Lecture 4, Part 1:

A Primer on Probability Theory

Robert Bamler · Summer Term of 2023

These slides are part of the course *"Data Compression With and Without Deep Probabilistic Models"* taught at University of Tübingen. More course materials—including video recordings, lecture notes, and problem sets with solutions—are publicly available at `https://robamler.github.io/teaching/compress23/`.

Recap: Why We Need Good Probabilistic Models

- Bound on practical compression performance: cross entropy

$$\text{expected bit rate} \geq H\big(p_{\text{data}}(\mathbf{x}), p_{\text{model}}(\mathbf{x})\big) := -\sum_{\mathbf{x}} p_{\text{data}}(\mathbf{x}) \log p_{\text{model}}(\mathbf{x})$$

- Overhead due to $p_{\text{model}} \neq p_{\text{data}}$: Kullback-Leibler divergence (aka relative entropy)

$$D_{\text{KL}}\big(p_{\text{data}}(\mathbf{x}) \,\big\|\, p_{\text{model}}(\mathbf{x})\big) := H\big(p_{\text{data}}(\mathbf{x}), p_{\text{model}}(\mathbf{x})\big) - H\big[p_{\text{data}}(\mathbf{x})\big]$$

  - For low overhead, we need p_{model} to approximate p_{data}
  - But so far: only simplistic p_{model}s that ignore *correlations* between symbols
- **This part:** mathematical language for probabilistic models
- **Next part:** information-theoretical quantification of correlations
- **Then:** machine learning models that describe correlations

Ingredients of a Probabilistic Model

- *sample space* Ω (abstract space of "all states of the world")
  - subsets $E \subseteq \Omega$: *"events"* ("event E occurs" $\iff$ "the world is in some state $\omega \in E$")
- *probability measure:* a function $P : \Sigma \to [0, 1]$ where
  - Σ is a so-called σ-algebra on Ω. (a set of all "expressible" events $E \subseteq \Omega$)
  - $P(\emptyset) = 0 \quad$ and $\quad P(\Omega) = 1$.
  - countable additivity: $P\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} P(E_i) \quad$ if all E_i are pairwise disjoint.
  - therefore, for finite sums: $P\left(\bigcup_{i=1}^{k} E_i\right) = \sum_{i=1}^{k} P(E_i) \quad$ if all E_i are pairwise disjoint.
  - therefore: $P(E) + P(\Omega \setminus E) = P(\Omega) = 1 \quad \forall E \in \Sigma$.
  - therefore: $P(E_1) \leq P(E_2)$ if $E_1 \subseteq E_2$ (and $E_1, E_2 \in \Sigma$)

Examples of Probability Measures

1. Simplified Game of Monopoly: (throw two fair three-sided dice)
   - sample space: $\Omega = \{1,2,3\}^2 = \big\{(1,1),(1,2),(1,3),(2,1),(2,2),(2,3),(3,1),(3,2),(3,3)\big\}$
   - sigma algebra: $\Sigma = 2^\Omega := \big\{\text{all subsets of } \Omega \text{ (including } \emptyset \text{ and } \Omega)\big\}$
   - probability measure P: for all $E \subseteq \Sigma$, let $P(E) := |E|/|\Omega| = |E|/9$

Examples of Probability Measures (cont'd)

1. Simplified Game of Monopoly
2. Wait times for the next three buses from "Sternwarte":
   - sample space (in a simple model): $\Omega = \{(x_1, x_2, x_3) \in \mathbb{R}^3 \quad \text{where} \quad 0 \le x_1 \le x_2 \le x_3\}$
   - sigma algebra: all "measurable subsets" of Ω
     (essentially, all subsets of Ω except for extremely pathological exceptions)
   - probability measure P: complicated function, but we know it satisfies certain relations, e.g.,
     $P(\text{"next bus departs in at most 5 minutes"}) = P(\text{"next bus departs in at most 2 minutes"}) + P(\text{"next bus departs in between 2 and 5 minutes"})$.
   - **Question:** what is the probability that the next bus departs in *exactly* 3 minutes?
     i.e., what is $P\big((\{3\text{ min}\} \times \mathbb{R}^2) \cap \Omega\big)$?
   - **Question:** what is the probability that the next bus departs in between 2 and 5 minutes?
     $$P\big((\underbrace{[2\text{ min}, 5\text{ min}]}_{=:\mathcal{I}} \times \mathbb{R}^2) \cap \Omega\big) = P\Big(\bigcup_{x_1 \in \mathcal{I}} \big((\{x_1\} \times \mathbb{R}^2) \cap \Omega\big)\Big) \overset{?}{=} \sum_{x_1 \in \mathcal{I}} P\big((\{x_1\} \times \mathbb{R}^2) \cap \Omega\big) = 0$$

