

STAD91 Bayesian Statistics

Lecture 1: Organization & Review

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UTSC

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Overview of the lecture

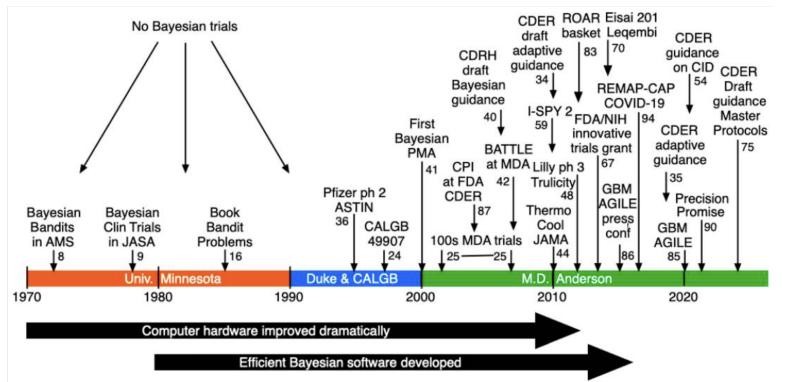
- First part: Organization of the course
 - Motivation
 - Course logistics
 - Assessment
- Second part: Background from Probability and Statistics

World War II

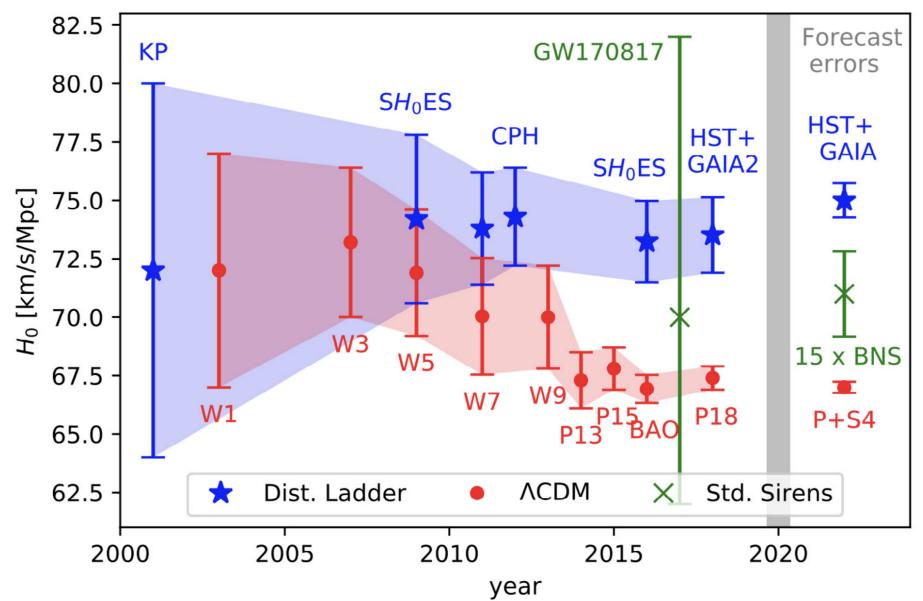


Search for plane wreck



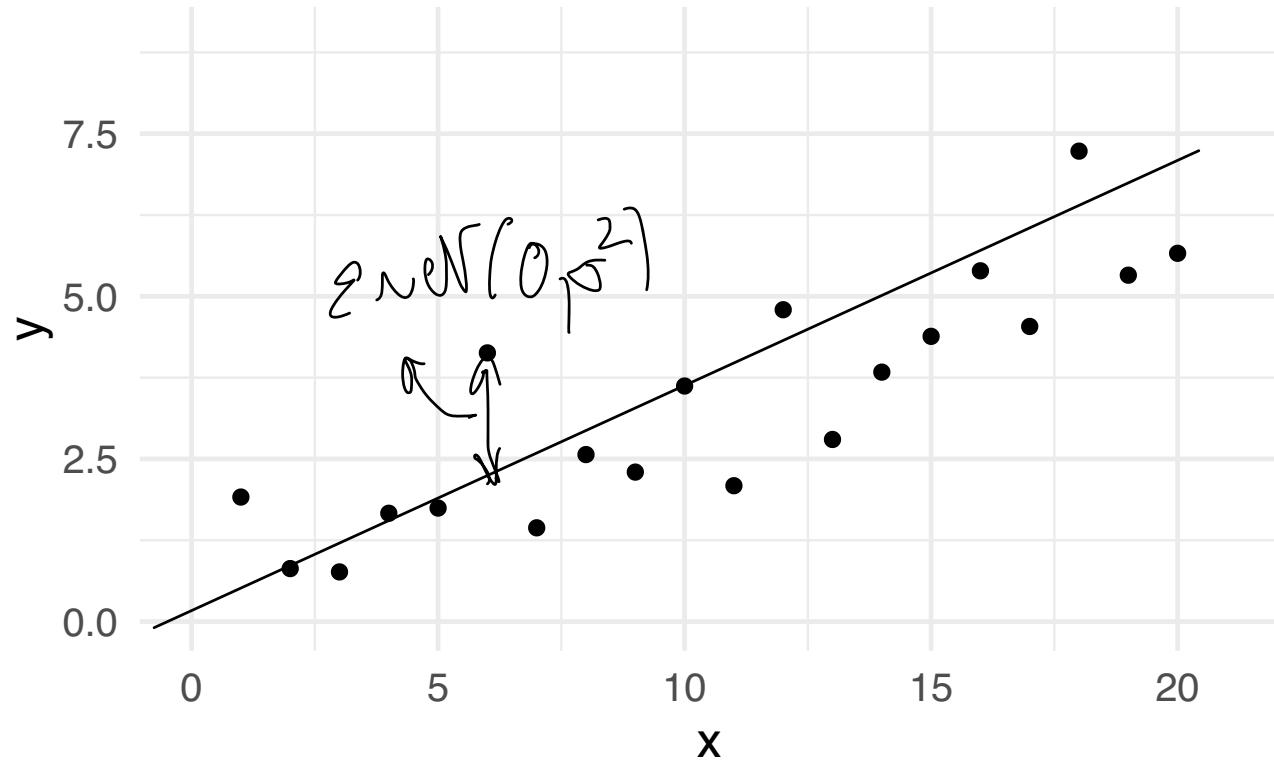


D. Berry, *Adaptive Bayesian Clinical Trials: The Past, Present, and Future of Clinical Research*, 2025



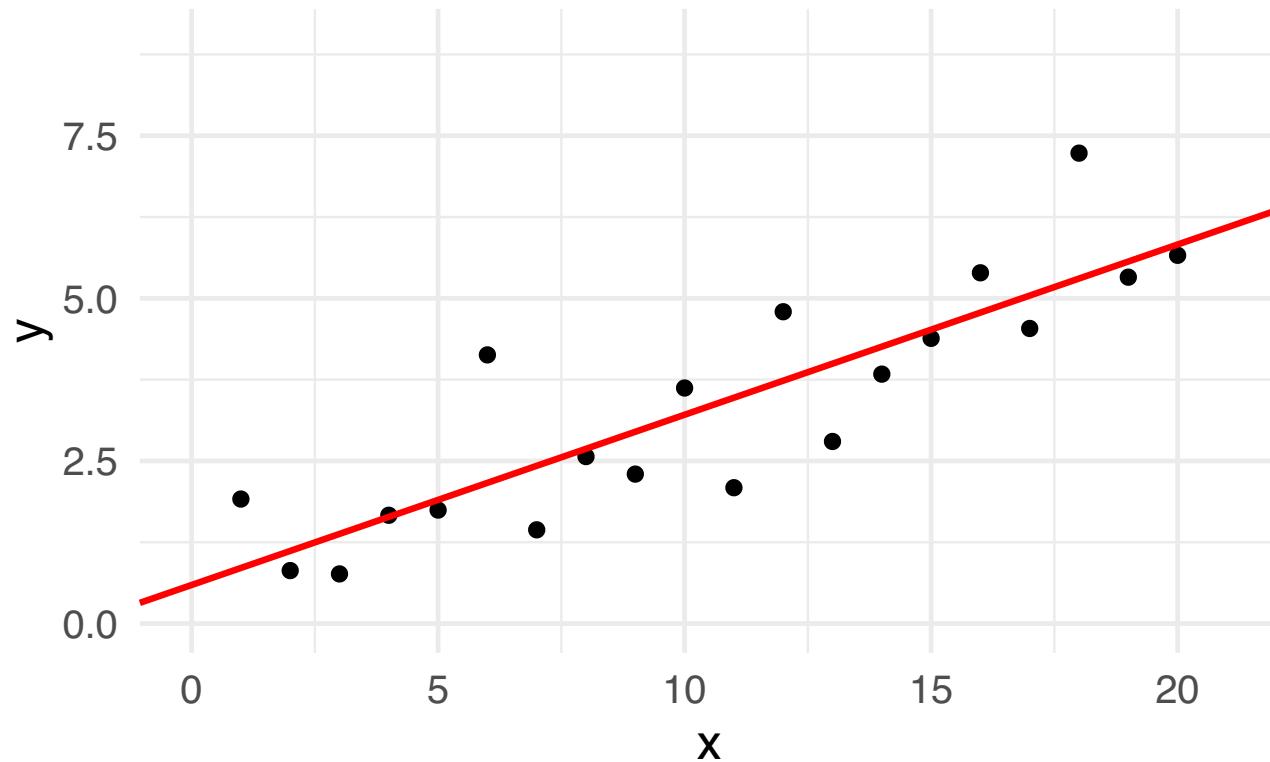
Uncertainty in modeling

Data



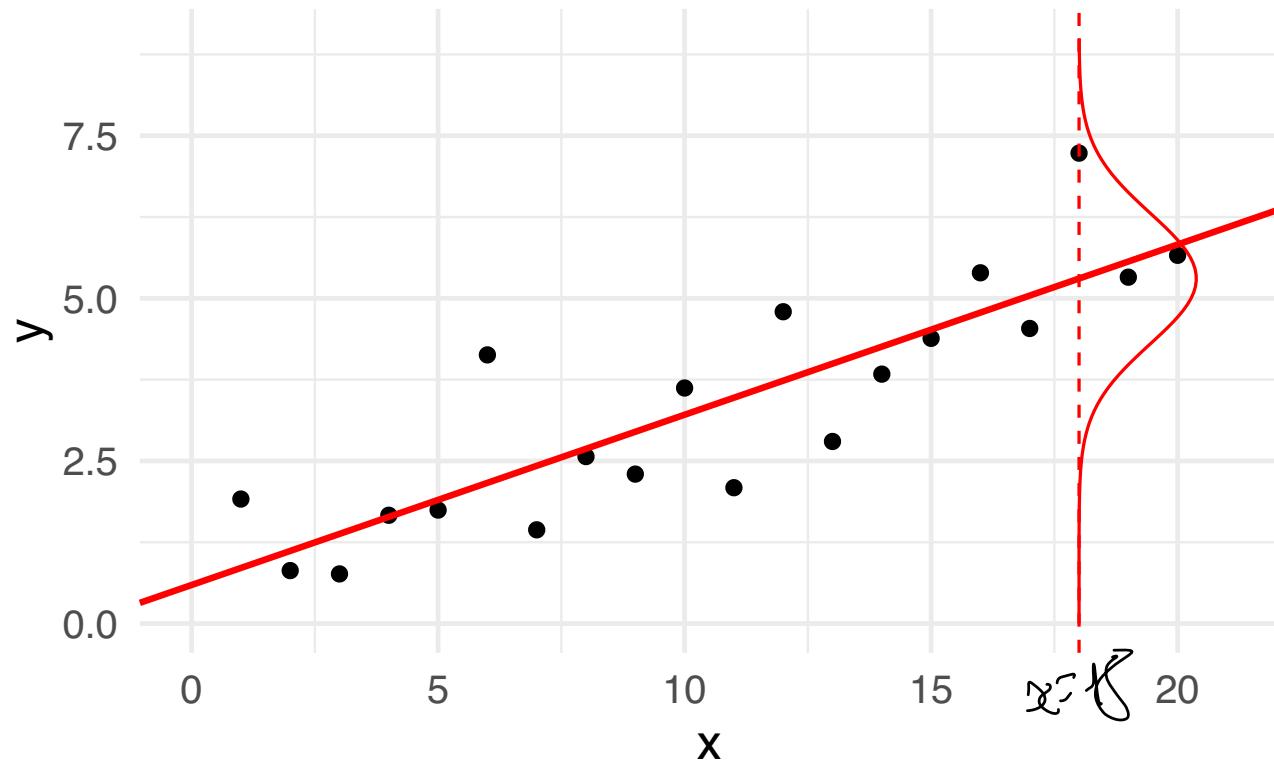
Uncertainty in modeling

Posterior mean



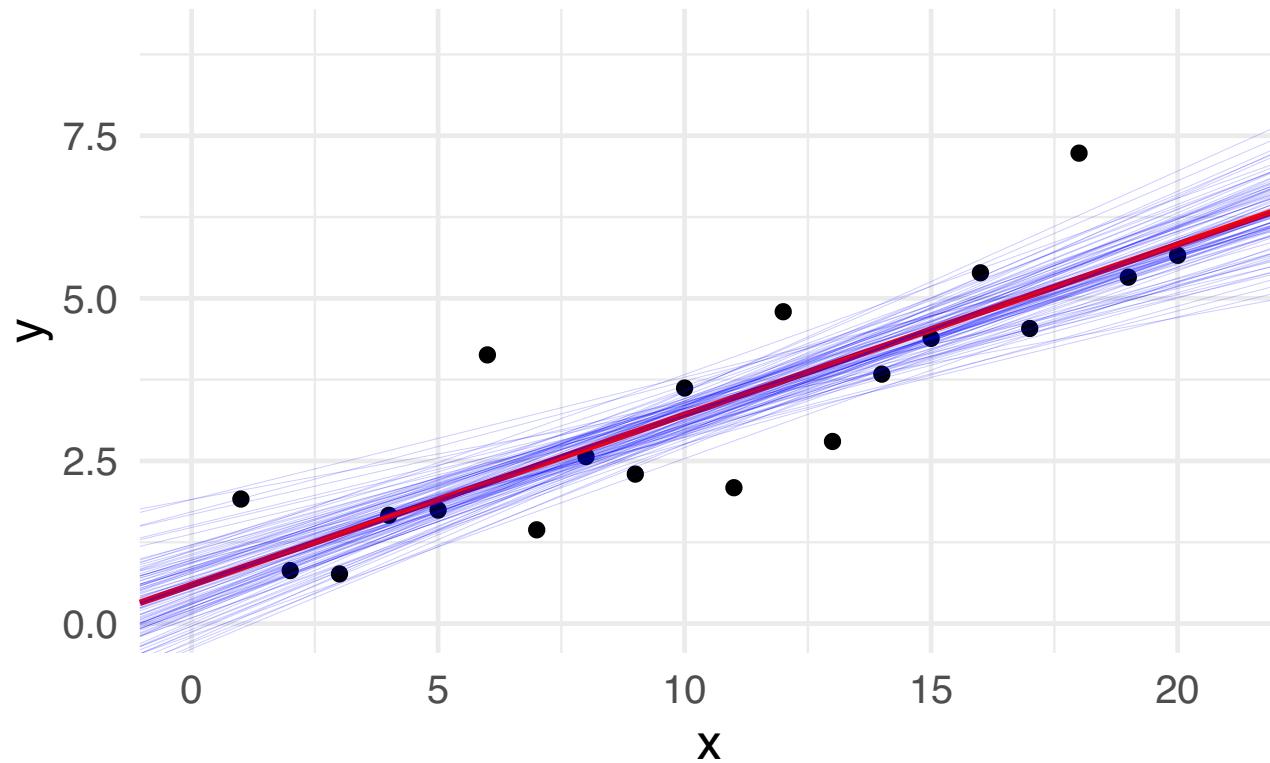
Uncertainty in modeling

Predictive distribution given posterior mean



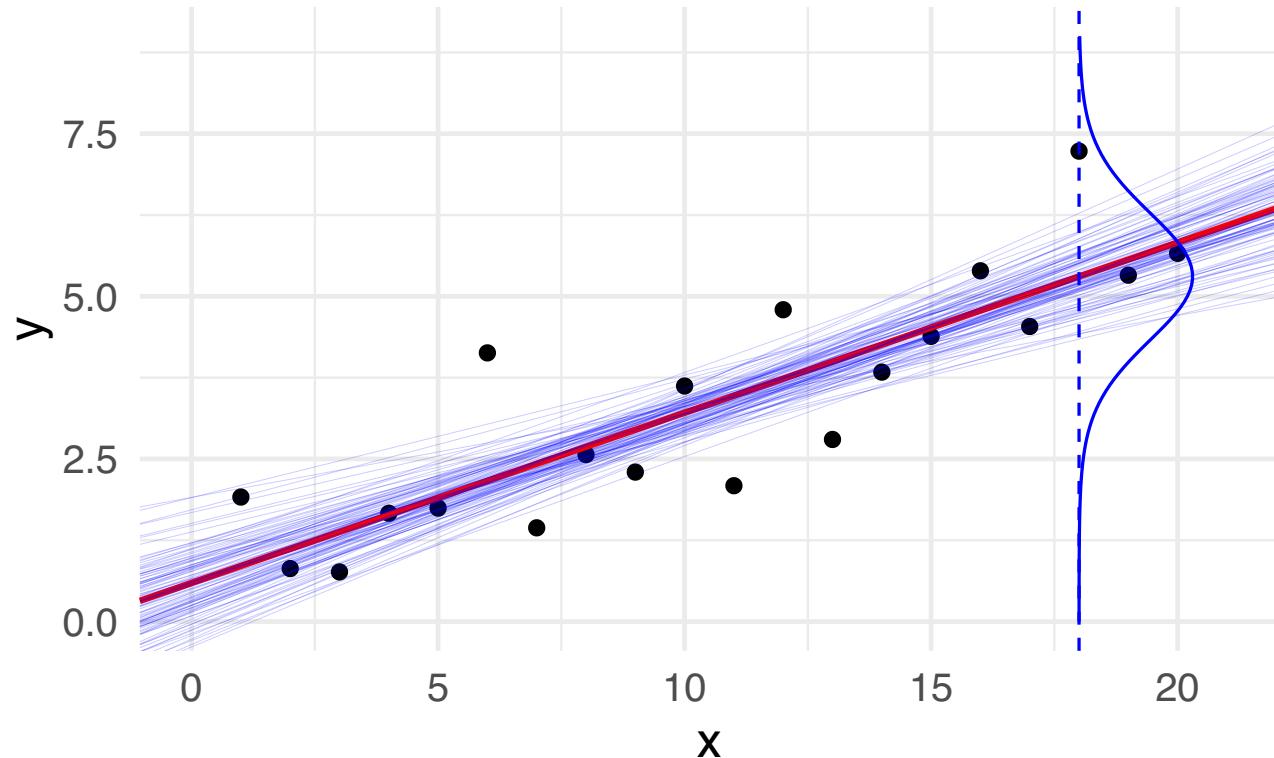
Uncertainty in modeling

Posterior draws



Uncertainty in modeling

Posterior draws and predictive distribution



Uncertainty and probabilistic modeling

- Representing uncertainty with **probabilities** + Updating **uncertainty**
- Two types of uncertainty: aleatoric and epistemic
- Aleatoric uncertainty due to randomness
 - we are not able to obtain observations which could reduce this uncertainty
- Epistemic uncertainty due to lack of knowledge
 - we are able to obtain observations which can reduce this uncertainty
 - two observers may have different epistemic uncertainty

Impact on society

Better modelling and quantification of uncertainty

- better science
- better informed decision making
in companies, government, and NGOs

Bayesian probability theory

expert information, previous experiments,...

Bayesian probability theory

expert information, previous experiments,...



mathematical model

+

uncertainty with probabilities

Bayesian probability theory

expert information, previous experiments,...

data



mathematical model

+

uncertainty with probabilities

Bayesian probability theory

expert information, previous experiments,...



mathematical model

+

uncertainty with probabilities

Bayesian probability theory

