Probabilistic (Graphical) Models

and inference

Oliver Obst · Autumn 2024

WESTERN SYDNEY
UNIVERSITY

Probabilistic (Graphical) Models and Inference

(PGM: Probabilistic Graphical Models: Principles and Techniques by Daphne Koller and Nir Friedman. MIT Press)
(PMLI: Probabilistic Machine Learning: An introduction by Kevin Murphy. MIT Press)

Week	Lecture	Required reading	Assessment
1 Monday, 4 March 2024	Introduction, Probability Theory	PGM Chapter 2, PMLI Chapter 6.1	
2 Monday, 11 March 2024	Directed and undirected networks introduction		Quiz 1
3 Monday, 18 March 2024	Variable elimination		
4 Monday, 25 March 2024	Belief propagation		Quiz 2
5 Monday, 1 April 2024	public holiday		
6 Monday, 8 April 2024	Message passing / Graph neural networks		
7 Monday, 15 April 2024	Sampling		Quiz 3
8 Monday, 22 April 2024	Mid-term break		
9 Monday, 29 April 2024	Variational inference		Intra-session exam
10 Monday, 6 May 2024	Autoregressive models		Quiz 4
11 Monday, 13 May 2024	Variational Auto-Encoders		
12 Monday, 20 May 2024	GANs		Quiz 5
13 Monday, 27 May 2024	Energy-based models		
14 Monday, 3 June 2024	Evaluating generative models		Quiz 6
Monday, 17 June 2024			Project due

Some material adapted from
- Sargur Srihari
- David Sontag
- Daphne Koller and Nir Friedman

What is Probabilistic Graphical Models

Probabilistic models explicitly allow us to

- Deal with uncertainty in the data that we use
- Predict events in the world with an understanding of data and model uncertainty

To make useful predictions for what will happen next, in a given situation, considering effects of actions that we will take, we need to model the world with probability distributions.

- Probabilistic Graphical Models help us to do just that

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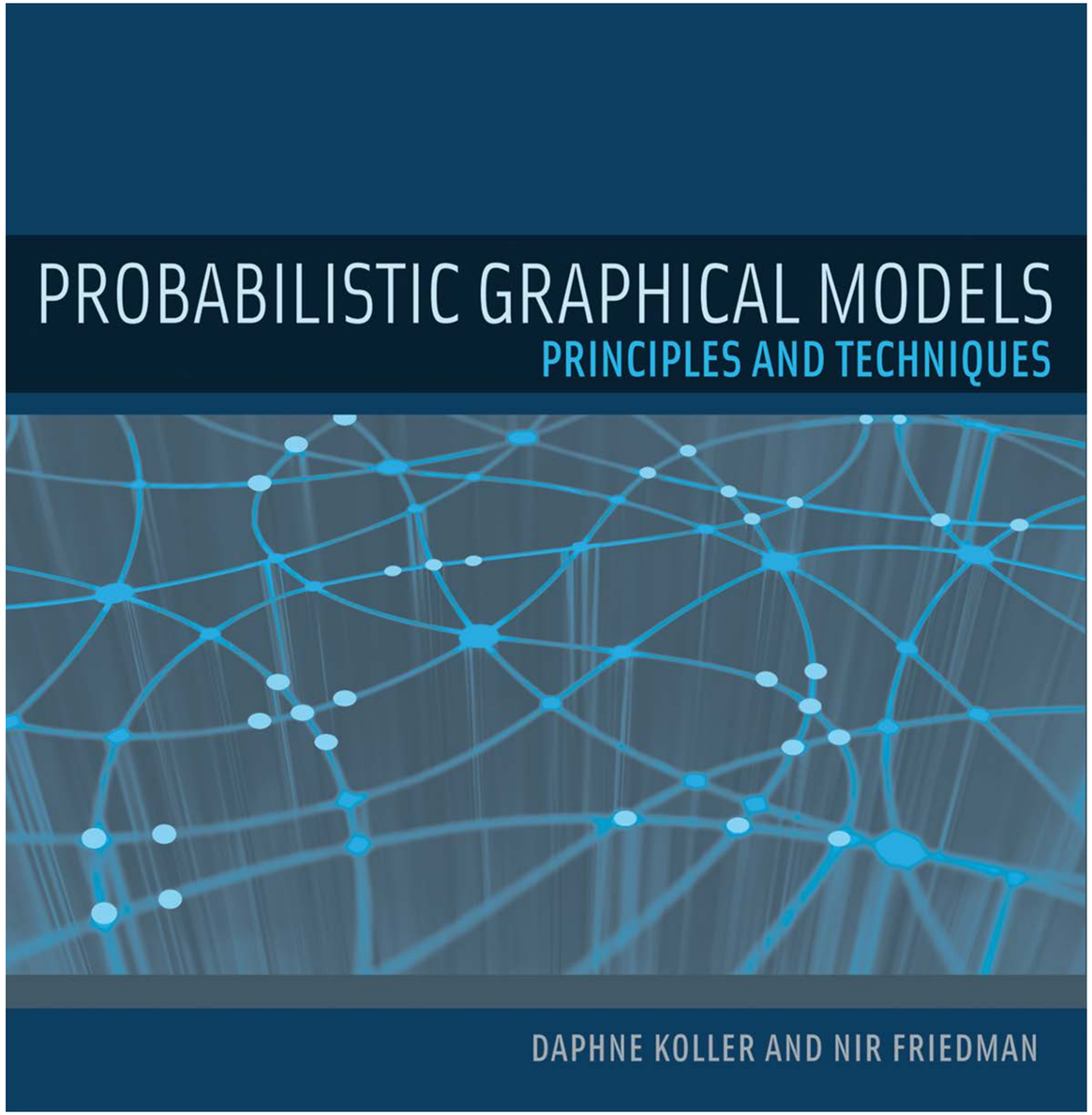
Why now?

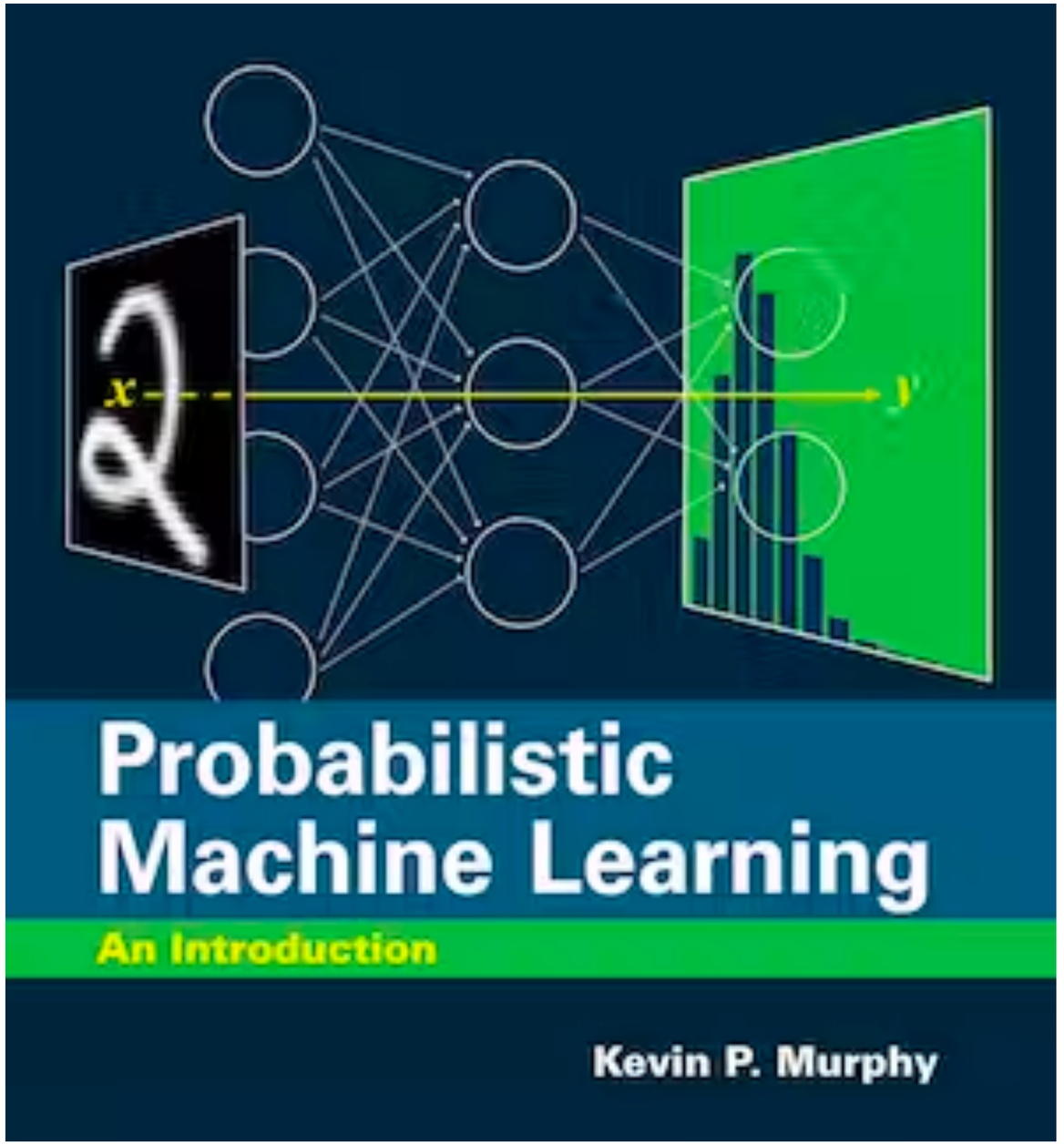
- PGM have been very popular in the ML community 10-15 years ago, then Deep Learning took over.
- Now that DL is used a lot in production, there is renewed interest to solve some of the problems that DL cannot solve.



