# Probabilistic Graphical Models

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# 1. Introduction

- Probabilistic graphical models

- Mathematical background
  Basic concepts in probability
  Random variables
  Set conditional independence
  Graphs

- Course information

# Outline

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# Probabilistic graphical models (PGMs)

**example**: medical diagnosis

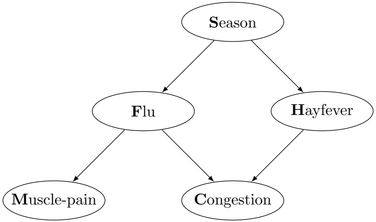
- 2 binary-valued diseases: $\mathbf{F}$lu and $\mathbf{H}$ayfever
- 4-valued variable: $\mathbf{S}$eason
- 2 binary-valued symptoms: $\mathbf{C}$ongestion and $\mathbf{M}$uscle-pain

- probability space: $2 \times 2 \times 4 \times 2 \times 2 = 64$ values
- diagnosis query: how likely the patient is to have the flu given that it is fall, and that she has sinus congestion but no muscle pain

$$\mathbf{P}(F = \text{true} \mid S = \text{fall}, C = \text{true}, M = \text{false})$$

# Probabilistic graphical models (PGMs)

graphical representation | independencies | factorization




$$(F \perp\!\!\!\perp H \mid S)$$
$$(C \perp\!\!\!\perp S \mid F, H)$$
$$(M \perp\!\!\!\perp H, C \mid F)$$
$$(M \perp\!\!\!\perp C \mid F)$$

$$\mathbf{P}(S, F, H, C, M) = \mathbf{P}(S)\mathbf{P}(F \mid S)$$
$$\mathbf{P}(H \mid S)\mathbf{P}(C \mid F, H)\mathbf{P}(M \mid F)$$

- parameter space: $4 + 4 \times 2 + 4 \times 2 + 2 \times 2 \times 2 + 2 \times 2 = 32$ values
- diagnosis query: $\mathbf{P}(C \mid F, H, S) = \mathbf{P}(C \mid F, H)$

# Probabilistic graphical models (PGMs)

- compact, tractable, transparent **representation** of variables and dependencies
  - human expert can understand and evaluate its semantics and properties
  - accurate reflection of our understanding of a domain
- effective **inference**
  - answering queries using the distribution as our model of the world
  - computing the posterior probability of some variables given evidence on others
- automatic **learning** of a model from data
  - provides a good approximation to our past experience
  - combining human expert knowledge and data information

# Real-world applications

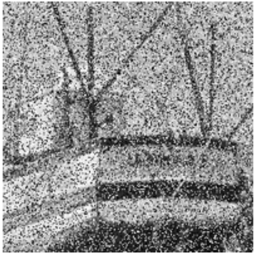
Where would you apply probabilistic graphical models?

# Real-world applications

- **images**: generation, denoising
- **language**: generation, translation
- **audio**: super-resolution, speech synthesis, speech recognition
- **economics**: causal inference
- **science**: error-correcting codes, computational biology, ecology
- **health care and medicine**: diagnosis

# Real-world applications

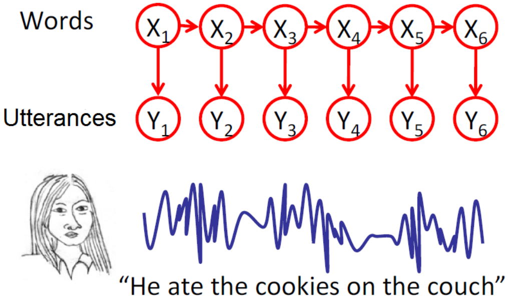
**image denoising**



- restore old photographs based on probabilistic graphical models that does a good job at modeling the posterior distribution $p(\text{original image} \mid \text{noisy image})$

# Real-world applications

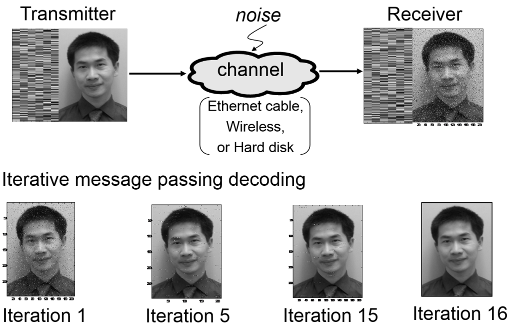
**speech recognition**




- infer spoken words from audio signals with variants of hidden Markov models

# Real-world applications

## error-correcting codes




- detect and correct communication errors with graphical models

# Deep learning and PGMs

Why do we still need PGMs in the age of deep learning?

