Advanced probabilistic methods

Lecture 1

Pekka Marttinen

Aalto University

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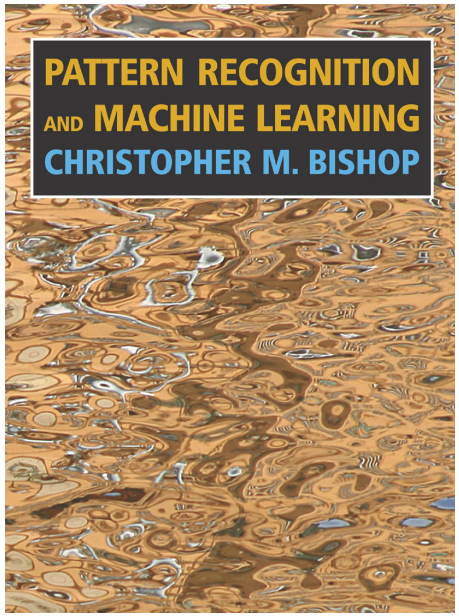
Lecture 1 overview

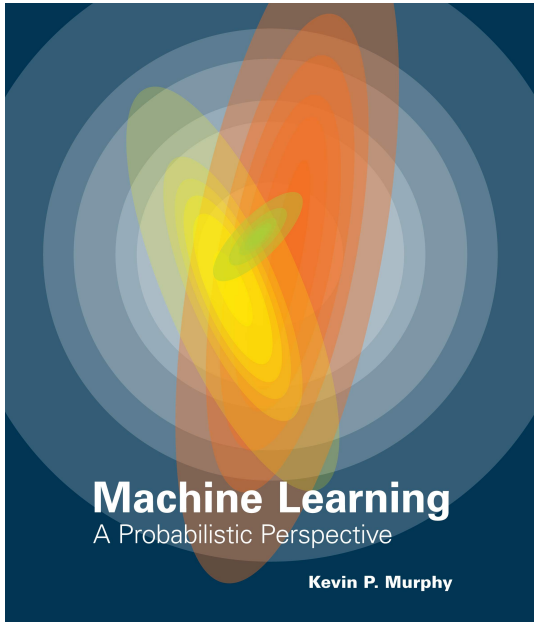
- Practical matters
  - Structure, grading, workload
  - Exercise format
  - Student feedback from previous years
- Course overview
- Basic probability calculus (Barber, Ch. 1)
- Basic graph concepts

Course structure

- Structure
  - Lectures 10×2 hours
  - Exercise sessions 9×2 hours
  - See *Timetable* in *myCourses/Lectures*
- Grading is based on the better of the following:
  - Exam (64%) + assignments (36%)
  - Exam (100%)
- *Preliminary* boundaries: 1:50%, 2:60%, 3:70%, 4:80%, 5:90%

Course books





- *Bayesian Reasoning and Machine Learning* available at *www.cs.ucl.ac.uk/staff/D.Barber/brml*
- *Pattern Recognition and Machine Learning* available at *www.microsoft.com/en-us/research/people/cmbishop/*

Estimated workload

- Lectures: 10×2h
- Preparation for lectures, reading the book (~ 200 pages): 9×4h
- Exercise sessions: 9×2h
- Doing the exercises: 9×5h
- Preparing for the exam: 12h
- Exam: 4h
- Total 135h. As credits $135/27 = 5$cr.

Implementation

- Lectures are given in-person.
- Previous years' recordings can be found in *MyCourses / Extra Materials*
  - These cover all the main topics.
- The course has a Slack workspace which is intended mainly for discussions about exercises
  - A link to Slack can be found in *MyCourses / General.*
  - See more information in the next slides.
- Important announcements will be posted in MyCourses