MIT Press, 2009

Another (newer) book

- https://probml.github.io/pml-book/book1.html



Readings

Probabilistic Graphical Models: Principles and Techniques by Daphne Koller and Nir Friedman, MIT Press (2009)

- For this lecture, if we refer to “Chapter X”, it means the chapter from this book

- It’s a big book! Daphne Koller also has a Coursera class (comprehensive, difficult)

Probabilistic Machine Learning: An Introduction by Kevin P. Murphy
https://probml.github.io/pml-book/book1.html

MacKay, D. J. C. (2003). Information theory, inference, and learning algorithms. Cambridge University Press.
http://www.inference.org.uk/itila/book.html

Introduction to Probability, 2nd ed (Joseph K. Blitzstein, Jessica Hwang)
Free course and book: https://projects.iq.harvard.edu/stat110/home

Mathematics for Machine Learning:
https://mml-book.github.io/book/mml-book.pdf.

RTFLG (read the fantastic learning guide)

Videos

Coursera Probabilistic Graphical Models Specialisation

The videos are optional / additional / not a replacement for our lectures.

- https://www.coursera.org/specializations/probabilistic-graphical-models

Programming in Python

You are (almost) a Data Scientist. Over your career, programming languages will change.

You may have learned another language before, like R. This one uses Python.

We cannot teach you programming in a lecture (similarly to how we cannot teach you swimming in a lecture) – you need to practice a lot for yourself.
You will need to learn new programming skills throughout your career.

Set yourself goals. We can help by giving you some ideas or exercises (not marked), but you have the time and energy to push through.

The internet is your friend.

Example first goals

For this week 1, work on the following things. These should be easy.

- How to install python on your machine?
- Python can make use of extra libraries that are not installed by default. Figure out if NumPy, matplotlib, pandas, torch are installed with python. Figure out how to install them if they are not.
- Write a Python program that
  - creates a random 3 x 3 matrix W, a random 3 x 1 vector x, and then prints the 3 x 1 vector $y = Wx$.
  - solves the practice quiz on vUWS (quiz 0 — unmarked).
- Try this for yourself first. If you get stuck, ask others in this class. It's a good idea to learn programming together with others.

Other steps till next time

- Revise some of the data science and programming introduction (previous units).
- Revise probabilities (it helps if you took advanced statistical methods)

- This is an advanced subject.
  We require you to know material from earlier units.
- You will have spend time practicing your skills — approx. 10h/week.

How can we gain **global insight** based on **local observations?**

(David Sontag)

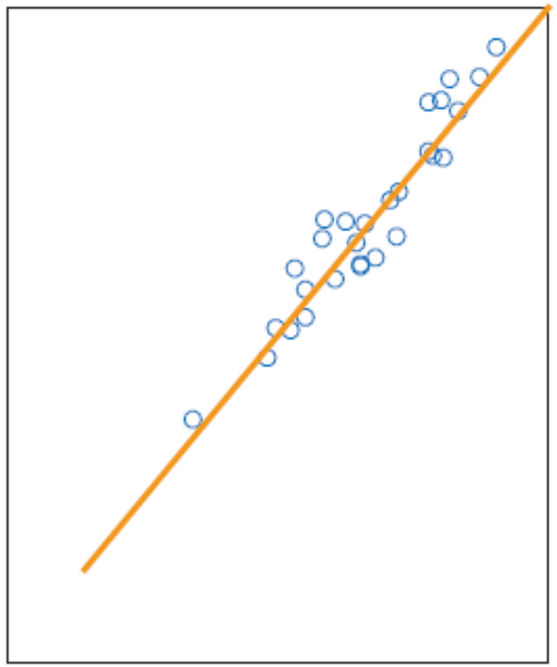
Key Idea

- **Represent** the world as a collection of random variables $X_1, \ldots, X_n$ with joint distribution $p(X_1, \ldots, X_n)$
- **Learn** the distribution from data
- Perform "**inference**" - i.e., compute conditional distributions $p(X_i \mid X_1 = x_1, \ldots, X_m = x_m)$

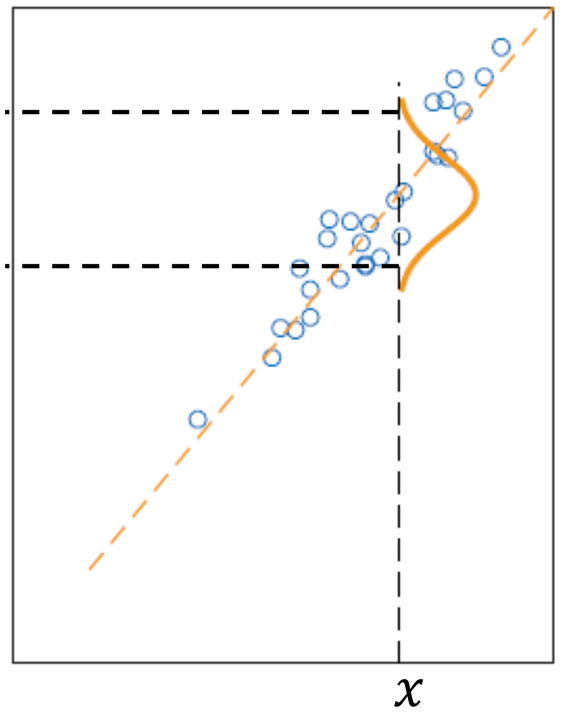
Reasoning under uncertainty

- We are continuously making predictions under uncertainty
- But uncertainty does not play a big role in “classical” AI and many of the machine learning approaches
- Probabilistic approaches enable us to do things that are not possible otherwise
- Different kinds of uncertainty:
  partial knowledge / noise / modelling limitations / inherent randomness