$$+ \quad \left\{ \begin{array}{l} p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)} \\ p(\tilde{y}|y) = \int p(\tilde{y}|\theta)p(\theta|y)d\theta \end{array} \right.$$

posterior distribution



data

Bayesian probability theory

expert information, previous experiments,...



mathematical model

+

uncertainty with probabilities

+

Bayesian probability theory

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta)p(\theta|y)d\theta$$



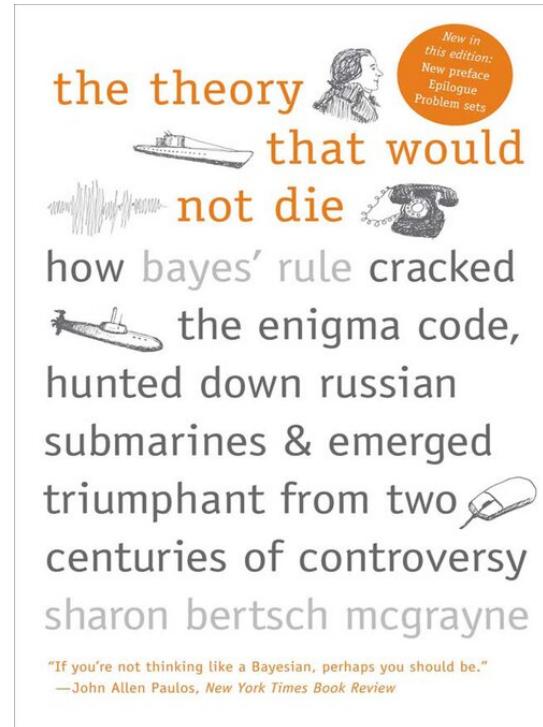
updated uncertainty

Bayesian probability theory

- Based on Bayesian probability theory
 - uncertainty is presented with probabilities
 - probabilities are updated based on new information
- Thomas Bayes (170?–1761)
 - English nonconformist, Presbyterian minister, (amateur) mathematician
 - considered the problem of *inverse probability*
→ single problem only
- Bayes did not invent all, but was first to solve problem of inverse probability in special case
- Laplace generalized the initial methods and applied it to scientific problems (e.g., astronomy)
- Modern Bayesian theory with rigorous proofs developed in 20th century

Bayesian probability theory

A nice book about history: Sharon Bertsch McGrayne, *The Theory That Would Not Die*, 2012.



Term Bayesian used first time in mid 20th century

- Earlier there was just "probability theory"
 - concept of the probability was not strictly defined, although it was close to modern Bayesian interpretation
 - in the end of 19th century there were increasing demand for more strict definition of probability (mathematical and philosophical problem) → Kolmogorov
- In the beginning of 20th century frequentist view gained popularity
 - accepts definition of probabilities only through frequencies
 - does not accept inverse probability or use of prior
 - gained popularity due to apparent objectivity and "cook book" like reference books
- R. A. Fisher used in 1950 first time term "Bayesian" to emphasize the difference to general term "probability theory"
 - term became quickly popular, because alternative descriptions were longer
- The probabilistic programming revolution started in early 1990's

Bayesian Statistics course

- Probability distributions as model building blocks

- need to understand the math part (prereq.)
- continuous vs discrete (prereq.)