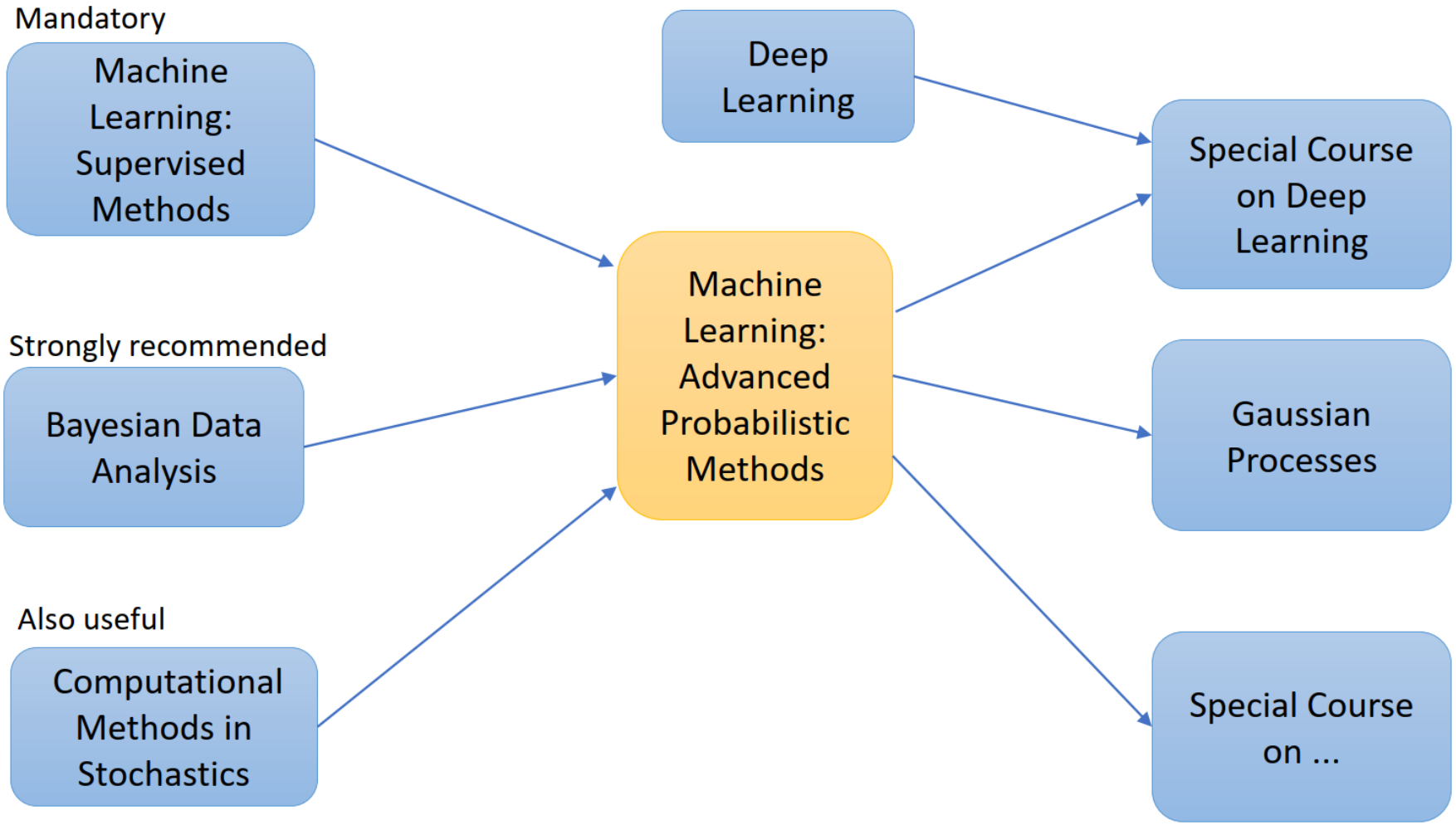
Exercises

- Exercises must be returned by the deadline using JupyterHub.
  - See instructions in *MyCourses / Assignments*.
  - Grading principle: **2p**→done, almost correct; **1p**→done, but something clearly missing/incorrect; **0p**→not done or completely incorrect (may be modified case-by-case).
  - Exercises are graded by the TAs, not corrected → Make sure you know the correct answer afterwards by attending the exercise sessions or checking the model solutions.
- Exercise session format
  - Help for getting started with next week's exercises
  - Possibility to ask about next week's exercises or previous week's solutions
  - Two assistants present

Exercises

- Slack
  - You can write questions and comments about exercises in dedicated Slack channels.
  - Students are encouraged to answer and give hints to each other's questions in the Slack; however, do not reveal the full answer.
  - The TAs will participate in the discussions at the times of the exercise sessions (and possibly at other times, see details in MyCourses)
- Other policies
  - Collaborating with your colleagues to solve the exercises is allowed and encouraged, but in the end you are expected to write your own solution (copy-paste from someone else is not allowed and will be checked for).
  - Sharing solutions online or the use of any such materials is prohibited. Suspected violations will be reported for further investigation.

Relation to other courses



Student feedback from previous years

- About prerequisites
  - *'Bayesian Data Analysis should be listed as a prerequisite'*
    $\rightarrow$See previous slide.
- About lectures
  - '*One of the courses where lecture attendance is really beneficial, I would definitely point this out in the intro lecture as students are trying to optimize their time between other lectures and exercise sessions*'
  - '*All lectures could be recorded*'
    $\rightarrow$Recordings from previous years are provided.

