Machine Learning

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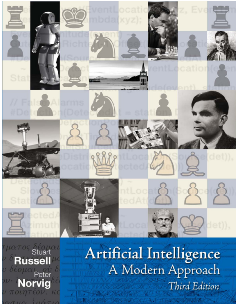
Chapter 1: Probabilities

- **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 $\quad X : \Omega \to \{\text{true,false}\}.$

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 $\{\omega \in \Omega : X(\omega) \leq x\}$

Boolen 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 $A(\omega) =$ true
  - event $\neg a$ = set of atomic events where $A(\omega) =$ false
  - event $a \wedge b$ = atomic events where $A(\omega) =$ true and $B(\omega) =$ true
- With Boolean variables, **event = propositional logic model**
  e.g., $A =$ true, $B =$ 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:
  $\mathbf{P}(Weather) = \langle 0.72, 0.1, 0.08, 0.1 \rangle$ (normalized, sums to 1)
- **Joint probability distribution** for a set of RVs gives the probability of every atomic event on those RVs:
  $\mathbf{P}(Weather, Cavity) =$ 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

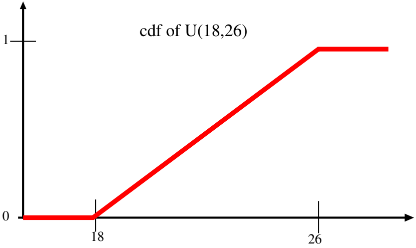
Suppose X describes some uncertain continuous quantity.
What is the probability that $a < X \leq b$?

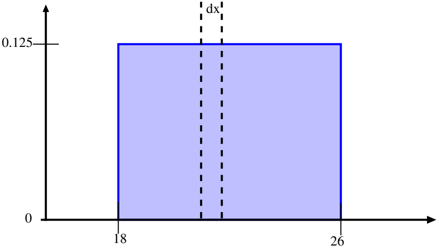
- define events $A = (X \leq a), B = (X \leq b), W = (a < X \leq b)$.
- $B = A \vee W$, A and W are **mutually exclusive**
  $\rightsquigarrow P(B) = P(A) + P(W) \rightsquigarrow P(W) = P(B) - P(A)$.
- Define the **cumulative distribution function (cdf)** as
  $F(q) := P(X \leq q)$: $P(W) = P(B) - P(A) = F(b) - F(a)$.
- 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
  $P(x < X \leq x + dx) \approx p(x)\, dx$.
- We require $p(x) \geq 0$, but it is possible for $p(x) > 1$, so long as the density integrates to 1.

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

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

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:
$$\begin{aligned} \text{var}[X] =: \sigma^2 &= E[(X-\mu)^2] = E[X^2 - 2X\mu + \mu^2] \\ &= E[X^2] - 2\mu E[X] + \mu^2 = E[X^2] - 2\mu^2 + \mu^2 = E[X^2] - \mu^2 \end{aligned}$$
- The square root $\sqrt{\text{var}[X]}$ is the **standard deviation**.

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 $\boldsymbol{X} = (X_1, X_2, \ldots X_K)$ 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.

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

Common discrete distributions: Empirical

- Given a set of data, $\mathcal{D} = \{x_1, \ldots, x_N\}$, define the **empirical distribution**, a.k.a. **empirical measure**:

$$p_{emp}(A) = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i}(A),$$

where

$$\delta_x(A) = \begin{cases} 0, & \text{if } x \notin A \\ 1, & \text{if } x \in A \end{cases}$$

- In general, we can associate **weights** with each sample:

$$p(x) = \sum_{i=1}^{N} w_i \delta_{x_i}(x)$$

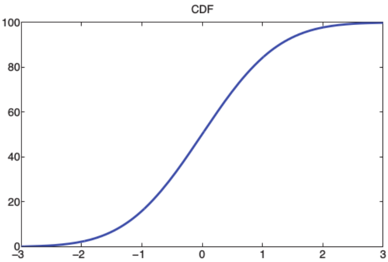
where we require $0 \leq w_i \leq 1$ and $\sum_{i=1}^{N} w_i = 1$.