- observation model, likelihood, prior
- constructing bigger models

- Computation

- We need to be able to compute expectations

marginalize, conditioning

$$E_{\theta|y}[g(\theta)] = \int p(\theta|y)g(\theta)d\theta$$

- when analytic solutions are not available, computational approximations with finite number of function evaluations
- importance sampling, Monte Carlo, Markov chain Monte Carlo, variational Bayes

- **Not in this course:** Diagnostics

Bayesian Statistics course

- *Bayesian inference* : process of statistical learning via Bayes' rule.

$$P(A|E) = \frac{P(E|A)P(A)}{P(E|A)P(A) + P(E|A^c)P(A^c)} = \frac{P(E|A)P(A)}{P(E)}$$

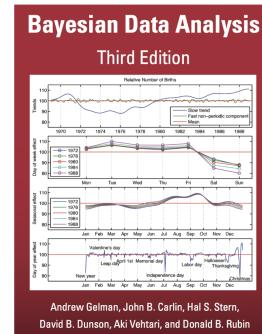
or

$$p(\theta|y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)p(y|\theta)}{p(y)}$$

- *Bayesian methods* are data analysis tools that are derived from the principles of Bayesian inference.
- Bayesian methods provide:
 - a rational method for updating beliefs in light of new information;
 - parameter estimates with good statistical properties;
 - predictions for missing data and forecasts of future data;
 - a computational framework for model estimation, selection and validation.

Course Logistics

- Course administered through [Quercus](#)
 - Syllabus, Lecture Notes, HW Problems, Quizzes, etc
 - Also look at the [course webpage](#)
- Textbook: [Bayesian Data Analysis](#) by Gelman, Carlin, Stern, Dunson, Vehtari & Rubin.



- Communication
 - For course content questions use [Piazza](#) or OH
 - For personal issues use email (with [STAD91] in the subject) or office hours (TH 10am-1pm @ IA 4064)

Assessment

Evaluation	Weight	Details
Weekly Quizzes (on Kahoot)	20%	<ul style="list-style-type: none">• Best 8/10• Cover previous week's material• At the end of the lecture
Homework Assignments	10%	<ul style="list-style-type: none">• Two Homework Assignments (5% each)• Date: After the midterm, TBD• Pen & paper derivations + Coding (Python/Numpy or R)
Term Test	25%	<ul style="list-style-type: none">• Covers first 5 weeks• Tentative Date: Feb 26 (Mar 10)
Final	45%	<ul style="list-style-type: none">• Cumulative• Final exam period

No make-up Quizzes/Term Tests; if you miss midterm you must **declare absence on ACORN** & mark will be replaced by final.