Student feedback from previous years

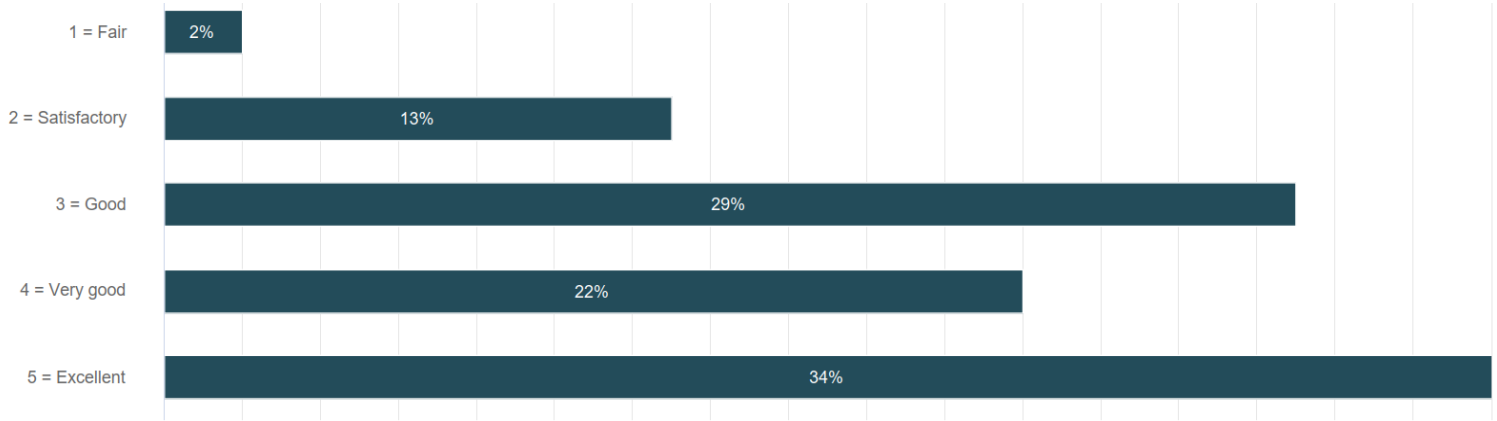
- About exercises (positive)
  - *'Participating in the exercise sessions was extremely useful and the course assistants were great'*
  - *'The exercises really helped me to understand the concepts related to this course, and I think that they played a huge role in my learning'*
  - *'The exercise sessions were very good. Without them I would never have been able to achieve that far.'*
- About exercises (things to improve)
  - *'A slack group would have been useful'*
    $\rightarrow$This exists now.

Student feedback from previous years

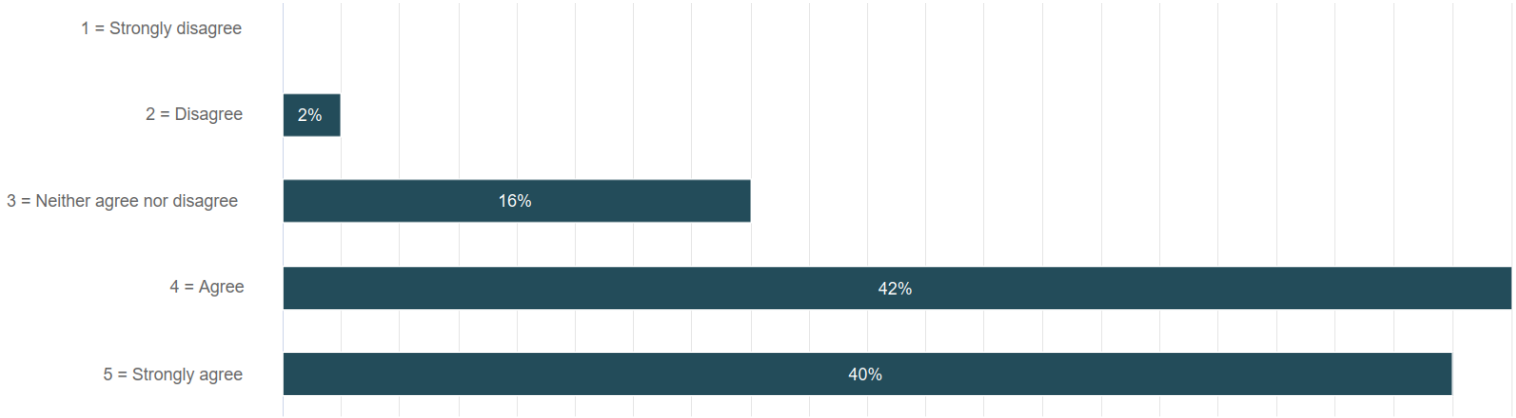
- About difficulty in general
  - *'At least to me there was steep curve in the topic difficulty starting from lecture 5. Compress lectures 1-4 and spend more time on the "new stuff"*
    $\rightarrow$Some changes in the material to this direction.
    $\rightarrow$Take a full advantage of the Exercise sessions (also and especially on the 2nd half).
    $\rightarrow$Ask clarifications and participate in discussions in the Slack.
- About contents
  - '*Add a small project*'
    $\rightarrow$We used to have one, but dropped that to keep the workload manageable.
  - '*How were these topics are chosen? Does the course aim to practical work life skills, or prepare for research career or is it just general background knowledge?*'
    $\rightarrow$See slides *Course contents*, *Course outline* and *What to expect* below.

