Machine Learning

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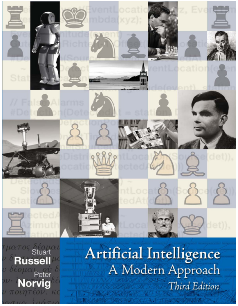
Chapter 1: Probabilities

- **Probability basics**
- **Some important probability distributions**
- **Bayes rule and conditional inference**
- **Origins of probabilities: Bayesian and frequentist interpretation**



Probabilities

Definition (Probability Space)

A probability space is the triple

$$(\Omega, S, P)$$

where

- Ω is the sample/outcome space, $\omega \in \Omega$ is a **sample point/atomic event**.
  Example: 6 possible rolls of a die: $\Omega = \{1, 2, 3, 4, 5, 6\}$
- S is a collection of **events** to which we are willing to assign probabilities. An **event** $a \in S$ is any subset of Ω, e.g., die roll < 4: $a = \{1, 2, 3\}$
- P is a mapping from events in S to $\mathbb{R}$ that satisfies the probability axioms.

Axioms of Probability

1. $P(a) \geq 0 \; \forall a \in S$: probabilities are not negative,
2. $P(\Omega) = 1$: "trivial" event has maximal possible prob 1,
3. $a, b \in S$ and $a \cap b = \{\,\} \Rightarrow P(a \cup b) = P(a) + P(b)$: probability of two mutually disjoint events is the sum of their probabilities.
   Example:
   $P(\text{die roll} < 4) = P(1) + P(2) + P(3) = 1/6 + 1/6 + 1/6 = 1/2.$

Random Variables

Definition (Random Variable)

A **random variable** X is a function from the sample points to some range, e.g., the reals

$$X : \Omega \to \mathbb{R},$$

or booleans $X : \Omega \to \{\text{true,false}\}.$

Real random variables are characterized by their distribution function.

Definition (Cumulative Distribution Function)

Let $X : \Omega \to \mathbb{R}$ be a real valued random variable. We define

$$F_X(x) = P(X \leq x).$$

This is the probability of the event $\{\omega \in \Omega : X(\omega) \leq x\}$

Boolean RVs and propositional logic

- Dentistry example: **Boolean** random variable (dental) *Cavity*
- Proposition: answer to question "do I have a cavity?"
  $\rightsquigarrow$ *Cavity* $=$ *true* **is a proposition, also written** *cavity*
- **Proposition**: event (=set of sample points / atomic events) where the **proposition is true.**
- Given Boolean random variables A and B:
  - event a = set of atomic events where $A(\omega) = \text{true}$
  - event $\neg a$ = set of atomic events where $A(\omega) = \text{false}$
  - event $a \wedge b$ = atomic events where $A(\omega) = \text{true}$ and $B(\omega) = \text{true}$
- With Boolean variables, **event = propositional logic model**
  e.g., $A = \text{true}$, $B = \text{false}$, or $a \wedge \neg b$.

Proposition = disjunction of events in which it is true
e.g., $(a \vee b) = (\neg a \wedge b) \vee (a \wedge \neg b) \vee (a \wedge b)$
$\Longrightarrow \; P(a \vee b) = P(\neg a \wedge b) + P(a \wedge \neg b) + P(a \wedge b)$

Syntax for Propositions

- **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., $Temp < 22.0$.

Probability distribution

- **Unconditional probabilities** of propositions
  e.g., $P(Weather = sunny) = 0.72$.
  Bayesian interpretation:
  Belief, prior to arrival of any (new) evidence
- **Probability distribution** gives values for all possible assignments:
  $P(Weather) = \langle 0.72, 0.1, 0.08, 0.1 \rangle$ (normalized, sums to 1)
- **Joint probability distribution** for a set of RVs gives the probability of every atomic event on those RVs:
  $P(Weather, Cavity) =$ a 4×2 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

Probability for continuous variables

Suppose X describes some uncertain continuous quantity.

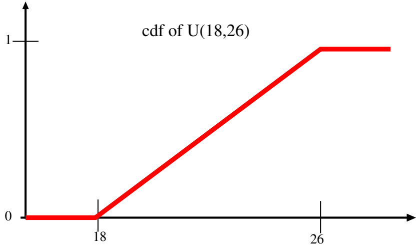
What is the probability of the event $a < X \leq b$?