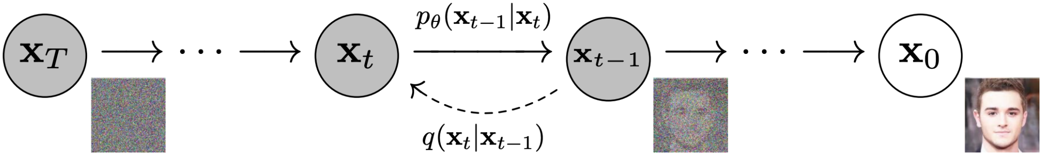
# Deep learning and PGMs

combining deep learning architectures and probabilistic modeling techniques can be advantageous in

- **generative models**: variational autoencoders (VAEs), diffusion models
- **inference**: estimating the distribution of unobserved variables given observed data
- **interpretability and uncertainty**: interpretable representation of data and XAI
- **causality**: causal discovery and causal-based learning

# Deep learning and PGMs

**diffusion models**



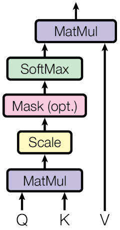

- directed Markov chain structure
- model a sequence of random variables $\{x_0, \ldots, x_T\}$
- each $x_t$ is an intermediate between a uniform random distribution and the data distribution

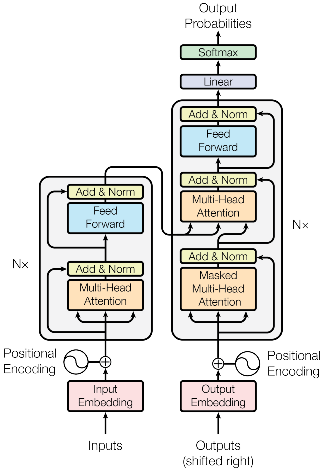
# Deep learning and PGMs

## transformer architecture

- fully connected graphical model
- scaled dot-product attention

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$



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# Basic concepts in probability

**axioms of probability**

- $0 \leq \mathbf{P}(A) \leq 1$
- $\mathbf{P}(\text{sure proposition}) = 1$
- $\mathbf{P}(A \text{ or } B) = \mathbf{P}(A) + \mathbf{P}(B)$ if $A$ and $B$ are mutually exclusive

**marginal probability**

$$\mathbf{P}(A) = \sum_{i=1}^{n} \mathbf{P}(A, B_i)$$

if $\{B_1, \ldots, B_n\}$ is a set of exhaustive and mutually exclusive propositions

# Basic concepts in probability

**conditional probability $\mathbf{P}(A \mid B)$**

- $A$ and $B$ are independent if $\mathbf{P}(A \mid B) = \mathbf{P}(A)$
- $A$ and $B$ are conditionally independent given $C$ if $\mathbf{P}(A \mid B, C) = \mathbf{P}(A \mid C)$

**product rule**

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

- chain rule

$$\mathbf{P}(E_1, \dots, E_n) = \mathbf{P}(E_1)\mathbf{P}(E_2 \mid E_1) \cdots \mathbf{P}(E_n \mid E_{n-1}, \dots, E_1)$$

# Basic concepts in probability

**Bayes' theorem**

$$\mathbf{P}(H \mid e) = \frac{\mathbf{P}(e \mid H)\mathbf{P}(H)}{\mathbf{P}(e)}$$

- $\mathbf{P}(H)$: prior probability
- $\mathbf{P}(e \mid H)$: likelihood
- $\mathbf{P}(H \mid e)$: posterior probability