Student feedback from 2022, overview

- Overall assessment

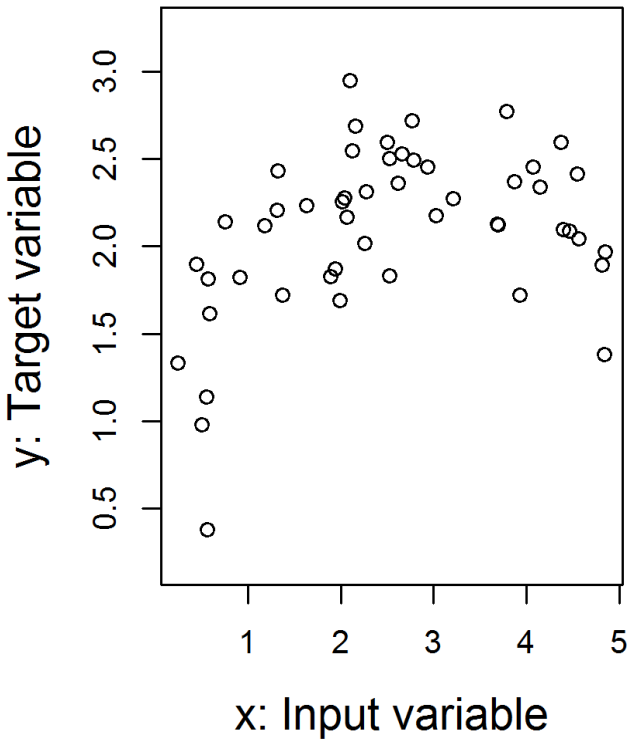


- I will benefit from things learnt on the course



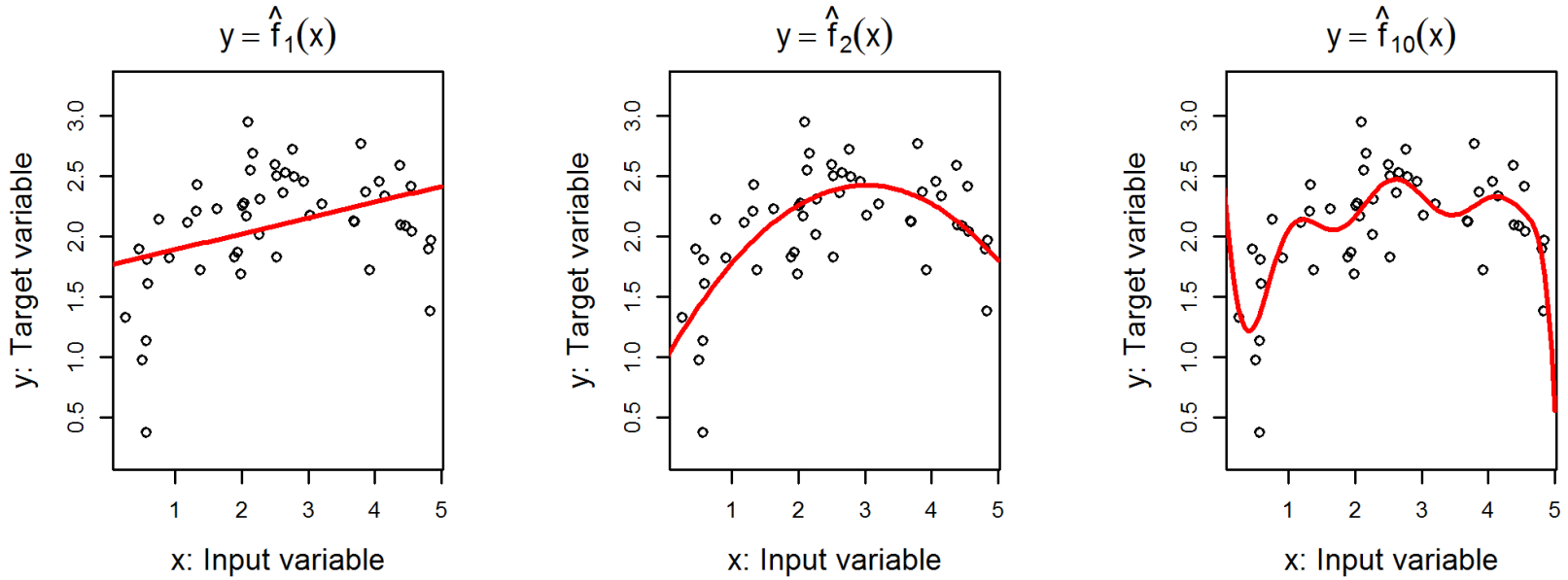
Probabilistic modeling overview (1/2)

- The goal of **probabilistic modeling** is to answer a question about the data:
  - Classify the samples into groups
  - Create prediction for future observations
  - Select between competing hypotheses
  - Estimate a parameter, such as the mean, of the population
  - ...
- and **quantify uncertainty** using probabilities.



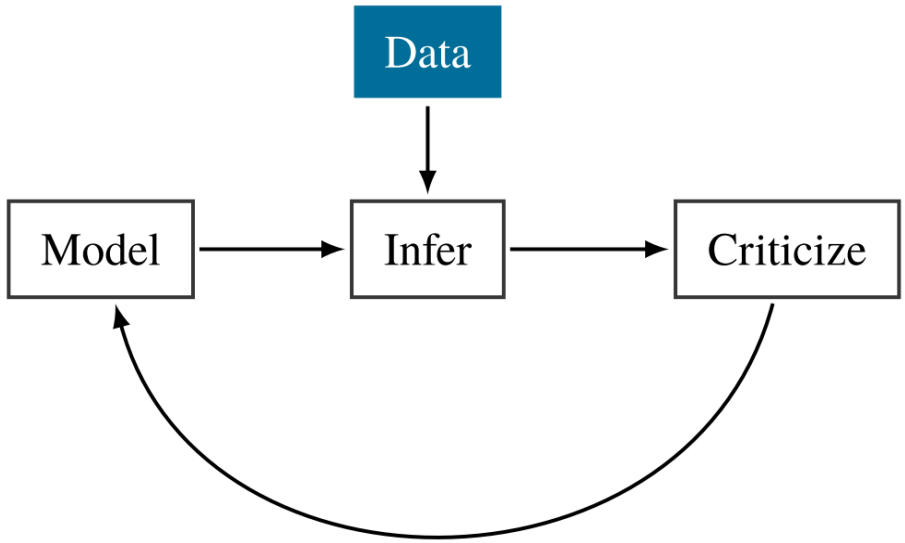
Probabilistic modeling overview (2/2)

