Probabilistic Modeling and Reasoning The Role of Uncertainty in Machine Learning

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ATHENA RC — HUA

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Program

- Course Overview
- 2 The Role of Uncertainty in Machine Learning
- Probabilistic Modeling and Reasoning
- 4 Key Rules of Probability
- Recap & What's Next

Course objective

Be able to apply probabilistic models to real-world problems.

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Be able to apply probabilistic models to real-world problems.

Be able to apply Bayesian models to real-world problems.

Course Overview

Course structure

- \bullet 6 sessions \times 1.5 hours
- Each session consists of:
 - ► Lecture (45') 30' lecture + 15' discussion
 - Exercises (45') 20' you work on exercises, 25' discussion
 - Either pen-and-paper or in R

Course material

- Slides, exercises and R code available on course website https://www.github.com/givasile/BAC
- Solutions to exercises will be provided after each session

Course Overview

Bridging Theory and Practice

- Sessions 1-3: Foundational concepts of Bayesian modeling
- Sessions 4-6: Application on regression and classification problems
- Session 1: Probabilistic Modeling and Reasoning
 - The Role of Uncertainty in Machine Learning
 - Probabilistic Modeling and Reasoning
 - Key Rules of Probability
- Session 2: Probabilities and Random Variables
 - Random Variables and Probability Distributions
 - Key properties: Expectation, Variance, Covariance
- Session 3: Bayesian Modeling: A Unified Framework
 - Probabilistic vs. Statistical vs. Bayesian Modeling
 - Prior, Posterior, Likelihood, Predictive Posterior



Course Overview

Bridging Theory and Practice

- Sessions 1-3: Foundational concepts of Bayesian modeling
- Sessions 4-6: Application on regression and classification problems
- Session 4: Bayesian Linear Regression
 - Linear Regression as a Probabilistic Model
 - Exact Inference with Conjugate Priors
- Session 5: Bayesian Logistic Regression
 - Logistic Regression as a Probabilistic Model
 - Approximate Inference:
 - ★ Laplace Approximation
 - ★ Importance Sampling
 - **★** MCMC
- Session 6: Real-world problem
 - Summary of all concepts
 - Application on a real-world problem

Material used in this course

This course is highly inspired (some parts are copied verbatim) from the following sources:

- Probabilistic Modeling and Reasoning
 University of Edinburgh, School of Informatics
 https://opencourse.inf.ed.ac.uk/pmr/course-material
- Machine Learning and Pattern Recognition
 University of Edinburgh, School of Informatics
 https://mlpr.inf.ed.ac.uk/2024/
- BayesRules book https://bayesrulesbook.com/
- Multivariate Statistics https://11annah-s-teachings.github.io/
- Mathematics of Machine Learning https://mml-book.github.io/

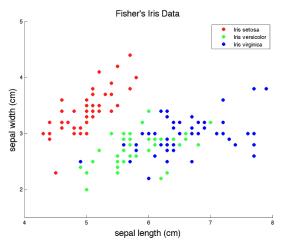


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Variability

- Variability is part of nature.
- Data for 3 species of iris, from Ronald Fisher (1936).



Variability

- Our handwriting is unique
- ullet Variability leads to uncertainty: e.g., distinguish $\{1,7\}$ and $\{4,9\}$

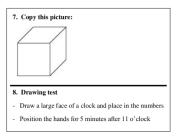
Variability

- ullet Variability $\stackrel{\text{leads to}}{\longrightarrow}$ uncertainty $\stackrel{\text{asks for}}{\longrightarrow}$ probabilistic modeling
- Reading handwritten text in a foreign language.



Example: Screening and Diagnostic Tests

- Early warning test for Alzheimer's disease (Scharre, 2010, 2014)
- Detects 'mild cognitive impairment'
- Takes 10–15 minutes
- Freely available
- Assume a 70-year-old man tests positive
- Should he be concerned?

