \mid parents(Z_i)) \prod_{i=1}^{m} P(e_i \mid parents(E_i))$$

$$= P(\mathbf{z}, \mathbf{e})$$
(14.9)

because the two products cover all the variables in the network, allowing us to use Equation (14.2) for the joint probability.

Now it is easy to show that likelihood weighting estimates are consistent. For any particular value x of X, the estimated posterior probability can be calculated as follows:

$$\begin{split} \hat{P}(x \,|\, \mathbf{e}) &= \alpha \sum_{\mathbf{y}} N_{WS}(x,\mathbf{y},\mathbf{e}) w(x,\mathbf{y},\mathbf{e}) & \text{from Likelihood-Weighting} \\ &\approx \alpha' \sum_{\mathbf{y}} S_{WS}(x,\mathbf{y},\mathbf{e}) w(x,\mathbf{y},\mathbf{e}) & \text{for large } N \\ &= \alpha' \sum_{\mathbf{y}} P(x,\mathbf{y},\mathbf{e}) & \text{by Equation (14.9)} \\ &= \alpha' P(x,\mathbf{e}) = P(x \,|\, \mathbf{e}) \;. \end{split}$$

Hence, likelihood weighting returns consistent estimates.

Because likelihood weighting uses all the samples generated, it can be much more efficient than rejection sampling. It will, however, suffer a degradation in performance as the number of evidence variables increases. This is because most samples will have very low weights and hence the weighted estimate will be dominated by the tiny fraction of samples that accord more than an infinitesimal likelihood to the evidence. The problem is exacerbated if the evidence variables occur late in the variable ordering, because then the nonevidence variables will have no evidence in their parents and ancestors to guide the generation of samples. This means the samples will be simulations that bear little resemblance to the reality suggested by the evidence.

# 14.5.2 Inference by Markov chain simulation

MARKOV CHAIN MONTE CARLO

**Markov chain Monte Carlo** (MCMC) algorithms work quite differently from rejection sampling and likelihood weighting. Instead of generating each sample from scratch, MCMC algorithms generate each sample by making a random change to the preceding sample. It is therefore helpful to think of an MCMC algorithm as being in a particular *current state* specifying a value for every variable and generating a *next state* by making random changes to the

GIBBS SAMPLING

current state. (If this reminds you of simulated annealing from Chapter 4 or WALKSAT from Chapter 7, that is because both are members of the MCMC family.) Here we describe a particular form of MCMC called **Gibbs sampling**, which is especially well suited for Bayesian networks. (Other forms, some of them significantly more powerful, are discussed in the notes at the end of the chapter.) We will first describe what the algorithm does, then we will explain why it works.

#### Gibbs sampling in Bayesian networks

The Gibbs sampling algorithm for Bayesian networks starts with an arbitrary state (with the evidence variables fixed at their observed values) and generates a next state by randomly sampling a value for one of the nonevidence variables  $X_i$ . The sampling for  $X_i$  is done conditioned on the current values of the variables in the Markov blanket of  $X_i$ . (Recall from page 517 that the Markov blanket of a variable consists of its parents, children, and children's parents.) The algorithm therefore wanders randomly around the state space—the space of possible complete assignments—flipping one variable at a time, but keeping the evidence variables fixed.

Consider the query  $\mathbf{P}(Rain \mid Sprinkler = true, WetGrass = true)$  applied to the network in Figure 14.12(a). The evidence variables Sprinkler and WetGrass are fixed to their observed values and the nonevidence variables Cloudy and Rain are initialized randomly—let us say to true and false respectively. Thus, the initial state is [true, true, false, true]. Now the nonevidence variables are sampled repeatedly in an arbitrary order. For example:

- 1. Cloudy is sampled, given the current values of its Markov blanket variables: in this case, we sample from  $\mathbf{P}(Cloudy \mid Sprinkler = true, Rain = false)$ . (Shortly, we will show how to calculate this distribution.) Suppose the result is Cloudy = false. Then the new current state is [false, true, false, true].
- 2. Rain is sampled, given the current values of its Markov blanket variables: in this case, we sample from  $\mathbf{P}(Rain \mid Cloudy = false, Sprinkler = true, WetGrass = true)$ . Suppose this yields Rain = true. The new current state is [false, true, true, true].

Each state visited during this process is a sample that contributes to the estimate for the query variable Rain. If the process visits 20 states where Rain is true and 60 states where Rain is false, then the answer to the query is NORMALIZE( $\langle 20, 60 \rangle$ ) =  $\langle 0.25, 0.75 \rangle$ . The complete algorithm is shown in Figure 14.16.

### Why Gibbs sampling works



We will now show that Gibbs sampling returns consistent estimates for posterior probabilities. The material in this section is quite technical, but the basic claim is straightforward: the sampling process settles into a "dynamic equilibrium" in which the long-run fraction of time spent in each state is exactly proportional to its posterior probability. This remarkable property follows from the specific **transition probability** with which the process moves from one state to another, as defined by the conditional distribution given the Markov blanket of the variable being sampled.

**function** GIBBS-ASK $(X, \mathbf{e}, bn, N)$  **returns** an estimate of  $\mathbf{P}(X|\mathbf{e})$ 

**local variables**: N, a vector of counts for each value of X, initially zero

 $\mathbf{Z}$ , the nonevidence variables in bn

x, the current state of the network, initially copied from e

initialize  $\mathbf{x}$  with random values for the variables in  $\mathbf{Z}$ 

for j = 1 to N do

for each  $Z_i$  in **Z** do

set the value of  $Z_i$  in **x** by sampling from  $P(Z_i|mb(Z_i))$ 

 $\mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1$  where x is the value of X in x

return NORMALIZE(N)

**Figure 14.16** The Gibbs sampling algorithm for approximate inference in Bayesian networks; this version cycles through the variables, but choosing variables at random also works.

MARKOV CHAIN

Let  $q(\mathbf{x} \to \mathbf{x}')$  be the probability that the process makes a transition from state  $\mathbf{x}$  to state  $\mathbf{x}'$ . This transition probability defines what is called a **Markov chain** on the state space. (Markov chains also figure prominently in Chapters 15 and 17.) Now suppose that we run the Markov chain for t steps, and let  $\pi_t(\mathbf{x})$  be the probability that the system is in state  $\mathbf{x}$  at time t. Similarly, let  $\pi_{t+1}(\mathbf{x}')$  be the probability of being in state  $\mathbf{x}'$  at time t+1. Given  $\pi_t(\mathbf{x})$ , we can calculate  $\pi_{t+1}(\mathbf{x}')$  by summing, for all states the system could be in at time t, the probability of being in that state times the probability of making the transition to  $\mathbf{x}'$ :

$$\pi_{t+1}(\mathbf{x}') = \sum_{\mathbf{x}} \pi_t(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}') .$$

STATIONARY DISTRIBUTION We say that the chain has reached its **stationary distribution** if  $\pi_t = \pi_{t+1}$ . Let us call this stationary distribution  $\pi$ ; its defining equation is therefore

$$\pi(\mathbf{x}') = \sum_{\mathbf{x}} \pi(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}') \qquad \text{for all } \mathbf{x}'.$$
 (14.10)

ERGODIC

Provided the transition probability distribution q is **ergodic**—that is, every state is reachable from every other and there are no strictly periodic cycles—there is exactly one distribution  $\pi$  satisfying this equation for any given q.

Equation (14.10) can be read as saying that the expected "outflow" from each state (i.e., its current "population") is equal to the expected "inflow" from all the states. One obvious way to satisfy this relationship is if the expected flow between any pair of states is the same in both directions; that is,

$$\pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}') = \pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x})$$
 for all  $\mathbf{x}, \mathbf{x}'$ . (14.11)

DETAILED BALANCE

When these equations hold, we say that  $q(\mathbf{x} \to \mathbf{x}')$  is in **detailed balance** with  $\pi(\mathbf{x})$ .

We can show that detailed balance implies stationarity simply by summing over  $\mathbf{x}$  in Equation (14.11). We have

$$\sum_{\mathbf{x}} \pi(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}') = \sum_{\mathbf{x}} \pi(\mathbf{x}') q(\mathbf{x}' \to \mathbf{x}) = \pi(\mathbf{x}') \sum_{\mathbf{x}} q(\mathbf{x}' \to \mathbf{x}) = \pi(\mathbf{x}')$$

where the last step follows because a transition from  $\mathbf{x}'$  is guaranteed to occur.

The transition probability  $q(\mathbf{x} \to \mathbf{x}')$  defined by the sampling step in GIBBS-ASK is actually a special case of the more general definition of Gibbs sampling, according to which each variable is sampled conditionally on the current values of *all* the other variables. We start by showing that this general definition of Gibbs sampling satisfies the detailed balance equation with a stationary distribution equal to  $P(\mathbf{x} \mid \mathbf{e})$ , (the true posterior distribution on the nonevidence variables). Then, we simply observe that, for Bayesian networks, sampling conditionally on all variables is equivalent to sampling conditionally on the variable's Markov blanket (see page 517).

To analyze the general Gibbs sampler, which samples each  $X_i$  in turn with a transition probability  $q_i$  that conditions on all the other variables, we define  $\overline{X_i}$  to be these other variables (except the evidence variables); their values in the current state are  $\overline{X_i}$ . If we sample a new value  $x_i'$  for  $X_i$  conditionally on all the other variables, including the evidence, we have

$$q_i(\mathbf{x} \to \mathbf{x}') = q_i((x_i, \overline{\mathbf{x}_i}) \to (x_i', \overline{\mathbf{x}_i})) = P(x_i' | \overline{\mathbf{x}_i}, \mathbf{e})$$
.