- Probabilistic modeling in a nutshell
  1. Select a **model**
  2. **Infer** the parameters of the model (train/fit the model)
  3. Use the fitted model to answer the question of interest
- Usually several models are considered, requiring **model selection**.
- For example: $f_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$



Course contents

- Ingredients of probabilistic modeling
  - **Models**: Bayesian networks, Sparse Bayesian linear regression, Gaussian mixture models, latent linear models
  - **Methods for inference**: maximum likelihood, maximum a posteriori (MAP), Laplace approximation, expectation maximization (EM), Variational Bayes (VB), Stochastic variational inference (SVI)
  - **Ways to select between models**



Box's loop (Blei, 2014)

Course outline

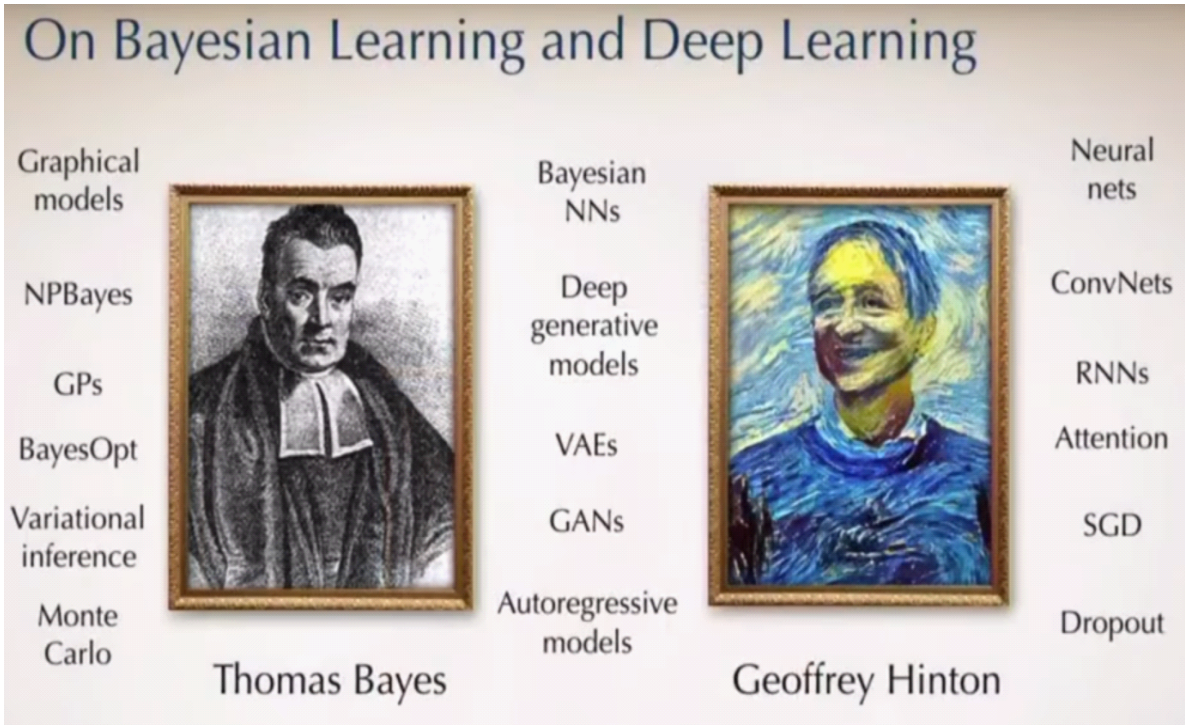
- "Probabilistic Modelling Course" (the last column) from the preface of Barber's book is used as the backbone. Deterministic approximate inference techniques (28) have been added to this, and correspondingly less weight is given to some other topics.

What to expect on the course

- More emphasis on
  - fundamental principles of probabilistic modeling and machine learning
  - introducing simple models that serve as building blocks for more complex (or realistic) models
  - building a detailed understanding of the algorithms through simple examples, which allows us to focus on the principles
  - enhancing mathematical skills to operate with probabilities
- Less emphasis on
  - hands-on learning on how to use a specific software package to fit 'advanced' models to a real-world data set (though we'll use *PyTorch* in some exercises to show how things are *nowadays* done 'in real life')
- Goal
  - knowledge needed to start understanding and applying probabilistic modeling using existing software packages, and those to come

Role of probabilistic machine learning today

- Keynote at *NeurIPS 2017* by Yee Whye Teh



https://www.youtube.com/watch?v=9saauSBgmcQ

- *NeurIPS 2020*: articles with a keyword in the title: *Bayes* (n=63), *Uncertainty* (n=18), *Variational* (n=36). Many of these coming from the major IT companies.