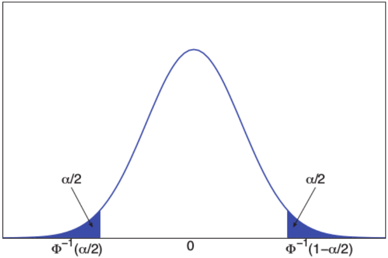
- We can think of this as a histogram, with "spikes" at the data points x_i, where w_i determines the height of spike i.
- This distribution assigns 0 probability to any point not in the data set.

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 a sum or integral:

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

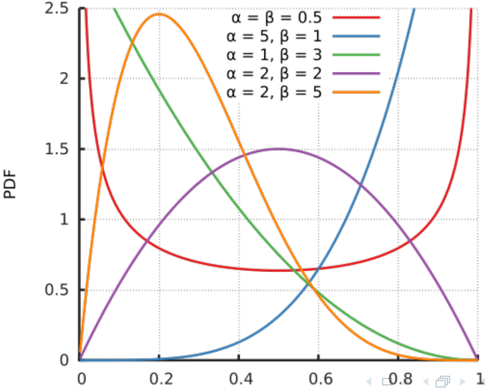
  since the integrand is only non-zero if $x - z = 0$.

Central Limit Theorem

- Under certain (fairly common) conditions, the sum of many random variables 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.

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

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

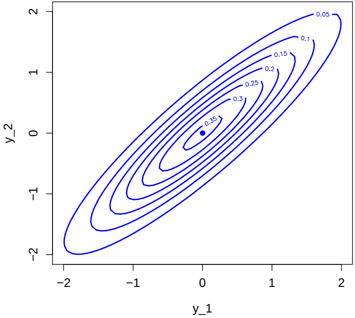
  where

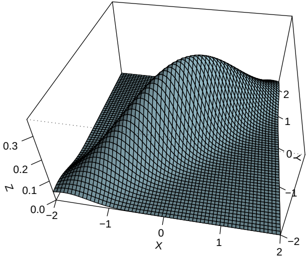
$$\mathrm{Cov}[X_i, X_j] = \mathrm{E}[(X_i - \mu_i)(X_j - \mu_j)].$$

- The inverse of the covariance matrix is the precision matrix $Q = \Sigma^{-1}$.
- 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 2D Normal distribution





Affine transformations:

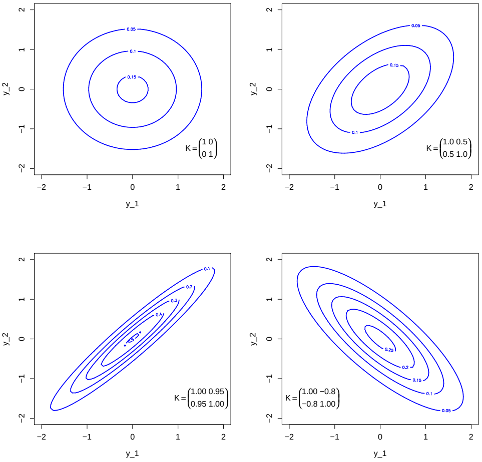
If $\boldsymbol{y} = \boldsymbol{c} + B\boldsymbol{x}$ is an affine transformation of $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$, then $\mathbf{Y} \sim \mathcal{N}\left(\boldsymbol{c} + B\boldsymbol{\mu}, B\Sigma B^{\mathrm{t}}\right)$

The 2D Gaussian distribution

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

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

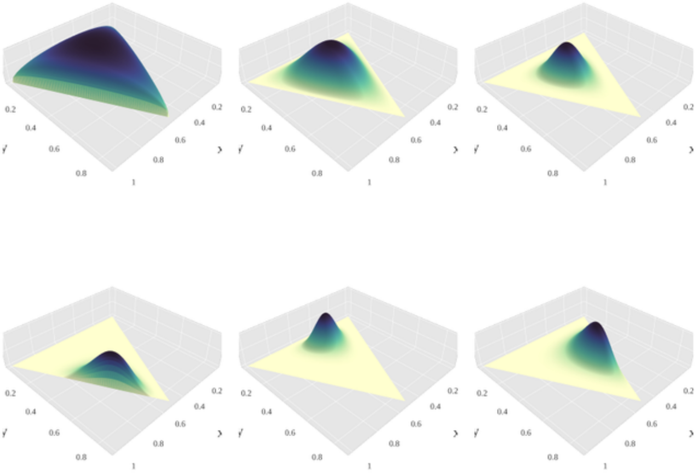
$$p(x_1, \ldots, x_K | \alpha_1, \ldots, \alpha_K) = \frac{1}{\mathrm{B}(\boldsymbol{\alpha})} \prod_{i=1}^{K} x_i^{\alpha_i - 1},$$

  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.
- Tne mean is $E[X_i] = \frac{a_i}{\sum_k (a_k)}$.