Random Variables

- Often, we we're not interested in a *full* description of the state $\omega \in \Omega$, but only in certain properties of it.
- **Definition:** "random variable": function $X : \Omega \to \mathbb{R}$ (not necessarily injective)

Examples:

1. Simplified Game of Monopoly; $\Omega = \big\{(a,b) \quad \text{where} \quad a,b \in \{1,2,3\}\big\}$
   - total value: $X_{\text{sum}}\big((a,b)\big) = a + b \in \{2,3,4,5,6\}$
   - value of the red die: $X_{\text{red}}\big((a,b)\big) = a$
   - value of the blue die: $X_{\text{blue}}\big((a,b)\big) = b$
2. In our bus schedule model from before; $\Omega = \{(x_1,x_2,x_3) \in \mathbb{R}^3 \quad \text{where} \quad 0 \le x_1 \le x_2 \le x_3\}$
   - Time between the next bus and the one after it: $X_{\text{gap}}\big((x_1,x_2,x_3)\big) = x_2 - x_1$

Properties of Individual Random Variables

- "Probability that a random variable X has some given value x":
  $P(X = x) := P\big(X^{-1}(x)\big) = P\big(\{\omega \in \Omega : X(\omega) = x\}\big)$
  - Example 1 (Simplified Game of Monopoly): $P(X_{\text{sum}} = 3) =$
  - Example 2 (bus schedule): $P(X_{\text{gap}} = 20 \text{ minutes}) =$
- When we write just $P(X)$, then we mean the *function* that maps $x \mapsto P(X = x)$.
  (more precisely: $P(X)$ denotes a *probability measure* on the space of X)
- **Expectation value** of a random variable X under a model P
  - discrete case: $\mathbb{E}_P[X] := \sum_{\omega \in \Omega} P(\{\omega\})\, X(\omega) = \sum_{x \in X(\Omega)} P(X{=}x)\, x$

    examples: $\mathbb{E}_P[X_{\text{red}}] =$; $\mathbb{E}_P[X_{\text{blue}}] =$; $\mathbb{E}_P[X_{\text{sum}}] =$
  - continuous case: $\mathbb{E}_P[X] := \int_\Omega X(\omega)\, dP(\omega)$ (see next slide)

Properties of Individual Random Variables (cont'd)

- *Cumulative Density Function (CDF):* $P(X \le x) := P\big(\{\omega \in \Omega : X(\omega) \le x\}\big)$
  - Example 1 (Simplified Game of Monopoly): $P(X_{\text{sum}} \le 3) =$
  - Example 2 (bus schedule): $P(X_{\text{gap}} \le 20 \text{ minutes}) \in [0, 1]$ (nonzero in general)
- Analogous definitions for: $P(X < x)$, $P(X \ge x)$, $P(X > x)$, $P(X \in \text{some set})$, ...
- *Probability Density Function (PDF)* of a real-valued random variable X:
  $p(x) := \frac{d}{dx} P(X \le x)$ (if derivative exists)
  $\rightarrow$ expectation value: $\mathbb{E}_P[X] = \int X(\omega)\, dP(\omega) = \int_{-\infty}^{\infty} x\, p(x)\, dx$
  (if a density $p(x)$ exists)

Multiple Random Variables

- **Definition:** *joint probability distribution* of two random variables X and Y:
  $P(X{=}x, Y{=}y) := P\big(\{\omega \in \Omega : X(\omega) = x \ \wedge \ Y(\omega) = y\}\big)$
- **Notation:** "$P(X, Y)$": function that maps $(x, y) \mapsto P(X{=}x, Y{=}x)$
  (more precisely: $P(X, Y)$ denotes a *probability measure* on the product space of X and Y)
- If we know $P(X, Y)$, then we can calculate $P(X) = \sum_y P(X, Y{=}y)$ (for discrete Y)
  - This process is called "marginalization".
  - for continuous random variables: $p(X) = \int p(X, y)\, dy$