Review of Key Concepts

Probability & inference topics you are expected to remember (quick recap)

Absolute continuity

Definition (absolute continuity)

Let P and μ be two σ -finite measures on a measurable space (E, \mathcal{E}) . We say that P is absolutely continuous with respect to μ , and write $P \ll \mu$, if

$$\forall A \in \mathcal{E}, \quad \mu(A) = 0 \implies P(A) = 0.$$

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Radon–Nikodym theorem

If $P \ll \mu$, then there exists a positive measurable function p such that for every $A \in \mathcal{E}$,

$$P(A) = \int_A p(x) d\mu(x).$$

The function p is called the *Radon–Nikodym derivative* of P with respect to μ and is denoted

$$p = \frac{dP}{d\mu}.$$

Absolute continuity

Notation

One may write, suggestively,

$$P(A) = \int_A dP(x) = \int_A \frac{dP(x)}{d\mu(x)} d\mu(x) = \int_A p(x) d\mu(x).$$

Discrete distributions

- On $E = \{0, 1\}$, the Bernoulli(θ) law has a density with respect to $\mu = \delta_0 + \delta_1$:

$$p(x) = (1 - \theta)\mathbf{1}_{\{x=0\}} + \theta\mathbf{1}_{\{x=1\}}.$$

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- On $E = \{0, 1, \dots, n\}$, the Binomial(n, θ) law is absolutely continuous with respect to the counting measure $\mu = \sum_{k=0}^n \delta_k$, with density

$$p(k) = \binom{n}{k} \theta^k (1 - \theta)^{n-k}, \quad k = 0, 1, \dots, n.$$

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- On $E = \mathbb{N}^*$, the geometric law with parameter p is absolutely continuous with respect to the counting measure $\mu = \sum_{k \geq 1} \delta_k$, with density

$$p(k) = (1 - p)^{k-1} p, \quad k \geq 1.$$

Continuous distributions

- The normal law $\mathcal{N}(\mu, \sigma^2)$ has density with respect to Lebesgue measure on \mathbb{R} :

$$x \longmapsto \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}.$$

- The exponential law with rate $\lambda > 0$ has density (with respect to Lebesgue on \mathbb{R})

$$x \longmapsto \lambda e^{-\lambda x} \mathbf{1}_{\{x \geq 0\}}.$$

Classical inequalities

Markov's inequality

Let X be a non-negative real random variable and $a > 0$. Then

$$\mathbb{P}(X \geq a) \leq \frac{\mathbb{E}[X]}{a}.$$

In particular, for a real random variable X and $p \in \mathbb{N}^*$, since $x \mapsto x^p$ is increasing on \mathbb{R}_+ ,

$$\mathbb{P}(|X| \geq a) = \mathbb{P}(|X|^p \geq a^p) \leq a^{-p} \mathbb{E}[|X|^p].$$

Chebyshev's inequality

Let X be a real random variable and $a > 0$. Then

$$\mathbb{P}(|X - \mathbb{E}[X]| \geq a) \leq \frac{\text{Var}(X)}{a^2}, \quad \text{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2].$$

Classical inequalities

Hoeffding's inequality

Let X_1, \dots, X_n be independent random variables, denote $\bar{X}_n = \frac{1}{n} \sum_{k=1}^n X_k$ and suppose $a_i \leq X_i \leq b_i$ a.s.. Then for all $\varepsilon \geq 0$,

$$\mathbb{P}(\underbrace{\bar{X}_n - \mathbb{E}[\bar{X}_n]}_{\hookrightarrow \mathbb{E}[X_1]} \geq \varepsilon) \leq \exp\left(-\frac{2\varepsilon^2 n^2}{\sum_{i=1}^n (b_i - a_i)^2}\right).$$

$$\mathbb{P}(|\bar{X}_n - \mathbb{E}[X_1]| \geq \varepsilon) \leq 2 \exp\left(-\frac{2\varepsilon^2 n^2}{\sum_{i=1}^n (b_i - a_i)^2}\right)$$

Classical inequalities

Example: Bernoulli sample mean

Let X_1, \dots, X_n be i.i.d. with Bernoulli(p) distribution and $\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i$. For every $\varepsilon > 0$,

Chebyshev's inequality:

$$\overbrace{\text{Var}(\bar{X}_n)}^{\text{I}\!\text{I}\!\text{I}} = \frac{1}{n} \text{Var}(X_1)$$

$$\mathbb{P}(|\bar{X}_n - p| > \varepsilon) \leq \frac{\text{Var}(\bar{X}_n)}{\varepsilon^2} = \frac{p(1-p)}{n\varepsilon^2}.$$

Since $0 \leq X_i \leq 1$, we can improve this using **Hoeffding's inequality**:

$$\mathbb{P}(|\bar{X}_n - p| > \varepsilon) \leq 2 \exp(-2n\varepsilon^2).$$

Chebyshev gives a bound of order $1/n$, whereas Hoeffding yields an exponentially small bound in n .

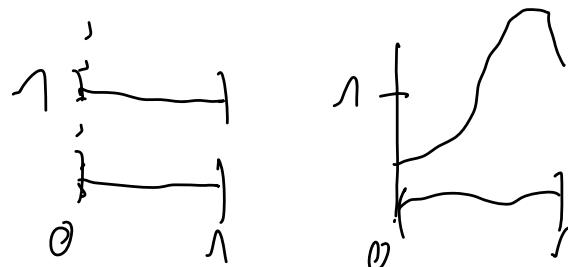
Gamma and Beta distributions

Gamma distribution

For $p, \lambda > 0$, a random variable Z has $\text{Gamma}(p, \lambda)$ distribution if it has density

$$f_Z(x) = \frac{\lambda^p}{\Gamma(p)} x^{p-1} e^{-\lambda x} \mathbf{1}_{\{x \geq 0\}}, \quad \Gamma(p) = \int_0^\infty z^{p-1} e^{-z} dz.$$

- $\mathbb{E}[Z] = \frac{p}{\lambda}$, $\text{Var}(Z) = \frac{p}{\lambda^2}$.
- Special case: $\Gamma(1, \lambda) = \text{Exp}(\lambda)$.



Beta distribution

For $a, b > 0$, a random variable X has $\text{Beta}(a, b)$ distribution if it has density

$$f_X(x) = \frac{1}{B(a, b)} x^{a-1} (1-x)^{b-1} \mathbf{1}_{\{0 \leq x \leq 1\}}, \quad B(a, b) = \int_0^1 z^{a-1} (1-z)^{b-1} dz = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}.$$

- $\mathbb{E}[X] = \frac{a}{a+b}$, $\text{Var}(X) = \frac{ab}{(a+b)^2(a+b+1)}$.
- Special case: $\text{Beta}(1, 1) = \mathcal{U}[0, 1]$.

Gamma and Beta: main properties

Additivity of Gamma

If $Y \sim \Gamma(p, \lambda)$ and $Z \sim \Gamma(q, \lambda)$ are independent, then

$$Y + Z \sim \Gamma(p + q, \lambda).$$

In particular, if E_1, \dots, E_n are i.i.d. $\text{Exp}(\lambda)$, then $\sum_{i=1}^n E_i \sim \Gamma(n, \lambda)$.

Scaling of Gamma

If $Y \sim \Gamma(p, \lambda)$ and $t > 0$, then $tY \sim \Gamma(p, \frac{\lambda}{t})$.

Gamma–Beta connection

If $X \sim \Gamma(a, \lambda)$ and $Y \sim \Gamma(b, \lambda)$ are independent, then $\frac{X}{X+Y} \sim \text{Beta}(a, b)$.
or $\Gamma(a, \lambda)$

As a special case, if E_1, E_2 are i.i.d. $\text{Exp}(\lambda)$, then

$$\frac{E_1}{E_1 + E_2} \sim \mathcal{U}[0, 1].$$

$$\frac{Y}{X+Y} \sim \text{Beta}(b, a)$$

Dirichlet distribution: definition and properties

Definition (Dirichlet distribution)

Let $K \geq 2$ and $\alpha_1, \dots, \alpha_K > 0$. A random vector $X = (X_1, \dots, X_K)$ has $\text{Dirichlet}(\alpha_1, \dots, \alpha_K)$ distribution if $X_i > 0$, $\sum_{i=1}^K X_i = 1$, and its density on the *simplex* is

$$f_X(x_1, \dots, x_K) = \frac{\Gamma(\sum_{i=1}^K \alpha_i)}{\prod_{i=1}^K \Gamma(\alpha_i)} \prod_{i=1}^K x_i^{\alpha_i - 1}, \quad (x_1, \dots, x_K) \in S_K = \{x \in [0, 1]^K : \sum_i x_i = 1\}$$