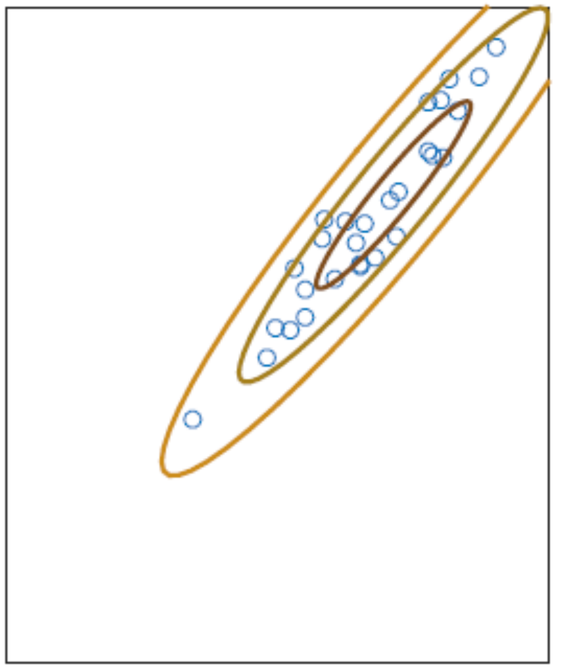
Types of Models



$\hat{y} = f(x)$



$P(y|x)$



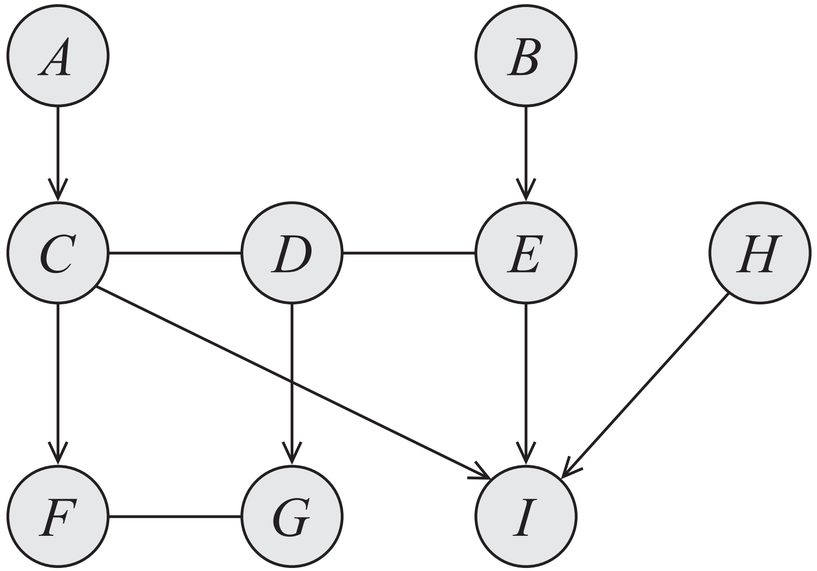
$P(x, y)$

Graphical models

- Graph – as in: a set of nodes connected with edges / vertices
- To organise and represent knowledge and relations
- If we have random variables $X_1, \ldots, X_n$ with joint distribution $p(X_1, \ldots, X_n)$, and every random variable could only take 2 values,
  a complete table would have 2^n rows.

Graphs

- A graph is a data structure G, consisting of a set of nodes / vertices, and a set of edges
- Graphs can be directed or undirected



Key challenges

1. **Represent** the world as a collection of random variables $X_1, \ldots, X_n$ with joint distribution $p(X_1, \ldots, X_n)$
   - How can we *compactly describe* this joint distribution?
   - Directed graphical models (Bayesian Networks)
   - Undirected graphical models (Markov random fields, factor graphs)
2. **Learn** the distribution from data
   - Maximum likelihood estimation, other estimation methods
   - How much data do we need?
   - How much computation does it take?
3. Perform "**inference**" - i.e., compute conditional distributions $p(X_i \mid X_1 = x_1, \ldots, X_m = x_m)$

Application of probabilities: Detecting generated texts

A watermark for language models

https://arxiv.org/abs/2301.10226 John Kirchenbauer et al.

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- without re-training the language model
- with an open-source approach, without publishing the language model

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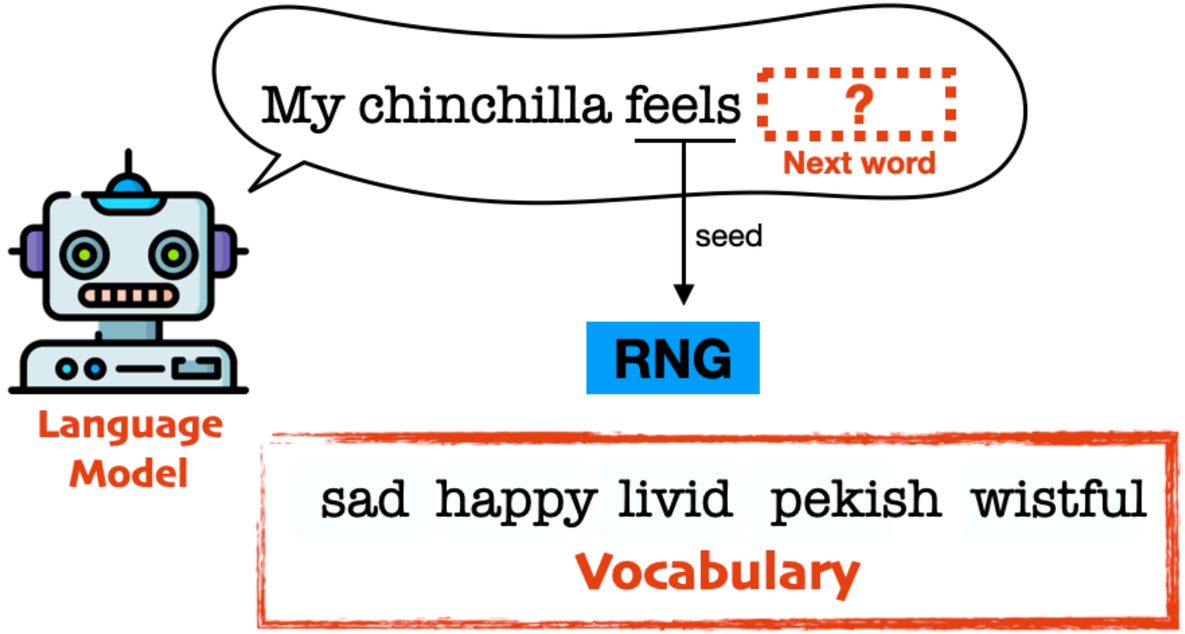

(Image: Tom Goldstein @tomgoldsteincs)

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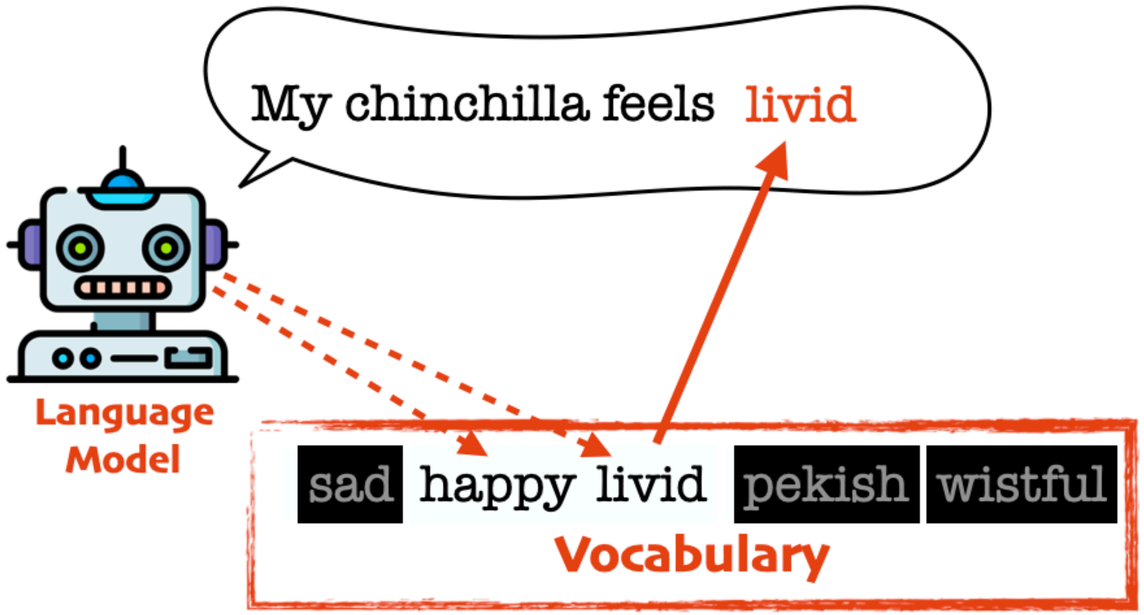

