QUANTIFYING UNCERTAINTY

Chapter 13

Chapter 13 1

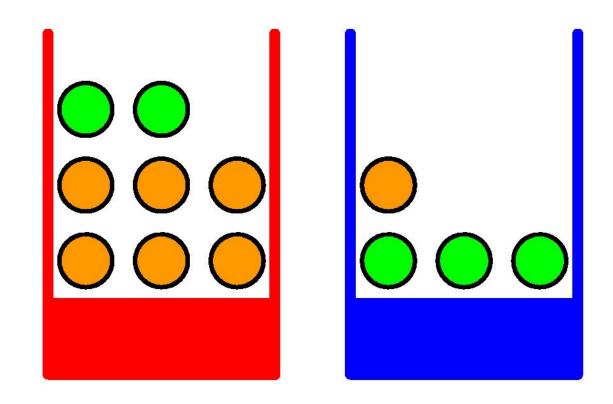
Outline

- \diamondsuit Uncertainty
- \diamond Probability
- \Diamond Inference
- \Diamond Independence
- \diamond Bayes' Rule

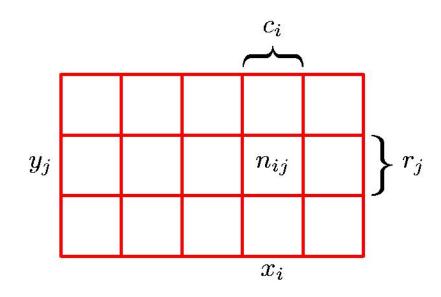
PATTERN RECOGNITION AND MACHINE LEARNING CHAPTER 1: INTRODUCTION

Probability Theory

Apples and Oranges



Probability Theory



Marginal Probability

$$p(X = x_i) = \frac{c_i}{N}.$$

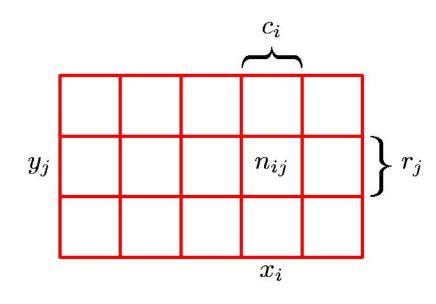
Joint Probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

Conditional Probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

Probability Theory

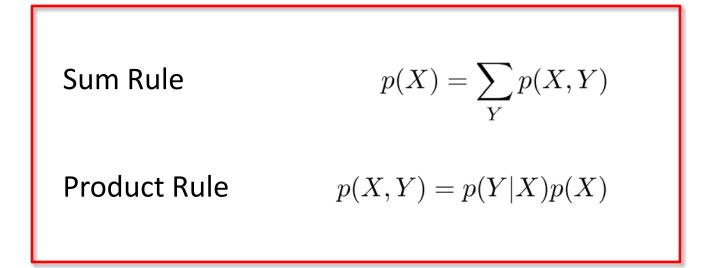


Sum Rule $p(X = x_i) = \frac{c_i}{N} = \frac{1}{N} \sum_{j=1}^{L} n_{ij}$ $= \sum_{j=1}^{L} p(X = x_i, Y = y_j)$

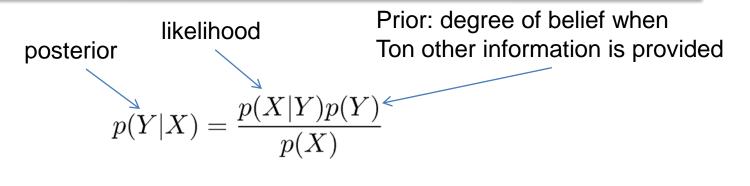
Product Rule

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$$
$$= p(Y = y_j | X = x_i) p(X = x_i)$$

