Bayesian data analysis (Aalto fall 2024)

- Book: Gelman, Carlin, Stern, Dunson, Vehtari & Rubin: Bayesian Data Analysis, Third Edition. (online pdf available)
- The course website has more detailed information https://avehtari.github.io/BDA_course_Aalto/Aalto2024.html
- Timetable: see the course website
- TAs: David Kohns, Mélanie Guhl, Noa Kallioinen, Anna Riha, Varun Shanmugam, Maksim Sinelnikov, Teemu Säilynoja



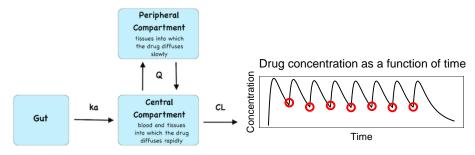
Uncertainty and decision making

• Predicting concrete quality



Uncertainty and decision making¹

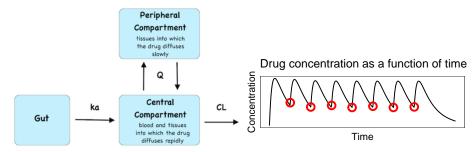
- Everolimus is immunosuppressant to prevent rejection of organ transplants
- Pharmacokinetic model of drug and body, optimal dosage depends on weight



¹with E. Siivola, Aalto and S. Weber, Novartis Pharma

Uncertainty and decision making¹

- Everolimus is immunosuppressant to prevent rejection of organ transplants
- Pharmacokinetic model of drug and body, optimal dosage depends on weight

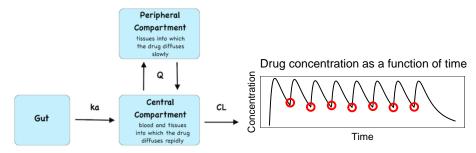


Model fitted with 500 adults, extrapolation to children?

¹with E. Siivola, Aalto and S. Weber, Novartis Pharma

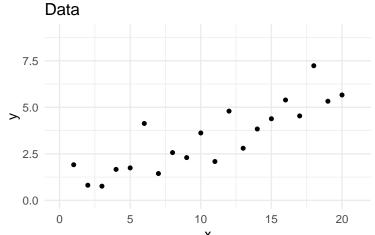
Uncertainty and decision making¹

- Everolimus is immunosuppressant to prevent rejection of organ transplants
- Pharmacokinetic model of drug and body, optimal dosage depends on weight

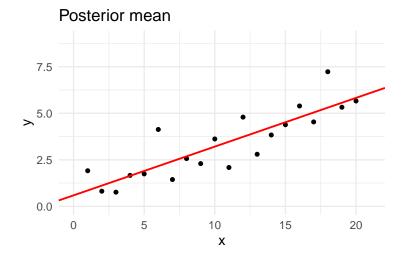


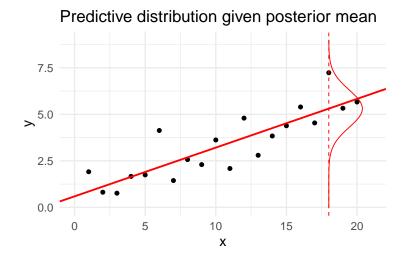
- Model fitted with 500 adults, extrapolation to children?
- Maturation effect, 17 observations from children

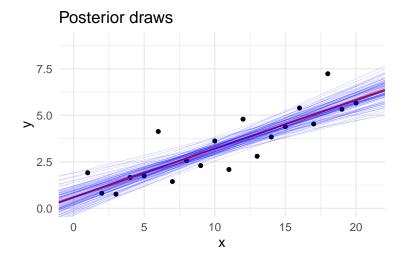
¹with E. Siivola, Aalto and S. Weber, Novartis Pharma

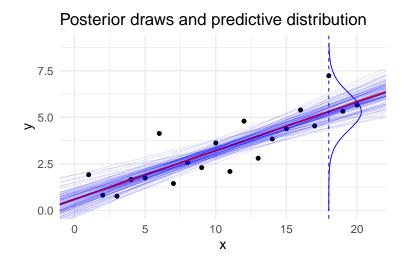


Х









expert information

```
expert information

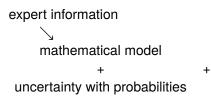
mathematical model

+

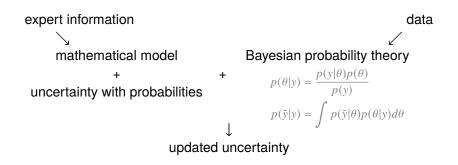
uncertainty with probabilities
```