Statistical Independence

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- **Definition:** X and Y are *(statistically) independent* iff: $P(X, Y) = P(X)\,P(Y)$
  (i.e., if $P(X \in \mathbb{X}, Y \in \mathbb{Y}) = P(X \in \mathbb{X})\,P(Y \in \mathbb{Y})\ \ \forall\, \mathbb{X}, \mathbb{Y}$)
- **Examples** (Simplified Game of Monopoly):
  - X_{red} and X_{blue} are statistically independent.
  - X_{red} and X_{sum} are *not* statistically independent. (proof: Problem 4.1)
- **Definition:** *conditional* independence of X and Y given Z: see later

Conditional Probability Distributions: Examples

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"X & Y are *not* statistically independent" $\iff$ "knowing X reveals something about Y"

Examples: (Simplified Game of Monopoly; $P(E) = \frac{|E|}{9}$)

	$x =$	1	2	3	4	5	6
What are the (marginal) probability distributions $P(X_{\text{red}})$ and $P(X_{\text{sum}})$ of the red die and the sum, respectively?	$P(X_{\text{red}} = x) =$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0
	$P(X_{\text{sum}} = x) =$	0	$\frac{1}{9}$	$\frac{2}{9}$	$\frac{1}{3}$	$\frac{2}{9}$	$\frac{1}{9}$
Assume that you only accept throws where the red die comes up with value 1, and you keep rethrowing both dice until this condition is satisfied. What is the probability distribution of X_{sum} in your first accepted throw? We call this the *conditional* probability distribution $P(X_{\text{sum}} \mid X_{\text{red}} = 1)$.	$P(X_{\text{sum}} = x \mid X_{\text{red}} = 1) =$						
Now you only accept throws where the sum of both dies is at least 5. What is the conditional probability distribution of X_{red}?	$P(X_{\text{red}} = x \mid X_{\text{sum}} \geq 5) =$						
Finally, assume you only accept throws where $X_{\text{blue}} = 1$. What is the conditional probability distribution of X_{red}?	$P(X_{\text{red}} = x \mid X_{\text{blue}} = 1) =$						

Conditional Probability Distributions: Definition

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- **Definition:** "conditional probability of event E_2 *given* event E_1": $P(E_2 \mid E_1) := \frac{P(E_1 \cap E_2)}{P(E_1)}$
  - Thus, $P(E_2 \mid E_1)$ is a (properly normalized) probability distribution w.r.t. the first parameter,
    i.e., $P(E_2 \mid E_1) + P(\Omega \setminus E_2 \mid E_1) = \dfrac{P(E_2 \cap E_1) + P((\Omega \setminus E_2) \cap E_1)}{P(E_1)} = \dfrac{P(E_1)}{P(E_1)} = 1.$
- **Definition:** "conditional probability distribution of a random variable Y *given* another random variable X": $P(Y \mid X) := \frac{P(X,Y)}{P(X)}$ i.e., $P(Y = y \mid X = x) := \frac{P(X=x, Y=y)}{P(X=x)}\ \ \forall x, y$
  - Thus, if X and Y are statistically independent *(but only then!)*:
    $P(Y \mid X) = \frac{P(X,Y)}{P(X)} = \frac{P(X)\,P(Y)}{P(X)} = P(Y)$ ("knowing X reveals no new information about Y")
  - In the general case: "chain rule" of probability theory: (follows directly from above definition)
    $P(X_1, X_2, X_3, \ldots) =$

Conditional Independence

- **Reminder:** X and Z are (statistically) independent $:\Longleftrightarrow P(X, Z) = P(X)\,P(Z)$
- **Analogous definition:**

  X and Z are *conditionally* independent *given* Y $:\Longleftrightarrow P(X, Z \mid Y) = P(X \mid Y)\,P(Z \mid Y)$

  - **equivalently:** chain rule simplifies:
    $P(X, Y, Z) = P(X)\,P(Y \mid X)\,P(Z \mid X, Y) = P(Y)\,P(X \mid Y)\,P(Z \mid Y)$

- **Problem Set 5:** comparison to normal (i.e., unconditional) independence
- **Problem Set 10:** propagation of information along $X \longrightarrow Y \longrightarrow Z$

Warning: Conditionality $\neq$ Causation

- We'll often specify a joint probability distribution as, e.g., $P(X, Y) = P(X)\,P(Y \mid X)$.
- But just because we write "$P(Y \mid X)$", this does *not* necessarily mean that X is the cause of Y.
- **Example:** (Simplified Game of Monopoly):
  - X_{red} and X_{blue} can be considered to cause X_{sum}.
  - But, in the examples three slides ago, we were still able to calculate, e.g., $P(X_{\text{red}} \mid X_{\text{sum}})$.
    (i.e., the probability of the *cause* X_{red} given its *effect* X_{sum})

    → This is called "posterior inference". (more in Lectures 7 and 8)
- Causality goes beyond the scope of a probabilistic model;
  understanding causal structures generally requires *interventions* in the generative process.