Now we show that the transition probability for each step of the Gibbs sampler is in detailed balance with the true posterior:

$$\pi(\mathbf{x})q_i(\mathbf{x} \to \mathbf{x}') = P(\mathbf{x} \mid \mathbf{e})P(x_i' \mid \overline{\mathbf{x}_i}, \mathbf{e}) = P(x_i, \overline{\mathbf{x}_i} \mid \mathbf{e})P(x_i' \mid \overline{\mathbf{x}_i}, \mathbf{e})$$

$$= P(x_i \mid \overline{\mathbf{x}_i}, \mathbf{e})P(\overline{\mathbf{x}_i} \mid \mathbf{e})P(x_i' \mid \overline{\mathbf{x}_i}, \mathbf{e}) \qquad \text{(using the chain rule on the first term)}$$

$$= P(x_i \mid \overline{\mathbf{x}_i}, \mathbf{e})P(x_i', \overline{\mathbf{x}_i} \mid \mathbf{e}) \qquad \text{(using the chain rule backward)}$$

$$= \pi(\mathbf{x}')q_i(\mathbf{x}' \to \mathbf{x}).$$

We can think of the loop "for each  $Z_i$  in  $\mathbf{Z}$  do" in Figure 14.16 as defining one large transition probability q that is the sequential composition  $q_1 \circ q_2 \circ \cdots \circ q_n$  of the transition probabilities for the individual variables. It is easy to show (Exercise 14.19) that if each of  $q_i$  and  $q_j$  has  $\pi$  as its stationary distribution, then the sequential composition  $q_i \circ q_j$  does too; hence the transition probability q for the whole loop has  $P(\mathbf{x} \mid \mathbf{e})$  as its stationary distribution. Finally, unless the CPTs contain probabilities of 0 or 1—which can cause the state space to become disconnected—it is easy to see that q is ergodic. Hence, the samples generated by Gibbs sampling will eventually be drawn from the true posterior distribution.

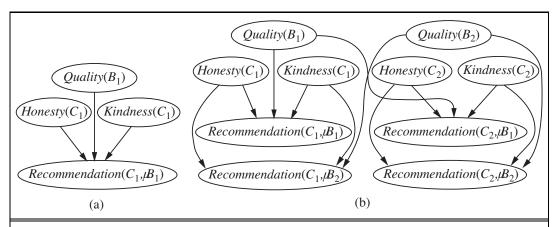
The final step is to show how to perform the general Gibbs sampling step—sampling  $X_i$  from  $\mathbf{P}(X_i | \overline{\mathbf{x}_i}, \mathbf{e})$ —in a Bayesian network. Recall from page 517 that a variable is independent of all other variables given its Markov blanket; hence,

$$P(x_i' | \overline{\mathbf{x}_i}, \mathbf{e}) = P(x_i' | mb(X_i)),$$

where  $mb(X_i)$  denotes the values of the variables in  $X_i$ 's Markov blanket,  $MB(X_i)$ . As shown in Exercise 14.7, the probability of a variable given its Markov blanket is proportional to the probability of the variable given its parents times the probability of each child given its respective parents:

$$P(x_i' \mid mb(X_i)) = \alpha P(x_i' \mid parents(X_i)) \times \prod_{Y_j \in Children(X_i)} P(y_j \mid parents(Y_j)) . (14.12)$$

Hence, to flip each variable  $X_i$  conditioned on its Markov blanket, the number of multiplications required is equal to the number of  $X_i$ 's children.



**Figure 14.17** (a) Bayes net for a single customer  $C_1$  recommending a single book  $B_1$ .  $Honest(C_1)$  is Boolean, while the other variables have integer values from 1 to 5. (b) Bayes net with two customers and two books.

# 14.6 RELATIONAL AND FIRST-ORDER PROBABILITY MODELS

In Chapter 8, we explained the representational advantages possessed by first-order logic in comparison to propositional logic. First-order logic commits to the existence of objects and relations among them and can express facts about *some* or *all* of the objects in a domain. This often results in representations that are vastly more concise than the equivalent propositional descriptions. Now, Bayesian networks are essentially propositional: the set of random variables is fixed and finite, and each has a fixed domain of possible values. This fact limits the applicability of Bayesian networks. *If we can find a way to combine probability theory with the expressive power of first-order representations, we expect to be able to increase dramatically the range of problems that can be handled.* 



Section 14.6.

For example, suppose that an online book retailer would like to provide overall evaluations of products based on recommendations received from its customers. The evaluation will take the form of a posterior distribution over the quality of the book, given the available evidence. The simplest solution to base the evaluation on the average recommendation, perhaps with a variance determined by the number of recommendations, but this fails to take into account the fact that some customers are kinder than others and some are less honest than others. Kind customers tend to give high recommendations even to fairly mediocre books, while dishonest customers give very high or very low recommendations for reasons other than quality—for example, they might work for a publisher.<sup>6</sup>

For a single customer  $C_1$ , recommending a single book  $B_1$ , the Bayes net might look like the one shown in Figure 14.17(a). (Just as in Section 9.1, expressions with parentheses such as  $Honest(C_1)$  are just fancy symbols—in this case, fancy names for random variables.)

<sup>&</sup>lt;sup>6</sup> A game theorist would advise a dishonest customer to avoid detection by occasionally recommending a good book from a competitor. See Chapter 17.

With two customers and two books, the Bayes net looks like the one in Figure 14.17(b). For larger numbers of books and customers, it becomes completely impractical to specify the network by hand.

Fortunately, the network has a lot of repeated structure. Each Recommendation(c, b) variable has as its parents the variables Honest(c), Kindness(c), and Quality(b). Moreover, the CPTs for all the Recommendation(c, b) variables are identical, as are those for all the Honest(c) variables, and so on. The situation seems tailor-made for a first-order language. We would like to say something like

$$Recommendation(c, b) \sim RecCPT(Honest(c), Kindness(c), Quality(b))$$

with the intended meaning that a customer's recommendation for a book depends on the customer's honesty and kindness and the book's quality according to some fixed CPT. This section develops a language that lets us say exactly this, and a lot more besides.

#### 14.6.1 Possible worlds

Recall from Chapter 13 that a probability model defines a set  $\Omega$  of possible worlds with a probability  $P(\omega)$  for each world  $\omega$ . For Bayesian networks, the possible worlds are assignments of values to variables; for the Boolean case in particular, the possible worlds are identical to those of propositional logic. For a first-order probability model, then, it seems we need the possible worlds to be those of first-order logic—that is, a set of objects with relations among them and an interpretation that maps constant symbols to objects, predicate symbols to relations, and function symbols to functions on those objects. (See Section 8.2.) The model also needs to define a probability for each such possible world, just as a Bayesian network defines a probability for each assignment of values to variables.

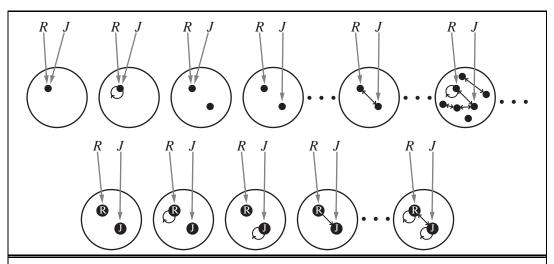
Let us suppose, for a moment, that we have figured out how to do this. Then, as usual (see page 485), we can obtain the probability of any first-order logical sentence  $\phi$  as a sum over the possible worlds where it is true:

$$P(\phi) = \sum_{\omega: \phi \text{ is true in } \omega} P(\omega) . \tag{14.13}$$

Conditional probabilities  $P(\phi | \mathbf{e})$  can be obtained similarly, so we can, in principle, ask any question we want of our model—e.g., "Which books are most likely to be recommended highly by dishonest customers?"—and get an answer. So far, so good.

There is, however, a problem: the set of first-order models is infinite. We saw this explicitly in Figure 8.4 on page 293, which we show again in Figure 14.18 (top). This means that (1) the summation in Equation (14.13) could be infeasible, and (2) specifying a complete, consistent distribution over an infinite set of worlds could be very difficult.

Section 14.6.2 explores one approach to dealing with this problem. The idea is to borrow not from the standard semantics of first-order logic but from the **database semantics** defined in Section 8.2.8 (page 299). The database semantics makes the **unique names assumption**—here, we adopt it for the constant symbols. It also assumes **domain closure**—there are no more objects than those that are named. We can then guarantee a finite set of possible worlds by making the set of objects in each world be exactly the set of constant



**Figure 14.18** Top: Some members of the set of all possible worlds for a language with two constant symbols, R and J, and one binary relation symbol, under the standard semantics for first-order logic. Bottom: the possible worlds under database semantics. The interpretation of the constant symbols is fixed, and there is a distinct object for each constant symbol.

RELATIONAL PROBABILITY MODEL symbols that are used; as shown in Figure 14.18 (bottom), there is no uncertainty about the mapping from symbols to objects or about the objects that exist. We will call models defined in this way **relational probability models**, or RPMs.<sup>7</sup> The most significant difference between the semantics of RPMs and the database semantics introduced in Section 8.2.8 is that RPMs do not make the closed-world assumption—obviously, assuming that every unknown fact is false doesn't make sense in a probabilistic reasoning system!