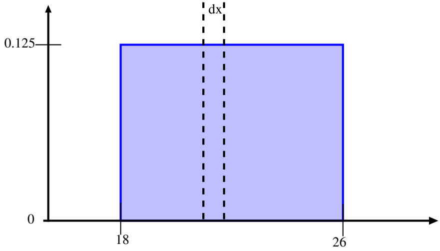
- define events $A = (X \leq a), B = (X \leq b), W = (a < X \leq b)$.
- $B = A \vee W$, A and W are **mutually exclusive**
  $\rightsquigarrow P(B) = P(A) + P(W) \rightsquigarrow P(W) = P(B) - P(A)$.
- Define the **cumulative distribution function (cdf)** as
  $F(q) := P(X \leq q)$: $P(W) = P(B) - P(A) = F(b) - F(a)$.
- Assume that F is absolutely continuous:
  define **probability density function (pdf) $p(x) := \frac{d}{dx}F(x)$.**
- Given a **pdf**, the probability of a continuous variable being **in a finite interval** is: $P(a < X \leq b) = \int_a^b p(x)\, dx$.
- As the size of the interval gets smaller, we can write
  $P(x < X \leq x + dx) \approx p(x)\, dx \;\Rightarrow\; p(x) \approx P(x < X \leq x + dx)/dx$.
  Finally: $p(x) = \lim_{dx \to 0} P(x < X \leq x + dx)/dx$.
- Note: $p(x) \geq 0$ and $\int_{-\infty}^{+\infty} p(x)\, dx = 1$, but $p(x) > 1$ is possible.

Probability for continuous variables

Example: uniform distribution:

$$\text{Unif}(a, b) = \frac{1}{b - a}\mathbb{I}(a \leq x \leq b).$$





$p(X = 20.5) = 0.125$ really means

$$\lim_{dx \to 0} P(20.5 < X \leq 20.5 + dx)/dx = 0.125$$

Mean and Variance

- Most familiar property of a distribution: **mean**, or **expected value**, denoted by μ or $E[X]$.
- Discrete RVs:
$$E[X] = \sum_{x \in \mathcal{X}} x p(x),$$
- Continuous RVs:
$$E[X] = \int_{\mathcal{X}} x p(x)\, dx.$$
If this integral is not finite, the mean is not defined.
- The **variance** is a measure of the **spread** of a distribution:
$$\begin{aligned}\mathrm{var}[X] =: \sigma^2 &= E[(X-\mu)^2] = E[X^2 - 2X\mu + \mu^2] \\ &= E[X^2] - 2\mu E[X] + \mu^2 = E[X^2] - 2\mu^2 + \mu^2 = E[X^2] - \mu^2\end{aligned}$$
- The square root $\sqrt{\mathrm{var}[X]}$ is the **standard deviation**.

Common continuous distributions: Normal

- The **pdf** of the **normal distribution** is

$$p(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}},$$

where μ is the **mean**, σ^2 is the **variance.**
The **inverse variance** is sometimes called **precision.**

- The **cdf** of the **standard normal distribution** is the integral

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-t^2/2}\, dt.$$

It has no closed form expression.

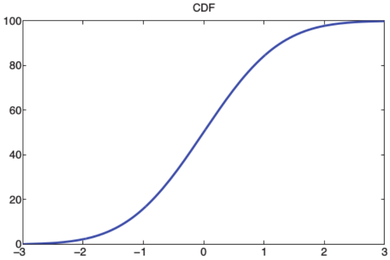
- The **cdf** is sometimes expressed in terms of the **error function**

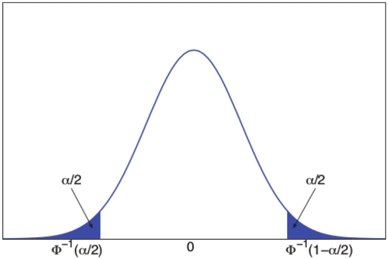
$$erf(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2}\, dt,$$

as follows:

$$\Phi(x) = \frac{1}{2}\left[1 + erf\left(\frac{x}{\sqrt{2}}\right)\right].$$

Probability for continuous variables





Left: **cdf** for the standard normal, $\mathcal{N}(0, 1)$. Right: corresponding **pdf.**

- Shaded regions each contain $\alpha/2$ of the probability mass
  $\rightsquigarrow$ nonshaded region contains $1 - \alpha$.
- Left cutoff point is $\Phi^{-1}(\alpha/2)$, Φ is cdf of standard Gaussian.
- By symmetry, the right cutoff point is $\Phi^{-1}(1 - \alpha/2) = -\Phi^{-1}(\alpha/2)$.
- If $\alpha = 0.05$, the central interval is 95%, left cutoff is -1.96, right cutoff is 1.96.

Common continuous distributions: Normal

- If σ tends to zero, $p(x)$ tends to zero at any $x \neq \mu$, but grows without limit if $x = \mu$, while its integral remains equal to 1.
- Can be defined as a generalized function: **Dirac's delta function δ** translated by the mean: $p(x) = \delta(x - \mu)$, where

$$\delta(x) = \begin{cases} +\infty, & x = 0 \\ 0, & x \neq 0, \end{cases}$$

  additionally constrained to satisfy the identity

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

- **Sifting property:** selecting out a single term from an integral:

$$\int_{-\infty}^{\infty} f(x)\delta(x - z)\, dx = f(z)$$

  since the integrand is only non-zero if $x - z = 0$.

Central Limit Theorem

- Under certain (fairly common) conditions, the **sum of many RVs** will have an **approximately normal distribution.**
- Let $X_1, \ldots, X_n$ be i.i.d. RVs with the same (arbitrary) distribution, zero mean, and variance σ^2.
- Let
$$Z = \sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right)$$
- Then, as n increases, the probability distribution of Z will tend to the **normal distribution** with zero mean and variance σ^2.