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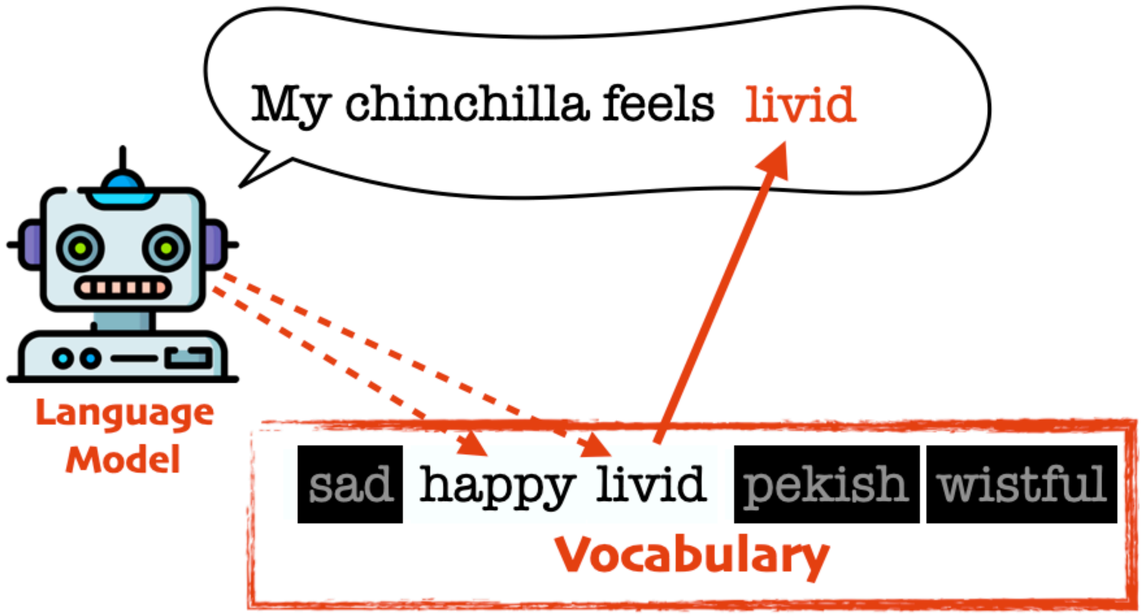

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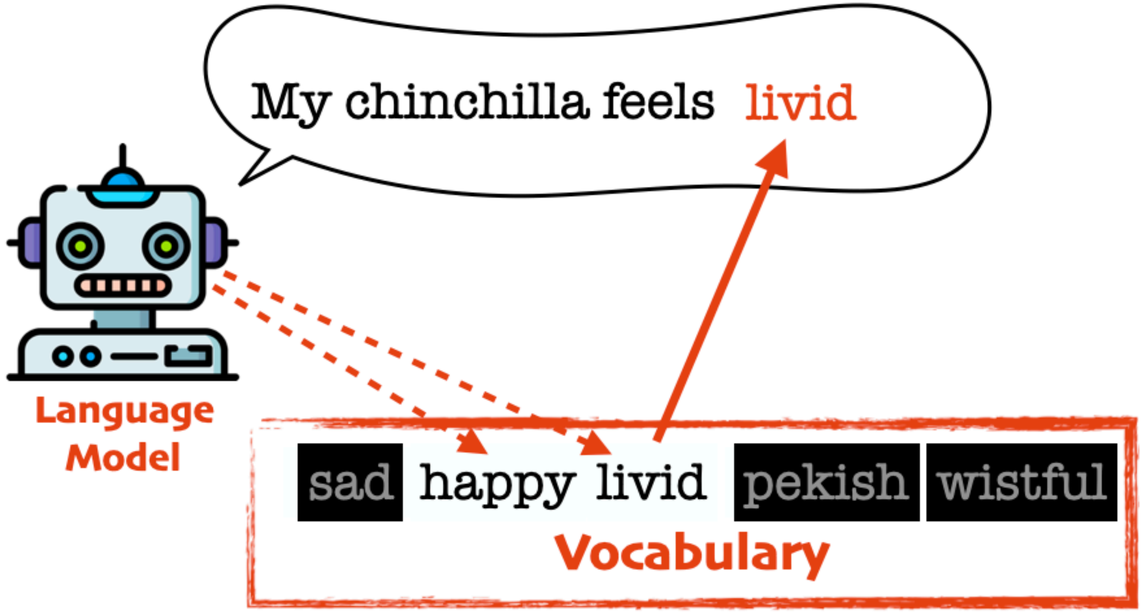

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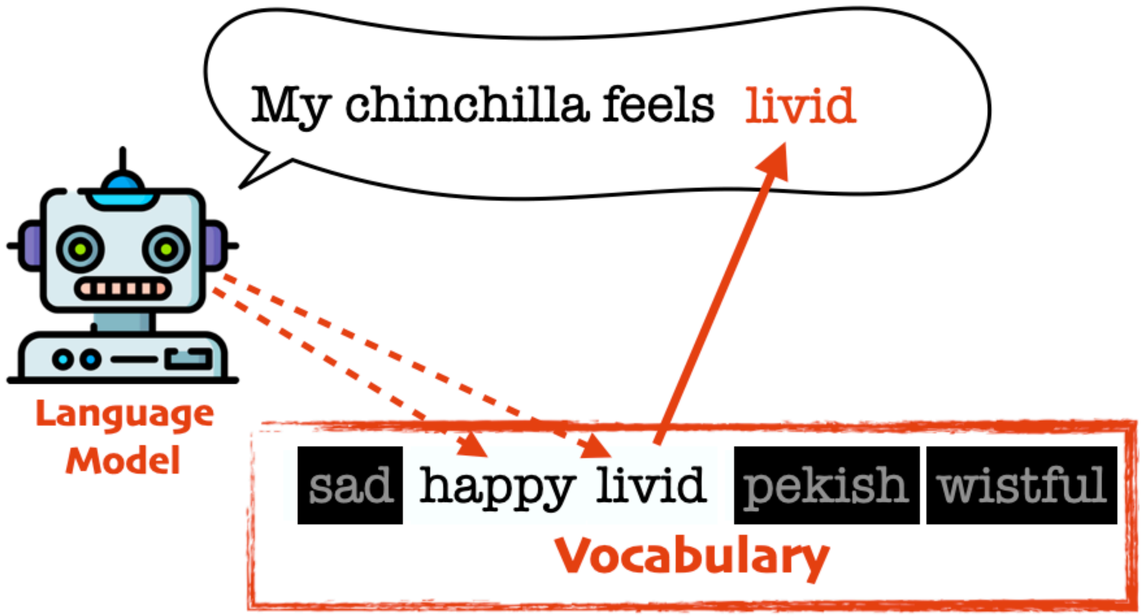

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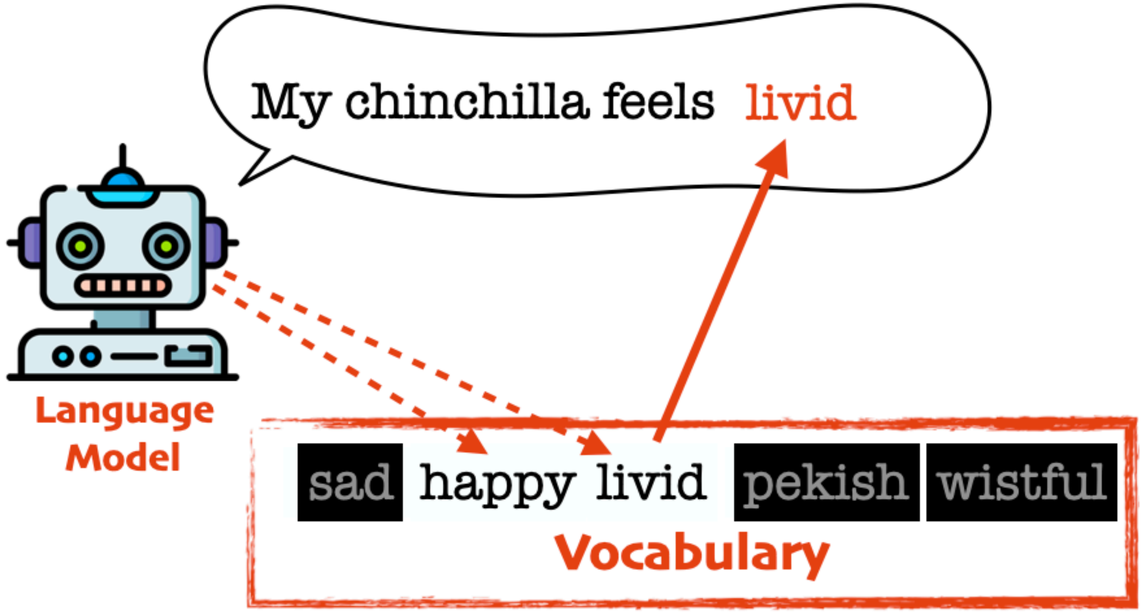

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For N words, this probability is 0.5^N.