Common continuous distributions: Dirichlet



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Conditional probability

- **Conditional** probabilities
  e.g., $P(cavity|toothache) = 0.8$
  i.e., **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:
$$\begin{aligned} & P(X_1, \ldots, X_n) = P(X_1, \ldots, X_{n-1})\ P(X_n|X_1, \ldots, X_{n-1}) \\ &= P(X_1, \ldots, X_{n-2})\ P(X_{n-1}|X_1, \ldots, X_{n-2})\ P(X_n|X_1, \ldots, X_{n-1}) \\ &= \ldots \\ &= \prod_{i=1}^{n} P(X_i|X_1, \ldots, X_{i-1}) \end{aligned}$$

Inference by enumeration

Start with the joint distribution:

	toothache		¬ *toothache*	
	catch	¬ *catch*	*catch*	¬ *catch*
cavity	**.108**	**.012**	**.072**	**.008**
¬ *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		¬ *toothache*	
	catch	¬ *catch*	*catch*	¬ *catch*
cavity	**.108**	**.012**	**.072**	**.008**
¬ *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:

$$P(\neg cavity | toothache) = \frac{P(\neg cavity \wedge toothache)}{P(toothache)}$$

$$= \frac{0.016 + 0.064}{0.108 + 0.012 + 0.016 + 0.064} = 0.4$$

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: $\prod_{i=1}^{n} |arity(x_i)|$.

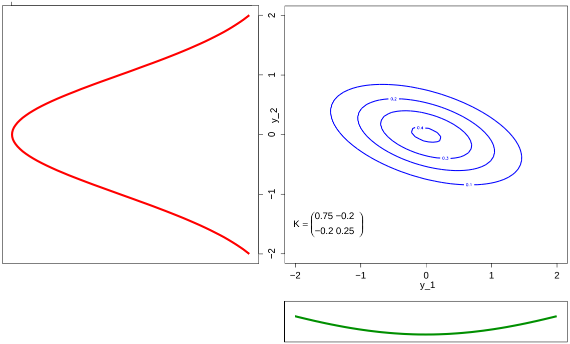
Obvious problems:

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???

Inference in Jointly Gaussian Distributions: Marginalization

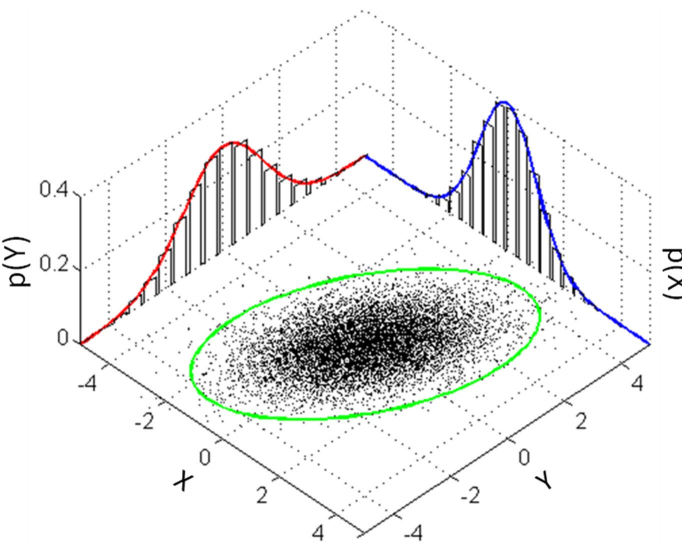
$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$. Let $\boldsymbol{x} = \begin{pmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{pmatrix}$ and $\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$.