# Random variables

given a random variable $X$ with $\mathbf{dom}(X) \subseteq \mathbf{R}$

- expected value of $X$:
$$\mathbf{E}[X] = \sum_x x\mathbf{P}(x)$$
- expectation of function $g$ of $X$:
$$\mathbf{E}[g(X)] = \sum_x g(x)\mathbf{P}(x).$$
- variance of $X$:
$$\mathbf{var}(X) = \mathbf{E}\left[(X - \mathbf{E}[X])^2\right]$$
  - standard deviation of $X$: $\sigma(X) = \sqrt{\mathbf{var}(X)}$

# Random variables

given two random variables $X, Y$ with $\mathbf{dom}(X), \mathbf{dom}(Y) \subseteq \mathbf{R}$

- covariance of $X$ and $Y$:

$$\mathbf{cov}(X,Y) = \mathbf{E}[(X - \mathbf{E}[X])(Y - \mathbf{E}[Y])]$$

- correlation coefficient of $X$ and $Y$:

$$\rho(X,Y) = \frac{\mathbf{cov}(X,Y)}{\sigma(X)\sigma(Y)}$$

- regression coefficient of $X$ on $Y$:

$$r(X,Y) = \rho(X,Y)\frac{\sigma(X)}{\sigma(Y)} = \frac{\mathbf{cov}(X,Y)}{\mathbf{var}(Y)}$$

# Random variables

## continuous random variables

$$\mathbf{P}(a \le X \le b) = \int_a^b p(x)\ dx$$

- $p(x)$: density function
- translation between discrete and continuous random variables:

$$\int_{-\infty}^{\infty} p(x)\ dx \Longleftrightarrow \sum_x \mathbf{P}(x)$$

- expected value of continuous random variable $X$:

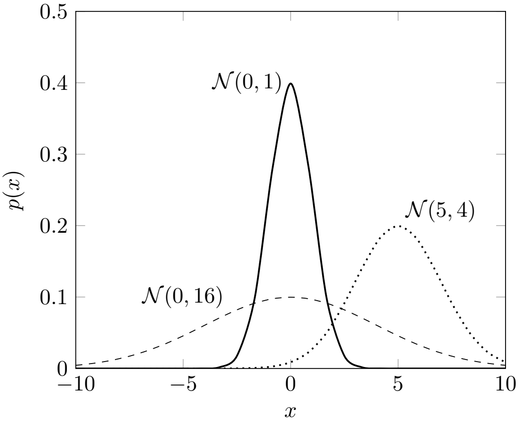
$$\mathbf{E}[X] = \int_{-\infty}^{\infty} xp(x)\ dx$$

# Random variables

**example**: Gaussian distribution $\mathcal{N}(\mu, \sigma^2)$

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- $\mu$: mean of random variable $X$
- $\sigma^2$: variance of random variable $X$
- standard Gaussian distribution: $\mathcal{N}(0,1)$



# Set conditional independence

let $V = \{V_1, V_2, \ldots\}$, and $X, Y, Z \subseteq V$

**conditionally independent** set $X$ and $Y$ given $Z$:

$$(X \perp\!\!\!\perp Y \mid Z) \implies \mathbf{P}(x \mid y, z) = \mathbf{P}(x \mid z), \quad \text{for all } \{y, z \mid \mathbf{P}(y, z) > 0\}$$

- marginal independence: $(X \perp\!\!\!\perp Y \mid \emptyset)$
- $(X \perp\!\!\!\perp Y \mid Z) \implies \mathbf{P}(V_i \mid V_j, Z) = \mathbf{P}(V_i \mid Z)$, for all $V_i \in X$, $V_j \in Y$
  - the converse is not necessarily true