Probability theory, basics

- Marginalization
- Independence
- Conditional distribution
- Conditional independence
- Continuous random variables

(To recap these, see *Additional Reading* in *myCourses/Materials*)

Notation (1/2)

- Random variables: $X, Y, Z, \ldots$
- Values these random variables can take: $x, y, z, \ldots$
- Probability
  - The following notations are used interchangeably

$$p(X = x) = p_X(x) = p(x)$$

  - All are interpreted as the probability that variable X is in state x

Notation (2/2)

- Domain
  - $dom(X)$ denotes all possible states for variable X.
- Distribution of a variable X consists of
  - its domain $dom(X)$
  - and full specification of probability values $p_X(x)$, for all possible $x \in dom(X)$
- Normalization
  - The summation over all the states

$$\sum_{x \in dom(X)} p(X = x) = 1$$

  - The sum can be written as: $\sum_x p(x) = 1$

Example - probability table

B	M	K	$p(b, m, k)$
1	1	1	0.012
1	1	0	0.108
1	0	1	0.288
1	0	0	0.192
0	1	1	0.016
0	1	0	0.064
0	0	1	0.096
0	0	0	0.224

- The probability table lists the probabilities of all possible combinations of the random variables.
- The *joint* distribution of B, M and K
- For example

$$p_{B,M,K}(1,1,0) = p(B=1, M=1, K=0) = 0.108$$

- Modified from Example 1.3 "Inspector Clouseau"
  M ='Maid is the murderer'
  B ='Butler is the murderer'
  K ='Knife is the murder weapon'

Marginalization

- Given a joint dist $p_{X,Y}(x, y)$, the marginal dist of X is defined by

$$p_X(x) = \sum_y p_{X,Y}(x, y)$$

- More generally,

$$p(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) = \sum_{x_i} p(x_1, \ldots, x_n)$$

Example - marginalization (1/2)

B	M	K	$p(b, m, k)$
1	1	1	0.012
1	1	0	0.108
1	0	1	0.288
1	0	0	0.192
0	1	1	0.016
0	1	0	0.064
0	0	1	0.096
0	0	0	0.224

- What is the marginal distribution of B and M?
- We need to compute $p_{B,M}(b, m)$, for all possible b and m.

Example - marginalization (2/2)

- Use

$$p_{B,M}(b,m) = \sum_{k=0}^{1} p_{B,M,K}(b,m,k)$$

- For example:

$$\begin{aligned} p_{B,M}(0,0) &= p_{B,M,K}(0,0,0) + p_{B,M,K}(0,0,1) \\ &= 0.096 + 0.224 = 0.32 \end{aligned}$$

- Doing this for all B, M combinations, we get the marginal probability table

B	M	$p(b,m)$
1	1	0.12
1	0	0.48
0	1	0.08
0	0	0.32

Independence

- Random variables X and Y are independent if

$$p_{X,Y}(x,y) = p_X(x)p_Y(y)$$

  for all x and y.
- Intuitively, this means that knowing the value of X does not provide any information about the value of Y.
- Notation: $X \perp\!\!\!\perp Y$
- More generally: $\mathcal{A} = \{A_1, \ldots, A_k\}$ and $\mathcal{B} = \{B_1, \ldots, B_l\}$ are independent if

$$\begin{aligned} &p_{A_1,\ldots,A_k,B_1,\ldots,B_l}(a_1, \ldots, a_k, b_1, \ldots, b_l) \\ &= p_{A_1,\ldots,A_k}(a_1, \ldots, a_k)p_{B_1,\ldots,B_l}(b_1, \ldots, b_l) \end{aligned}$$

Example - Independence (1/2)

B	M	$p(b, m)$
1	1	0.12
1	0	0.48
0	1	0.08
0	0	0.32

- Are B and M independent?

Example - Independence (2/2)

- Marginal distributions

B	$p(b)$
1	0.6
0	0.4

and

M	$p(m)$
1	0.2
0	0.8

- Direct computation gives

B	M	$p(b)p(m)$	$p(b,m)$
1	1	0.12	0.12
1	0	0.48	0.48
0	1	0.08	0.08
0	0	0.32	0.32

- Hence, B and M are (marginally) independent

Statistical vs. causal independence

- D='number of people drowned', A='amount of ice-cream sold'
  - Are D and A independent?
  - Are D and A causally dependent?

Conditional distribution

- Conditional distribution

$$p_{X|Y}(x|y) = \frac{p_{X,Y}(x,y)}{p_Y(y)}$$

specifies the probability of each possible value x of X given that we have observed variable Y in state y.