The Rules of Probability



Bayes' Theorem

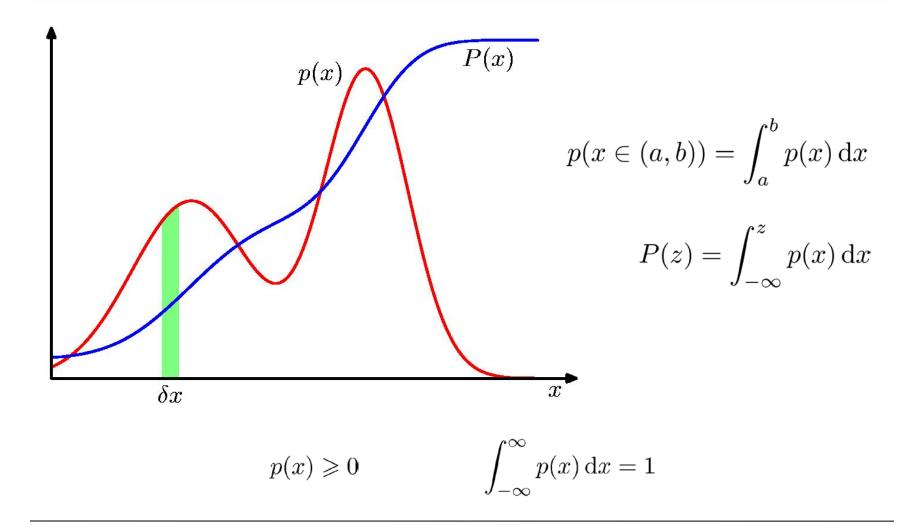


$$p(X) = \sum_{Y} p(X|Y)p(Y)$$

posterior ∞ likelihood x prior

Bayesian terms: Y: cause | not observed X: effect | observed

Probability Densities



Expectations

$$\mathbb{E}[f] = \sum_{x} p(x) f(x)$$

$$\mathbb{E}[f] = \int p(x)f(x) \,\mathrm{d}x$$

$$\mathbb{E}_{x}[f|y] = \sum_{x} p(x|y)f(x)$$

Conditional Expectation (discrete)

$$\mathbb{E}[f] \simeq \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

Approximate Expectation (discrete and continuous)

$$\operatorname{var}[f] = \mathbb{E}\left[\left(f(x) - \mathbb{E}[f(x)]\right)^2\right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

$$\begin{array}{lll} \operatorname{cov}[x,y] &= & \mathbb{E}_{x,y} \left[\left\{ x - \mathbb{E}[x] \right\} \left\{ y - \mathbb{E}[y] \right\} \right] \\ &= & \mathbb{E}_{x,y}[xy] - \mathbb{E}[x] \mathbb{E}[y] \end{array}$$

$$\begin{aligned} \operatorname{cov}[\mathbf{x}, \mathbf{y}] &= & \mathbb{E}_{\mathbf{x}, \mathbf{y}} \left[\{ \mathbf{x} - \mathbb{E}[\mathbf{x}] \} \{ \mathbf{y}^{\mathrm{T}} - \mathbb{E}[\mathbf{y}^{\mathrm{T}}] \} \right] \\ &= & \mathbb{E}_{\mathbf{x}, \mathbf{y}}[\mathbf{x} \mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{x}] \mathbb{E}[\mathbf{y}^{\mathrm{T}}] \end{aligned}$$

The Gaussian Distribution

Gaussian Mean and Variance

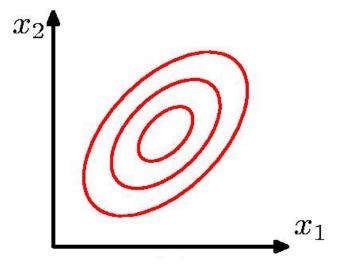
$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x \, \mathrm{d}x = \mu$$

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x^2 \,\mathrm{d}x = \mu^2 + \sigma^2$$