When the underlying assumptions of database semantics fail to hold, RPMs won't work well. For example, a book retailer might use an ISBN (International Standard Book Number) as a constant symbol to name each book, even though a given "logical" book (e.g., "Gone With the Wind") may have several ISBNs. It would make sense to aggregate recommendations across multiple ISBNs, but the retailer may not know for sure which ISBNs are really the same book. (Note that we are not reifying the *individual copies* of the book, which might be necessary for used-book sales, car sales, and so on.) Worse still, each customer is identified by a login ID, but a dishonest customer may have thousands of IDs! In the computer security field, these multiple IDs are called **sibyls** and their use to confound a reputation system is called a **sibyl attack**. Thus, even a simple application in a relatively well-defined, online domain involves both **existence uncertainty** (what are the real books and customers underlying the observed data) and **identity uncertainty** (which symbol really refer to the same object). We need to bite the bullet and define probability models based on the standard semantics of first-order logic, for which the possible worlds vary in the objects they contain and in the mappings from symbols to objects. Section 14.6.3 shows how to do this.

SIBYL ATTACK
EXISTENCE
UNCERTAINTY
IDENTITY
UNCERTAINTY

<sup>&</sup>lt;sup>7</sup> The name *relational probability model* was given by Pfeffer (2000) to a slightly different representation, but the underlying ideas are the same.

# 14.6.2 Relational probability models

TYPE SIGNATURE

Like first-order logic, RPMs have constant, function, and predicate symbols. (It turns out to be easier to view predicates as functions that return true or false.) We will also assume a **type signature** for each function, that is, a specification of the type of each argument and the function's value. If the type of each object is known, many spurious possible worlds are eliminated by this mechanism. For the book-recommendation domain, the types are Customer and Book, and the type signatures for the functions and predicates are as follows:

```
Honest: Customer \rightarrow \{true, false\} Kindness: Customer \rightarrow \{1, 2, 3, 4, 5\}

Quality: Book \rightarrow \{1, 2, 3, 4, 5\}

Recommendation: Customer \times Book \rightarrow \{1, 2, 3, 4, 5\}
```

The constant symbols will be whatever customer and book names appear in the retailer's data set. In the example given earlier (Figure 14.17(b)), these were  $C_1$ ,  $C_2$  and  $B_1$ ,  $B_2$ .

Given the constants and their types, together with the functions and their type signatures, the random variables of the RPM are obtained by instantiating each function with each possible combination of objects:  $Honest(C_1)$ ,  $Quality(B_2)$ ,  $Recommendation(C_1, B_2)$ , and so on. These are exactly the variables appearing in Figure 14.17(b). Because each type has only finitely many instances, the number of basic random variables is also finite.

To complete the RPM, we have to write the dependencies that govern these random variables. There is one dependency statement for each function, where each argument of the function is a logical variable (i.e., a variable that ranges over objects, as in first-order logic):

```
Honest(c) \sim \langle 0.99, 0.01 \rangle

Kindness(c) \sim \langle 0.1, 0.1, 0.2, 0.3, 0.3 \rangle

Quality(b) \sim \langle 0.05, 0.2, 0.4, 0.2, 0.15 \rangle

Recommendation(c, b) \sim RecCPT(Honest(c), Kindness(c), Quality(b))
```

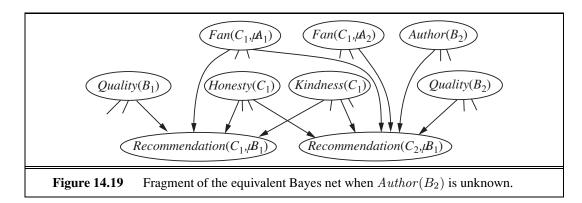
where RecCPT is a separately defined conditional distribution with  $2 \times 5 \times 5 = 50$  rows, each with 5 entries. The semantics of the RPM can be obtained by instantiating these dependencies for all known constants, giving a Bayesian network (as in Figure 14.17(b)) that defines a joint distribution over the RPM's random variables.<sup>8</sup>

We can refine the model by introducing a **context-specific independence** to reflect the fact that dishonest customers ignore quality when giving a recommendation; moreover, kindness plays no role in their decisions. A context-specific independence allows a variable to be independent of some of its parents given certain values of others; thus, Recommendation(c, b) is independent of Kindness(c) and Quality(b) when Honest(c) = false:

```
Recommendation(c,b) \sim \quad \textbf{if } Honest(c) \quad \textbf{then}  HonestRecCPT(Kindness(c), Quality(b))   \textbf{else } \langle 0.4, 0.1, 0.0, 0.1, 0.4 \rangle \ .
```

CONTEXT-SPECIFIC INDEPENDENCE

<sup>&</sup>lt;sup>8</sup> Some technical conditions must be observed to guarantee that the RPM defines a proper distribution. First, the dependencies must be *acyclic*, otherwise the resulting Bayesian network will have cycles and will not define a proper distribution. Second, the dependencies must be *well-founded*, that is, there can be no infinite ancestor chains, such as might arise from recursive dependencies. Under some circumstances (see Exercise 14.6), a fixed-point calculation yields a well-defined probability model for a recursive RPM.



This kind of dependency may look like an ordinary if—then—else statement on a programming language, but there is a key difference: the inference engine *doesn't necessarily know the value of the conditional test*!

We can elaborate this model in endless ways to make it more realistic. For example, suppose that an honest customer who is a fan of a book's author always gives the book a 5, regardless of quality:

```
Recommendation(c,b) \sim \quad \text{if } Honest(c) \text{ then} \\ \\ \text{if } Fan(c,Author(b)) \text{ then } Exactly(5) \\ \\ \text{else } HonestRecCPT(Kindness(c),Quality(b)) \\ \\ \text{else } \langle 0.4,0.1,0.0,0.1,0.4 \rangle
```

Again, the conditional test Fan(c, Author(b)) is unknown, but if a customer gives only 5s to a particular author's books and is not otherwise especially kind, then the posterior probability that the customer is a fan of that author will be high. Furthermore, the posterior distribution will tend to discount the customer's 5s in evaluating the quality of that author's books.

In the preceding example, we implicitly assumed that the value of Author(b) is known for every b, but this may not be the case. How can the system reason about whether, say,  $C_1$  is a fan of  $Author(B_2)$  when  $Author(B_2)$  is unknown? The answer is that the system may have to reason about  $all\ possible\ authors$ . Suppose (to keep things simple) that there are just two authors,  $A_1$  and  $A_2$ . Then  $Author(B_2)$  is a random variable with two possible values,  $A_1$  and  $A_2$ , and it is a parent of  $Recommendation(C_1, B_2)$ . The variables  $Fan(C_1, A_1)$  and  $Fan(C_1, A_2)$  are parents too. The conditional distribution for  $Recommendation(C_1, B_2)$  is then essentially a multiplexer in which the  $Author(B_2)$  parent acts as a selector to choose which of  $Fan(C_1, A_1)$  and  $Fan(C_1, A_2)$  actually gets to influence the recommendation. A fragment of the equivalent Bayes net is shown in Figure 14.19. Uncertainty in the value of  $Author(B_2)$ , which affects the dependency structure of the network, is an instance of relational uncertainty.

In case you are wondering how the system can possibly work out who the author of  $B_2$  is: consider the possibility that three other customers are fans of  $A_1$  (and have no other favorite authors in common) and all three have given  $B_2$  a 5, even though most other customers find it quite dismal. In that case, it is extremely likely that  $A_1$  is the author of  $B_2$ .

MULTIPLEXER

RELATIONAL UNCERTAINTY The emergence of sophisticated reasoning like this from an RPM model of just a few lines is an intriguing example of how probabilistic influences spread through the web of interconnections among objects in the model. As more dependencies and more objects are added, the picture conveyed by the posterior distribution often becomes clearer and clearer.

The next question is how to do inference in RPMs. One approach is to collect the evidence and query and the constant symbols therein, construct the equivalent Bayes net, and apply any of the inference methods discussed in this chapter. This technique is called **unrolling**. The obvious drawback is that the resulting Bayes net may be very large. Furthermore, if there are many candidate objects for an unknown relation or function—for example, the unknown author of  $B_2$ —then some variables in the network may have many parents.

Fortunately, much can be done to improve on generic inference algorithms. First, the presence of repeated substructure in the unrolled Bayes net means that many of the factors constructed during variable elimination (and similar kinds of tables constructed by clustering algorithms) will be identical; effective caching schemes have yielded speedups of three orders of magnitude for large networks. Second, inference methods developed to take advantage of context-specific independence in Bayes nets find many applications in RPMs. Third, MCMC inference algorithms have some interesting properties when applied to RPMs with relational uncertainty. MCMC works by sampling complete possible worlds, so in each state the relational structure is completely known. In the example given earlier, each MCMC state would specify the value of  $Author(B_2)$ , and so the other potential authors are no longer parents of the recommendation nodes for  $B_2$ . For MCMC, then, relational uncertainty causes no increase in network complexity; instead, the MCMC process includes transitions that change the relational structure, and hence the dependency structure, of the unrolled network.

All of the methods just described assume that the RPM has to be partially or completely unrolled into a Bayesian network. This is exactly analogous to the method of **proposition-alization** for first-order logical inference. (See page 322.) Resolution theorem-provers and logic programming systems avoid propositionalizing by instantiating the logical variables only as needed to make the inference go through; that is, they *lift* the inference process above the level of ground propositional sentences and make each lifted step do the work of many ground steps. The same idea applied in probabilistic inference. For example, in the variable elimination algorithm, a lifted factor can represent an entire set of ground factors that assign probabilities to random variables in the RPM, where those random variables differ only in the constant symbols used to construct them. The details of this method are beyond the scope of this book, but references are given at the end of the chapter.