Conditional probability

- **Conditional** probabilities
  e.g., $P(cavity|toothache) = 0.8$
  "Prob. of cavity is 80%, **given that** *toothache* **is all I know**"
  NOT "if *toothache* then 80% chance of *cavity*"
- Notation for conditional distributions:
  $P(Cavity|Toothache)$ = 2-element vector of 2-elem. vectors.
- 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**:
  $P(cavity|toothache, die\ roll = 3) = P(cavity|toothache) = 0.8$

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.,
$P(Weather, Cavity) = P(Weather|Cavity)P(Cavity)$
- **Chain rule** is derived by successive application of product rule:
$$\begin{aligned} & P(X_1, \dots, X_n) = P(X_1, \dots, X_{n-1})\ P(X_n|X_1, \dots, X_{n-1}) \\ = & P(X_1, \dots, X_{n-2})\ P(X_{n-1}|X_1, \dots, X_{n-2})\ P(X_n|X_1, \dots, X_{n-1}) \\ = & \dots \\ = & \prod_{i=1}^n P(X_i|X_1, \dots, X_{i-1}) \end{aligned}$$

Bayes Rule

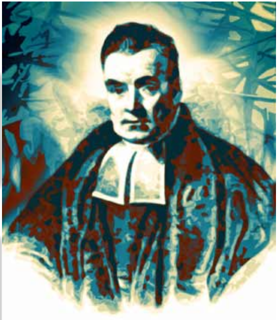
Bayes Rule

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

Proof.

$$P(A|B)P(B) = P(A,B) = P(B|A)P(A)$$

□



Thomas Bayes (1701 - 1761)

Bayes Rule (cont'd)

- Useful for assessing **diagnostic** probability from **causal** probability:

$$P(Cause|Effect) = \frac{\overbrace{P(Effect|Cause)}^{\text{Prob(symptoms)}}\overbrace{P(Cause)}^{\text{Prevalence}}}{P(Effect)}$$

- E.g., let M **be meningitis** (acute inflammation of the protective membranes covering the brain and spinal cord), S **be stiff neck**. Assume the doctor knows that the **prevalence of meningitis** is $P(m) = 1/50000$, that the **prior probability of a stiff neck** is $p(s) = 0.01$, and that the **symptom stiff neck** occurs with a probability of 0.7.

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

- Note: the posterior probability of meningitis is still very small (1 in 700 patients)!

Bayes rule (cont'd)

Question: Why should it be easier to estimate the conditional probabilities in the causal direction $P(Effect|Cause)$, as compared to the diagnostic direction, $P(Cause|Effect)$?

There are two possible answers (in a medical setting):

- We might have access to a **collection of health records** for patients having meningitis $\rightsquigarrow$ we can estimate $P(s|m)$.
  For directly estimating $P(m|s)$ we would need a database of all cases of the **very unspecific symptom**.
- Diagnostic knowledge might be **more fragile** than causal knowledge.
  - Assume a doctor has directly estimated $P(m|s)$.
    Sudden epidemic $\rightsquigarrow$ $P(m)$ will go up...but how to update $P(m|s)$??
  - Other doctor uses Bayes rule, he knows that $P(m|s) \propto p(s|m)p(m)$ should go up proportionately with $p(m)$.
    Note that causal information $P(s|m)$ is **unaffected by the epidemic** (it simply reflects the way how meningitis works)!

Origins of probabilities

Historically speaking, probabilities have been regarded in a number of different ways:

- **Frequentist position:** probabilities come from **measurements**.
  - The assertion $P(cavity) = 0.05$ means that 0.05 is the fraction that would be observed in the limit of infinitely many samples.
  - From a finite sample, we can estimate this true fraction and also the accuracy of this estimate.
- **Objectivist view:** probabilities are actual **properties of the universe**
  - An excellent example: quantum phenomena.
  - A less clear example: coin flipping – the uncertainty is probably due to our uncertainty about the initial conditions of the coin.

Origins of probabilities

- **Subjectivist view**: probabilities are an **agent's degrees of belief**, rather than having any external physical significance.
- The **Bayesian view** allows any self-consistent ascription of prior probabilities to propositions, but then insists on proper **Bayesian updating** as evidence arrives.
  For example $P(cavity) = 0.05$ denotes the degree of belief that a random person has a cavity **before we make any actual observation** of that person.
  Updating in the light of **further evidence** "person has a *toothache*":

$$P(cavity|toothache) = \alpha\, P(toothache|cavity)P(cavity)$$

The reference class problem

- Bayesian viewpoint is often criticized because of the use of subjective believes...
  ...**but even a strict frequentist position involves subjective analysis!**
- **Example:** Say a doctor takes a frequentist approach to diagnosis. She examines a large number of people to establish the probability of whether or not they have heart disease.
- To be accurate she tries to measure "similar people" (she knows for example that gender might be important) $\rightsquigarrow$ "reference class".
- ...but probably other variables might also be important...
- Taken to an extreme, all people are different
  $\rightsquigarrow$ **reference class is empty**.
- Some subjective assumptions must be involved in the design of nonempty reference classes...a tricky problem in the philosophy of science.