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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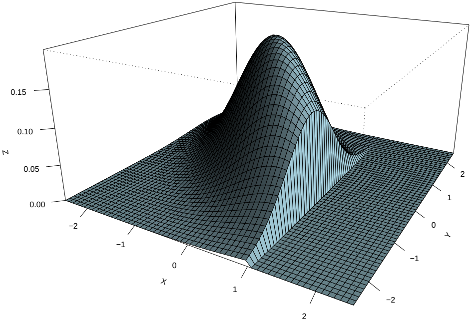
Inference in Jointly Gaussian Distributions

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

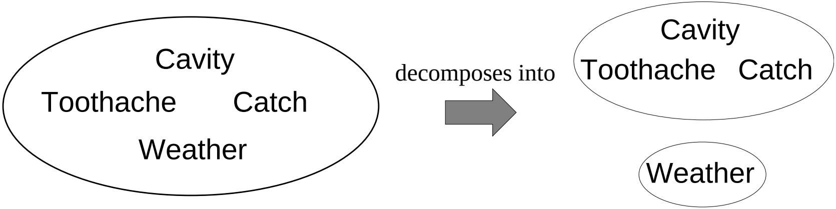


Conditionals of Gaussians are again Gaussian!

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.

Often, 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

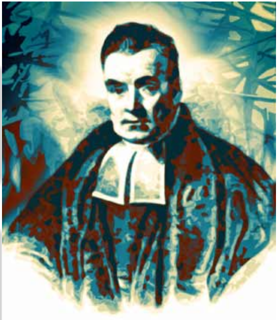
Bayes Rule

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

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 $P(\mathit{Effect}|\mathit{Cause})$, as compared to the diagnostic direction, $P(\mathit{Cause}|\mathit{Effect})$?
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)!

Bayes' Rule and conditional independence

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

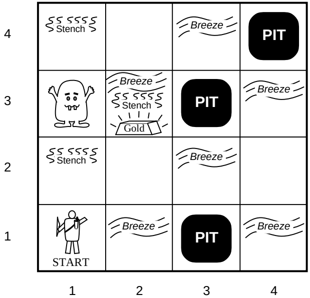
This is an example of a **naive Bayes** model:

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

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

Example: Wumpus World

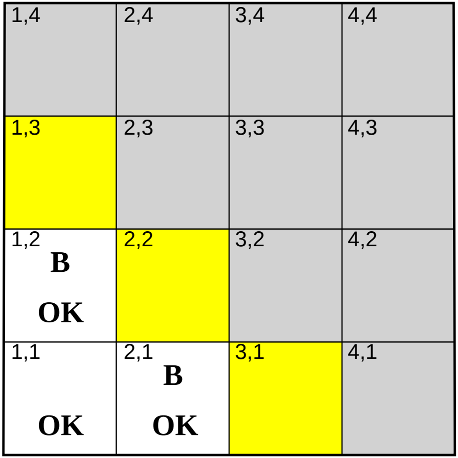
- The **wumpus** is a beast that eats anyone who enters the room.
- Some rooms contain bottomless **pits** that will trap anyone entering the room (except for the wumpus, which is too big to fall in!)
- The only positive aspect is the possibility of finding **gold**...



Squares adjacent to wumpus are **smelly**.
Squares adjacent to pit are **breezy**.
Glitter if and only if gold is in the same square.
Shooting kills the wumpus if you are facing it.
Shooting uses up the only **arrow**.
Grabbing picks up the gold if in the same square.
Releasing drops the gold in the same square.

Goal: Get gold back to start without entering pit or wumpus square

Wumpus World



$P_{ij} = true$ iff $[i, j]$ contains a pit
$B_{ij} = true$ iff $[i, j]$ is breezy
Include only $B_{1,1}, B_{1,2}, B_{2,1}$ in the probability model

Specifying the probability model

The full joint distribution is $\mathbf{P}(P_{1,1}, \ldots, P_{4,4}, B_{1,1}, B_{1,2}, B_{2,1})$
Apply product rule: $\mathbf{P}(B_{1,1}, B_{1,2}, B_{2,1} \mid P_{1,1}, \ldots, P_{4,4})\mathbf{P}(P_{1,1}, \ldots, P_{4,4})$
(Do it this way to get $P(Effect|Cause)$.)
First term: 1 if pits are adjacent to breezes, 0 otherwise
Second term: pits are placed randomly, probability 0.2 per square:

$$\mathbf{P}(P_{1,1}, \ldots, P_{4,4}) = \prod_{i,j=1,1}^{4,4} \mathbf{P}(P_{i,j}) = 0.2^n \times 0.8^{16-n}$$

for n pits.