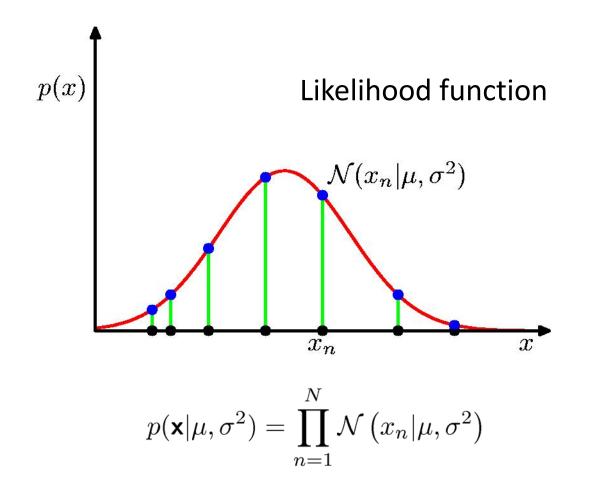
 $\operatorname{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$

The Multivariate Gaussian

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$



Gaussian Parameter Estimation



Maximum (Log) Likelihood

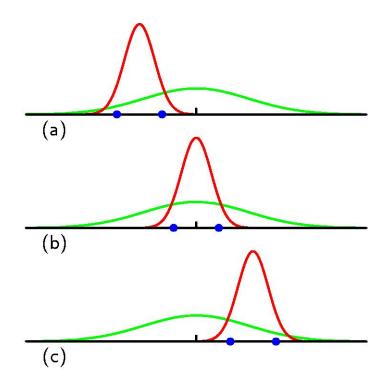
$$\ln p\left(\mathbf{x}|\mu,\sigma^{2}\right) = -\frac{1}{2\sigma^{2}} \sum_{n=1}^{N} (x_{n}-\mu)^{2} - \frac{N}{2} \ln \sigma^{2} - \frac{N}{2} \ln(2\pi)$$

$$\mu_{\rm ML} = \frac{1}{N} \sum_{n=1}^{N} x_n \qquad \qquad \sigma_{\rm ML}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2$$

Properties of $\mu_{ m ML}$ and $\sigma_{ m ML}^2$

 $)^{2}$

$$\mathbb{E}[\mu_{\mathrm{ML}}] = \mu$$
$$\mathbb{E}[\sigma_{\mathrm{ML}}^2] = \left(\frac{N-1}{N}\right)\sigma^2$$
$$\widetilde{\sigma}^2 = \frac{N}{N-1}\sigma_{\mathrm{ML}}^2$$
$$= \frac{1}{N-1}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}})$$



Maximum Likelihood

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathbf{w}), \beta^{-1}\right)$$

. .

$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\underbrace{\frac{\beta}{2} \sum_{n=1}^{N} \left\{ y(x_n, \mathbf{w}) - t_n \right\}^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

Determine \mathbf{w}_{ML} by minimizing sum-of-squares error, $E(\mathbf{w})$.

$$\frac{1}{\beta_{\rm ML}} = \frac{1}{N} \sum_{n=1}^{N} \{ y(x_n, \mathbf{w}_{\rm ML}) - t_n \}^2$$

Decision Theory

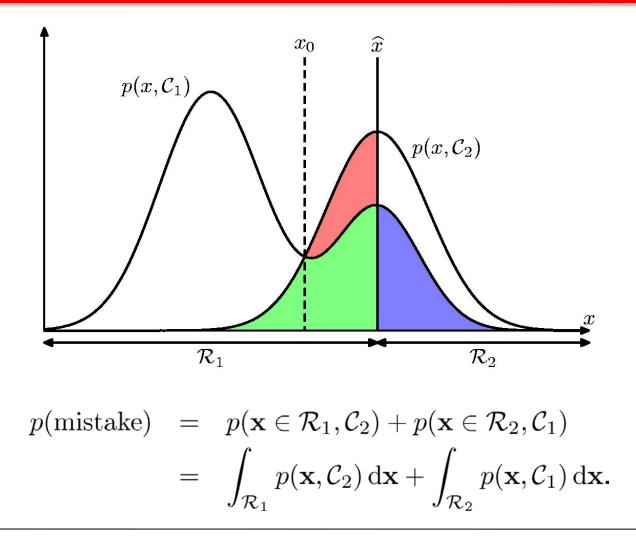
Inference step

Determine either $p(t|\mathbf{x})$ or $p(\mathbf{x}, t)$.