A tweet of 25 words, with only words from whitelists, is 99.99999997% generated.

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Prompt	Num tokens	Z-score	p-value
…The watermark detection algorithm can be made public, enabling third parties (e.g., social media platforms) to run it themselves, or it can be kept private and run behind an API. We seek a watermark with the following properties:			
No watermark Extremely efficient on average term lengths and word frequencies on synthetic, microamount text (as little as 25 words) Very small and low-resource key/hash (e.g., 140 bits per key is sufficient for 99.999999999% of the Synthetic Internet	56	.31	.38
With watermark - minimal marginal probability for a detection attempt. - Good speech frequency and energy rate reduction. - messages indiscernible to humans. - easy for humans to verify.	36	7.4	6e-14

Figure 1. Outputs of a language model, both with and without the application of a watermark. The watermarked text, if written by a human, is expected to contain 9 “whitelisted” tokens, yet it contains 28. The probability of this happening by random chance is $\approx 6 \times 10^{-14}$, leaving us *extremely* certain that this text is machine generated. Whitelist words are green, blacklist words are red. The model is OPT-6.7B using multinomial sampling. Watermark parameters are $\gamma, \delta = (0.25, 2)$. The prompt is the whole blue paragraph marked in blue below.

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“Synonym attacks” need to replace impractically large parts of the generated text.

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plagiarism

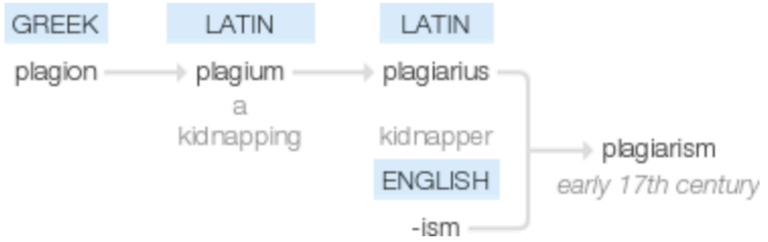
/ˈpleɪdʒərɪz(ə)m/

noun

noun: **plagiarism**; plural noun: **plagiarisms**

the practice of taking someone else's work or ideas and passing them off as one's own.
"there were accusations of plagiarism"
synonyms: copying, infringement of copyright, piracy, theft, stealing, poaching, appropriation;
informal cribbing
"there were accusations of plagiarism"

Origin



early 17th century: from Latin *plagiarius* ‘kidnapper’ (from *plagium* ‘a kidnapping’, from Greek *plagion*) + -ism.

Translate plagiarism to Choose language

Use over time for: plagiarism

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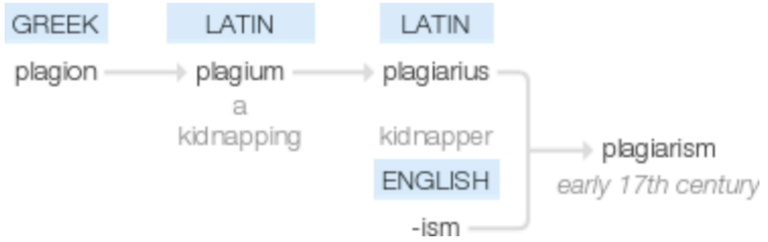

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Academic misconduct

Unit *Philosophy*

- “Understanding” assumes some knowledge that you may have from school or earlier classes, mostly linear algebra, calculus, stats.
- “Applying” means that you will have to program (usually short pieces of code). I will use Python for examples and questions, but (unless specifically requested to use python) you can also use R or Matlab if you prefer.
- We will explain and revise some of the programming, but this is not an introductory Maths or Programming class. If you don’t understand or don’t know how to do things at first, persist and try to figure things out.
- (As usual in my classes) we aim to not be overly prescriptive: there are often multiple ways to solve problems. Treat it like a job – solve the problem. Do not just copy/paste!

Assessment Items

	Due	Weight
In-tutorial quizzes (6 overall)	11 Mar, 25 Mar, 15 Apr, 6 May, 20 May, 3 Jun	30%
Applied project	17 June 5pm	40%
Practical exam	Week 9: 29 Apr, in tutorial	30%

To pass, you will need to attempt every item, and achieve at least 50% overall.

This unit is 10 credit points, and will likely be perceived a difficult unit by most. This unit will require 10 hours of study per week. This time includes the time spent within classes during lectures, tutorials / practicals.
I recommend to not take more than 4 units over the semester, and less if you are working full time.

The usual questions

- Will lecture X / topic Y / something we do in a practical be part of the exam?
  Yes, possibly.

- Will the exam be open book?
  You can use your own notes and code, books, websites, no chatGPT, don’t call your mum.

- Will we have to program, can we use our own computer?
  Yes, and most MacOs/Windows/Linux computers should work.

- Can we have a practice exam?
  There will be no “practice” exam to show you what the exam could or will look like. The quizzes will be a preparation for the exam.

What should I do with my time?

(not a usual question, but glad that you asked)

- Read the relevant chapters of the book, each week. Ideally before the lecture, but after the lecture is also good.

- You will get much better at this topic with practice, so .. please practice.

- There are heaps of resources (tutorials, data sets, competitions) online

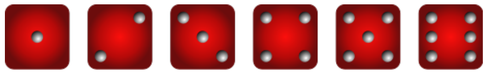
- Find practice problems for yourself to solve

- I will suggest online material from time to time

Basics (recap)

Probability: outcomes

(PGM chapter 2)



Probability: outcomes

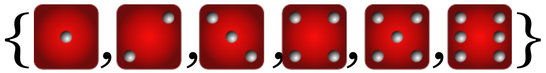
(PGM chapter 2)

- An outcome space specifies the possible outcomes that we would like to reason about, for example:
  - $\Omega =$ {  ,  } coin toss
  - $\Omega =$ {  } die toss

Probability: outcomes

(PGM chapter 2)

- An outcome space specifies the possible outcomes that we would like to reason about, for example:

  - $\Omega =$ {  ,  } coin toss
  - $\Omega =$ {  } die toss

- We specify a probability $p(\omega)$ for each outcome ω such that

  - $$p(\omega) \geq 0, \qquad \sum_{\omega \in \Omega} p(\omega) = 1$$

For example: p() = 0.6, p() = 0.4

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For example, $P(E) = p($  $) + p($  $) + p($  $) = \frac{1}{2}$, for fair dice.

Discrete random variables

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(e.g., “age”, “gender”, “hasPneumonia”, “hasDiabetes”)

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- $\mathrm{Val}(X)$: set D of all values assumed by X (“values” or “states” of X)

Probability measures and spaces

- A probability measure maps from a set of events to a real number (probability)

  $P : E \mapsto [0,1]$, for example $P(\{1\}) = 1/6,\ P(\{1,2\}) = 1/3, \ldots$

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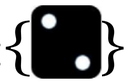
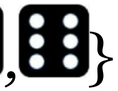
- Example:{  } is an atomic event, for a single die, {  ,  ,  } is not.

σ - algebra

(sigma-algebra)

Let E be a set of elementary events. Consider a power set of E, written as 2^E.