# **14.6.3** Open-universe probability models

We argued earlier that database semantics was appropriate for situations in which we know exactly the set of relevant objects that exist and can identify them unambiguously. (In particular, all observations about an object are correctly associated with the constant symbol that names it.) In many real-world settings, however, these assumptions are simply untenable. We gave the examples of multiple ISBNs and sibyl attacks in the book-recommendation domain (to which we will return in a moment), but the phenomenon is far more pervasive:

UNROLLING

- A vision system doesn't know what exists, if anything, around the next corner, and may not know if the object it sees now is the same one it saw a few minutes ago.
- A text-understanding system does not know in advance the entities that will be featured in a text, and must reason about whether phrases such as "Mary," "Dr. Smith," "she," "his cardiologist," "his mother," and so on refer to the same object.
- An intelligence analyst hunting for spies never knows how many spies there really are and can only guess whether various pseudonyms, phone numbers, and sightings belong to the same individual.

In fact, a major part of human cognition seems to require learning what objects exist and being able to connect observations—which almost never come with unique IDs attached—to hypothesized objects in the world.

OPEN UNIVERSE

Section 14.6.

For these reasons, we need to be able to write so-called **open-universe** probability models or OUPMs based on the standard semantics of first-order logic, as illustrated at the top of Figure 14.18. A language for OUPMs provides a way of writing such models easily while guaranteeing a unique, consistent probability distribution over the infinite space of possible worlds.

The basic idea is to understand how ordinary Bayesian networks and RPMs manage to define a unique probability model and to transfer that insight to the first-order setting. In essence, a Bayes net *generates* each possible world, event by event, in the topological order defined by the network structure, where each event is an assignment of a value to a variable. An RPM extends this to entire sets of events, defined by the possible instantiations of the logical variables in a given predicate or function. OUPMs go further by allowing generative steps that *add objects* to the possible world under construction, where the number and type of objects may depend on the objects that are already in that world. That is, the event being generated is not the assignment of a value to a variable, but the very *existence* of objects.

One way to do this in OUPMs is to add statements that define conditional distributions over the numbers of objects of various kinds. For example, in the book-recommendation domain, we might want to distinguish between *customers* (real people) and their *login IDs*. Suppose we expect somewhere between 100 and 10,000 distinct customers (whom we cannot observe directly). We can express this as a prior log-normal distribution<sup>9</sup> as follows:

$$\# Customer \sim LogNormal[6.9, 2.3^2]()$$
.

We expect honest customers to have just one ID, whereas dishonest customers might have anywhere between 10 and 1000 IDs:

ORIGIN FUNCTION

This statement defines the number of login IDs for a given owner, who is a customer. The *Owner* function is called an **origin function** because it says where each generated object came from. In the formal semantics of BLOG (as distinct from first-order logic), the domain elements in each possible world are actually generation histories (e.g., "the fourth login ID of the seventh customer") rather than simple tokens.

A distribution  $LogNormal[\mu, \sigma^2](x)$  is equivalent to a distribution  $N[\mu, \sigma^2](x)$  over  $\log_e(x)$ .

Subject to technical conditions of acyclicity and well-foundedness similar to those for RPMs, open-universe models of this kind define a unique distribution over possible worlds. Furthermore, there exist inference algorithms such that, for every such well-defined model and every first-order query, the answer returned approaches the true posterior arbitrarily closely in the limit. There are some tricky issues involved in designing these algorithms. For example, an MCMC algorithm cannot sample directly in the space of possible worlds when the size of those worlds is unbounded; instead, it samples finite, partial worlds, relying on the fact that only finitely many objects can be relevant to the query in distinct ways. Moreover, transitions must allow for merging two objects into one or splitting one into two. (Details are given in the references at the end of the chapter.) Despite these complications, the basic principle established in Equation (14.13) still holds: the probability of any sentence is well defined and can be calculated.

Research in this area is still at an early stage, but already it is becoming clear that first-order probabilistic reasoning yields a tremendous increase in the effectiveness of AI systems at handling uncertain information. Potential applications include those mentioned above—computer vision, text understanding, and intelligence analysis—as well as many other kinds of sensor interpretation.

## 14.7 OTHER APPROACHES TO UNCERTAIN REASONING

Other sciences (e.g., physics, genetics, and economics) have long favored probability as a model for uncertainty. In 1819, Pierre Laplace said, "Probability theory is nothing but common sense reduced to calculation." In 1850, James Maxwell said, "The true logic for this world is the calculus of Probabilities, which takes account of the magnitude of the probability which is, or ought to be, in a reasonable man's mind."

Given this long tradition, it is perhaps surprising that AI has considered many alternatives to probability. The earliest expert systems of the 1970s ignored uncertainty and used strict logical reasoning, but it soon became clear that this was impractical for most real-world domains. The next generation of expert systems (especially in medical domains) used probabilistic techniques. Initial results were promising, but they did not scale up because of the exponential number of probabilities required in the full joint distribution. (Efficient Bayesian network algorithms were unknown then.) As a result, probabilistic approaches fell out of favor from roughly 1975 to 1988, and a variety of alternatives to probability were tried for a variety of reasons:

• One common view is that probability theory is essentially numerical, whereas human judgmental reasoning is more "qualitative." Certainly, we are not consciously aware of doing numerical calculations of degrees of belief. (Neither are we aware of doing unification, yet we seem to be capable of some kind of logical reasoning.) It might be that we have some kind of numerical degrees of belief encoded directly in strengths of connections and activations in our neurons. In that case, the difficulty of conscious access to those strengths is not surprising. One should also note that qualitative reason-

ing mechanisms can be built directly on top of probability theory, so the "no numbers" argument against probability has little force. Nonetheless, some qualitative schemes have a good deal of appeal in their own right. One of the best studied is **default reasoning**, which treats conclusions not as "believed to a certain degree," but as "believed until a better reason is found to believe something else." Default reasoning is covered in Chapter 12.

- Rule-based approaches to uncertainty have also been tried. Such approaches hope to
  build on the success of logical rule-based systems, but add a sort of "fudge factor" to
  each rule to accommodate uncertainty. These methods were developed in the mid-1970s
  and formed the basis for a large number of expert systems in medicine and other areas.
- One area that we have not addressed so far is the question of **ignorance**, as opposed to uncertainty. Consider the flipping of a coin. If we know that the coin is fair, then a probability of 0.5 for heads is reasonable. If we know that the coin is biased, but we do not know which way, then 0.5 for heads is again reasonable. Obviously, the two cases are different, yet the outcome probability seems not to distinguish them. The **Dempster–Shafer theory** uses **interval-valued** degrees of belief to represent an agent's knowledge of the probability of a proposition.
- Probability makes the same ontological commitment as logic: that propositions are true or false in the world, even if the agent is uncertain as to which is the case. Researchers in **fuzzy logic** have proposed an ontology that allows **vagueness**: that a proposition can be "sort of" true. Vagueness and uncertainty are in fact orthogonal issues.

The next three subsections treat some of these approaches in slightly more depth. We will not provide detailed technical material, but we cite references for further study.

# 14.7.1 Rule-based methods for uncertain reasoning

Rule-based systems emerged from early work on practical and intuitive systems for logical inference. Logical systems in general, and logical rule-based systems in particular, have three desirable properties:

LOCALITY

• Locality: In logical systems, whenever we have a rule of the form  $A \Rightarrow B$ , we can conclude B, given evidence A, without worrying about any other rules. In probabilistic systems, we need to consider all the evidence.

DETACHMENT

• **Detachment**: Once a logical proof is found for a proposition B, the proposition can be used regardless of how it was derived. That is, it can be **detached** from its justification. In dealing with probabilities, on the other hand, the source of the evidence for a belief is important for subsequent reasoning.

TRUTH-FUNCTIONALITY • **Truth-functionality**: In logic, the truth of complex sentences can be computed from the truth of the components. Probability combination does not work this way, except under strong global independence assumptions.

There have been several attempts to devise uncertain reasoning schemes that retain these advantages. The idea is to attach degrees of belief to propositions and rules and to devise purely local schemes for combining and propagating those degrees of belief. The schemes



are also truth-functional; for example, the degree of belief in  $A \vee B$  is a function of the belief in A and the belief in B.

The bad news for rule-based systems is that the properties of *locality, detachment, and* truth-functionality are simply not appropriate for uncertain reasoning. Let us look at truth-functionality first. Let  $H_1$  be the event that a fair coin flip comes up heads, let  $T_1$  be the event that the coin comes up tails on that same flip, and let  $H_2$  be the event that the coin comes up heads on a second flip. Clearly, all three events have the same probability, 0.5, and so a truth-functional system must assign the same belief to the disjunction of any two of them. But we can see that the probability of the disjunction depends on the events themselves and not just on their probabilities:

P(A)	P(B)	$P(A \vee B)$
$P(H_1) = 0.5$	$P(H_1) = 0.5$ $P(T_1) = 0.5$ $P(H_2) = 0.5$	$P(H_1 \lor H_1) = 0.50 P(H_1 \lor T_1) = 1.00 P(H_1 \lor H_2) = 0.75$

It gets worse when we chain evidence together. Truth-functional systems have **rules** of the form  $A \mapsto B$  that allow us to compute the belief in B as a function of the belief in the rule and the belief in A. Both forward- and backward-chaining systems can be devised. The belief in the rule is assumed to be constant and is usually specified by the knowledge engineer—for example, as  $A \mapsto_{0.9} B$ .

Consider the wet-grass situation from Figure 14.12(a) (page 529). If we wanted to be able to do both causal and diagnostic reasoning, we would need the two rules

$$Rain \mapsto WetGrass$$
 and  $WetGrass \mapsto Rain$ .

These two rules form a feedback loop: evidence for *Rain* increases the belief in *WetGrass*, which in turn increases the belief in *Rain* even more. Clearly, uncertain reasoning systems need to keep track of the paths along which evidence is propagated.