Decision step For given x, determine optimal t.

Decision theory = **probability** theory + **utility** theory

Minimum Misclassification Rate



Minimum Expected Loss

Example: classify medical images as 'cancer' or 'normal'

 $\begin{array}{c} \text{Decision} \\ \text{cancer normal} \\ \begin{array}{c} \text{pcancer} \\ \text{normal} \end{array} \begin{pmatrix} 0 & 1000 \\ 1 & 0 \end{pmatrix} \end{array}$

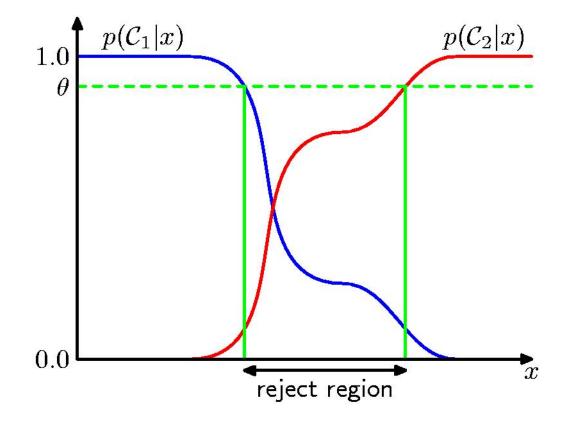
Minimum Expected Loss

$$\mathbb{E}[L] = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) \, \mathrm{d}\mathbf{x}$$

Regions \mathcal{R}_j are chosen to minimize

$$\mathbb{E}[L] = \sum_{k} L_{kj} p(\mathcal{C}_k | \mathbf{x})$$

Reject Option



Why Separate Inference and Decision?

- Minimizing risk (loss matrix may change over time)
- Reject option
- Unbalanced class priors
- Combining models

Uncertainty

Example: Let action A_t = leave for airport t minutes before flight Will A_t get me there on time? 13

Possible source of uncertainty:

- 1) partial observability (road state, other drivers' plans, etc.)
- 2) noisy sensors (traffic reports)
- 3) uncertainty in action outcomes (flat tire, etc.)
- * Immense complexity of modelling and predicting traffic

Hence a purely logical approach either

- 1) risks falsehood: " A_{25} will get me there on time"
- or 2) leads to conclusions that are too weak for decision making:

" A_{25} will get me there on time if there's no accident on the bridge and it doesn't rain and my tires remain intact etc etc."

The rational decision depends on both the relative importance of various goals and the likelihood that, and degree to which, they will be achieved.

Example of uncertain reasoning

Problem: diagnosing a dental paient's toohache.

Propositional logic:

 $\begin{aligned} Toothache \ \Rightarrow \ Cavity \text{ is wrong.} \\ Toothache \ \Rightarrow \ Cavity \lor GumProblem \lor Abscess \dots \text{ is still wrong.} \end{aligned}$

Failure points:

Laziness: too much work and too hard to use.

Theoretical ignorange: Medical science has no complete therory

Pratical ignorance: even if we have the complete rule,

we may not know complete information about the patient.

Solutions to the qualification problem:

Use probability theory to specify degree of belief of relavent sentences.

Making decisions under uncertainty

Suppose I believe the following:

 $P(A_{25} \text{ gets me there on time}|...) = 0.04$ $P(A_{90} \text{ gets me there on time}|...) = 0.70$ $P(A_{120} \text{ gets me there on time}|...) = 0.95$ $P(A_{1440} \text{ gets me there on time}|...) = 0.9999$

Which action to choose?

Depends on my preferences for missing flight vs. airport cuisine, etc.

Utility theory is used to represent and infer preferences of agents about the possible outcomes of the various plans.