Outlook

- **Problem 4.1:** probability measures & statistical independence
- **Next part:**
  - information-theoretical quantification of *correlations*
  - machine-learning models that can capture correlations

Lecture 4, Part 2:

Mutual Information and Taxonomy of Probabilistic (Machine-Learning) Models

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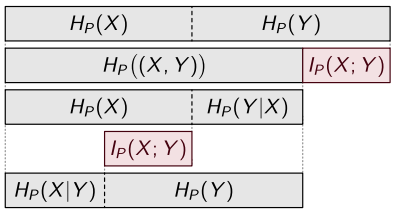
Recap: Random Variables, Conditional Probabilities

- **Random variables**: (uppercase letters $X, Y, Z, \ldots$)
  - Think "placeholders" for values: $P(X_i)$ is a probability measure for symbol X_i.
  - $P(X=x)$: probability ($\in [0,1]$) that the random variable X assumes value x.
  - *Expectation value:* $\mathbb{E}_P[f(X)] = \sum_x P(X=x)\, f(x)$ (discrete case)
- **Multiple random variables:**
  - *joint distribution:* $P(X, Y)$
  - *marginal distributions:* $P(X)$, $P(Y)$
  - *conditional distribution:* $P(Y \mid X) = \frac{P(X,Y)}{P(X)}$ ("How is Y distributed if I know the value of X?")
- **Statistical (in-)dependencies between random variables:**
  - *(unconditional) (statistical) independence:* if $P(X, Y) = P(X)\, P(Y)$ $(\iff P(Y \mid X) = P(Y))$
  - *conditional independence:* if $P(X, Z \mid Y) = P(X \mid Y)\, P(Y \mid Y)$ $(\iff P(Z \mid X, Y) = P(Z \mid Y))$
- **Goal now:** *quantify* statistical dependencies

Quantification of Statistical Dependencies

- **Use information theory:**
  - information content of the statement "$X = x$":
  - entropy of a random variable X under a model P: $H_P(X) :=$
  - analogously: joint and conditional information content and entropy (see Problems 4.2 and 4.3).
- **Entropy is *subadditive*:** $\forall$ random variables X & Y:

  $$\boxed{H_P\big((X, Y)\big) \leq H_P(X) + H_P(Y)}$$ (proof: Problem 4.4)
  - equality holds iff X and Y are statistically independent (proof: Problem 2.3 (b))



(figure adapted from MacKay book)

- **Thus:** *wrongfully* assuming independence (to simplify a model) leads to an overhead in bit rate:

  Def. *"mutual information"*: $\boxed{I_P(X;Y) := H_P(X) + H_P(Y) - H_P\big((X, Y)\big) \geq 0}$ (Problem 4.4)

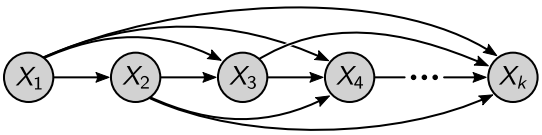
Modeling Statistical Dependencies

- Assume that the message is a sequence of symbols: $\mathbf{X} = (X_1, X_2, \ldots, X_k)$
- Subadditivity of entropies: $H(\mathbf{X}) \leq \sum_{i=1}^{k} H(X_i)$

- **Thus:** instead of modeling each symbol X_i independently, we should model the message $\mathbf{X}$ *as a whole* (without completely sacrificing computational efficiency).
  - autoregressive models (e.g., Problem 3.3)
  - latent variable models (planned for Problem Set 6; also: basis for variational autoencoders)

Probabilistic Models at Scale

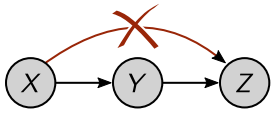
- *All* probability distributions P over messages $\mathbf{X} = (X_1, X_2, \ldots, X_k)$ satisfy the *chain rule:*
  $P(\mathbf{X}) = P(X_1)\, P(X_2 \,|\, X_1)\, P(X_3 \,|\, X_1, X_2)\, P(X_4 \,|\, X_1, X_2, X_3) \cdots P(X_k \,|\, X_1, X_2, \ldots, X_{k-1})$



- **Example:** assume each symbol is from alphabet $\mathfrak{X} = \{1, 2, 3\}$.
  - How many model parameters do we need to specify an arbitrary distribution $P(X_1)$?
  - How many parameters for an arbitrary conditional distribution $P(X_2 \,|\, X_1)$?
  - How many parameters for an arbitrary conditional distribution $P(X_k \,|\, X_1, X_2, \ldots, X_k)$?