A subset $\mathcal{F} \subseteq 2^E$ is called a σ-algebra if it satisfies the following properties:

1. $E \in \mathcal{F}$, i.e., the algebra contains all elementary events.
2. $\mathcal{F}$ is closed under complementation: If $A \in \mathcal{F}$, then so is its complement, $A^c \in \mathcal{F}$.
3. $\mathcal{F}$ is closed under countable unions: If $A_1, A_2, \ldots, \in \mathcal{F}$, then $A_1 \cup A_2 \cup \ldots \in \mathcal{F}$.

Probability measure

For the set E with the σ-algebra $\mathscr{F}$, a non-negative real function $P : \mathscr{F} \mapsto \mathbb{R}_0^+$ is called a **measure** if it satisfies the following properties:

1. $P(\varnothing) = 0$

2. If $A_1, A_2, \ldots \in \mathscr{F}$ are pairwise disjoint, then $P(\cup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i)$.

A measure P is called a **probability measure** if

3. $P(E) = 1$.

We call $(E, \mathscr{F}, P)$ a probability space.

Sum rule

Foundations of the theory of probability, A. N. Kolmogorov, 1933

From $A + \neg A = E$ we can see that

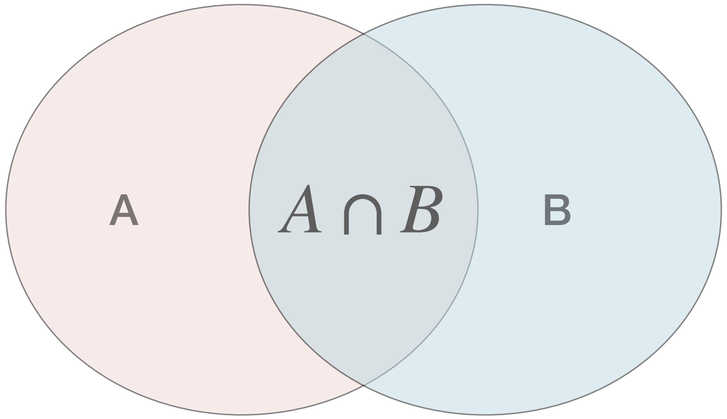
$$P(A) + P(\neg A) = P(E) = 1, \text{ so } \quad P(A) = 1 - P(\neg A).$$

From $A = A \cap (B + \neg B)$ and using the notation $P(A, B) = P(A \cap B)$ for the joint probability of A and B, we get the **sum rule**:

$$P(A) = P(A, B) + P(A, \neg B).$$

Conditional Probability

Foundations of the theory of probability, A. N. Kolmogorov, 1933



If $P(A) > 0$, the quotient

$$P(B \mid A) = \frac{P(A, B)}{P(A)}$$

is called the **conditional probability** of B given A.

$$P(A, B) = P(B \mid A)\, P(A) = P(A \mid B)\, P(B).$$

1) $\sum_{\omega \in S} p(\omega \mid S) = 1$

2) If A and B are independent, then $P(B \mid A) = P(B)$.

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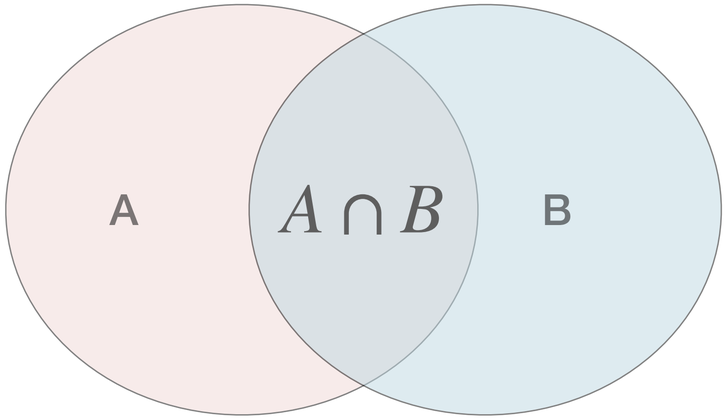

1) $\sum_{\omega \in S} p(\omega \,|\, S) = 1.$

- $P(A \,|\, A) = \dfrac{P(A \cap A)}{P(A)} = 1$
- $P(E \,|\, A) = 1$

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

2) If A and B are independent, then $P(B \,|\, A) = P(B)$.

- for $B \cap C = \varnothing$: $P(B \cup C \,|\, A) = P(B \,|\, A) + P(C \,|\, A)$

3) For a given (fixed) A, $(E, \mathscr{F}, P(\,\cdot\,|\, A))$ is a probability space.

Law of total probability

Let $A_1 \cup A_2 + \ldots + A_n = E$, and $A_i \cap A_j = \varnothing$ for all $i \neq j$.

For any $X \in \mathscr{F}$,

$$P(X) = \sum_{i=1}^{n} P(X \mid A_i)\, P(A_i).$$

Bayes' Theorem

Let $A_1 \cup A_2 + \ldots + A_n = E$, and $A_i \cap A_j = \varnothing$ for all $i \neq j$.

For any $X \in \mathscr{F}$,

$$P(A_i \mid X) = \frac{P(A_i)\, P(X \mid A_i)}{\sum_{j=1}^{n} P(A_j)\, P(X \mid A_j)}.$$

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We write $X_1 \perp X_2$ if the two random variables are independent:

$$p(X_1 = x_1, X_2 = x_2) = p(X_1 = x_1)\, p(X_2 = x_2),$$

for all values $x_1 \in \mathrm{Val}(X_1)$ and $x_2 \in \mathrm{Val}(X_2)$.

- Sum rule:

$$P(A) = P(A, B) + P(A, \neg B)$$

- Product rule:

$$P(A, B) = P(A \mid B)\, P(B) = P(B \mid A)\, P(A)$$

- Bayes' theorem:

$$P(A \mid B) = \frac{P(B \mid A)\, P(A)}{P(B)} = \frac{P(B \mid A)\, P(A)}{P(B, A) + P(B, \neg A)}$$

Bayes' theorem

Terminology

$$\underbrace{P(X \mid D)}_{\text{posterior for X given D}} = \frac{\overbrace{P(X)}^{\text{prior for X}} \quad \overbrace{P(D \mid X)}^{\text{likelihood for X}}}{\underbrace{P(D)}_{\text{evidence for the model}}} = \frac{P(X)\,P(D \mid X)}{\sum_{x \in \mathcal{X}} P(D \mid x)\,P(x)}$$

- $P(D \mid X)$ is the likelihood of X, but the conditional probability for D, given X.
- The prior is the marginal distribution $P(X) = \sum_{d \in \mathcal{D}} P(X, d)$ under all possible data.

Expectation, Variance

- Expectation $\mathbb{E}[X]$ is the random variable X's "average" value
  - $\mathbb{E}[X] = \sum_{x \in \text{Val}(X)} x\, P(X = x)$ or $\mathbb{E}[X] = \int_x x\, P(x)\, dx$

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e.g., for $c = 10$: probability that a value is more than 10 standard deviations away from expectation is less than 0.01.

Entropy

(PMLI, Chapter 6.1)

For discrete random variables:

$$\mathbb{H}(X) = -\sum_{k=1}^{K} p(X=k)\ \log_2 p(X=k) = -\mathbb{E}_X[\log_2 p(X)]$$

The entropy of a distribution: amount of uncertainty, “disorder”.

For a discrete distribution, entropy is maximised for the uniform distribution.

How would a discrete minimum entropy distribution look like (and what is it’s value)?

Multivariate distributions

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- Conditioning, chain rule, Bayes' rule, etc. all apply

Examples

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$2^3 - 1$

x_1	x_2	x_3	$p(x_1x_2x_3)$
0	0	0	0.11
0	0	1	0.02
	…		
1	1	1	0.05

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joint distribution	Very high	High
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- $p(Y = p) = ? = 0.85$

Marginalisation

Suppose we have a joint distribution $p(X_1, \ldots, X_n)$.
Then,

$$p(X_i = x_i) = \sum_{x_1} \sum_{x_2} \ldots \sum_{x_{i-1}} \sum_{x_{i+1}} \ldots \sum_{x_n} p(x_1, \ldots, x_n)$$

Marginalisation means: summing away all but the random variable(s) of interest

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Compute the conditional probability

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$$= \frac{0.7}{0.7 + 0.1} = 0.875$$

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The Quick Medical Reference (QMR-DT) model has 600 diseases and 4000 symptoms.