Example - Conditional distribution

- For example:

$$p(K = 1|B = 1, M = 1) = \frac{p(B = 1, M = 1, K = 1)}{p(B = 1, M = 1)} = 0.1$$

$$p(K = 0|B = 1, M = 1) = 0.9$$

- All conditional probabilities in the last column

B	M	K	$p(b, m, k)$	$p(k\|b, m)$
1	1	1	0.012	0.1
1	1	0	0.108	0.9
1	0	1	0.288	0.6
1	0	0	0.192	0.4
0	1	1	0.016	0.2
0	1	0	0.064	0.8
0	0	1	0.096	0.3
0	0	0	0.224	0.7

Conditional independence

- $X \perp\!\!\!\perp Y|Z$ denotes that variables X and Y are conditionally independent of each other, given the state of variable Z. This is formally defined by condition

$$p_{X,Y|Z}(x, y|z) = p_{X|Z}(x|z)p_{Y|Z}(y|z)$$

  for all states x, y, z of variables X, Y, Z.
- Intuitively, this means that if we know the value of Z, knowing in addition the value of Y does not provide any information about the value of X. Indeed, provided $p(y, z) > 0$, we have

$$X \perp\!\!\!\perp Y|Z \Longrightarrow p_{X|Y,Z}(x|y, z) = p_{X|Z}(x|z)$$

Conditional independence

$$X \perp\!\!\!\perp Y|Z \implies p_{X|Y,Z}(x|y,z) = p_{X|Z}(x|z)$$

- Proof

$$\begin{aligned} p(x|y,z) &= \frac{p(x,y,z)}{p(y,z)} = \frac{p(x,y|z)p(z)}{p(z)p(y|z)} \\ &= \frac{p(x|z)p(y|z)p(z)}{p(z)p(y|z)} = p(x|z) \end{aligned}$$

- The general *chain rule of probability*

$$p(x,y,z) = p(x|y,z)p(y|z)p(z),$$

follows from iterative use of the definition of conditional probability.

Example - Conditional independence (1/3)

B	M	K	$p(b, m, k)$
1	1	1	0.012
1	1	0	0.108
1	0	1	0.288
1	0	0	0.192
0	1	1	0.016
0	1	0	0.064
0	0	1	0.096
0	0	0	0.224

- Are M and B conditionally independent, given K?
- We need to compare
  - $p_{M|K}(m|k)p_{B|K}(b|k)$
  - $p_{B,M|K}(b, m|k)$

  for all m, b, k.

Example - Conditional independence (2/3)

- For example,

$$p(B=1, M=1|K=1) = \frac{p(B=1, M=1, K=1)}{p(K=1)}$$
$$= \frac{0.012}{0.012 + 0.288 + 0.016 + 0.096} \approx 0.0291$$

- Similarly,

$$p(M=1|K=1) = \frac{p(M=1, K=1)}{p(K=1)}$$
$$= \frac{0.012 + 0.016}{0.012 + 0.288 + 0.016 + 0.096} \approx 0.0508$$

and

$$p(B=1|K=1) = \ldots \approx 0.7110$$

Example - Conditional independence (3/3)

B	M	K	$p(b,m\|k)$	$p(b\|k)$	$p(m\|k)$	$p(b\|k)p(m\|k)$
1	1	1	**0.029**	**0.711**	**0.051**	**0.036**
0	1	1	...	...	...	...
1	0	1				
0	0	1				
1	1	0				
0	1	0				
1	0	0				
0	0	0				

- Because $0.029 \neq 0.036$, it follows that B and M are not conditionally independent given K.

Intuition for independence and conditional independence (1/2)

- Let $X_1, X_2, \ldots, X_n$ denote the cumulative sum of n dice throws, such that $dom(X_1) = \{1, \ldots, 6\}$, $dom(X_2) = \{2, \ldots, 12\}$, etc.
  - Is X_{n+1} independent of X_{n-1}?
  - Is X_{n+1} conditionally independent of X_{n-1} given X_n?
- X='Location of an airplane now', Y='Location of the plane 15s ago', Z='Location 15s from now'
  - Is Y independent of Z?
  - Is Y conditionally independent of Z given X?

Intuition for independence and conditional independence (2/2)

- S='sunshine', D='number of people drowned', A='amount of ice-cream sold'
  - Are D and A independent?
  - Are D and A conditionally independent given S?
- A='The alarm is on', B=There is a burglar in the house", T='A truck passes the house'
  - Suppose that the alarm can be triggered either by a burglar or by a passing truck
  - Are B and T independent?
  - Are B and T conditionally independent given A

Continuous random variables (1/3)

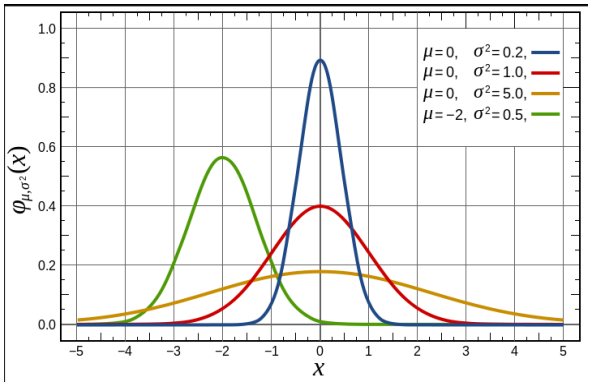
- Probability density function (pdf) for a continuous variable X, $f_X()$