# Graphs

A graph $G$ consists of

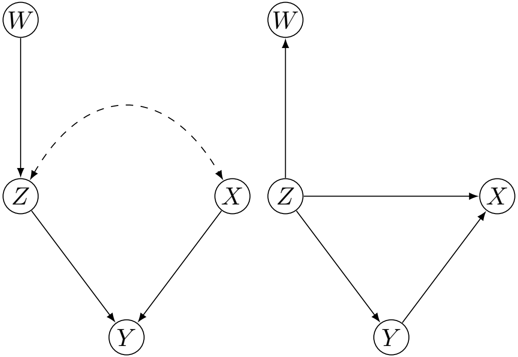
- a set $V$ of vertices (or nodes)
- a set $E$ of edges (or links)
  - directed or undirected

**path**: $((W,Z),(Z,Y),(Y,X),(X,Z))$

- directed: $((W,Z),(Z,Y))$
- undirected: $((W,Z),(Z,Y),(Y,X))$

**directed acyclic graph (DAG)**

- a directed graph without directed cycles



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# Contents


1. Introduction
2. Bayesian classifiers
3. Markov models
4. Bayesian networks
5. Inference with Monte Carlo methods
6. Markov decision problems
7. Control as probabilistic inference
8. Graphical causal models
9. Deep learning and graphical models

# Organization

- 6 ETCS
- course number: 11E13MO-1228
- every Tuesday 16:15 – 17:45 and Wednesday 12:15 – 13:45
- course material and forum on ILIAS
- exam:
  - open-book
  - date: tbd (probably some day between Sep. 9th and Sep. 13th)

# Exercises

- **not** mandatory
- sample solutions will be presented on Wednesdays, 1 week after exercise release
- answer questions of others and ask your own questions in the ILIAS forum
- time management options:

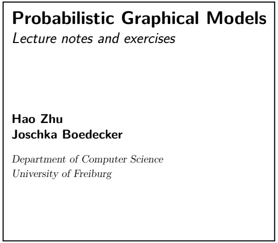
| | | |
|---|---|---|
| 7 – 9 hours per ex. | little exam prep. | **RECOMMENDED** |
| 5 – 6 hours per ex. | more exam prep. | MINIMUM |
| 0 hours per ex. | $\infty$ exam prep. | **IMPOSSIBLE** |

# Team

Joschka Boedecker

Hao Zhu

# Textbook


**Probabilistic Graphical Models**
*Lecture notes and exercises*

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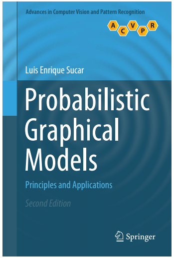
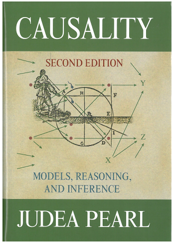
Lecture notes and exercises



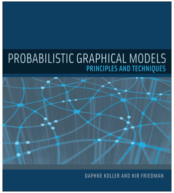

Probabilistic Graphical Models: Principles and Applications (2nd edition)
Luis Enrique Sucar (2021)
https://link.springer.com/book/10.1007/978-3-030-61943-5

# Other useful materials




Causality (2nd edition)
Judea Pearl (2009)
http://bayes.cs.ucla.edu/BOOK-2K

Probabilistic Graphical Models: Principles and Techniques
Daphne Koller and Nir Friedman (2009)
https://mitpress.mit.edu/9780262013192/probabilistic-graphical-models



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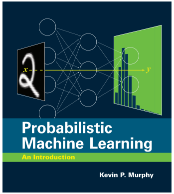
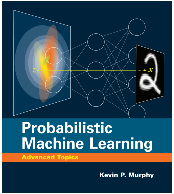



Probabilistic Machine Learning: An introduction
Kevin P. Murphy (2022)
hhttps://probml.github.io/pml-book/book1.html

Probabilistic Machine Learning: Advanced Topics
Kevin P. Murphy (2023)
https://probml.github.io/pml-book/book2.html



## Other useful materials

- Probabilistic Graphical Models Specialization (Coursera)
  - Probabilistic Graphical Models 1: Representation
  - Probabilistic Graphical Models 2: Inference
  - Probabilistic Graphical Models 3: Learning
- notes from CS228 - Probabilistic Graphical Models (Stanford University)