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This would also defeat the purpose of probabilistic modelling, which is to make predictions with *previously unseen observations*.

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This is a simple, yet powerful model.

Example: naîve Bayes for classification

Classify emails as spam ($Y = 1$) or not spam ($Y = 0$).

- $i : 1 \ldots n$ index the words in our vocabulary (e.g., all English words)
- $X_i = 1$ if word i appears in an email, and 0 otherwise
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math7002
advanced statistical methods

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Philosophy: Nearly all probabilistic models are “wrong”, but many are nonetheless useful.

Graphical models

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Graphs with only undirected edges are *undirected graphs*, denoted with H.

- We can get the undirected version of a graph $K = (V, E)$ by replacing all edges with undirected edges: $H = (V, E')$, where $E' = \{X - Y : X \leftrightharpoons Y \in E\}$.

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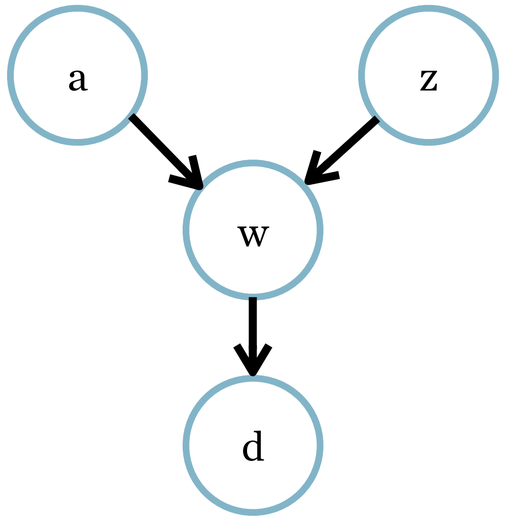
The set of all parents and neighbours of X combined, $\mathrm{Pa}(X) \cup \mathrm{Nb}(X)$, is called the *boundary* of X.

Notation: $\mathrm{Boundary}_X$

Topological ordering

For directed graphs

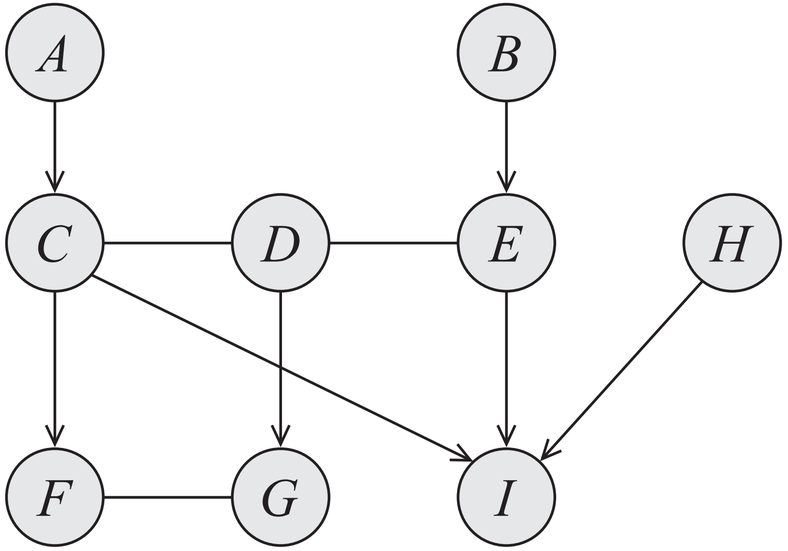
- A linear ordering of the nodes so that
  for every edge from u to v the node u comes before v in the ordering.
- This requires the graph to have no cycles, i.e., requires directed acyclic graphs (DAG).
- In general, multiple topological orderings are possible for the same graph.

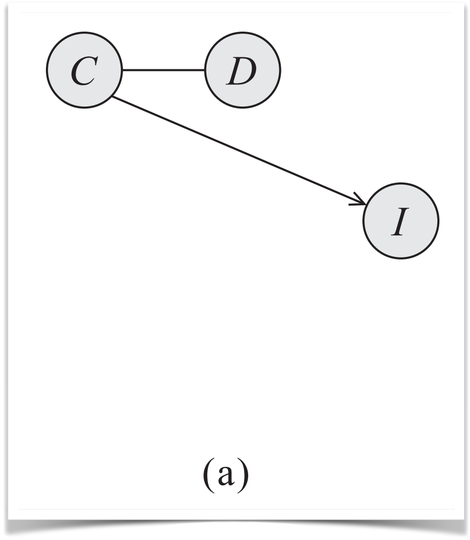


Solutions:
(a, z, w, d) (z, a, w, d)

Not a solution:
(a, w, d, z)

(or anything else, really)





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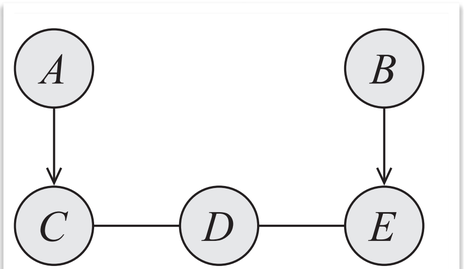

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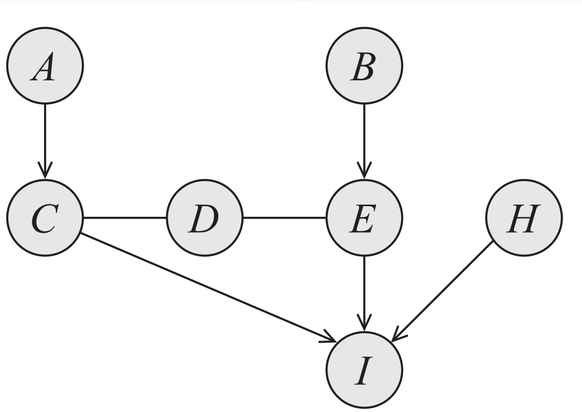