Decision theory = utility theory + probability theory

Probability basics: In logical perspective

Begin with a set Ω -the sample space set of all possible states that are mutually exclusive and exhaustive $\omega \in \Omega$ is a sample point/possible world/atomic event e.g., 6 possible rolls of a die.

A probability model is a sample space with an assignment $P(\omega)$ (probability value) for every $\omega \in \Omega$ s.t. $0 \leq P(\omega) \leq 1$ and $\Sigma_{\omega}P(\omega) = 1$ e.g., P(1) = P(2) = P(3) = P(4) = P(5) = P(6) = 1/6.

An event A is any subset of Ω

 $P(A) = \sum_{\{\omega \in A\}} P(\omega)$

(The Sum Rule) E.g., P(die roll < 4) = P(1) + P(2) + P(3) = 1/6 + 1/6 + 1/6 = 1/2

Random variables

A random variable (r.v.) is variables in probability theory and their names begin with uppercase letter.

A domain of r.v. is the set pf possible values it can take.

P induces a probability distribution for any r.v. X:

 $P(X = x_i) = \sum_{\{\omega: X(\omega) = x_i\}} P(\omega)$

e.g., P(Odd = true) = P(1) + P(3) + P(5) = 1/6 + 1/6 + 1/6 = 1/2

Propositions

Propositions are set of events (set of sample points) in the sample space where the proposition is true

Given Boolean random variables A and B: event $a = \text{set of sample points where } A(\omega) = true$ event $\neg a = \text{set of sample points where } A(\omega) = false$ event $a \land b = \text{points where } A(\omega) = true$ and $B(\omega) = true$

With Boolean variables, sample point = propositional logic model e.g., A = true, B = false, or $a \land \neg b$. Proposition = disjunction of atomic events in which it is true

e.g.,
$$(a \lor b) \equiv (\neg a \land b) \lor (a \land \neg b) \lor (a \land b)$$

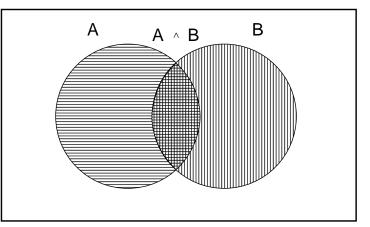
 $\Rightarrow P(a \lor b) = P(\neg a \land b) + P(a \land \neg b) + P(a \land b)$

Why use probability?

The definitions imply that certain logically related events must have related probabilities

E.g.,
$$P(a \lor b) = P(a) + P(b) - P(a \land b)$$

True



Syntax for propositions

Propositional or Boolean random variables e.g., Cavity (do I have a cavity?) Cavity = true is a proposition, also written cavity Discrete random variables (finite or infinite) e.g., Weather is one of $\langle sunny, rain, cloudy, snow \rangle$ Weather = rain is a proposition Values must be exhaustive and mutually exclusive

Continuous random variables (bounded or unbounded) e.g., Temp = 21.6; also allow, e.g., Temp < 22.0.

Arbitrary Boolean combinations of basic propositions

Syntax for probability distributions

Prepresent a discrete probability distribution as a vector of probabilit values: $\mathbf{P}(Weather) = \langle 0.72, 0.1, 0.08, 0.1 \rangle \text{ (normalized, i.e., sums to 1)}$

Joint probability distribution for a set of r.v.s gives the probability of every atomic event on those r.v.s (i.e., every sample point) $\mathbf{P}(Weather, Cavity) = a \ 4 \times 2$ matrix of values:

Weather =	sunny	rain	cloudy	snow
Cavity = true	0.144	0.02	0.016	0.02
Cavity = false	0.576	0.08	0.064	0.08

Sum Rule: For any proposition ϕ ,

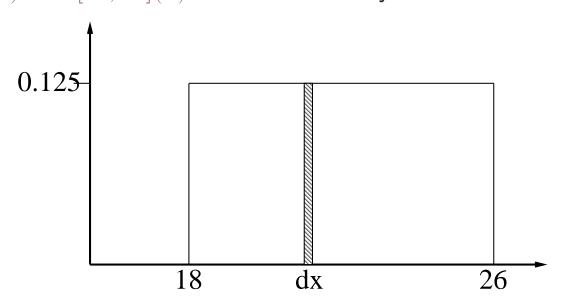
 $P(\phi) = \sum_{\omega \in \phi} P(\omega)$