Intercausal reasoning (or explaining away) is also tricky. Consider what happens when we have the two rules

$$Sprinkler \mapsto WetGrass$$
 and  $WetGrass \mapsto Rain$ .

Suppose we see that the sprinkler is on. Chaining forward through our rules, this increases the belief that the grass will be wet, which in turn increases the belief that it is raining. But this is ridiculous: the fact that the sprinkler is on explains away the wet grass and should *reduce* the belief in rain. A truth-functional system acts as if it also believes  $Sprinkler \mapsto Rain$ .

Given these difficulties, how can truth-functional systems be made useful in practice? The answer lies in restricting the task and in carefully engineering the rule base so that undesirable interactions do not occur. The most famous example of a truth-functional system for uncertain reasoning is the **certainty factors** model, which was developed for the MYCIN medical diagnosis program and was widely used in expert systems of the late 1970s and 1980s. Almost all uses of certainty factors involved rule sets that were either purely diagnostic (as in MYCIN) or purely causal. Furthermore, evidence was entered only at the "roots" of the rule set, and most rule sets were singly connected. Heckerman (1986) has shown that,

CERTAINTY FACTOR

under these circumstances, a minor variation on certainty-factor inference was exactly equivalent to Bayesian inference on polytrees. In other circumstances, certainty factors could yield disastrously incorrect degrees of belief through overcounting of evidence. As rule sets became larger, undesirable interactions between rules became more common, and practitioners found that the certainty factors of many other rules had to be "tweaked" when new rules were added. For these reasons, Bayesian networks have largely supplanted rule-based methods for uncertain reasoning.

## 14.7.2 Representing ignorance: Dempster–Shafer theory

DEMPSTER-SHAFER
THEORY

BELIEF FUNCTION

The **Dempster-Shafer theory** is designed to deal with the distinction between **uncertainty** and **ignorance**. Rather than computing the probability of a proposition, it computes the probability that the evidence supports the proposition. This measure of belief is called a **belief function**, written Bel(X).

We return to coin flipping for an example of belief functions. Suppose you pick a coin from a magician's pocket. Given that the coin might or might not be fair, what belief should you ascribe to the event that it comes up heads? Dempster–Shafer theory says that because you have no evidence either way, you have to say that the belief Bel(Heads) = 0 and also that  $Bel(\neg Heads) = 0$ . This makes Dempster–Shafer reasoning systems skeptical in a way that has some intuitive appeal. Now suppose you have an expert at your disposal who testifies with 90% certainty that the coin is fair (i.e., he is 90% sure that P(Heads) = 0.5). Then Dempster–Shafer theory gives  $Bel(Heads) = 0.9 \times 0.5 = 0.45$  and likewise  $Bel(\neg Heads) = 0.45$ . There is still a 10 percentage point "gap" that is not accounted for by the evidence.

The mathematical underpinnings of Dempster–Shafer theory have a similar flavor to those of probability theory; the main difference is that, instead of assigning probabilities to possible worlds, the theory assigns **masses** to *sets* of possible world, that is, to events. The masses still must add to 1 over all possible events. Bel(A) is defined to be the sum of masses for all events that are subsets of (i.e., that entail) A, including A itself. With this definition, Bel(A) and  $Bel(\neg A)$  sum to *at most* 1, and the gap—the interval between Bel(A) and A and A are subsets of the interpreted as bounding the probability of A.

As with default reasoning, there is a problem in connecting beliefs to actions. Whenever there is a gap in the beliefs, then a decision problem can be defined such that a Dempster–Shafer system is unable to make a decision. In fact, the notion of utility in the Dempster–Shafer model is not yet well understood because the meanings of masses and beliefs themselves have yet to be understood. Pearl (1988) has argued that Bel(A) should be interpreted not as a degree of belief in A but as the probability assigned to all the possible worlds (now interpreted as logical theories) in which A is provable. While there are cases in which this quantity might be of interest, it is not the same as the probability that A is true.

A Bayesian analysis of the coin-flipping example would suggest that no new formalism is necessary to handle such cases. The model would have two variables: the Bias of the coin (a number between 0 and 1, where 0 is a coin that always shows tails and 1 a coin that always shows heads) and the outcome of the next Flip. The prior probability distribution for Bias

MASS

would reflect our beliefs based on the source of the coin (the magician's pocket): some small probability that it is fair and some probability that it is heavily biased toward heads or tails. The conditional distribution  $\mathbf{P}(Flip \mid Bias)$  simply defines how the bias operates. If  $\mathbf{P}(Bias)$  is symmetric about 0.5, then our prior probability for the flip is

Chapter

$$P(Flip = heads) = \int_0^1 P(Bias = x)P(Flip = heads \mid Bias = x) dx = 0.5$$
.

This is the same prediction as if we believe strongly that the coin is fair, but that does *not* mean that probability theory treats the two situations identically. The difference arises *after* the flips in computing the posterior distribution for *Bias*. If the coin came from a bank, then seeing it come up heads three times running would have almost no effect on our strong prior belief in its fairness; but if the coin comes from the magician's pocket, the same evidence will lead to a stronger posterior belief that the coin is biased toward heads. Thus, a Bayesian approach expresses our "ignorance" in terms of how our beliefs would change in the face of future information gathering.

## 14.7.3 Representing vagueness: Fuzzy sets and fuzzy logic

FUZZY SET THEORY

Fuzzy set theory is a means of specifying how well an object satisfies a vague description. For example, consider the proposition "Nate is tall." Is this true if Nate is 5' 10''? Most people would hesitate to answer "true" or "false," preferring to say, "sort of." Note that this is not a question of uncertainty about the external world—we are sure of Nate's height. The issue is that the linguistic term "tall" does not refer to a sharp demarcation of objects into two classes—there are degrees of tallness. For this reason, fuzzy set theory is not a method for uncertain reasoning at all. Rather, fuzzy set theory treats Tall as a fuzzy predicate and says that the truth value of Tall(Nate) is a number between 0 and 1, rather than being just true or false. The name "fuzzy set" derives from the interpretation of the predicate as implicitly defining a set of its members—a set that does not have sharp boundaries.

FUZZY LOGIC

**Fuzzy logic** is a method for reasoning with logical expressions describing membership in fuzzy sets. For example, the complex sentence  $Tall(Nate) \wedge Heavy(Nate)$  has a fuzzy truth value that is a function of the truth values of its components. The standard rules for evaluating the fuzzy truth, T, of a complex sentence are

$$T(A \wedge B) = \min(T(A), T(B))$$
  

$$T(A \vee B) = \max(T(A), T(B))$$
  

$$T(\neg A) = 1 - T(A)$$

Fuzzy logic is therefore a truth-functional system—a fact that causes serious difficulties. For example, suppose that T(Tall(Nate)) = 0.6 and T(Heavy(Nate)) = 0.4. Then we have  $T(Tall(Nate) \wedge Heavy(Nate)) = 0.4$ , which seems reasonable, but we also get the result  $T(Tall(Nate) \wedge \neg Tall(Nate)) = 0.4$ , which does not. Clearly, the problem arises from the inability of a truth-functional approach to take into account the correlations or anticorrelations among the component propositions.

FUZZY CONTROL

**Fuzzy control** is a methodology for constructing control systems in which the mapping between real-valued input and output parameters is represented by fuzzy rules. Fuzzy control has been very successful in commercial products such as automatic transmissions, video

Section 14.8. Summary 551

cameras, and electric shavers. Critics (see, e.g., Elkan, 1993) argue that these applications are successful because they have small rule bases, no chaining of inferences, and tunable parameters that can be adjusted to improve the system's performance. The fact that they are implemented with fuzzy operators might be incidental to their success; the key is simply to provide a concise and intuitive way to specify a smoothly interpolated, real-valued function.

There have been attempts to provide an explanation of fuzzy logic in terms of probability theory. One idea is to view assertions such as "Nate is Tall" as discrete observations made concerning a continuous hidden variable, Nate's actual Height. The probability model specifies  $P(\text{Observer says Nate is tall} \mid Height)$ , perhaps using a **probit distribution** as described on page 522. A posterior distribution over Nate's height can then be calculated in the usual way, for example, if the model is part of a hybrid Bayesian network. Such an approach is not truth-functional, of course. For example, the conditional distribution

P(Observer says Nate is tall and heavy | Height, Weight)

allows for interactions between height and weight in the causing of the observation. Thus, someone who is eight feet tall and weighs 190 pounds is very unlikely to be called "tall and heavy," even though "eight feet" counts as "tall" and "190 pounds" counts as "heavy."

Fuzzy predicates can also be given a probabilistic interpretation in terms of **random** sets—that is, random variables whose possible values are sets of objects. For example, Tall is a random set whose possible values are sets of people. The probability  $P(Tall = S_1)$ , where  $S_1$  is some particular set of people, is the probability that exactly that set would be identified as "tall" by an observer. Then the probability that "Nate is tall" is the sum of the probabilities of all the sets of which Nate is a member.

Both the hybrid Bayesian network approach and the random sets approach appear to capture aspects of fuzziness without introducing degrees of truth. Nonetheless, there remain many open issues concerning the proper representation of linguistic observations and continuous quantities—issues that have been neglected by most outside the fuzzy community.

### 14.8 SUMMARY

This chapter has described **Bayesian networks**, a well-developed representation for uncertain knowledge. Bayesian networks play a role roughly analogous to that of propositional logic for definite knowledge.