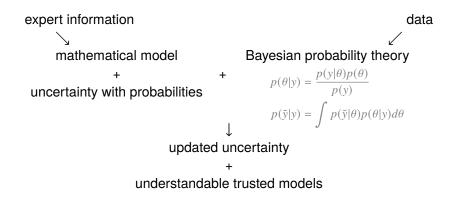
expert information $\overline{\ }$ mathematical model + uncertainty with probabilities

data



data Bayesian probability theory $p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$ $p(\tilde{y}|y) = \int p(\tilde{y}|\theta)p(\theta|y)d\theta$





Bayesian inference with computers

mathematical model to computer

probabilistic programming

computation, automatic inference algorithms

limitations of computers

Yes, but did it work?

computation + inference diagnostics

model diagnostics

limitations of mathematical models

improve and iterate

Bayesian Workflow

All the pieces put together

Probabilistic programming and Stan

Stan is a probabilistic programming framework and ecosystem 40+ developers, 100+ contributors, 200K+ users



mc-stan.org

Bayesian Data Analysis 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

Bayesian Data Analysis 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

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

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

Bayesian Data Analysis 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

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

- when analytic solutions are not available, computational approximations with finite number of function evaluations
- grid, importance sampling, Monte Carlo, Markov chain Monte Carlo
- Workflow
 - steps of model building, inference, and diagnostics

Impact on society

Better modelling and quantification of uncertainty

 \rightarrow better science

→ better informed decision making in companies, government, and NGOs

- 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, mathematician
 - considered the problem of *inverse probability*
 - significant part of the Bayesian 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, mathematician
 - considered the problem of inverse probability
 - significant part of the Bayesian theory
- Bayes did not invent all, but was first to solve problem of inverse probability in special case
- Modern Bayesian theory with rigorous proofs developed in 20th century

- 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, mathematician
 - considered the problem of inverse probability
 - significant part of the Bayesian theory
- Bayes did not invent all, but was first to solve problem of inverse probability in special case
- Modern Bayesian theory with rigorous proofs developed in 20th century
- A nice book about history: Sharon Bertsch McGrayne, *The Theory That Would Not Die*, 2012.

- 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)

- 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)
- 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

- 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)
- 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

- 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)
- 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

Uncertainty and probabilistic modeling

- Two types of uncertainty: aleatoric and epistemic
- Representing uncertainty with probabilities
- Updating uncertainty

Two types of uncertainty

• Aleatoric uncertainty due to randomness

• Epistemic uncertainty due to lack of knowledge

Two types of uncertainty

- Aleatoric uncertainty due to randomness
 - we are not able to obtain observations which could reduce this uncertainty
- Epistemic uncertainty due to lack of knowledge

Two types of uncertainty

- 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

Updating uncertainty

• Probability of red $\frac{\text{#red}}{\text{#red}+\text{#yellow}} = \theta$

• Probability of red
$$\frac{\text{#red}}{\text{#red}+\text{#yellow}} = \theta$$

• $p(y = \#red|\theta) = \theta$ aleatoric uncertainty

- Probability of red $\frac{\text{#red}}{\text{#red}+\text{#yellow}} = \theta$
- $p(y = \#red|\theta) = \theta$ aleatoric uncertainty
- $p(\theta)$ epistemic uncertainty

- Probability of red $\frac{\text{#red}}{\text{#red}+\text{#yellow}} = \theta$
- $p(y = \#red|\theta) = \theta$ aleatoric uncertainty
- $p(\theta)$ epistemic uncertainty
- Picking many chips updates our uncertainty about the proportion
- $p(\theta|y = \#red, \#yellow, \#red, \#red, ...) =?$

- Probability of red $\frac{\text{#red}}{\text{#red}+\text{#yellow}} = \theta$
- $p(y = \#red|\theta) = \theta$ aleatoric uncertainty
- $p(\theta)$ epistemic uncertainty
- Picking many chips updates our uncertainty about the proportion
- $p(\theta|\mathbf{y} = \# \text{red}, \# \text{yellow}, \# \text{red}, \# \text{red}, \ldots) = ?$

• Bayes rule
$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{\int p(y|\theta)p(\theta)d\theta}$$

Model vs. likelihood

- Bayes rule $p(\theta|y) \propto p(y|\theta)p(\theta)$
- Model: *p*(y|θ) as a function of y given fixed θ describes the aleatoric uncertainty
- Likelihood: *p*(*y*|θ) as a function of θ given fixed *y* provides information about epistemic uncertainty, but is not a probability distribution