A possible world is defined to be an assignment of values to all of the r.v. under consideration. This means that probability model is completely determined by the joint distribution for all of the r.v. – full joint probability

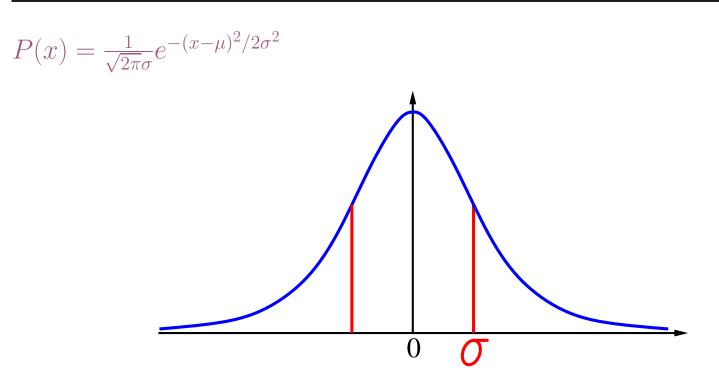
distribution

Probability for continuous variables

Express distribution as a parameterized function of value: P(X = x) = U[18, 26](x) = uniform density between 18 and 26



Gaussian density



Conditional probability

Conditional or posterior probabilities

e.g., P(cavity|toothache) = 0.8

i.e., **given that** *toothache* is true and we have no **further informa-tion** conclude that **cavity** is true with prob. 0.8.

NOT "if *toothache* then prob. that *cavity* is true is 0.8"

If we know more, e.g., *cavity* is also given, then we have

P(cavity|toothache, cavity) = 1

Note: the less specific belief **remains valid** after more evidence arrives, but is not always **useful**

New evidence may be irrelevant, allowing simplification, e.g., P(cavity|toothache, 49ersWin) = P(cavity|toothache) = 0.8

Conditional probability

Definition of conditional probability:

 $P(a|b) = \frac{P(a \wedge b)}{P(b)} \text{ if } P(b) \neq 0$

Product rule gives an alternative formulation: $P(a \wedge b) = P(a|b)P(b) = P(b|a)P(a)$

A general version holds for whole distributions, e.g., $\mathbf{P}(Weather, Cavity) = \mathbf{P}(Weather|Cavity)\mathbf{P}(Cavity)$ (View as a 4×2 set of equations, **not** matrix mult.)

Chain rule is derived by successive application of product rule: $\mathbf{P}(X_1, \dots, X_n) = \mathbf{P}(X_1, \dots, X_{n-1}) \mathbf{P}(X_n | X_1, \dots, X_{n-1})$ $= \mathbf{P}(X_1, \dots, X_{n-2}) \mathbf{P}(X_{n-1} | X_1, \dots, X_{n-2}) \mathbf{P}(X_n | X_1, \dots, X_{n-1})$ $= \dots$ $= \prod_{i=1}^n \mathbf{P}(X_i | X_1, \dots, X_{i-1})$

probabilisic inference: the computation of posterior probabilities for query propositions given obsrved evidence.

For simple cases, we can use the full joint distribution as he "knowledge base".