$$\int_{x \in \mathcal{R}} f_X(x)dx = 1$$

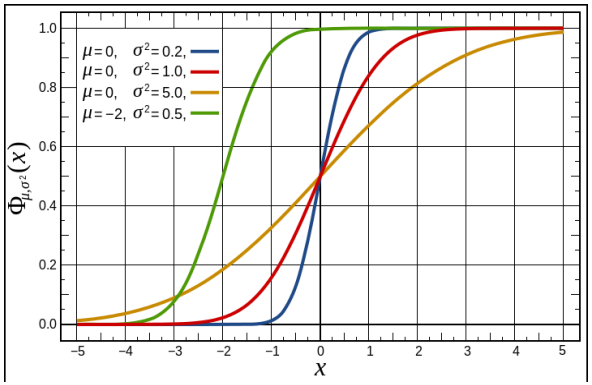
$$p(X \in [a, b]) = \int_{x=a}^{b} f_X(x)dx$$

- Cumulative distribution function (cdf)

$$F_X(x) = p(X \leq x) = \int_{t=-\infty}^{x} f_X(t)dt$$



$N(\mu, \sigma^2)$ pdf (Wikip.)



$N(\mu, \sigma^2)$ cdf (Wikip.)

Continuous random variables (2/3)

- Concepts presented can be generalized to continuous random variables
- Marginalization
  - Discrete: $p_X(x) = \sum_y p_{X,Y}(x, y)$
  - Continuous: $f_X(x) = \int_y f_{X,Y}(x, y)dy$
- Expected value
  - Discrete: $E(X) = \sum_x x\, p_X(x)$
  - Continuous: $E(X) = \int_x x\, f_X(x)\, dx$

Continuous random variables (3/3)

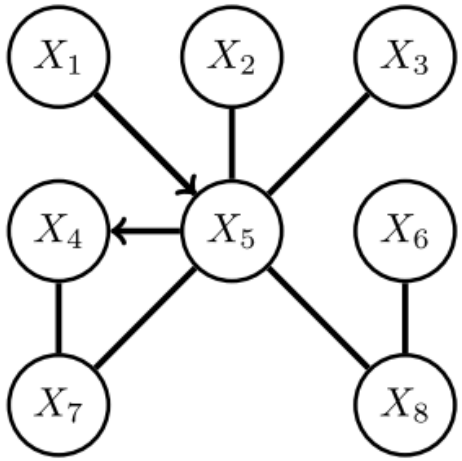
- Conditional distribution

$$f_{Y|X}(y|x) = \frac{f_{X,Y}(x,y)}{f_X(x)}$$

- (conditional) independence: $X \perp\!\!\!\perp Y|Z$, if

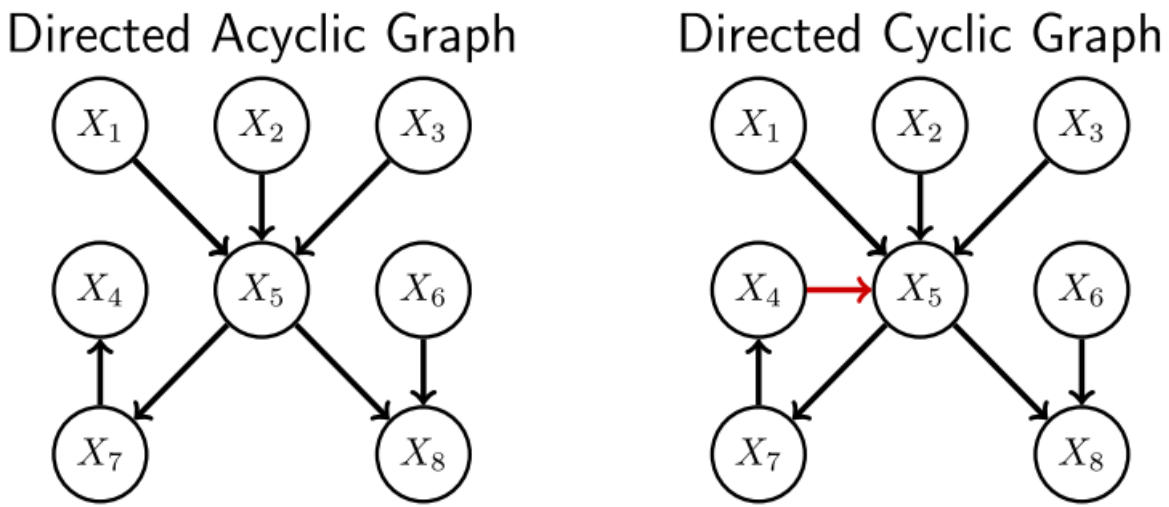
$$f_{X,Y|Z}(x,y|z) = f_{X|Z}(x|z) f_{Y|Z}(y|z)$$

Basic graph definitions



- A **graph** consists of **nodes** (vertices) and undirected of directed **edges** (links) between nodes.
- A path from X_i to X_j is a sequence of connected nodes starting at X_i and ending at X_j.

Directed graphs



- A Directed Acyclic Graph (**DAG**) is a directed graph without cycles
- **Parents, Children, Ancestors, Descendants,...** (see Ch. 2)

Important points

- marginalization
- conditional distribution
- conditional/marginal independence
- probability density function, cumulative distribution function
- Basic graph concepts