Frequentist and Bayesian view: a simple example

- Assume $x_1, \dots, x_n$ are drawn i.i.d. from normal $\mathcal{N}(\mu, \sigma^2)$ with known variance σ^2. What can be said about μ?
- Frequentist view: no further probabilistic assumptions
  $\rightsquigarrow$ **treat μ as an unknown constant**.
- **Theorem:** Let X and Y be independent normal RVs, then their sum is also normally distributed. i.e., if

  $$X \sim \mathcal{N}(\mu_X, \sigma_X^2), \quad Y \sim \mathcal{N}(\mu_Y, \sigma_Y^2)$$
  $$Z = X + Y, \text{ then } Z \sim \mathcal{N}(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2).$$

- **Theorem:** If $y = c + bx$ is an **affine transformation** of $X \sim \mathcal{N}(\mu, \sigma^2)$, then $Y \sim \mathcal{N}\left(c + b\mu, b^2\sigma^2\right)$
- The **sample mean** $\bar{x} = \sum_i x_i / n$ is the observed value of the RV $\bar{X} \sim \mathcal{N}(\mu, \bar{\sigma}^2), \quad \text{with } \bar{\sigma}^2 = n\sigma^2/n^2 = \sigma^2/n.$

Frequentist and Bayesian view: a simple example

- Now define the **transformed random variable**

$$B := \frac{\mu - \bar{X}}{\bar{\sigma}} \sim \mathcal{N}(0,1), \text{ (i.e. standard normal).}$$

- Use normal cdf $\Phi(k_c) = P(B < k_c)$ to derive an **upper limit for μ:**

$$\begin{aligned} P(B < k_c) &= \Phi(k_c) = 1 - c \\ &= P(-\bar{\sigma} B > -\bar{\sigma} k_c) \\ &= P(\underbrace{\mu - \bar{\sigma} B}_{\bar{X}} > \mu - \bar{\sigma} k_c) \\ &= P(\bar{X} + \bar{\sigma} k_c > \mu). \\ \Rightarrow \quad P(\mu < \bar{X} + \bar{\sigma} k_c) &= 1 - c \end{aligned}$$

- Define $B' = -B \rightsquigarrow$ **lower limit.**

Frequentist and Bayesian view: a simple example

- The statement $P(\mu < \bar{X} + \bar{\sigma} k_c) = 1 - c$ can be interpreted as specifying a **hypothetical long run of statements** about the **constant μ, a portion $1 - c$ of which is correct.**
- Note that $\bar{X}$ is a RV that takes **one specific value** $\bar{x}$ for one dataset of n observations $\{x_1, \ldots, x_n\}$.
- For the **actually observed** $\bar{x}$, the statement $\mu < \bar{x} + \bar{\sigma} k_c$ can be interpreted as **one** of a long run of such statements about μ.
- Arguments involving probability **only via its (hypothetical) long-run frequency interpretation** are called **frequentist.**
- In the frequentist world we define procedures for assessing evidence that are calibrated by how they would perform **were they used repeatedly.**

Frequentist and Bayesian view: a simple example

- From the Bayesian viewpoint, we treat μ as having a probability distribution **both with and without the data:**
  $\rightsquigarrow$ **treat μ as a random variable.**
- Bayes' theorem: $p(\mu|\bar{x}) \propto p(\bar{x}|\mu)p(\mu)$.
- Intuitive idea:
  - all relevant information about μ is in the conditional distribution, given the data;
  - this distribution is determined by the elementary formulae of probability theory;
  - remaining problems are solely computational.
- Example: choose $p(\mu) = \mathcal{N}(m, \nu^2) \rightsquigarrow p(\mu|x) = \mathcal{N}(\tilde{m}, \tilde{\nu}^2)$ with

$$\tilde{m} = \frac{\bar{x}/\bar{\sigma}^2 + m/\nu^2}{1/\bar{\sigma}^2 + 1/\nu^2}, \quad \tilde{\nu}^2 = \frac{1}{1/\bar{\sigma}^2 + 1/\nu^2}$$

"Normal likelihood times normal prior gives normal posterior"