Start with the full joint distribution:

	toothache		¬ toothache	
	catch	\neg catch	catch	\neg catch
cavity	.108	.012	.072	.008
\neg cavity	.016	.064	.144	.576

* the table sums to one

Start with the full joint distribution:

	toothache		¬ toothache	
	catch	\neg catch	catch	\neg catch
cavity	.108	.012	.072	.008
\neg cavity	.016	.064	.144	.576

Marginalization (or summing out):

For any proposition $\phi,$ sum the atomic events where it is true: $P(\phi) = \sum_{\omega:\omega\models\phi} P(\omega)$

EX¿ Compute the marginal probability of toothache: P(toothache) = 0.108 + 0.012 + 0.016 + 0.064 = 0.2

Start with the joint distribution:

	toothache		¬ toothache	
	catch	\neg catch	catch	\neg catch
cavity	.108	.012	.072	.008
\neg cavity	.016	.064	.144	.576

For any proposition $\phi,$ sum the atomic events where it is true: $P(\phi)=\sum_{\omega:\omega\models\phi}P(\omega)$

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

Start with the joint distribution:

	toothache		¬ toothache	
	catch	\neg catch	catch	\neg catch
cavity	.108	.012	.072	.008
\neg cavity	.016	.064	.144	.576

Can also compute conditional probabilities:

$$P(\neg cavity | toothache) = \frac{P(\neg cavity \land toothache)}{P(toothache)} \\ = \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4$$

Normalization

	toothache		<i>¬ toothache</i>	
	catch	\neg catch	catch	\neg catch
cavity	.108	.012	.072	.008
\neg cavity	.016	.064	.144	.576

Denominator can be viewed as a normalization constant $\boldsymbol{\alpha}$

 $\mathbf{P}(Cavity|toothache) = \alpha \mathbf{P}(Cavity, toothache)$

- $= \alpha \left[\mathbf{P}(Cavity, toothache, catch) + \mathbf{P}(Cavity, toothache, \neg catch) \right]$
- $= \alpha [\langle 0.108, 0.016 \rangle + \langle 0.012, 0.064 \rangle]$
- $= \alpha \left< 0.12, 0.08 \right> = \left< 0.6, 0.4 \right>$

General idea: compute distribution on query variable by fixing evidence variables and summing over hidden variables

Inference by enumeration, contd.

Let \mathbf{X} be all the variables. Typically, we want the posterior joint distribution of the query variables \mathbf{Y} given specific values \mathbf{e} for the evidence variables \mathbf{E}

Let the hidden variables be $\mathbf{H}=\mathbf{X}-\mathbf{Y}-\mathbf{E}$

Then the required summation of joint entries is done by summing out the hidden variables:

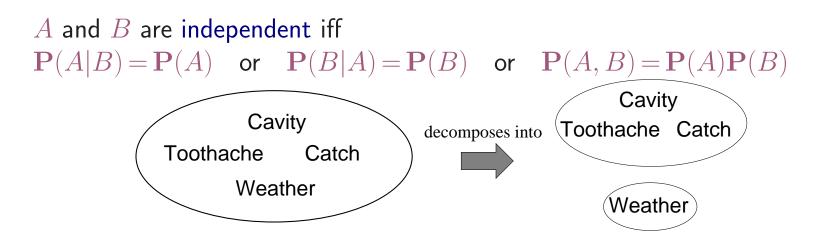
 $\mathbf{P}(\mathbf{Y}|\mathbf{E}\!=\!\mathbf{e}) = \alpha \mathbf{P}(\mathbf{Y},\mathbf{E}\!=\!\mathbf{e}) = \alpha \Sigma_{\mathbf{h}} \mathbf{P}(\mathbf{Y},\mathbf{E}\!=\!\mathbf{e},\mathbf{H}\!=\!\mathbf{h})$

i.e., sum over every possible combination of values $h = < h_1, \ldots, h_n >$ of the hidden variabes $H = < H_1, \ldots, H_n >$

Obvious problems with the enumeration method:

- 1) Worst-case time complexity $O(d^n)$ where d is the largest arity
- 2) Space complexity $O(d^n)$ to store the joint distribution
- 3) How to find the numbers for $O(d^n)$ entries???

Independence



$$\begin{split} \mathbf{P}(Toothache, Catch, Cavity, Weather) \\ &= \mathbf{P}(Toothache, Catch, Cavity) \mathbf{P}(Weather) \end{split}$$

32 entries reduced to 12; for n independent biased coins, $2^n \rightarrow n$

Absolute independence powerful but rare

Dentistry is a large field with hundreds of variables, none of which are independent. What to do?