- A Bayesian network is a directed acyclic graph whose nodes correspond to random variables; each node has a conditional distribution for the node, given its parents.
- Bayesian networks provide a concise way to represent conditional independence relationships in the domain.
- A Bayesian network specifies a full joint distribution; each joint entry is defined as the
  product of the corresponding entries in the local conditional distributions. A Bayesian
  network is often exponentially smaller than an explicitly enumerated joint distribution.
- Many conditional distributions can be represented compactly by canonical families of

RANDOM SET

distributions. **Hybrid Bayesian networks**, which include both discrete and continuous variables, use a variety of canonical distributions.

- Inference in Bayesian networks means computing the probability distribution of a set
  of query variables, given a set of evidence variables. Exact inference algorithms, such
  as variable elimination, evaluate sums of products of conditional probabilities as efficiently as possible.
- In **polytrees** (singly connected networks), exact inference takes time linear in the size of the network. In the general case, the problem is intractable.
- Stochastic approximation techniques such as **likelihood weighting** and **Markov chain Monte Carlo** can give reasonable estimates of the true posterior probabilities in a network and can cope with much larger networks than can exact algorithms.
- Probability theory can be combined with representational ideas from first-order logic to
  produce very powerful systems for reasoning under uncertainty. Relational probability models (RPMs) include representational restrictions that guarantee a well-defined
  probability distribution that can be expressed as an equivalent Bayesian network. Openuniverse probability models handle existence and identity uncertainty, defining probability distributions over the infinite space of first-order possible worlds.
- Various alternative systems for reasoning under uncertainty have been suggested. Generally speaking, **truth-functional** systems are not well suited for such reasoning.

## BIBLIOGRAPHICAL AND HISTORICAL NOTES

The use of networks to represent probabilistic information began early in the 20th century, with the work of Sewall Wright on the probabilistic analysis of genetic inheritance and animal growth factors (Wright, 1921, 1934). I. J. Good (1961), in collaboration with Alan Turing, developed probabilistic representations and Bayesian inference methods that could be regarded as a forerunner of modern Bayesian networks—although the paper is not often cited in this context.<sup>10</sup> The same paper is the original source for the noisy-OR model.

The **influence diagram** representation for decision problems, which incorporated a DAG representation for random variables, was used in decision analysis in the late 1970s (see Chapter 16), but only enumeration was used for evaluation. Judea Pearl developed the message-passing method for carrying out inference in tree networks (Pearl, 1982a) and polytree networks (Kim and Pearl, 1983) and explained the importance of causal rather than diagnostic probability models, in contrast to the certainty-factor systems then in vogue.

The first expert system using Bayesian networks was CONVINCE (Kim, 1983). Early applications in medicine included the MUNIN system for diagnosing neuromuscular disorders (Andersen *et al.*, 1989) and the PATHFINDER system for pathology (Heckerman, 1991). The CPCS system (Pradhan *et al.*, 1994) is a Bayesian network for internal medicine consisting

<sup>&</sup>lt;sup>10</sup> I. J. Good was chief statistician for Turing's code-breaking team in World War II. In 2001: A Space Odyssey (Clarke, 1968a), Good and Minsky are credited with making the breakthrough that led to the development of the HAL 9000 computer.

of 448 nodes, 906 links and 8,254 conditional probability values. (The front cover shows a portion of the network.)

Applications in engineering include the Electric Power Research Institute's work on monitoring power generators (Morjaria *et al.*, 1995), NASA's work on displaying time-critical information at Mission Control in Houston (Horvitz and Barry, 1995), and the general field of **network tomography**, which aims to infer unobserved local properties of nodes and links in the Internet from observations of end-to-end message performance (Castro *et al.*, 2004). Perhaps the most widely used Bayesian network systems have been the diagnosis-and-repair modules (e.g., the Printer Wizard) in Microsoft Windows (Breese and Heckerman, 1996) and the Office Assistant in Microsoft Office (Horvitz *et al.*, 1998). Another important application area is biology: Bayesian networks have been used for identifying human genes by reference to mouse genes (Zhang *et al.*, 2003), inferring cellular networks Friedman (2004), and many other tasks in bioinformatics. We could go on, but instead we'll refer you to Pourret *et al.* (2008), a 400-page guide to applications of Bayesian networks.

Ross Shachter (1986), working in the influence diagram community, developed the first complete algorithm for general Bayesian networks. His method was based on goal-directed reduction of the network using posterior-preserving transformations. Pearl (1986) developed a clustering algorithm for exact inference in general Bayesian networks, utilizing a conversion to a directed polytree of clusters in which message passing was used to achieve consistency over variables shared between clusters. A similar approach, developed by the statisticians David Spiegelhalter and Steffen Lauritzen (Lauritzen and Spiegelhalter, 1988), is based on conversion to an undirected form of graphical model called a **Markov network**. This approach is implemented in the HUGIN system, an efficient and widely used tool for uncertain reasoning (Andersen *et al.*, 1989). Boutilier *et al.* (1996) show how to exploit context-specific independence in clustering algorithms.

The basic idea of variable elimination—that repeated computations within the overall sum-of-products expression can be avoided by caching—appeared in the symbolic probabilistic inference (SPI) algorithm (Shachter *et al.*, 1990). The elimination algorithm we describe is closest to that developed by Zhang and Poole (1994). Criteria for pruning irrelevant variables were developed by Geiger *et al.* (1990) and by Lauritzen *et al.* (1990); the criterion we give is a simple special case of these. Dechter (1999) shows how the variable elimination idea is essentially identical to **nonserial dynamic programming** (Bertele and Brioschi, 1972), an algorithmic approach that can be applied to solve a range of inference problems in Bayesian networks—for example, finding the **most likely explanation** for a set of observations. This connects Bayesian network algorithms to related methods for solving CSPs and gives a direct measure of the complexity of exact inference in terms of the tree width of the network. Wexler and Meek (2009) describe a method of preventing exponential growth in the size of factors computed in variable elimination; their algorithm breaks down large factors into products of smaller factors and simultaneously computes an error bound for the resulting approximation.

The inclusion of continuous random variables in Bayesian networks was considered by Pearl (1988) and Shachter and Kenley (1989); these papers discussed networks containing only continuous variables with linear Gaussian distributions. The inclusion of discrete variables has been investigated by Lauritzen and Wermuth (1989) and implemented in the

MARKOV NETWORK

NONSERIAL DYNAMIC PROGRAMMING

cHUGIN system (Olesen, 1993). Further analysis of linear Gaussian models, with connections to many other models used in statistics, appears in Roweis and Ghahramani (1999) The probit distribution is usually attributed to Gaddum (1933) and Bliss (1934), although it had been discovered several times in the 19th century. Bliss's work was expanded considerably by Finney (1947). The probit has been used widely for modeling discrete choice phenomena and can be extended to handle more than two choices (Daganzo, 1979). The logit model was introduced by Berkson (1944); initially much derided, it eventually became more popular than the probit model. Bishop (1995) gives a simple justification for its use.

Cooper (1990) showed that the general problem of inference in unconstrained Bayesian networks is NP-hard, and Paul Dagum and Mike Luby (1993) showed the corresponding approximation problem to be NP-hard. Space complexity is also a serious problem in both clustering and variable elimination methods. The method of **cutset conditioning**, which was developed for CSPs in Chapter 6, avoids the construction of exponentially large tables. In a Bayesian network, a cutset is a set of nodes that, when instantiated, reduces the remaining nodes to a polytree that can be solved in linear time and space. The query is answered by summing over all the instantiations of the cutset, so the overall space requirement is still linear (Pearl, 1988). Darwiche (2001) describes a recursive conditioning algorithm that allows a complete range of space/time tradeoffs.

The development of fast approximation algorithms for Bayesian network inference is a very active area, with contributions from statistics, computer science, and physics. The rejection sampling method is a general technique that is long known to statisticians; it was first applied to Bayesian networks by Max Henrion (1988), who called it **logic sampling**. Likelihood weighting, which was developed by Fung and Chang (1989) and Shachter and Peot (1989), is an example of the well-known statistical method of **importance sampling**. Cheng and Druzdzel (2000) describe an adaptive version of likelihood weighting that works well even when the evidence has very low prior likelihood.

Markov chain Monte Carlo (MCMC) algorithms began with the Metropolis algorithm, due to Metropolis *et al.* (1953), which was also the source of the simulated annealing algorithm described in Chapter 4. The Gibbs sampler was devised by Geman and Geman (1984) for inference in undirected Markov networks. The application of MCMC to Bayesian networks is due to Pearl (1987). The papers collected by Gilks *et al.* (1996) cover a wide variety of applications of MCMC, several of which were developed in the well-known Bugs package (Gilks *et al.*, 1994).

There are two very important families of approximation methods that we did not cover in the chapter. The first is the family of **variational approximation** methods, which can be used to simplify complex calculations of all kinds. The basic idea is to propose a reduced version of the original problem that is simple to work with, but that resembles the original problem as closely as possible. The reduced problem is described by some **variational parameters**  $\lambda$  that are adjusted to minimize a distance function D between the original and the reduced problem, often by solving the system of equations  $\partial D/\partial \lambda = 0$ . In many cases, strict upper and lower bounds can be obtained. Variational methods have long been used in statistics (Rustagi, 1976). In statistical physics, the **mean-field** method is a particular variational approximation in which the individual variables making up the model are assumed

VARIATIONAL APPROXIMATION

VARIATIONAL PARAMETER

MEAN FIELD

to be completely independent. This idea was applied to solve large undirected Markov networks (Peterson and Anderson, 1987; Parisi, 1988). Saul *et al.* (1996) developed the mathematical foundations for applying variational methods to Bayesian networks and obtained accurate lower-bound approximations for sigmoid networks with the use of mean-field methods. Jaakkola and Jordan (1996) extended the methodology to obtain both lower and upper bounds. Since these early papers, variational methods have been applied to many specific families of models. The remarkable paper by Wainwright and Jordan (2008) provides a unifying theoretical analysis of the literature on variational methods.