Frequentist and Bayesian view: a simple example

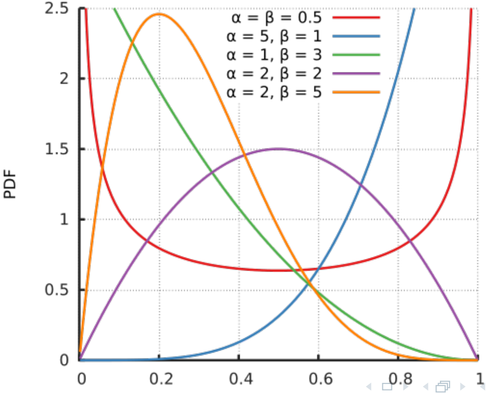
- Same reasoning as before: define transformed $\tilde{B} := \frac{\mu - \tilde{m}}{\tilde{\nu}} \sim \mathcal{N}(0,1)$
- Upper limit for μ: $P(\mu < \tilde{m} + k_c \tilde{\nu}) = 1 - c$.
- If the **prior variance** $\nu^2 \gg \bar{\sigma}^2$ and the **prior mean** m **is not too different from** $\bar{X}$, **this limit agrees closely with the one obtained by the frequentist method** (because then $\tilde{m} \approx \bar{x}$ and $\tilde{\nu} \approx \bar{\sigma}$).
- Note that this approximation becomes exact in the limit as $n \to \infty$, since then $\bar{\sigma}^2 = \sigma^2/n \to 0$.
- This broad parallel is in no way specific to the normal distribution (mainly due to the **central limit theorem**).
- **Warning:** there **are** situations in which there are fundamental differences!
- See the discussion of the "likelihood principle" in `https://en.wikipedia.org/wiki/Likelihood_principle`, or the paper "The Interplay of Bayesian and Frequentist Analysis" by M. J. Bayarri and J. O. Berger, or the book (D.R. Cox, Principles of statistical inference, Cambridge, 2006).

Common continuous distributions: Beta

- The beta distribution is supported on the unit interval $[0, 1]$
- For $0 \leq x \leq 1$, and shape parameters $\alpha, \beta > 0$, the pdf is

$$p(x|\alpha, \beta) = \frac{1}{\mathrm{B}(\alpha, \beta)} x^{\alpha-1}(1-x)^{\beta-1}.$$

The **beta function**, B, is a normalization constant to ensure that the total probability is 1. Note: $\mu[\text{Beta}(\alpha, \beta)] = \frac{\alpha}{\alpha+\beta}$



Common continuous distributions: Multivariate Normal

- The multivariate normal distribution of a k-dimensional random vector $\boldsymbol{X} = (X_1, \ldots, X_k)^t$ can be written as: $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$, with k-dimensional **mean vector**

$$\boldsymbol{\mu} = \mathrm{E}[\mathbf{X}] = [\mathrm{E}[X_1], \mathrm{E}[X_2], \ldots, \mathrm{E}[X_k]]^{\mathrm{t}}$$

  and $k \times k$ **covariance matrix**

$$\Sigma =: \mathrm{E}[(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^{\mathrm{t}}] = [\mathrm{Cov}[X_i, X_j]; 1 \leq i, j \leq k],$$

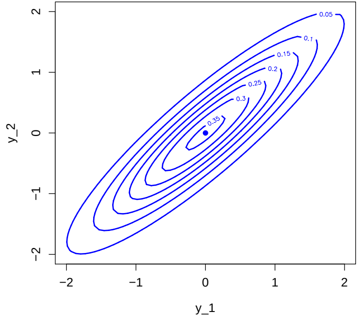
  where

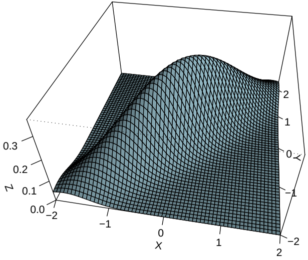
$$\mathrm{Cov}[X_i, X_j] = \mathrm{E}[(X_i - \mu_i)(X_j - \mu_j)].$$

- The inverse of the covariance matrix is called **precision matrix**
- The pdf of the multivariate normal distribution is

$$p(x_1, \ldots, x_k | \boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{(2\pi)^k |\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^{\mathrm{t}} \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

The multivariate Normal distribution





Affine transformations:
If $\mathbf{Y} = \boldsymbol{c} + B\mathbf{X}$ is an affine transformation of $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$, then $\mathbf{Y} \sim \mathcal{N}\left(\boldsymbol{c} + B\boldsymbol{\mu}, B\Sigma B^{\mathrm{t}}\right)$. Why?

$$\boldsymbol{\mu}_{\mathbf{Y}} = \mathrm{E}[\boldsymbol{c} + B\mathbf{X}] = \boldsymbol{c} + B\,\mathrm{E}[\mathbf{X}] = \boldsymbol{c} + B\boldsymbol{\mu}$$

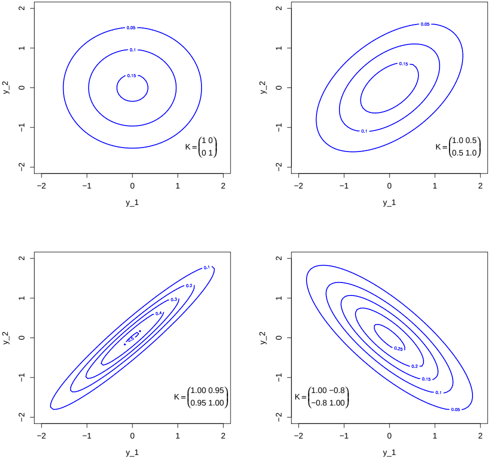
$$\Sigma_{\mathbf{Y}} = \mathrm{E}[(\boldsymbol{c} + B\mathbf{X} - \boldsymbol{c} + B\boldsymbol{\mu})(\boldsymbol{c} + B\mathbf{X} - \boldsymbol{c} + B\boldsymbol{\mu})^t]$$
$$= \mathrm{E}[B(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^t B^t] = B\Sigma B^t$$