Key properties

- **Beta as a special case:** for $K = 2$, $\text{Dir}(\alpha_1, \alpha_2)$ is the $\text{Beta}(\alpha_1, \alpha_2)$ distribution.
- **Marginals are Beta:** if $X \sim \text{Dir}(\alpha_1, \dots, \alpha_K)$, then

$$X_i \sim \text{Beta}\left(\alpha_i, \sum_{k=1}^K \alpha_k - \alpha_i\right), \quad \mathbb{E}[X_i] = \frac{\alpha_i}{\sum_{k=1}^K \alpha_k}$$

- **Gamma representation:** If $Z_i \sim \Gamma(\alpha_i, \lambda)$ are independent and $Z = \sum_{k=1}^K Z_k$, then

$$\left(\frac{Z_1}{Z}, \dots, \frac{Z_K}{Z}\right) \sim \text{Dir}(\alpha_1, \dots, \alpha_K).$$

Modes of convergence of random variables

Convergence in probability

Let X_1, \dots, X_n, \dots and X be random variables taking values in \mathbb{R}^d , defined on the same probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The sequence (X_n) *converges in probability* to X , written $X_n \xrightarrow{\mathbb{P}} X$, if

$$\forall \varepsilon > 0, \quad \mathbb{P}(\|X_n - X\| > \varepsilon) \xrightarrow{n \rightarrow \infty} 0.$$

Convergence in L^2

In the same setting, we say that (X_n) *converges in L^2* to X , written $X_n \xrightarrow{L^2} X$, if

$$\mathbb{E} [\|X_n - X\|^2] \xrightarrow{n \rightarrow \infty} 0.$$

Modes of convergence of random variables (II)

Almost sure convergence

With the same notation, the sequence (X_n) *converges almost surely* to X , written $X_n \xrightarrow{\text{a.s.}} X$ if

$$\mathbb{P} \left(\left\{ \omega \in \Omega : X_n(\omega) \xrightarrow[n \rightarrow \infty]{} X(\omega) \right\} \right) = 1.$$

Proposition

We have the implications

$$X_n \xrightarrow{\text{a.s.}} X \implies X_n \xrightarrow{\mathbb{P}} X,$$

and

$$X_n \xrightarrow{L^2} X \implies X_n \xrightarrow{\mathbb{P}} X.$$

Convergence in distribution

Convergence in distribution / in law

Let $(X_n)_{n \geq 1}$ and X be random variables with values in \mathbb{R}^d . We say that X_n *converges in distribution* (or in law) to X , written $X_n \xrightarrow{\mathcal{L}} X$, if for every **bounded continuous** function $f : \mathbb{R}^d \rightarrow \mathbb{R}$,

$$\mathbb{E}[f(X_n)] \xrightarrow{n \rightarrow \infty} \mathbb{E}[f(X)].$$

Similarly, we say that (X_n) converges in distribution to a probability measure P on \mathbb{R}^d if

$$\mathbb{E}[f(X_n)] \xrightarrow{n \rightarrow \infty} \mathbb{E}[f(X)]$$

for $X \sim P$ and every bounded continuous function f .

Central Limit Theorem in \mathbb{R}^d

Multivariate Central Limit Theorem

Let (X_n) be a sequence of i.i.d. random variables with values in \mathbb{R}^d , such that $\mathbb{E}[\|X_1\|^2] < \infty$.

Let

$$\mu = \mathbb{E}[X_1], \quad \Sigma = \mathbb{E}[(X_1 - \mathbb{E}[X_1])(X_1 - \mathbb{E}[X_1])^T].$$

Then

$$\sqrt{n} (\bar{X}_n - \mu) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \Sigma).$$
$$= \frac{1}{n} \sum_{i=1}^n X_i$$

Continuous mapping theorem, Slutsky's lemma

Continuous mapping theorem

Let X_n, X be random variables taking values in \mathbb{R}^d and $g : \mathbb{R}^d \rightarrow \mathbb{R}^k$ a continuous function.

- If $X_n \xrightarrow{\mathcal{L}} X$, then $g(X_n) \xrightarrow{\mathcal{L}} g(X)$.
- If $X_n \xrightarrow{\mathbb{P}} X$, then $g(X_n) \xrightarrow{\mathbb{P}} g(X)$.
- If $X_n \xrightarrow{\text{a.s.}} X$, then $g(X_n) \xrightarrow{\text{a.s.}} g(X)$.

Slutsky's lemma

Let (X_n) and (Y_n) be sequences of real-valued random variables, X a real-valued random variable, and $a \in \mathbb{R}$.

$$X_n \xrightarrow{\mathcal{L}} X \quad \text{and} \quad Y_n \xrightarrow{\mathbb{P}} a \implies (X_n, Y_n) \xrightarrow{\mathcal{L}} (X, a).$$

Remark

For a **constant** a , we have

$$Z_n \xrightarrow{\mathcal{L}} a \iff Z_n \xrightarrow{\mathbb{P}} a.$$

Statistical experiment and model

A *statistical experiment* consists of

- a random variable X defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with values in a measurable space (E, \mathcal{E}) ;
- a family of probability measures on (E, \mathcal{E}) , called a *statistical model*,

$$\mathcal{P} = \{P_\theta : \theta \in \Theta\},$$

where Θ is the *parameter space*.

$\hookrightarrow \mathbb{R}^d$ for instance

In the *frequentist approach* one assumes that the law of X belongs to the model:

$$\exists \theta_0 \in \Theta, \quad X \sim P_{\theta_0}.$$

Statistical inference aims at learning about θ_0 from an observation of X .

Sample model

In practice X is often an n -tuple of random variables

$$X = (X_1, \dots, X_n)$$

Also, often X_i are i.i.d.

Example 2: $((x_1, y_1), \dots, (x_n, y_n))$

Then the sample space and the model depend on n .

Example: n -sample model

When $X = (X_1, \dots, X_n)$, one often works with the **n -sample model**

$$\mathcal{P}_n = \{P_\theta^{\otimes n} : \theta \in \Theta\},$$

where

$$P_\theta^{\otimes n} = \underbrace{P_\theta \otimes \cdots \otimes P_\theta}_{n \text{ times}}.$$

This corresponds to assuming that X_1, \dots, X_n are i.i.d. with common distribution P_θ .

Identifiability and dominated models

Identifiable model

A statistical model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ is *identifiable* if for all $\theta, \theta' \in \Theta$,

$$P_\theta = P_{\theta'} \implies \theta = \theta'.$$

Equivalently, the mapping $\theta \mapsto P_\theta$ is injective. This guarantees that each distribution in the model corresponds to a unique parameter value.

Dominated model

The model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ is *dominated* if there exists a σ -finite measure μ on E such that, for all $\theta \in \Theta$, $P_\theta \ll \mu$. Then every P_θ admits a density p_θ with respect to μ :

$$dP_\theta(x) = p_\theta(x) d\mu(x).$$

In what follows we often work with dominated, *parametric models* with $\Theta \subset \mathbb{R}^d$.

I have a family of densities $\{p_\theta : \theta \in \Theta\}$

Example 1: Bernoulli model

Consider $E = \{0, 1\}$ and parameter space $\Theta = (0, 1)$. For $\theta \in \Theta$ let

$$P_\theta(X = 1) = \theta, \quad P_\theta(X = 0) = 1 - \theta.$$

The model is

$$\mathcal{P} = \{P_\theta : \theta \in (0, 1)\}.$$

- This is a dominated model with respect to the counting measure on $\{0, 1\}$; the density is

$$p_\theta(x) = (1 - \theta)\mathbf{1}_{\{0\}}(x) + \theta\mathbf{1}_{\{1\}}(x).$$

- The model is identifiable: $P_\theta = P_{\theta'}$ implies $\theta = P_\theta(X = 1) = P_{\theta'}(X = 1) = \theta'$.

Example 2: Gaussian model with unknown mean

Let $E = \mathbb{R}$, $\Theta = \mathbb{R}$ and fix $\sigma^2 > 0$. For $\theta \in \Theta$ define P_θ as the normal law

$$P_\theta = \mathcal{N}(\theta, \sigma^2).$$

The model is

$$\mathcal{P} = \{\mathcal{N}(\theta, \sigma^2) : \theta \in \mathbb{R}\}.$$

- This model is dominated by Lebesgue measure λ on \mathbb{R} with density

$$p_\theta(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\theta)^2}{2\sigma^2}\right).$$

- It is identifiable: equality of the densities (or distributions) for all x forces the means to be equal.

$$\text{if } P_\theta = P_{\theta'}, \quad P_\theta = P_{\theta'} \Rightarrow \theta = \theta'$$

Estimators in a statistical experiment

Estimator

Consider the statistical experiment (X, \mathcal{P}) . An *estimator* of the parameter θ is a measurable function

$$\hat{\theta} = \hat{\theta}(X)$$

with values in the parameter space Θ (more precisely, $\hat{\theta}$ is measurable from (E, \mathcal{E}) to $(\Theta, \mathcal{B}(\Theta))$, where $\mathcal{B}(\Theta)$ is the Borel σ -algebra).