Expressive Yet Efficient Probabilistic Models

- **Goal:** Find approximation to arbitrary models $P(\mathbf{X})$ that
  - captures relevant correlations
  - but is still *computationally efficient*:
    → *reasonably compact* representation of the model in memory
    → *reasonably efficient evaluation* of probabilities $P(\mathbf{X} = \mathbf{x})$
    → suitable for entropy coding (later)
- **General Strategy:** enforce *conditional independence*:
  X & Z are *conditionally independent given* Y $:\Longleftrightarrow P(X, Z \,|\, Y) = P(X \,|\, Y)\, P(Z \,|\, Y)$
  $\Longleftrightarrow P(X, Y, Z) = P(X)\, P(Y \,|\, X)\, P(Z \,|\, Y)$ (proof: Problem 5.1 (a))



Four Kinds of Scalable Probabilistic Models

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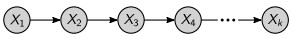
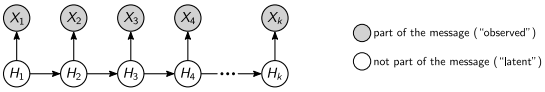
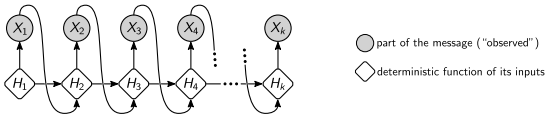
(1) Markov Process



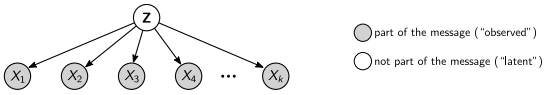
(2) Hidden Markov Model



(3) Autoregressive Model



(4) Latent Variable Model



(1) Markov Process

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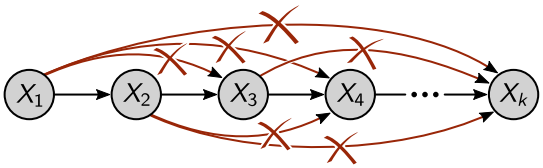
Modeling assumption: symbols X_i are generated by a *memoryless* process.

- Each symbol X_i depends on its immediate precessor X_{i-1} but not on any earlier symbols:



$$P(\mathbf{X}) = P(X_1)\,P(X_2 \mid X_1)\,P(X_3 \mid X_2)\,P(X_4 \mid X_3)\cdots P(X_k \mid X_{k-1})$$

- i.e., for all $j < i$, the symbols X_{i+1} and X_j are *conditionally independent* given X_i.

☺ only $O(k\,|\mathfrak{X}|^2)$ (or even $O(|\mathfrak{X}|^2)$) model parameters;

☹ simplistic assumption; e.g., in English text, the string "the" is very frequent.
$\Rightarrow P_{\text{data}}(X_i = \text{'e'} \mid X_{i-2} = \text{'t'}, X_{i-1} = \text{'h'}) > P_{\text{data}}(X_i = \text{'e'} \mid X_{i-1} = \text{'h'})$ (i.e., *not* cond. indep.)

(2) Hidden Markov Model

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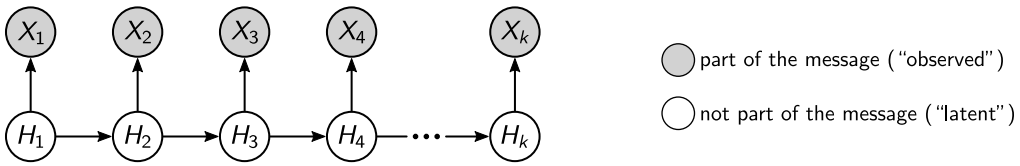
Modeling assumption: there is some memoryless *hidden* process, which is observed *indirectly*.