Conditional independence

 $\mathbf{P}(Toothache, Cavity, Catch)$ has $2^3 - 1 = 7$ independent entries

If I have a cavity, the probability that the probe catches in it doesn't depend on whether I have a toothache:

(1) P(catch|toothache, cavity) = P(catch|cavity)

The same independence holds if I haven't got a cavity: (2) $P(catch|toothache, \neg cavity) = P(catch|\neg cavity)$

 $\begin{aligned} Catch \text{ is conditionally independent of } Toothache \text{ given } Cavity: \\ \mathbf{P}(Catch|Toothache, Cavity) = \mathbf{P}(Catch|Cavity) \end{aligned}$

Equivalent statements:

$$\begin{split} \mathbf{P}(Toothache|Catch,Cavity) &= \mathbf{P}(Toothache|Cavity) \\ \mathbf{P}(Toothache,Catch|Cavity) &= \mathbf{P}(Toothache|Cavity) \mathbf{P}(Catch|Cavity) \end{split}$$

Conditional independence contd.

Write out full joint distribution using chain rule: P(Toothache, Catch, Cavity) = P(Toothache|Catch, Cavity)P(Catch, Cavity) = P(Toothache|Catch, Cavity)P(Catch|Cavity)P(Cavity) = P(Toothache|Cavity)P(Catch|Cavity)P(Cavity)

I.e., 2 + 2 + 1 = 5 independent numbers (equations 1 and 2 remove 2)

In most cases, the use of conditional independence reduces the size of the representation of the joint distribution from exponential in n to linear in n.

Conditional independence is our most basic and robust form of knowledge about uncertain environments.

Bayes' Rule

Product rule $P(a \land b) = P(a|b)P(b) = P(b|a)P(a)$

$$\Rightarrow$$
 Bayes' rule $P(a|b) = \frac{P(b|a)P(a)}{P(b)}$

or in distribution form

$$\mathbf{P}(Y|X) = \frac{\mathbf{P}(X|Y)\mathbf{P}(Y)}{\mathbf{P}(X)} = \alpha \mathbf{P}(X|Y)\mathbf{P}(Y)$$

Useful for assessing diagnostic probability from causal probability:

$$P(Cause | Effect) = \frac{P(Effect | Cause)P(Cause)}{P(Effect)}$$

E.g., let M be meningitis, ${\cal S}$ be stiff neck:

$$P(m|s) = \frac{P(s|m)P(m)}{P(s)} = \frac{0.8 \times 0.0001}{0.1} = 0.0008$$

Note: posterior probability of meningitis still very small!

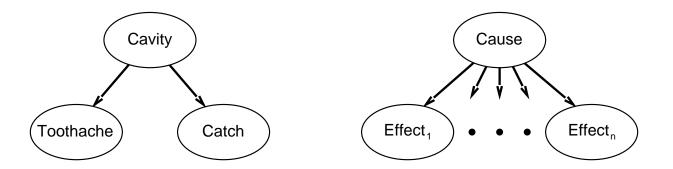
Bayes' Rule and conditional independence

 $\mathbf{P}(Cavity|toothache \wedge catch)$

- $= \alpha \mathbf{P}(toothache \wedge catch | Cavity) \mathbf{P}(Cavity)$
- $= \alpha \mathbf{P}(toothache|Cavity)\mathbf{P}(catch|Cavity)\mathbf{P}(Cavity)$

This is an example of a naive Bayes model:

 $\mathbf{P}(Cause, Effect_1, \dots, Effect_n) = \mathbf{P}(Cause)\Pi_i \mathbf{P}(Effect_i | Cause)$



Total number of parameters is **linear** in n

Summary

Probability is a rigorous formalism for uncertain knowledge Joint probability distribution specifies probability of every atomic event Queries can be answered by summing over atomic events For nontrivial domains, we must find a way to reduce the joint size Independence and conditional independence provide the tools