Sequence of experiments

In practice we often have a sequence of experiments $(X^{(n)}, \mathcal{P}_n)$, $n = 1, 2, \dots$

This leads to a sequence of estimators $(\hat{\theta}_n)$.

↳ e.g., n is the sample size

Likelihood and maximum likelihood estimator

Assume a dominated model with respect to a measure μ : for each $\theta \in \Theta$,

$$dP_\theta(x) = p_\theta(x) d\mu(x).$$

Let $X = (X_1, \dots, X_n) \sim P_\theta^{\otimes n}$. The **joint density** of X is

$$p_\theta^{\otimes n}(x_1, \dots, x_n) = \prod_{i=1}^n p_\theta(x_i).$$

Viewed as a function of θ for the observed data X , this is the *likelihood function*

$$L_\theta(X) = \prod_{i=1}^n p_\theta(X_i).$$

Often we work instead with the *log-likelihood*

$$\ell_\theta(X) = \log L_\theta(X) = \sum_{i=1}^n \log p_\theta(X_i).$$

Maximum likelihood estimator (MLE)

Definition (MLE)

In a dominated model, a *maximum likelihood estimator (MLE)* is, when it exists, a value $\hat{\theta}(X) \in \Theta$ such that

$$\hat{\theta}(X) \in \arg \max_{\theta \in \Theta} L_\theta(X), \quad \text{or equivalently} \quad \hat{\theta}(X) \in \arg \max_{\theta \in \Theta} \ell_\theta(X).$$

Example / exercise (Bernoulli model). In the Bernoulli model $\mathcal{P} = \{\mathcal{B}(\theta)^{\otimes n} : \theta \in [0, 1]\}$, show that the MLE of θ is unique and given by the empirical mean

$$\hat{\theta}(X) = \bar{X}_n.$$

Maximum likelihood estimator (MLE)

$$P_{\theta}^{\otimes n}(x) = \prod_{i=1}^N P_{\theta}(x_i) = \prod_{i=1}^N \theta^{x_i} (1-\theta)^{1-x_i}$$

$$\log P_{\theta}^{\otimes n}(x) = \sum_{i=1}^n [x_i \log \theta + (1-x_i) \log (1-\theta)]$$

$$= [\log \theta] \left[\sum_{i=1}^n x_i \right] + [N - \sum_{i=1}^n x_i] \log (1-\theta)$$

$$\frac{\partial \dots}{\partial \theta} = \frac{\sum_{i=1}^n x_i}{\theta} - \frac{[N - \sum_{i=1}^n x_i]}{1-\theta} = 0$$

$$\Rightarrow \frac{\theta}{\sum_{i=1}^n x_i} = \frac{1-\theta}{N - \sum_{i=1}^n x_i} \Rightarrow \frac{\theta}{1-\theta} = \frac{\bar{x}_n}{1-\bar{x}_n} \quad \text{and } \alpha \mapsto \frac{x}{1-x}$$

is bijective

Consistency and asymptotic normality

Consistency

Consider a sequence of experiments $(X^{(n)}, \mathcal{P}_n)$ with

$$\mathcal{P}_n = \{P_\theta^{\otimes n} : \theta \in \Theta\}.$$

A sequence of estimators $(\hat{\theta}_n)$ is *consistent* if, for every $\theta \in \Theta$, when $X^{(n)} \sim P_\theta^{\otimes n}$,

$$\hat{\theta}_n(X^{(n)}) \xrightarrow[n \rightarrow \infty]{\mathbb{P}} \theta. \quad \Leftrightarrow \quad \hat{\theta}_m(X^{(n)}) \xrightarrow[m \rightarrow +\infty]{\mathcal{D}} \oplus$$

$\in \mathbb{R}$

Asymptotic normality

In the same setting, $(\hat{\theta}_n)$ is *asymptotically normal* if for each $\theta \in \Theta$ there exists a symmetric positive semi-definite matrix Σ_θ such that, when $X^{(n)} \sim P_\theta^{\otimes n}$,

$$\sqrt{n} (\hat{\theta}_n(X^{(n)}) - \theta) \xrightarrow[n \rightarrow \infty]{\mathcal{D}} \mathcal{N}(0, \Sigma_\theta).$$

Consistency and asymptotic normality

Exercise. Show that if $(\hat{\theta}_n)$ is asymptotically normal, then it is consistent.

$$\sqrt{n}(\hat{\theta}_n(X^{(n)}) - \theta) \xrightarrow[n \rightarrow \infty]{\mathcal{L}} \mathcal{N}(0, \Sigma_\theta).$$

$$\rightarrow (\hat{\theta}_n - \theta) = \frac{1}{\sqrt{n}} \times \underbrace{\sqrt{n}(\hat{\theta}_n - \theta)}_{\xrightarrow{\mathcal{D}} \mathcal{N}(0, \Sigma_\theta)}$$

Similarly $\Rightarrow \left(\frac{1}{\sqrt{n}}, \sqrt{n}(\hat{\theta}_n - \theta) \right) \xrightarrow{\mathcal{D}} (0, \mathcal{N}(0, \Sigma_\theta))$

Apply $f: \mathbb{R}^2 \rightarrow \mathbb{R}$ with continuous mapping theorem:
 $(x, y) \mapsto xy$

$$\hat{\theta}_n - \theta \xrightarrow{\mathcal{D}} 0 \iff \hat{\theta}_n - \theta \xrightarrow{\mathcal{D}} 0 \text{ as } 0 \text{ is a constant}$$

Quadratic risk of an estimator

Definition (Quadratic risk)

Let (X, \mathcal{P}) be a statistical experiment with $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ and let $\hat{\theta}$ be an estimator. The *quadratic risk* of $\hat{\theta}$ at θ is

$$R(\theta, \hat{\theta}) = \mathbb{E}_\theta \left[\left\| \hat{\theta}(X) - \theta \right\|^2 \right] = \int_E \left\| \hat{\theta}(x) - \theta \right\|^2 dP_\theta(x).$$

Example: Scalar parameter case

When $\Theta \subset \mathbb{R}$, the quadratic risk reduces to

$$R(\theta, \hat{\theta}) = \mathbb{E}_\theta \left[(\hat{\theta}(X) - \theta)^2 \right] = \int_E (\hat{\theta}(x) - \theta)^2 dP_\theta(x).$$

A "good" estimator typically has small quadratic risk, but remember that $R(\theta, \hat{\theta})$ is a function of θ and may be small for some parameter values and large for others.

Bias–variance decomposition

Proposition (Bias–variance decomposition)

Let (X, \mathcal{P}) be a statistical experiment with $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ and let $\hat{\theta}$ be an estimator. For every $\theta \in \Theta$, if $X \sim P_\theta$,

$$R(\theta, \hat{\theta}) = \mathbb{E}_\theta \left[\left\| \hat{\theta}(X) - \mathbb{E}_\theta[\hat{\theta}(X)] \right\|^2 \right] + \left\| \mathbb{E}_\theta[\hat{\theta}(X)] - \theta \right\|^2.$$

The function

$$\theta \longmapsto \mathbb{E}_\theta[\hat{\theta}(X)] - \theta$$

is called the *bias* of $\hat{\theta}$.

Scalar parameter case

If $\Theta \subset \mathbb{R}$, then

$$R(\theta, \hat{\theta}) = \text{Var}_\theta(\hat{\theta}(X)) + (\mathbb{E}_\theta[\hat{\theta}(X)] - \theta)^2.$$

Example: Bernoulli model and empirical mean

Setting

Let (X, \mathcal{P}) with $\mathcal{P} = \{\mathcal{B}(\theta)^{\otimes n} : \theta \in [0, 1]\}$, where $X = (X_1, \dots, X_n)$ and X_i are i.i.d. $\text{Bernoulli}(\theta)$.

A natural estimator of θ is the empirical mean

$$\hat{\theta}_n(X) = \bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i.$$

- By the (strong) law of large numbers, $\hat{\theta}_n(X) \rightarrow \theta$ almost surely, hence $\hat{\theta}_n$ is consistent.
- By the central limit theorem, $\sqrt{n}(\hat{\theta}_n(X) - \theta) \xrightarrow{\mathcal{L}} \mathcal{N}(0, \theta(1 - \theta))$, so $\hat{\theta}_n$ is asymptotically normal.
- Since $\mathbb{E}_{\theta}[\hat{\theta}_n(X)] = \theta$, the estimator is unbiased and

$$R(\theta, \hat{\theta}_n) = \mathbb{E}_{\theta}[(\hat{\theta}_n(X) - \theta)^2] = \text{Var}_{\theta}(\hat{\theta}_n(X)) = \frac{\theta(1 - \theta)}{n}.$$

Risk and probability of large error

For any estimator $\hat{\theta}$ and any $\varepsilon > 0$, the quadratic risk controls the probability of a large error:

$$\mathbb{P}_\theta \left(|\hat{\theta}(X) - \theta| \geq \varepsilon \right) \leq \frac{\mathbb{E}_\theta \left[(\hat{\theta}(X) - \theta)^2 \right]}{\varepsilon^2} = \frac{R(\theta, \hat{\theta})}{\varepsilon^2}.$$

This follows from Markov's (or Chebyshev's) inequality.