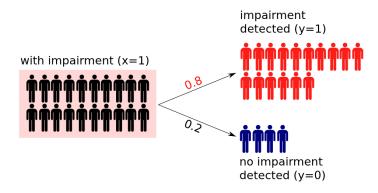


(Example from sagetest.osu.edu)



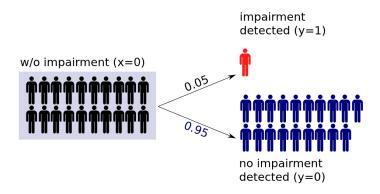
Accuracy of the Test

- Sensitivity of 0.8 and specificity of 0.95 (Scharre, 2010).
- 80% correct for people with impairment.



Accuracy of the Test

- Sensitivity of 0.8 and specificity of 0.95 (Scharre, 2010).
- 95% correct for people without impairment.



Variability Implies Uncertainty

- People of the same group do not have the same test results
 - ▶ Test outcome is subject to variability.
 - ► The data are noisy.
- Variability leads to uncertainty.
 - ▶ Positive test ≡ true positive?
 - Positive test ≡ false positive?
- What can we safely conclude from a positive test result?
- How should we analyze such ambiguous data?

Probabilistic Approach

- $P(y \mid x)$: model of the test specified in terms of (conditional) probabilities.
- $x \in \{0,1\}$: quantity of interest (cognitive impairment or not).
- $y \in \{0,1\}$: test outcome (negative or positive).
- The test outcomes y can be described with probabilities:
 - ► Sensitivity = 0.8

$$\star \Rightarrow P(y = 1 | x = 1) = 0.8$$

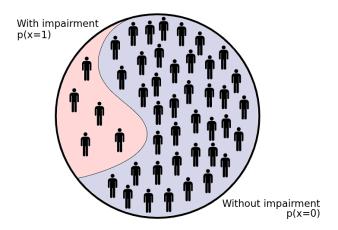
$$\star \Rightarrow P(y=0 \mid x=1) = 0.2$$

- ► Specificity = 0.95
 - $\star \Rightarrow P(y = 0 | x = 0) = 0.95$
 - $\star \Rightarrow P(y=1 \mid x=0) = 0.05$



Prior Information

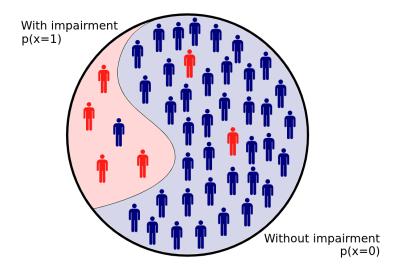
• Among people like the patient, $P(x=1) = \frac{5}{45} \approx 11\%$ have a cognitive impairment (plausible range: 3% - 22%, Geda, 2014).



Probabilistic Model

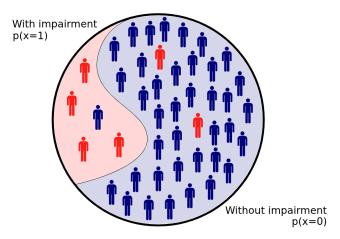
- Reality:
 - Properties/characteristics of the group of people like the patient
 - Properties/characteristics of the test
- Probabilistic model:
 - P(x = 1): probability of cognitive impairment
 - ▶ P(y = 1|x = 1) or P(y = 0|x = 1): probability of positive or negative test given cognitive impairment
 - ▶ P(y = 1|x = 0) or P(y = 0|x = 0): probability of positive or negative test given no cognitive impairment
 - Fully specified by three numbers.
- A probabilistic model is an abstraction of reality that uses probability theory to quantify the chance of uncertain events.





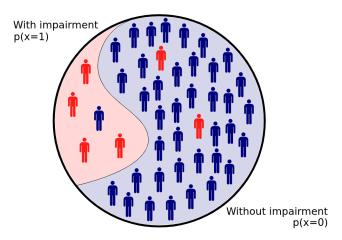
• Fraction of people who are impaired and test positive:

$$P(x = 1, y = 1) = P(y = 1 | x = 1)P(x = 1) = 0.8 \cdot \frac{5}{45} = \frac{4}{45} \approx 9\%$$