The multivariate normal distribution

2D Gaussian: $p(\boldsymbol{x}|\boldsymbol{\mu}=\mathbf{0},\Sigma)=\frac{1}{\sqrt{2\pi|\Sigma|}}\exp(-\frac{1}{2}\boldsymbol{x}^t\Sigma^{-1}\boldsymbol{x})$

Covariance
(also written "co-variance")
is a measure of how much **two random variables vary together**:

- **positive**: positive linear coherence,
- **negative**: negative linear coherence,
- **0**: no linear coherence.



Common continuous distributions: Dirichlet

- The Dirichlet distribution of order $K \geq 2$ with parameters $\alpha_1, \ldots, \alpha_K > 0$ is a multivariate generalization of the beta distribution.
- Its pdf on $\mathbb{R}^{K-1}$ is

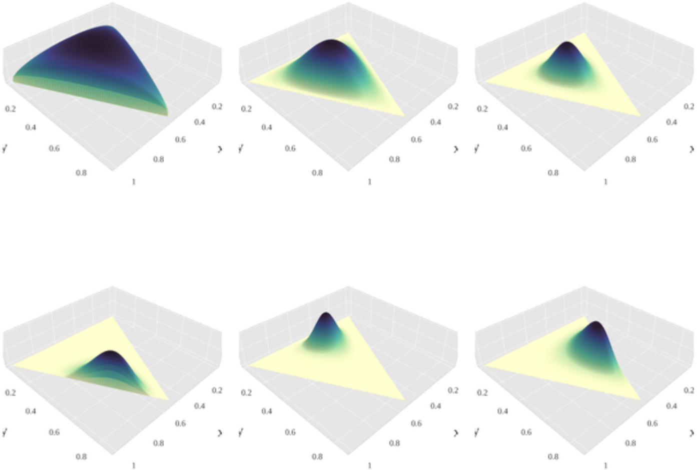
$$p(x_1, \ldots, x_K | \alpha_1, \ldots, \alpha_K) = \frac{1}{\mathrm{B}(\boldsymbol{\alpha})} \prod_{i=1}^{K} x_i^{\alpha_i - 1},$$

  where $\{x_i\}_{i=1}^{K}$ belong to the standard $K-1$ simplex:

$$\sum_{i=1}^{K} x_i = 1 \text{ and } x_i \geq 0$$

- The normalizing constant is the **multivariate beta function.**
- The mean is $E[X_i] = \frac{a_i}{\sum_k (a_k)}$.

Common continuous distributions: Dirichlet



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Common discrete distributions: Binomial and Bernoulli

- Toss a coin n times. Let $X \in \{0, 1, \ldots, n\}$ be the number of heads.
- If the probability of heads is θ, then we say the RV X has a **binomial distribution**, $X \sim \text{Bin}(n, \theta)$:

$$\text{Bin}(X = k | n, \theta) = \binom{n}{k} \theta^{k} (1 - \theta)^{n-k}.$$

- Special case for $n = 1$: **Bernoulli distribution.**
  Let $X \in \{0, 1\} \rightsquigarrow$ binary random variable.
  Let θ be the probability of **success**. We write $X \sim \text{Ber}(\theta)$.

$$\text{Ber}(x | \theta) = \theta^{\mathbb{I}(x=1)} (1 - \theta)^{\mathbb{I}(x=0)};$$

where $\mathbb{I}(x)$ is the indicator function of a binary x:

$$\text{Ber}(x|\theta) = \begin{cases} \theta, & \text{if } x = 1 \\ 1 - \theta, & \text{if } x = 0. \end{cases}$$

Common discrete distributions: Multinomial

- Tossing a K-sided die $\rightsquigarrow$ can use the **multinomial distribution**.
- Let $\boldsymbol{X} = (X_1, X_2, \dots X_K)$ be a **random vector**.
  Let x_j be the number of times side j of the die occurs.

$$\mathrm{Mu}(\boldsymbol{x}|n, \boldsymbol{\theta}) = \binom{n}{x_1 \cdots x_K} \prod_{j=1}^{K} \theta_j^{x_j},$$

  where θ_j is the probability that side j shows up, and

$$\binom{n}{x_1 \cdots x_K} = \frac{n!}{x_1! x_2! \cdots x_K!}$$

  is the **multinomial coefficient** (the number of ways to divide a set of size $n = \sum_{k=1}^{K} x_k$ into subsets with sizes x_1 up to x_K).