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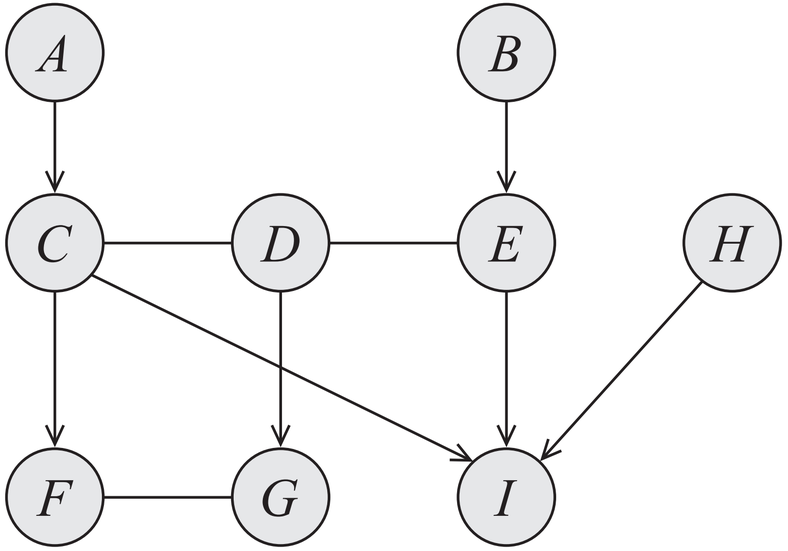
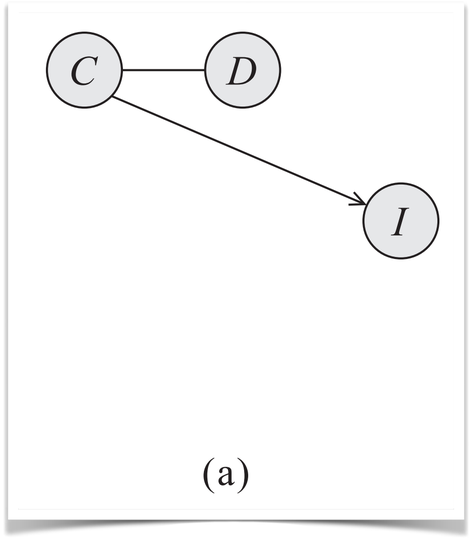
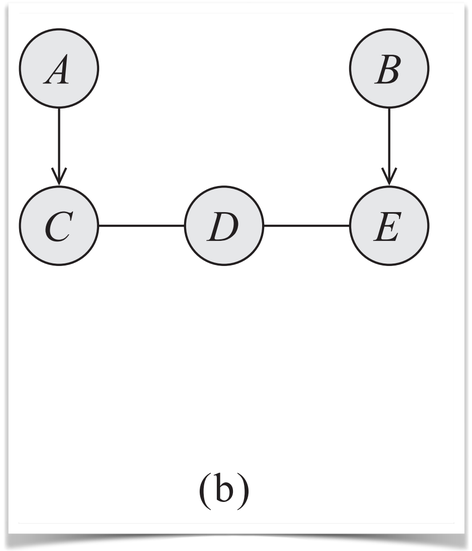
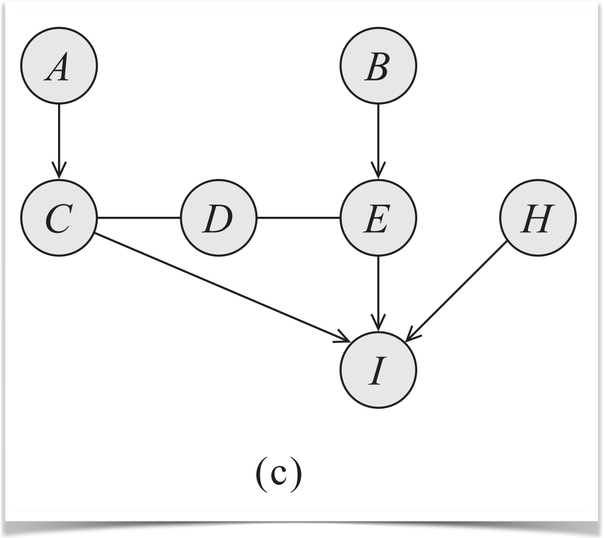


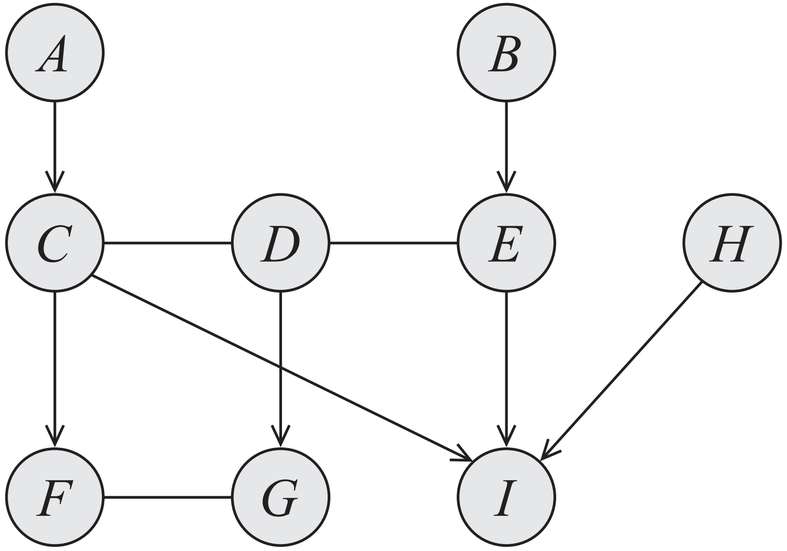


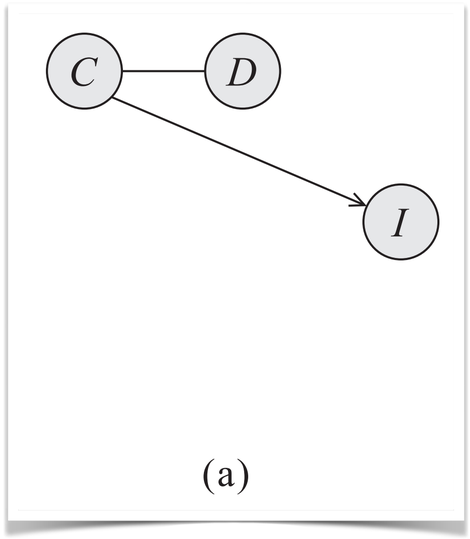


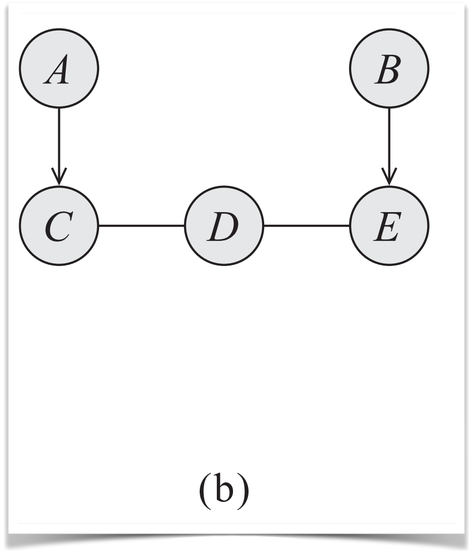


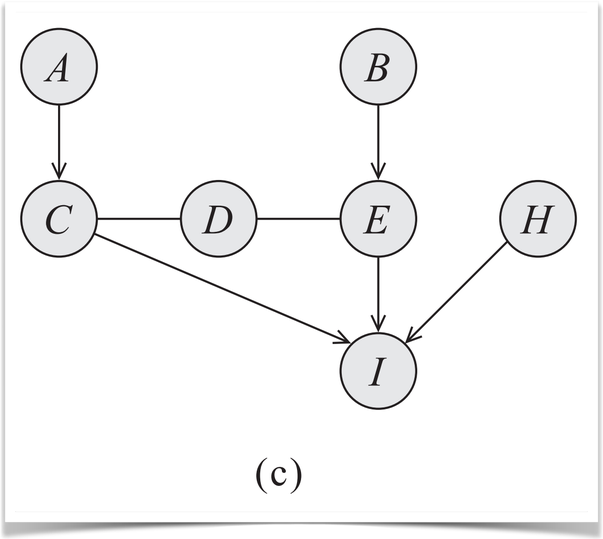
(a) $K = (V, E)$; let $\boldsymbol{X} \in V$. The induced subgraph $K[\boldsymbol{X}]$ is the graph $(\boldsymbol{X}, E')$, where E' are all the edges $X \leftrightharpoons Y \in E$ such that $X, Y \in \boldsymbol{X}$.
(example: $K[C, D, I]$)

- A subgraph over $\boldsymbol{X}$ is complete if every two nodes in $\boldsymbol{X}$ are connected by some edge.The set $\boldsymbol{X}$ is often called a clique; we say a clique $\boldsymbol{X}$ is maximal if for any superset of nodes $\boldsymbol{Y} \supset \boldsymbol{X}$, $\boldsymbol{Y}$ is not a clique.









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(b) and (c) A subset of nodes $\boldsymbol{X} \in V$ is upwardly closed in K if, for any $X \in \boldsymbol{X}$, we have that $\text{Boundary}_X \subset \boldsymbol{X}$. The upward closure of $\boldsymbol{X}$ is the minimal upwardly closed subset $\boldsymbol{Y}$ that contains $\boldsymbol{X}$. The upwardly closed subgraph of $\boldsymbol{X}$, denoted $K^+[\boldsymbol{X}]$, is the induced subgraph over $\boldsymbol{Y}$, $K[\boldsymbol{Y}]$.

Bayesian networks

PGM chapter 3

A Bayesian network is specified by a directed acyclic graph $G = (V, E)$ with:

1. One node $i \in V$ for each random variable X_i
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Powerful framework for designing algorithms to perform probability computations.

That’s it for today

Please also go to your tutorials!