Observations and query

We know the following facts:

$b = \neg b_{1,1} \wedge b_{1,2} \wedge b_{2,1}$

$known = \neg p_{1,1} \wedge \neg p_{1,2} \wedge \neg p_{2,1}$

Query is $\mathbf{P}(P_{1,3}|known, b)$

Define $Unknown = P_{ij}$s other than $P_{1,3}$ and $Known$

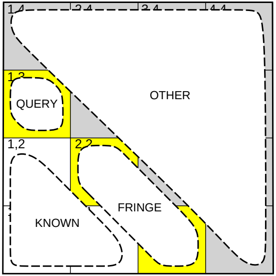
For inference by enumeration, we have

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

Grows exponentially with number of squares!

Using conditional independence

Basic insight: observations are conditionally independent of other hidden squares given neighbouring hidden squares



Define $\mathit{Unknown} = \mathit{Fringe} \cup \mathit{Other}$
$\mathbf{P}(b|P_{1,3}, \mathit{Known}, \mathit{Unknown}) = \mathbf{P}(b|P_{1,3}, \mathit{Known}, \mathit{Fringe})$
Manipulate query into a form where we can use this!

Using conditional independence contd.

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

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

$$= \alpha \sum_{fringe} \sum_{other} \mathbf{P}(b|known, P_{1,3}, fringe, other)\mathbf{P}(P_{1,3}, known, fringe, other)$$

$$= \alpha \sum_{fringe} \sum_{other} \mathbf{P}(b|known, P_{1,3}, fringe)\mathbf{P}(P_{1,3}, known, fringe, other)$$

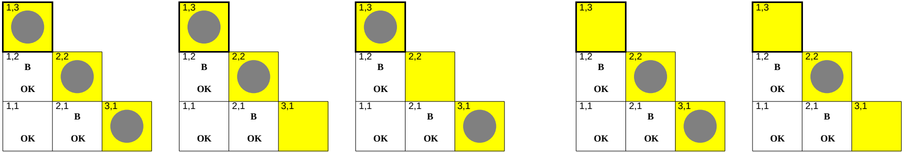
$$= \alpha \sum_{fringe} \mathbf{P}(b|known, P_{1,3}, fringe) \sum_{other} \mathbf{P}(P_{1,3}, known, fringe, other)$$

$$= \alpha \sum_{fringe} \mathbf{P}(b|known, P_{1,3}, fringe) \sum_{other} \mathbf{P}(P_{1,3})P(known)P(fringe)P(other)$$

$$= \alpha\, P(known)\mathbf{P}(P_{1,3}) \sum_{fringe} \mathbf{P}(b|known, P_{1,3}, fringe)P(fringe) \sum_{other} P(other)$$

$$= \alpha'\, \mathbf{P}(P_{1,3}) \sum_{fringe} \mathbf{P}(b|known, P_{1,3}, fringe)P(fringe)$$

Using conditional independence contd.



0.2 x 0.2 = 0.04 | 0.2 x 0.8 = 0.16 | 0.8 x 0.2 = 0.16 | 0.2 x 0.2 = 0.04 | 0.2 x 0.8 = 0.16

$$
\begin{aligned}
\mathbf{P}(P_{1,3} | known, b) &= \alpha' \langle 0.2(0.04 + 0.16 + 0.16),\ 0.8(0.04 + 0.16) \rangle \\
&\approx \langle 0.31, 0.69 \rangle
\end{aligned}
$$

$$
\mathbf{P}(P_{2,2} | known, b) \approx \langle 0.86, 0.14 \rangle
$$

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 criticised 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 asuumptions 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 $x_1, \ldots, x_n$ 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**.
- Thm: Let X and Y be independent normal RVs, then their sum is also normally distributed. i.e., if

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

- Remember: 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

$$\bar{X} \sim \mathcal{N}(\mu, \bar{\sigma}^2), \quad \text{with } \bar{\sigma}^2 = n\sigma^2/n^2 = \sigma^2/n.$$

- Now define the transformed random variable

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

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

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 $\{x_1, \ldots, x_n\}$.
- Plugging in 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**.
- That is, 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 transfomed $\tilde{B} := \frac{\mu - \tilde{m}}{\tilde{\nu}} \sim \mathcal{N}(0, 1)$
- 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 between the different types of analysis 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), or....