Common discrete distributions: Multinoulli

- Special case for $n = 1$: **Mutinoulli distribution.**
- Rolling a K-sided dice once, so $\boldsymbol{x}$ will be a vector of 0s and 1s, in which only one bit can be turned on.
- If the dice shows up as face k, then the k'th bit will be on $\rightsquigarrow$ think of x as being a scalar categorical random variable with K states, and $\boldsymbol{x}$ is its **dummy encoding**.
- Example: $K = 3$, encode the states 1, 2 and 3 as $(1, 0, 0), (0, 1, 0)$, and $(0, 0, 1)$.
- Also called a **one-hot encoding**, since we imagine that only one of the K "wires" is "hot" or on.

$$\mathrm{Mu}(\boldsymbol{x}|1, \boldsymbol{\theta}) = \prod_{j=1}^{K} \theta_j^{\mathbb{I}(x_j=1)}.$$

Empirical distribution

- Suppose that we perform N identical random experiments for fixed P
- We observe $\mathcal{D} = \{x_1, \dots, x_N\}$.
- Compute frequency of occurrences of event A:

$$\epsilon_N(A) = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i}(A), \qquad \delta_x(A) = \begin{cases} 0, & \text{if } x \notin A \\ 1, & \text{if } x \in A \end{cases}$$

$\Rightarrow \epsilon_N(A) =$ **fraction of experiments in which event A occurs.**

Example: **Event $A =$ die roll < 4**, we observed
$\mathcal{D} = \{4, \mathbf{2}, 5, 6, 4, \mathbf{3}, 5\} \Rightarrow \epsilon_N(A) = 2/7$.

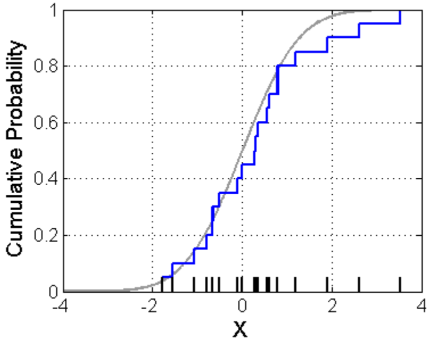
- Given dataset $\mathcal{D}$ of size N, define the **empirical distribution** as $p_{emp}(A) = \epsilon_N(A)$.
- $p_{emp}(A)$ assigns 0 probability to any point not in the data set $\rightsquigarrow$ essentially a discrete probability, even if sample space is not discrete.
- Can think of this as a histogram, with "spikes" at the data points x_i.

Empirical CDF

Let our sample $\mathcal{D} = \{x_1, \ldots, x_N\}$ be a collection of independent, identically distributed (iid) random data points with common cdf $F(t)$. Then the empirical distribution function is defined as

$$\hat{F}_N(t) = \frac{\#(\text{elements in the sample} \le t)}{N} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}\{x_i \le t\},$$

where $\mathbb{I}\{A\}$ is the indicator of event A.



Discrete distributions: Inference by enumeration

Start with the joint distribution:

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

For any proposition ϕ, sum the atomic events where it is true:
$P(toothache) = 0.108 + 0.012 + 0.016 + 0.064 = 0.2$

Inference by enumeration

Start with the joint distribution:

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

For any proposition ϕ, sum the atomic events where it is true:
$P(cavity \vee toothache) = 0.108 + 0.012 + 0.072 + 0.008 + 0.016 + 0.064 = 0.28$

Inference by enumeration

Start with the joint distribution:

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

Denominator can be viewed as a **normalization constant** α

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

$$= \alpha\,[\mathbf{P}(Cavity, toothache, catch) + \mathbf{P}(Cavity, toothache, \neg catch)]$$

$$= \alpha\,[\langle 0.108, 0.016\rangle + \langle 0.012, 0.064\rangle]$$

$$= \alpha\,\langle 0.12, 0.08\rangle = \langle 0.6, 0.4\rangle$$

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**:

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

Joint probability $p(x) = p(x_1, \ldots, x_n) \rightsquigarrow$ number of states: $\prod_{i=1}^{n} |arity(x_i)|$.

Obvious problems:

1) Worst-case time complexity $O(d^n)$ where d is the largest arity

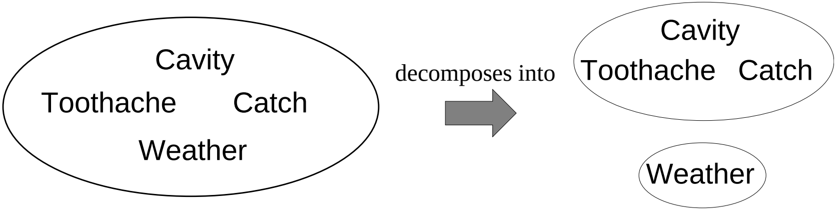
2) Space complexity $O(d^n)$ to store the joint distribution

3) How to find the numbers for $O(d^n)$ entries???

Independence

A and B are **independent** iff

$\mathbf{P}(A|B) = \mathbf{P}(A)$ or $\mathbf{P}(B|A) = \mathbf{P}(B)$ or $\mathbf{P}(A, B) = \mathbf{P}(A)\mathbf{P}(B)$



$\mathbf{P}(Toothache, Catch, Cavity, Weather)$
$= \mathbf{P}(Toothache, Catch, Cavity)\mathbf{P}(Weather)$
$\rightsquigarrow 4 \cdot 8 = 32$ entries reduced to $4 + 8 = 12$.