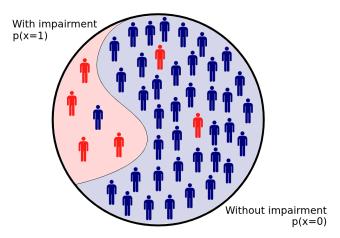
• Fraction of people who are not impaired and test positive:

$$P(x = 0, y = 1) = P(y = 1|x = 0)P(x = 0) = 0.05 \cdot \frac{40}{45} = \frac{2}{45} \approx 4\%$$



• Fraction of people where the test is positive:

$$P(y = 1) = P(x = 1, y = 1) + P(x = 0, y = 1) = \frac{4}{45} + \frac{2}{45} = \frac{6}{45} \approx 13\%$$



Putting Everything Together

• Among those with a positive test, fraction with impairment:

$$P(x = 1|y = 1) = \frac{P(y = 1|x = 1)P(x = 1)}{P(y = 1)} = \frac{4}{6} = \frac{2}{3}$$

Fraction without impairment:

$$P(x = 0|y = 1) = \frac{P(y = 1|x = 0)P(x = 0)}{P(y = 1)} = \frac{2}{6} = \frac{1}{3}$$

- Equations are examples of Bayes' rule.
- Positive test increased probability of cognitive impairment from 11% (prior belief) to 67%, or from 6% to 51%.
- 51% (coin flip)



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Probabilistic Modeling and Reasoning

 Bayesian analysis is probabilistic modeling and reasoning using Bayes' rule.

Probabilistic modeling:

- Model the world (events) using probabilities and random variables.
- Example random variables:
 - ★ y: test outcome
 - * x: cognitive impairment

Probabilistic reasoning (inference):

- Compute probabilities of events given other events.
- Infer probabilities of unobserved events from observed data.
- Use Bayes' rule to update beliefs based on evidence.

Probabilistic Modeling and Reasoning

- In our example:
 - ▶ Unobserved/uncertain event: cognitive impairment x = 1
 - ▶ Observed event (evidence): test result y = 1
 - **Prior**: probability before seeing evidence, e.g., P(x = 1)
 - **Posterior**: updated probability after evidence, e.g., P(x = 1|y = 1)
- Key idea: The posterior quantifies what we believe about x after seeing the test result y.

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Key Rules of Probability

Product rule:

- P(x = 1, y = 1) = P(y = 1|x = 1)P(x = 1)
- P(x = 1, y = 1) = P(x = 1|y = 1)P(y = 1)
- Sum rule:
 - P(y=1) = P(x=1, y=1) + P(x=0, y=1)
- Bayes' rule (conditioning) as consequence of product rule:

$$P(x=1|y=1) = \frac{P(x=1,y=1)}{P(y=1)} = \frac{P(y=1|x=1)P(x=1)}{P(y=1)}$$

Denominator from sum rule and product rule:

$$P(y=1) = P(y=1|x=1)P(x=1) + P(y=1|x=0)P(x=0)$$

Key Rules of Probability

- The rules generalize to multivariate random variables
 - $\mathbf{x} = (x_1, x_2, \ldots)$: vector of random variables
 - $\mathbf{y} = (y_1, y_2, \ldots)$: vector of random variables
- The rules generalize to continuous random variables
- Product rule:
 - $P(\mathbf{x},\mathbf{y}) = P(\mathbf{y}|\mathbf{x})P(\mathbf{x})$
 - $P(\mathbf{x}, \mathbf{y}) = P(\mathbf{x}|\mathbf{y})P(\mathbf{y})$
- Sum rule:
 - $P(y) = \sum_{x} P(x, y)$ (discrete case)
 - ▶ $P(y) = \int P(x, y) dx$ (continuous case)

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Recap & What's Next

Recap:

- Probabilistic Modeling:
 - ► The art of quantifying real-world phenomena with probabilities.
 - Example: Diagnosing Alzheimer's with a medical test.
- Probabilistic Reasoning (Inference):
 - Infer probabilities of unobserved events from observed data.
- Bayesian Analysis:
 - Bayes' rule updates our beliefs with new evidence.
 - Applied in the Alzheimer's test case.
- Core Probability Rules:
 - Product rule, Sum rule, Bayes' rule.
 - ▶ These simple rules help us make informed conclusions.

Next Session: Dive deeper into probabilities and random variables.

Complex phenomena require high dimensional random variables.