A second important family of approximation algorithms is based on Pearl's polytree message-passing algorithm (1982a). This algorithm can be applied to general networks, as suggested by Pearl (1988). The results might be incorrect, or the algorithm might fail to terminate, but in many cases, the values obtained are close to the true values. Little attention was paid to this so-called **belief propagation** (or BP) approach until McEliece *et al.* (1998) observed that message passing in a multiply connected Bayesian network was exactly the computation performed by the **turbo decoding** algorithm (Berrou *et al.*, 1993), which provided a major breakthrough in the design of efficient error-correcting codes. The implication is that BP is both fast and accurate on the very large and very highly connected networks used for decoding and might therefore be useful more generally. Murphy *et al.* (1999) presented a promising empirical study of BP's performance, and Weiss and Freeman (2001) established strong convergence results for BP on linear Gaussian networks. Weiss (2000b) shows how an approximation called loopy belief propagation works, and when the approximation is correct. Yedidia *et al.* (2005) made further connections between loopy propagation and ideas from statistical physics.

The connection between probability and first-order languages was first studied by Carnap (1950). Gaifman (1964) and Scott and Krauss (1966) defined a language in which probabilities could be associated with first-order sentences and for which models were probability measures on possible worlds. Within AI, this idea was developed for propositional logic by Nilsson (1986) and for first-order logic by Halpern (1990). The first extensive investigation of knowledge representation issues in such languages was carried out by Bacchus (1990). The basic idea is that each sentence in the knowledge base expressed a *constraint* on the distribution over possible worlds; one sentence entails another if it expresses a stronger constraint. For example, the sentence  $\forall x \ P(Hungry(x)) > 0.2$  rules out distributions in which any object is hungry with probability less than 0.2; thus, it entails the sentence  $\forall x \ P(Hungry(x)) > 0.1$ . It turns out that writing a *consistent* set of sentences in these languages is quite difficult and constructing a unique probability model nearly impossible unless one adopts the representation approach of Bayesian networks by writing suitable sentences about conditional probabilities.

Beginning in the early 1990s, researchers working on complex applications noticed the expressive limitations of Bayesian networks and developed various languages for writing "templates" with logical variables, from which large networks could be constructed automatically for each problem instance (Breese, 1992; Wellman *et al.*, 1992). The most important such language was Bugs (Bayesian inference Using Gibbs Sampling) (Gilks *et al.*, 1994), which combined Bayesian networks with the **indexed random variable** notation common in

BELIEF PROPAGATION

TURBO DECODING

INDEXED RANDOM VARIABLE

statistics. (In Bugs, an indexed random variable looks like X[i], where i has a defined integer range.) These languages inherited the key property of Bayesian networks: every well-formed knowledge base defines a unique, consistent probability model. Languages with well-defined semantics based on unique names and domain closure drew on the representational capabilities of logic programming (Poole, 1993; Sato and Kameya, 1997; Kersting  $et\ al.$ , 2000) and semantic networks (Koller and Pfeffer, 1998; Pfeffer, 2000). Pfeffer (2007) went on to develop IBAL, which represents first-order probability models as probabilistic programs in a programming language extended with a randomization primitive. Another important thread was the combination of relational and first-order notations with (undirected) Markov networks (Taskar  $et\ al.$ , 2002; Domingos and Richardson, 2004), where the emphasis has been less on knowledge representation and more on learning from large data sets.

Initially, inference in these models was performed by generating an equivalent Bayesian network. Pfeffer *et al.* (1999) introduced a variable elimination algorithm that cached each computed factor for reuse by later computations involving the same relations but different objects, thereby realizing some of the computational gains of lifting. The first truly lifted inference algorithm was a lifted form of variable elimination described by Poole (2003) and subsequently improved by de Salvo Braz *et al.* (2007). Further advances, including cases where certain aggregate probabilities can be computed in closed form, are described by Milch *et al.* (2008) and Kisynski and Poole (2009). Pasula and Russell (2001) studied the application of MCMC to avoid building the complete equivalent Bayes net in cases of relational and identity uncertainty. Getoor and Taskar (2007) collect many important papers on first-order probability models and their use in machine learning.

RECORD LINKAGE

Probabilistic reasoning about identity uncertainty has two distinct origins. In statistics, the problem of record linkage arises when data records do not contain standard unique identifiers—for example, various citations of this book might name its first author "Stuart Russell" or "S. J. Russell" or even "Stewart Russle," and other authors may use the some of the same names. Literally hundreds of companies exist solely to solve record linkage problems in financial, medical, census, and other data. Probabilistic analysis goes back to work by Dunn (1946); the Fellegi-Sunter model (1969), which is essentially naive Bayes applied to matching, still dominates current practice. The second origin for work on identity uncertainty is multitarget tracking (Sittler, 1964), which we cover in Chapter 15. For most of its history, work in symbolic AI assumed erroneously that sensors could supply sentences with unique identifiers for objects. The issue was studied in the context of language understanding by Charniak and Goldman (1992) and in the context of surveillance by (Huang and Russell, 1998) and Pasula et al. (1999). Pasula et al. (2003) developed a complex generative model for authors, papers, and citation strings, involving both relational and identity uncertainty, and demonstrated high accuracy for citation information extraction. The first formally defined language for open-universe probability models was BLOG (Milch et al., 2005), which came with a complete (albeit slow) MCMC inference algorithm for all well-defined mdoels. (The program code faintly visible on the front cover of this book is part of a BLOG model for detecting nuclear explosions from seismic signals as part of the UN Comprehensive Test Ban Treaty verification regime.) Laskey (2008) describes another open-universe modeling language called multi-entity Bayesian networks.

As explained in Chapter 13, early probabilistic systems fell out of favor in the early 1970s, leaving a partial vacuum to be filled by alternative methods. Certainty factors were invented for use in the medical expert system MYCIN (Shortliffe, 1976), which was intended both as an engineering solution and as a model of human judgment under uncertainty. The collection *Rule-Based Expert Systems* (Buchanan and Shortliffe, 1984) provides a complete overview of MYCIN and its descendants (see also Stefik, 1995). David Heckerman (1986) showed that a slightly modified version of certainty factor calculations gives correct probabilistic results in some cases, but results in serious overcounting of evidence in other cases. The PROSPECTOR expert system (Duda *et al.*, 1979) used a rule-based approach in which the rules were justified by a (seldom tenable) global independence assumption.

Dempster–Shafer theory originates with a paper by Arthur Dempster (1968) proposing a generalization of probability to interval values and a combination rule for using them. Later work by Glenn Shafer (1976) led to the Dempster-Shafer theory's being viewed as a competing approach to probability. Pearl (1988) and Ruspini *et al.* (1992) analyze the relationship between the Dempster–Shafer theory and standard probability theory.

Fuzzy sets were developed by Lotfi Zadeh (1965) in response to the perceived difficulty of providing exact inputs to intelligent systems. The text by Zimmermann (2001) provides a thorough introduction to fuzzy set theory; papers on fuzzy applications are collected in Zimmermann (1999). As we mentioned in the text, fuzzy logic has often been perceived incorrectly as a direct competitor to probability theory, whereas in fact it addresses a different set of issues. **Possibility theory** (Zadeh, 1978) was introduced to handle uncertainty in fuzzy systems and has much in common with probability. Dubois and Prade (1994) survey the connections between possibility theory and probability theory.

POSSIBILITY THEORY

The resurgence of probability depended mainly on Pearl's development of Bayesian networks as a method for representing and using conditional independence information. This resurgence did not come without a fight; Peter Cheeseman's (1985) pugnacious "In Defense of Probability" and his later article "An Inquiry into Computer Understanding" (Cheeseman, 1988, with commentaries) give something of the flavor of the debate. Eugene Charniak helped present the ideas to AI researchers with a popular article, "Bayesian networks without tears" (1991), and book (1993). The book by Dean and Wellman (1991) also helped introduce Bayesian networks to AI researchers. One of the principal philosophical objections of the logicists was that the numerical calculations that probability theory was thought to require were not apparent to introspection and presumed an unrealistic level of precision in our uncertain knowledge. The development of qualitative probabilistic networks (Wellman, 1990a) provided a purely qualitative abstraction of Bayesian networks, using the notion of positive and negative influences between variables. Wellman shows that in many cases such information is sufficient for optimal decision making without the need for the precise specification of probability values. Goldszmidt and Pearl (1996) take a similar approach. Work by Adnan Darwiche and Matt Ginsberg (1992) extracts the basic properties of conditioning and evidence combination from probability theory and shows that they can also be applied in logical and default reasoning. Often, programs speak louder than words, and the ready avail-

<sup>11</sup> The title of the original version of the article was "Pearl for swine."

ability of high-quality software such as the Bayes Net toolkit (Murphy, 2001) accelerated the adoption of the technology.

The most important single publication in the growth of Bayesian networks was undoubtedly the text *Probabilistic Reasoning in Intelligent Systems* (Pearl, 1988). Several excellent texts (Lauritzen, 1996; Jensen, 2001; Korb and Nicholson, 2003; Jensen, 2007; Darwiche, 2009; Koller and Friedman, 2009) provide thorough treatments of the topics we have covered in this chapter. New research on probabilistic reasoning appears both in mainstream AI journals, such as *Artificial Intelligence* and the *Journal of AI Research*, and in more specialized journals, such as the *International Journal of Approximate Reasoning*. Many papers on graphical models, which include Bayesian networks, appear in statistical journals. The proceedings of the conferences on Uncertainty in Artificial Intelligence (UAI), Neural Information Processing Systems (NIPS), and Artificial Intelligence and Statistics (AISTATS) are excellent sources for current research.