Thus, a small quadratic risk implies that $\hat{\theta}(X)$ is close to θ with high probability.

Example: Gaussian mean, two estimators

Setting

Let X_1, \dots, X_n be i.i.d. $\mathcal{N}(\theta, 1)$ with $\theta \in \mathbb{R}$.

We compare two estimators:

- a constant estimator $\tilde{\theta}_n = \theta_0$ for some fixed $\theta_0 \in \mathbb{R}$.

$$R(\theta, \tilde{\theta}_n) = \mathbb{E}_{\theta}[(\theta_0 - \theta)^2] = (\theta - \theta_0)^2.$$

This risk is zero at $\theta = \theta_0$, but positive elsewhere and does not decrease with n .

- the empirical mean $\hat{\theta}_n(X) = \bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i$, for which $\mathbb{E}_{\theta}[\hat{\theta}_n(X)] = \theta$ (unbiased) and

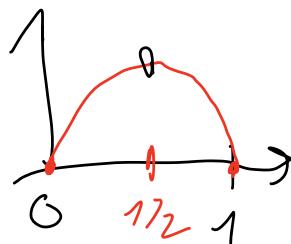
$$R(\theta, \hat{\theta}_n) = \text{Var}_{\theta}(\hat{\theta}_n(X)) = \frac{1}{n}.$$

The risk is independent of θ and decreases at rate $1/n$.

Consistency and asymptotic normality

Exercise. For $X \sim \text{Bin}(n, \theta)$ and $\hat{\theta} = X/n$, show that $R(\theta, \hat{\theta}) \leq 1/(4n)$ for all $\theta \in [0, 1]$.

$$\begin{aligned} R(\theta, \hat{\theta}) &= \underbrace{\text{bias}^2}_{\geq 0} + \text{Var}(\hat{\theta}) \\ &= \frac{n \theta(1-\theta)}{n^2} = \frac{\theta(1-\theta)}{n} \leq \frac{1}{4n} \\ \mathbb{E}[\hat{\theta}] &= n^{-1} \mathbb{E}[X] \\ &= n^{-1} n \theta = \theta \end{aligned}$$



Exact confidence intervals and regions

Let $\alpha > 0$.

Definition (exact confidence interval / region)

- **Case $\Theta \subset \mathbb{R}$.** A (random) interval $I(X) = [a(X), b(X)]$ is a *confidence interval of level (at least) $1 - \alpha$* if

$$\forall \theta \in \Theta, \quad \mathbb{P}_\theta(\theta \in I(X)) \geq 1 - \alpha.$$

- **Case $\Theta \subset \mathbb{R}^d$.** A random subset $\mathcal{R}(X) \subset \Theta$ is a *confidence region of level (at least) $1 - \alpha$* if

$$\forall \theta \in \Theta, \quad \mathbb{P}_\theta(\theta \in \mathcal{R}(X)) \geq 1 - \alpha.$$

⚠ The interval $I(X)$ cannot depend on the unknown parameter θ ; it may only depend on known quantities (such as α , the sample size n , and the data X).

Example: normal mean, exact confidence interval

- Gaussian model

We observe $X = (X_1, \dots, X_n)$ i.i.d. with $X_i \sim \mathcal{N}(\theta, 1)$, $\theta \in \mathbb{R}$. Let $\hat{\theta}(X) = \bar{X}_n = n^{-1} \sum_{i=1}^n X_i$. Then

$$\sqrt{n} (\bar{X}_n - \theta) \sim \mathcal{N}(0, 1).$$

Example: normal mean, exact confidence interval

- Gaussian model

We observe $X = (X_1, \dots, X_n)$ i.i.d. with $X_i \sim \mathcal{N}(\theta, 1)$, $\theta \in \mathbb{R}$. Let

$\hat{\theta}(X) = \bar{X}_n = n^{-1} \sum_{i=1}^n X_i$. Then

$$\sqrt{n} (\bar{X}_n - \theta) \sim \mathcal{N}(0, 1).$$

Denote by Φ the c.d.f. of $\mathcal{N}(0, 1)$ and set $q_\alpha = \Phi^{-1}(1 - \alpha/2)$, so that

$$\mathbb{P}(|\mathcal{N}(0, 1)| > q_\alpha) = \alpha.$$

Example: normal mean, exact confidence interval

- Gaussian model

We observe $X = (X_1, \dots, X_n)$ i.i.d. with $X_i \sim \mathcal{N}(\theta, 1)$, $\theta \in \mathbb{R}$. Let $\hat{\theta}(X) = \bar{X}_n = n^{-1} \sum_{i=1}^n X_i$. Then

$$\sqrt{n}(\bar{X}_n - \theta) \sim \mathcal{N}(0, 1).$$

Denote by Φ the c.d.f. of $\mathcal{N}(0, 1)$ and set $q_\alpha = \underbrace{\Phi^{-1}(1 - \alpha/2)}$, so that $\mathbb{P}(|\mathcal{N}(0, 1)| > q_\alpha) = \alpha$.

- Resulting confidence interval

We have

$$\begin{aligned} \hat{\theta}(x) - \frac{q_\alpha}{\sqrt{n}} \leq \hat{\theta}(x) + \frac{q_\alpha}{\sqrt{n}} \\ \mathbb{P}_{\theta}\left(\left|\sqrt{n}(\hat{\theta}(X) - \theta)\right| > q_\alpha\right) = \alpha. \end{aligned}$$

Equivalently,

$$I(X) = \left[\hat{\theta}(X) \pm \frac{q_\alpha}{\sqrt{n}} \right]$$

is an **exact** level $1 - \alpha$ confidence interval for θ .

Asymptotic confidence intervals

Sometimes the finite-sample distribution of an estimator is unknown, but its limiting distribution as $n \rightarrow \infty$ is known. This leads to asymptotic confidence intervals/regions.

Definition (asymptotic confidence interval/region)

- **Case $\Theta \subset \mathbb{R}$.** A random interval $I(X^{(n)})$ is an *asymptotic confidence interval of level (at least) $1 - \alpha$* if

$$\forall \theta \in \Theta, \quad \liminf_{n \rightarrow \infty} \mathbb{P}_\theta(\theta \in I(X^{(n)})) \geq 1 - \alpha.$$

- **Case $\Theta \subset \mathbb{R}^d$.** A random set $\mathcal{R}(X^{(n)}) \subset \Theta$ is an *asymptotic confidence region of level (at least) $1 - \alpha$* if

$$\forall \theta \in \Theta, \quad \liminf_{n \rightarrow \infty} \mathbb{P}_\theta(\theta \in \mathcal{R}(X^{(n)})) \geq 1 - \alpha.$$

General construction from an asymptotically normal estimator

Proposition (asymptotic CI from asymptotic normality)

Assume $\Theta \subset \mathbb{R}$ and let $\hat{\theta}_n = \hat{\theta}_n(X)$ be an estimator such that

$$\sqrt{n} (\hat{\theta}_n - \theta) \xrightarrow[n \rightarrow \infty]{\mathcal{L}} \mathcal{N}(0, \sigma^2(\theta)),$$

where the function $\theta \mapsto \sigma^2(\theta)$ is continuous.]

Let $q_\alpha > 0$ satisfy

$$\mathbb{P}(|\mathcal{N}(0, 1)| \leq q_\alpha) = 1 - \alpha \quad (\text{so } q_\alpha = \Phi^{-1}(1 - \alpha/2)).$$

Define

$$I(X) = \left[\hat{\theta}_n(X) - \frac{q_\alpha \sigma(\hat{\theta}_n(X))}{\sqrt{n}}, \hat{\theta}_n(X) + \frac{q_\alpha \sigma(\hat{\theta}_n(X))}{\sqrt{n}} \right].$$

Then $I(X)$ is an **asymptotic confidence interval of level exactly $1 - \alpha$** .