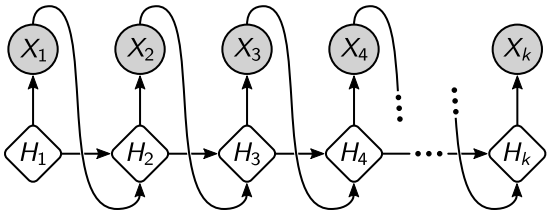
$$P(\mathbf{X}) = \int P(\mathbf{X}, \mathbf{H})\,d\mathbf{H} \quad \text{with} \quad P(\mathbf{X}, \mathbf{H}) = P(H_1)\,P(X_1 \mid H_1) \prod_{i=2}^{k} P(H_i \mid H_{i-1})\,P(X_i \mid H_i)$$

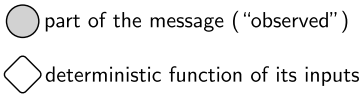
☺ can model long-range correlations, i.e., X_i, X_{i-2} *not* cond. indep. given X_{i-1} (exercise);

☹ bit-rate overhead: in order to model $P(X_i \mid H_i)$, decoder has to first decode H_i, even though it's not part of the message (solution: "bits-back coding", see Lecture 7).

(3) Autoregressive Model

Modeling assumption: memoryless hidden process with (typically) *deterministic* transitions;
but: transitions are also conditioned on the previous *symbol*.





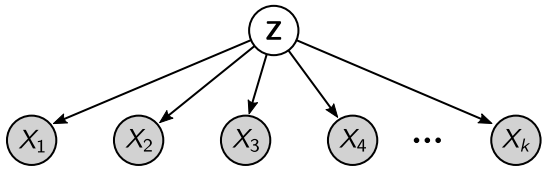
$$P(\mathbf{X}) = \prod_{i=1}^{k} P(X_i \mid H_i) \quad \text{where} \quad H_1 = \text{fixed}; \quad H_i = f(H_{i-1}, X_{i-1})$$

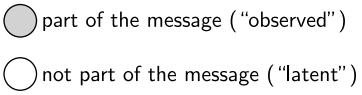
☺ no compression overhead for reconstructing H_i (see Problem 3.3);

☹ encoding & decoding are not parallelizable ($\Rightarrow$ slow on modern hardware).

(4) Latent Variable Model

Modeling assumption: there is some unobserved higher level of abstraction $\mathbf{Z}$.





$$P(\mathbf{X}) = \int P(\mathbf{X}, \mathbf{Z})\, d\mathbf{Z} \quad \text{where} \quad P(\mathbf{X}, \mathbf{Z}) = P(\mathbf{Z}) \prod_{i=1}^{k} P(X_i \mid \mathbf{Z})$$

☺ can model long-range correlations (see Problem 5.2 (c));

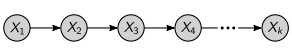
☺ parallelizable;

☹ bit-rate overhead for encoding $\mathbf{Z}$ (solution: "bits-back coding", see Lecture 7).

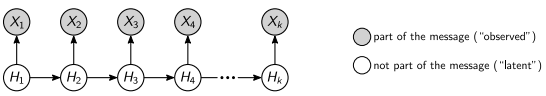
Summary: 4 Kinds of Scalable Probabilistic Models

- Each architecture makes different assumption about conditional independence of symbols.

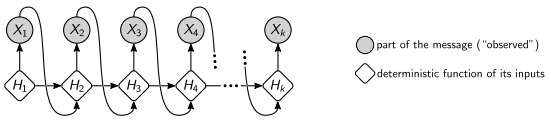
(1) Markov Process



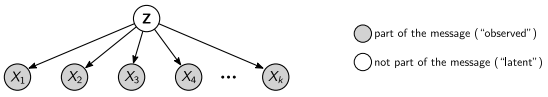
(2) Hidden Markov Model



(3) Autoregressive Model

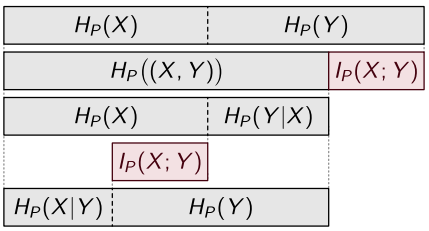


(4) Latent Variable Model



Outlook

- **Problem Set 4:**



- **Next 4 lectures:** lossless compression with deep probabilistic models
  - Different model architectures require different entropy coding algorithms.
- **Afterwards:** Lossy compression