#### **EXERCISES**

- 14.1 We have a bag of three biased coins a, b, and c with probabilities of coming up heads of 20%, 60%, and 80%, respectively. One coin is drawn randomly from the bag (with equal likelihood of drawing each of the three coins), and then the coin is flipped three times to generate the outcomes  $X_1$ ,  $X_2$ , and  $X_3$ .
  - a. Draw the Bayesian network corresponding to this setup and define the necessary CPTs.
  - **b**. Calculate which coin was most likely to have been drawn from the bag if the observed flips come out heads twice and tails once.
- **14.2** Equation (14.1) on page 513 defines the joint distribution represented by a Bayesian network in terms of the parameters  $\theta(X_i | Parents(X_i))$ . This exercise asks you to derive the equivalence between the parameters and the conditional probabilities  $\mathbf{P}(X_i | Parents(X_i))$  from this definition.
  - **a.** Consider a simple network  $X \to Y \to Z$  with three Boolean variables. Use Equations (13.3) and (13.6) (pages 485 and 492) to express the conditional probability  $P(z \mid y)$  as the ratio of two sums, each over entries in the joint distribution  $\mathbf{P}(X, Y, Z)$ .
  - **b.** Now use Equation (14.1) to write this expression in terms of the network parameters  $\theta(X)$ ,  $\theta(Y \mid X)$ , and  $\theta(Z \mid Y)$ .
  - c. Next, expand out the summations in your expression from part (b), writing out explicitly the terms for the true and false values of each summed variable. Assuming that all network parameters satisfy the constraint  $\sum_{x_i} \theta(x_i \mid parents(X_i)) = 1$ , show that the resulting expression reduces to  $\theta(x \mid y)$ .
  - **d**. Generalize this derivation to show that  $\theta(X_i | Parents(X_i)) = \mathbf{P}(X_i | Parents(X_i))$  for any Bayesian network.

Exercises 559

ARC REVERSAL

**14.3** The operation of **arc reversal** in a Bayesian network allows us to change the direction of an arc  $X \to Y$  while preserving the joint probability distribution that the network represents (Shachter, 1986). Arc reversal may require introducing new arcs: all the parents of X also become parents of Y, and all parents of Y also become parents of X.

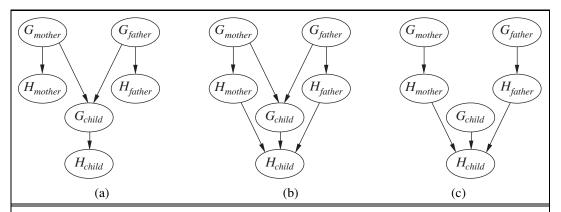
- a. Assume that X and Y start with m and n parents, respectively, and that all variables have k values. By calculating the change in size for the CPTs of X and Y, show that the total number of parameters in the network cannot decrease during arc reversal. (*Hint*: the parents of X and Y need not be disjoint.)
- **b**. Under what circumstances can the total number remain constant?
- c. Let the parents of X be  $U \cup V$  and the parents of Y be  $V \cup W$ , where U and W are disjoint. The formulas for the new CPTs after arc reversal are as follows:

$$\mathbf{P}(Y \mid \mathbf{U}, \mathbf{V}, \mathbf{W}) = \sum_{x} \mathbf{P}(Y \mid \mathbf{V}, \mathbf{W}, x) \mathbf{P}(x \mid \mathbf{U}, \mathbf{V})$$

$$\mathbf{P}(X \mid \mathbf{U}, \mathbf{V}, \mathbf{W}, Y) = \mathbf{P}(Y \mid X, \mathbf{V}, \mathbf{W}) \mathbf{P}(X \mid \mathbf{U}, \mathbf{V}) / \mathbf{P}(Y \mid \mathbf{U}, \mathbf{V}, \mathbf{W}).$$

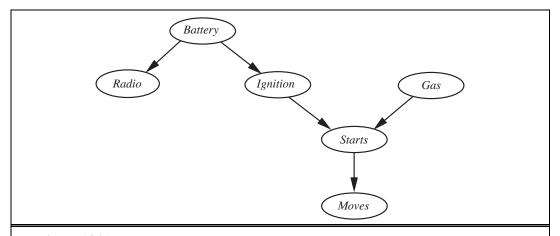
Prove that the new network expresses the same joint distribution over all variables as the original network.

- **14.4** Consider the Bayesian network in Figure 14.2.
  - **a.** If no evidence is observed, are *Burglary* and *Earthquake* independent? Prove this from the numerical semantics and from the topological semantics.
  - **b.** If we observe Alarm = true, are Burglary and Earthquake independent? Justify your answer by calculating whether the probabilities involved satisfy the definition of conditional independence.
- **14.5** Suppose that in a Bayesian network containing an unobserved variable Y, all the variables in the Markov blanket MB(Y) have been observed.
  - **a.** Prove that removing the node Y from the network will not affect the posterior distribution for any other unobserved variable in the network.
  - **b**. Discuss whether we can remove *Y* if we are planning to use (i) rejection sampling and (ii) likelihood weighting.
- 14.6 Let  $H_x$  be a random variable denoting the handedness of an individual x, with possible values l or r. A common hypothesis is that left- or right-handedness is inherited by a simple mechanism; that is, perhaps there is a gene  $G_x$ , also with values l or r, and perhaps actual handedness turns out mostly the same (with some probability s) as the gene an individual possesses. Furthermore, perhaps the gene itself is equally likely to be inherited from either of an individual's parents, with a small nonzero probability m of a random mutation flipping the handedness.
  - a. Which of the three networks in Figure 14.20 claim that  $\mathbf{P}(G_{father}, G_{mother}, G_{child}) = \mathbf{P}(G_{father})\mathbf{P}(G_{mother})\mathbf{P}(G_{child})$ ?
  - **b**. Which of the three networks make independence claims that are consistent with the hypothesis about the inheritance of handedness?



**Figure 14.20** Three possible structures for a Bayesian network describing genetic inheritance of handedness.

- **c**. Which of the three networks is the best description of the hypothesis?
- **d**. Write down the CPT for the  $G_{child}$  node in network (a), in terms of s and m.
- e. Suppose that  $P(G_{father} = l) = P(G_{mother} = l) = q$ . In network (a), derive an expression for  $P(G_{child} = l)$  in terms of m and q only, by conditioning on its parent nodes.
- **f**. Under conditions of genetic equilibrium, we expect the distribution of genes to be the same across generations. Use this to calculate the value of q, and, given what you know about handedness in humans, explain why the hypothesis described at the beginning of this question must be wrong.
- **14.7** The **Markov blanket** of a variable is defined on page 517. Prove that a variable is independent of all other variables in the network, given its Markov blanket and derive Equation (14.12) (page 538).



**Figure 14.21** A Bayesian network describing some features of a car's electrical system and engine. Each variable is Boolean, and the true value indicates that the corresponding aspect of the vehicle is in working order.

Exercises 561

- **14.8** Consider the network for car diagnosis shown in Figure 14.21.
  - **a.** Extend the network with the Boolean variables *IcyWeather* and *StarterMotor*.
  - **b**. Give reasonable conditional probability tables for all the nodes.
  - c. How many independent values are contained in the joint probability distribution for eight Boolean nodes, assuming that no conditional independence relations are known to hold among them?
  - d. How many independent probability values do your network tables contain?
  - **e**. The conditional distribution for *Starts* could be described as a **noisy-AND** distribution. Define this family in general and relate it to the noisy-OR distribution.
- **14.9** Consider the family of linear Gaussian networks, as defined on page 520.
  - **a.** In a two-variable network, let  $X_1$  be the parent of  $X_2$ , let  $X_1$  have a Gaussian prior, and let  $\mathbf{P}(X_2 \mid X_1)$  be a linear Gaussian distribution. Show that the joint distribution  $P(X_1, X_2)$  is a multivariate Gaussian, and calculate its covariance matrix.
  - **b**. Prove by induction that the joint distribution for a general linear Gaussian network on  $X_1, \ldots, X_n$  is also a multivariate Gaussian.
- **14.10** The probit distribution defined on page 522 describes the probability distribution for a Boolean child, given a single continuous parent.
  - **a**. How might the definition be extended to cover multiple continuous parents?
  - **b.** How might it be extended to handle a *multivalued* child variable? Consider both cases where the child's values are ordered (as in selecting a gear while driving, depending on speed, slope, desired acceleration, etc.) and cases where they are unordered (as in selecting bus, train, or car to get to work). (*Hint*: Consider ways to divide the possible values into two sets, to mimic a Boolean variable.)
- 14.11 In your local nuclear power station, there is an alarm that senses when a temperature gauge exceeds a given threshold. The gauge measures the temperature of the core. Consider the Boolean variables A (alarm sounds),  $F_A$  (alarm is faulty), and  $F_G$  (gauge is faulty) and the multivalued nodes G (gauge reading) and T (actual core temperature).
  - **a.** Draw a Bayesian network for this domain, given that the gauge is more likely to fail when the core temperature gets too high.
  - **b**. Is your network a polytree? Why or why not?
  - c. Suppose there are just two possible actual and measured temperatures, normal and high; the probability that the gauge gives the correct temperature is x when it is working, but y when it is faulty. Give the conditional probability table associated with G.
  - **d**. Suppose the alarm works correctly unless it is faulty, in which case it never sounds. Give the conditional probability table associated with A.
  - **e**. Suppose the alarm and gauge are working and the alarm sounds. Calculate an expression for the probability that the temperature of the core is too high, in terms of the various conditional probabilities in the network.