General construction from an asymptotically normal

proof: $\sqrt{n}(\hat{\theta}_n - \theta) \xrightarrow[n \rightarrow \infty]{\mathcal{L}} \mathcal{N}(0, \sigma^2(\theta))$, \rightarrow consistency estimator

$$\frac{\sqrt{n}(\hat{\theta}_m - \theta)}{\sigma(\hat{\theta}_m)} = \frac{\sigma(\theta)}{\sigma(\hat{\theta}_m)} \times \frac{\sqrt{n}(\hat{\theta}_m - \theta)}{\sigma(\theta)} \xrightarrow{\mathcal{L}} \mathcal{N}(0, 1)$$

$\xrightarrow{\text{LR}} 1 \quad \xrightarrow{\text{Z}} \mathcal{N}(0, 1)$

$$\lim_{n \rightarrow +\infty} \mathbb{P}\left(\left| \frac{\sqrt{n}(\hat{\theta}_m - \theta)}{\sigma(\hat{\theta}_m)} \right| > q_\alpha \right) \leq \alpha$$

$$\Leftrightarrow \theta \in \left[\hat{\theta}_m \pm \frac{q_\alpha \sigma(\hat{\theta}_m)}{\sqrt{n}} \right]$$

Conditional distribution (discrete case)

Definition (discrete conditional law)

Let X and Y be discrete random variables on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, with values respectively in sets E and F . For $x \in E$ such that $\mathbb{P}(X = x) > 0$, the **conditional distribution** of Y given $X = x$, denoted $\mathcal{L}(Y | X = x)$, is defined for all $y \in F$ by

$$\mathbb{P}(Y = y | X = x) = \frac{\mathbb{P}(Y = y, X = x)}{\mathbb{P}(X = x)}. \quad (\text{Bayes' rule})$$

This defines, for each fixed x , a probability distribution on F .

Let
 ↑ sample space for X
 ↗ same but for Y

Joint densities and marginals

- (E, \mathcal{E}) and (F, \mathcal{F}) be measurable spaces;
- α a σ -finite positive measure on (E, \mathcal{E}) , and β a σ -finite positive measure on (F, \mathcal{F}) ;
- X an E -valued random variable and Y an F -valued random variable.

Assume the pair (X, Y) has a joint density $h(x, y)$ with respect to $\alpha \otimes \beta$, i.e.

$$dP(x, y) = h(x, y) d\alpha(x) d\beta(y).$$

↙ ↘ \hookrightarrow α im Radon-
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The marginal law of X is the (probability) density

$$f(x) = \int_F h(x, y) d\beta(y),$$

and the marginal law of Y is the (probability) density

$$g(y) = \int_E h(x, y) d\alpha(x).$$

Note: $\underbrace{\mathcal{E}}_{\alpha} \times \underbrace{\mathcal{F}}_{\beta}$
 $\alpha \otimes \beta(A \times B)$
 $= \alpha(A) \beta(B)$

Conditional density (continuous case)

Definition (conditional density for fixed x)

Assume $f(x) > 0$ for some $x \in E$. The conditional law of Y given $X = x$, denoted $\mathcal{L}(Y | X = x)$, is the probability measure on F with density (w.r.t. β)

$$g_x(y) = \frac{h(x, y)}{f(x)} = \frac{h(x, y)}{\int_F h(x, y) d\beta(y)}.$$

We may sometimes write $g(y | x)$ instead of $g_x(y)$ when there is no risk of confusion.

Remark

For points where $f(x) = 0$ we can define g_x arbitrarily (e.g. 0); these x typically form a set of $\mathcal{L}(X)$ -measure zero, so they do not affect integrals.

Random conditional density and joint density factorization

Random conditional density

By extension, we define the conditional density of Y given X as the random density

$$g_X(y) = g(y | X) = \begin{cases} \frac{h(X, y)}{f(X)}, & f(X) > 0, \\ 0, & f(X) = 0. \end{cases}$$

Since $f(X) > 0$ almost surely, one usually just writes

$$g_X(y) = \frac{h(X, y)}{f(X)}.$$

Conditional expectation via conditional density

Definition (conditional expectation)

Let $\varphi : F \rightarrow \mathbb{R}$ be measurable with $\mathbb{E}[\varphi(Y)] < \infty$. The conditional expectation of $\varphi(Y)$ given X is

$$\mathbb{E}[\varphi(Y) | X] = \int_F \varphi(y) g(y | X) d\beta(y).$$

This is a random variable measurable with respect to $\sigma(X)$.

Law of total expectation

For any measurable $\psi : E \times F \rightarrow \mathbb{R}$ such that $\psi(X, Y)$ is integrable,

$$\mathbb{E}[\psi(X, Y)] = \mathbb{E}[\mathbb{E}[\psi(X, Y) | X]].$$

In particular, if $\psi(X, Y) = \psi_1(X)\psi_2(Y)$ with integrable $\psi_1(X)$ and $\psi_2(Y)$, then

$$\mathbb{E}[\psi_1(X)\psi_2(Y)] = \mathbb{E}[\psi_1(X) \mathbb{E}[\psi_2(Y) | X]].$$

Conditional expectation as best L^2 predictor

Projection property (orthogonality)

In the previous setting, let Y be square integrable: $\mathbb{E}[Y^2] < \infty$. Then

$$\inf_{\varphi: E \rightarrow \mathbb{R}, \mathbb{E}[\varphi(X)^2] < \infty} \mathbb{E}[(Y - \varphi(X))^2] = \mathbb{E}[(Y - \mathbb{E}[Y | X])^2].$$

Thus $\mathbb{E}[Y | X]$ is the **best mean-square predictor** of Y among all (square integrable) functions of X .

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Thus $\mathbb{E}[Y | X]$ is the **best mean-square predictor** of Y among all (square integrable) functions of X .

Proof:

For any measurable $\varphi : E \rightarrow \mathbb{R}$ with $\mathbb{E}[\varphi(X)^2] < \infty$,

$$\mathbb{E}[(Y - \varphi(X))^2] = \mathbb{E}[(Y - \mathbb{E}[Y | X])^2] + \mathbb{E}[(\mathbb{E}[Y | X] - \varphi(X))^2].$$

The cross-term is zero because

$$\mathbb{E}[(Y - \mathbb{E}[Y | X])(\mathbb{E}[Y | X] - \varphi(X))] = \mathbb{E}[\mathbb{E}[Y - \mathbb{E}[Y | X] | X](\mathbb{E}[Y | X] - \varphi(X))] = 0.$$

Square integrability of $\mathbb{E}[Y | X]$

To justify the previous result we need $\mathbb{E}[\mathbb{E}[Y | X]^2] < \infty$.

By the conditional Jensen inequality,

$$\mathbb{E}[\mathbb{E}[Y | X]^2] \leq \mathbb{E}[\mathbb{E}[Y^2 | X]] = \mathbb{E}[Y^2] < \infty.$$

Hence $\mathbb{E}[Y | X]$ is square integrable and the projection property makes sense in L^2 .

Frequentist approach

In the frequentist approach, we assume that there exists a *true but unknown* parameter value $\theta_0 \in \Theta$ such that the data X follow the law P_{θ_0} :

$$\exists \theta_0 \in \Theta \quad \text{s.t.} \quad X \sim P_{\theta_0}.$$

Gaussian model

Let

$$X = (X_1, \dots, X_n), \quad \mathcal{P} = \{\mathcal{N}(\theta, 1)^{\otimes n} : \theta \in \mathbb{R}\}.$$

The frequentist assumption is that for some $\theta_0 \in \mathbb{R}$, the data are i.i.d. $\mathcal{N}(\theta_0, 1)$. One can then estimate θ_0 by the empirical mean \bar{X}_n ; by the law of large numbers, $\bar{X}_n \xrightarrow{\mathbb{P}} \theta_0$.

- **Estimation:** construct an estimator $\hat{\theta}(X)$ close to θ_0 .
- **Confidence sets:** build random sets $\mathcal{R}(X) \subset \Theta$ with $\theta_0 \in \mathcal{R}(X)$ with high probability under P_{θ_0} .
- **Tests:** answer "true/false" to a property of θ_0 via tests $\varphi(X) \in \{0, 1\}$.

Bayesian approach: intuition

In the Bayesian approach, **all unknown quantities** are modeled as random variables.

Prior and posterior

- Before observing data, our uncertainty about θ is described by a **prior distribution** Π_0 on Θ .
- After observing X , we update this prior using Bayes' formula to obtain the **posterior distribution** $\Pi(\cdot | X)$.

The posterior combines:

- prior knowledge (or belief) about θ ;
- the information contained in the data X .

Coin tossing: frequentist vs Bayesian view

Let $\theta \in [0, 1]$ be the probability of "heads".

- **Frequentist**: θ is fixed; with many tosses, the empirical frequency \bar{X}_n converges to θ (LLN, CLT).
- **Bayesian**: before any toss, we put a prior on θ (e.g. uniform on $[0, 1]$). Each new observation updates the prior to a posterior that reflects both prior belief and data.