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) $P(catch|toothache, \neg cavity) = P(catch|\neg cavity)$

Catch is **conditionally independent** of *Toothache* given *Cavity*:

$\mathbf{P}(Catch|Toothache, Cavity) = \mathbf{P}(Catch|Cavity)$

Equivalent statements:

$\mathbf{P}(Toothache|Catch, Cavity) = \mathbf{P}(Toothache|Cavity)$

$\mathbf{P}(Toothache, Catch|Cavity) = \mathbf{P}(Toothache|Cavity)\mathbf{P}(Catch|Cavity)$

Conditional independence, contd.

Write out full joint distribution using chain rule:

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

$= \mathbf{P}(Toothache|Catch, Cavity)\mathbf{P}(Catch, Cavity)$

$= \mathbf{P}(Toothache|Catch, Cavity)\mathbf{P}(Catch|Cavity)\mathbf{P}(Cavity)$

$= \mathbf{P}(Toothache|Cavity)\mathbf{P}(Catch|Cavity)\mathbf{P}(Cavity)$

I.e., only $2 + 2 + 1 = 5$ independent numbers.

Sometimes, 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 and conditional independence

$$\begin{aligned} &P(Cavity|toothache \wedge catch) \\ &= \alpha\, P(toothache \wedge catch|Cavity)P(Cavity) \\ &= \alpha\, P(toothache|Cavity)P(catch|Cavity)P(Cavity) \end{aligned}$$

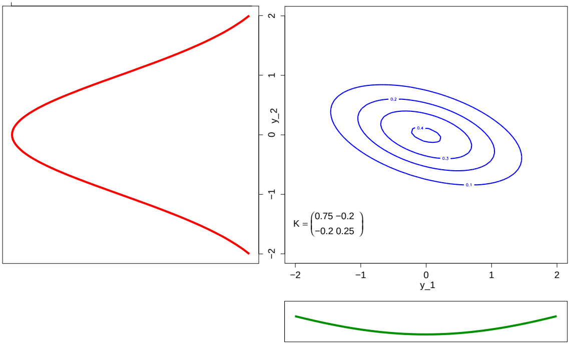
This is an example of a **naive Bayes** model:

$$P(Cause, Effect_1, \ldots, Effect_n) = P(Cause)\prod_i P(Effect_i|Cause)$$

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

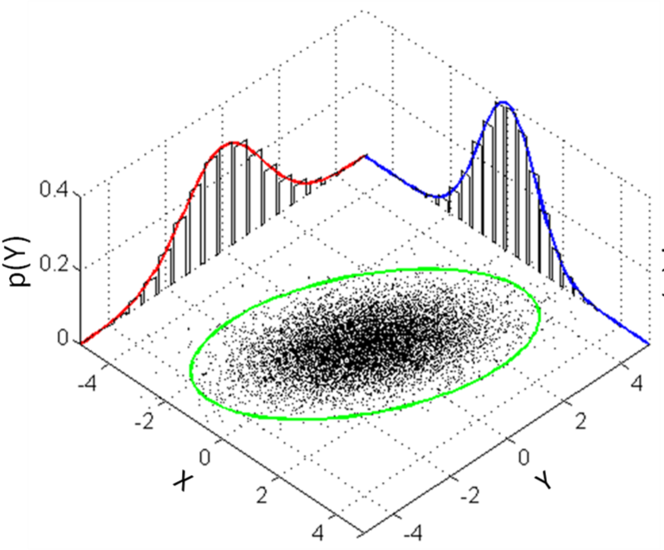
Inference in Jointly Gaussian Distributions: Marginalization

$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$. Let $\boldsymbol{x} = \begin{pmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{pmatrix}$ and $\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$.
Then $\boldsymbol{x}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \Sigma_{11})$ and $\boldsymbol{x}_2 \sim \mathcal{N}(\boldsymbol{\mu}_2, \Sigma_{22})$.



Marginals of Gaussians are again Gaussian!

Inference in Jointly Gaussian Distributions



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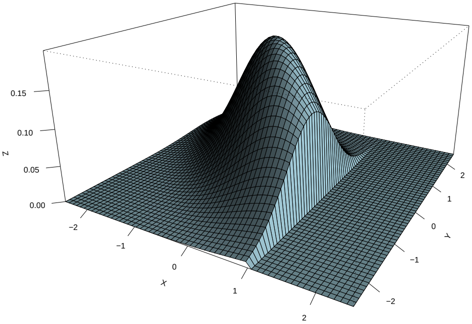
Inference in Jointly Gaussian Distributions

$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$. Let $\boldsymbol{x} = \begin{pmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{pmatrix}$ and $\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$.

Then $\boldsymbol{x}_2 | \boldsymbol{x}_1 \sim \mathcal{N}(\boldsymbol{\mu}_2 + \Sigma_{21}\Sigma_{11}^{-1}(\boldsymbol{x}_1 - \boldsymbol{\mu}_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})$.



Conditionals of Gaussians are again Gaussian!