Model vs. likelihood

- Bayes rule $p(\theta|y) \propto p(y|\theta)p(\theta)$
- Model: *p*(y|θ) as a function of y given fixed θ describes the aleatoric uncertainty
- Likelihood: *p*(*y*|*θ*) as a function of *θ* given fixed *y* provides information about epistemic uncertainty, but is not a probability distribution
- Bayes rule combines the likelihood with prior uncertainty $p(\theta)$ and transforms them to updated posterior uncertainty

The art of probabilistic modeling

 The art of probabilistic modeling is to describe in a mathematical form (model and prior distributions) what we already know and what we don't know

The art of probabilistic modeling

- The art of probabilistic modeling is to describe in a mathematical form (model and prior distributions) what we already know and what we don't know
- "Easy" part is to use Bayes rule to update the uncertainties
 - computational challenges

The art of probabilistic modeling

- The art of probabilistic modeling is to describe in a mathematical form (model and prior distributions) what we already know and what we don't know
- "Easy" part is to use Bayes rule to update the uncertainties
 - computational challenges
- Other parts of the art of probabilistic modeling are, for example,
 - model checking: is data in conflict with our prior knowledge?
 - presentation: presenting the model and the results to the application experts

• Drop a ball from different heights and measure time

- Drop a ball from different heights and measure time
 - Newton
 - air resistance, air pressure, shape and surface structure of the ball
 - relativity

- Drop a ball from different heights and measure time
 - Newton
 - air resistance, air pressure, shape and surface structure of the ball
 - relativity
- Taking into account the accuracy of the measurements, how accurate model is needed?

- Drop a ball from different heights and measure time
 - Newton
 - air resistance, air pressure, shape and surface structure of the ball
 - relativity
- Taking into account the accuracy of the measurements, how accurate model is needed?
 - often simple models are adequate and useful
 - All models are wrong, but some of them are useful, George P. Box

Reminder: Uncertainty and probabilistic modeling

- Two types of uncertainty: aleatoric and epistemic
- Representing uncertainty with probabilities
- Updating uncertainty

Chapter 1

Reading instructions

- 1.1-1.3 important terms
- 1.4 a useful example
- 1.5 foundations
- 1.6 & 1.7 examples (can be skipped, but may be useful to read)
- 1.8 & 1.9 background material, good to read before doing the exercises
- 1.10 a point of view for using Bayesian inference

Part of the assignment 1

Refresh your memory on these concepts!

- probability
- probability density
- probability mass
- probability density function (pdf)
- probability mass function (pmf)
- probability distribution
- discrete probability distribution
- continuous probability distribution
- cumulative distribution function (cdf)
- likelihood
- Bayes rule

Ambiguous notation in statistics

Find this in the Chapter 1 reading instructions on the course web page! In $p(y \mid \theta)$

- y can be variable or value
 - we could clarify by using $p(Y \mid \theta)$ or $p(y \mid \theta)$
- θ can be variable or value
 - we could clarify by using $p(y \mid \Theta)$ or $p(y \mid \theta)$
- p can be a discrete or continuous function of y or θ we could clarify by using P_Y, P_{Θ}, p_Y or p_{Θ}
- $P_Y(Y \mid \Theta = \theta)$ is a probability mass function, sampling distribution, observation model
- $P(Y = y | \Theta = \theta)$ is a probability
- $P_{\Theta}(Y = y \mid \Theta)$ is a likelihood function (can be discrete or continuous)
- $p_Y(Y \mid \Theta = \theta)$ is a probability density function, sampling distrbution, observation model
- $p(Y = y | \Theta = \theta)$ is a density
- $p_{\Theta}(Y = y \mid \Theta)$ is a likelihood function (can be discrete or continuous)
- y and θ can also be mix of continuous and discrete
- due to the sloppines sometimes likelihood is used to refer $P_{Y,\theta}(Y \mid \Theta), p_{Y,\theta}(Y \mid \Theta)$

• Pick a number between 1–5

- Pick a number between 1–5
 - raise as many fingers

- Pick a number between 1–5
 - raise as many fingers
 - is the number of fingers raised random (by you or by others)?

- Pick a number between 1–5
 - raise as many fingers
 - is the number of fingers raised random (by you or by others)?
- If we build a robot with very fast vision which can observe the rotating coin accurately, is the throw random for the robot?

- Pick a number between 1–5
 - raise as many fingers
 - is the number of fingers raised random (by you or by others)?
- If we build a robot with very fast vision which can observe the rotating coin accurately, is the throw random for the robot?
- What is your own example with both aleatoric and epistemic uncertainty?