67800: Probabilistic Methods in AI

Recitation 0: Background

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0.1 Probability Theory

Recommended reading:

- PGM Book, Chapter 2 [2]
- Standford CS 229 Course / Probability notes [3]
- Notes in Hebrew by Gal Chechnik et al [1]

0.1.1 Basic Definitions

Sample space Ω – all possible outcomes e.g. single dice throw: $\Omega = \{1, 2, 3, 4, 5, 6\}$

Event e – a subset of the sample space $e \subseteq \Omega$ e.g. odd throw result: $e = \{1, 3, 5\}$

Event space S – a set of all relevant events, including \emptyset and Ω

Probability measure $P: S \to \mathbb{R}^+$

Basic properties:

- $\forall a \in S, P(a) \ge 0, P(\Omega) = 1, P(\Omega \setminus a) = 1 P(a)$
- $a \subseteq b \implies P(a) \le P(b)$
- $P(a \cap b) \leq min(P(a), P(b))$
- Union bound: $P(\bigcup_i a_i) \leq \sum_i P(a_i)$ (equal if $\{a_i\}$ are disjoint events)

Conditional probability:

$$P(a \mid b) = \frac{P(a \cap b)}{P(b)}$$

The chain rule:

$$P(\bigcap_{i} a_i) = P(a_1)P(a_2 \mid a_1) \cdots P(a_k \mid a_1 \cap \ldots \cap a_{k-1})$$

Bayes rule:

$$P(a \mid b) = \frac{P(b \mid a)P(a)}{P(b)}$$

Independent events:

- $P \models (a \perp b) \iff P(a \cap b) = P(a)P(b)$, or equivalently: $P(a \mid b) = P(a)$
- Conditional independence: $P \models (a \perp b \mid c) \iff P(a \mid b \cap c) = P(a \mid c)$

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¹Original LaTeX template courtesy of UC Berkeley.

0.1.2 Random Variables

A random variable X is a function $X : \Omega \to \mathbb{R}$, (or to one of possible set of values).

Example 0.1 Two dice roll $\Omega = \{(1,1), (1,2), \dots, (6,6)\}$ $X((n_1, n_2)) = n_1 + n_2 - a$ random variable describing the roll sum.

Probability distribution of a random variable:

$$P(X = x) = P_X = P(\{\omega \subseteq \Omega : X(\omega) = x\})$$

 P_X is a new probability distribution function associated with the random variable X. It only records the probability of different values of X.

Discrete random variable:

$$\sum_{x \in Val(X)} P(X = x) = \sum_{x} P_X(x) = 1$$

0.1.2.1 Moments – Expectation and Variance

Expectation (for discrete variables): $\mathbb{E}_P[X] = \Sigma_x x P_X(x)$

Linearity of expectation:

 $\mathbb{E}[X+Y] = \mathbb{E}[X] + \mathbb{E}[Y], \quad \mathbb{E}[aX] = a\mathbb{E}[X]$ Variance: $\operatorname{Var}_{P}[X] = \mathbb{E}[(X - \mathbb{E}[X])^{2}] = \mathbb{E}[X^{2}] - (\mathbb{E}[X])^{2}]$

Proof:

$$\operatorname{Var}_{P}[X] = \mathbb{E}[(X - \mathbb{E}[X])^{2}]$$

= $\mathbb{E}[X^{2} - 2X \cdot \mathbb{E}[X] + (\mathbb{E}[X])^{2}]$
= $\mathbb{E}[X^{2}] - 2 \cdot \mathbb{E}[X] \cdot \mathbb{E}[X] + (\mathbb{E}[X])^{2}$ (inner $\mathbb{E}[X]$ is considered as constant)
= $\mathbb{E}[X^{2}] - (\mathbb{E}[X])^{2}]$

 $\operatorname{Var}[aX + b] = a^2 \operatorname{Var}[X]$

X, Y are independent $\implies \mathbb{E}[X \cdot Y] = \mathbb{E}[X] \cdot \mathbb{E}[Y], \text{ Var}[X + Y] = \text{Var}[X] + \text{Var}[Y]$ Chebyshev inequality:

$$P(|X - \mathbb{E}[X]| \ge t) \le \frac{\operatorname{Var}[X]}{t^2}$$

0.1.3 Multivariate Distributions

0.1.3.1 Joint and Marginal Probability

The explicit joint distribution (for two discrete random variables X and Y) is a table assigning a probability value for every combination of $Val(X) \times Val(Y)$, for example:

Example 0.2

There are $(|Val(X)| \times |Val(Y)| - 1)$ degrees of freedom in the general joint probability table.

The joint probability should be consistent with the marginal probabilities (sums of rows or columns):

$$\Sigma_x P_{X,Y}(x,y) = P_Y(y)$$
 and $\Sigma_y P_{X,Y}(x,y) = P_X(x)$

0.1.3.2 Conditional Probability of Random Variables

 $P(X \mid Y = y)$ is the conditional distribution over the outcomes defined by X given the knowledge that Y = y. $P(X \mid Y)$ assigns a probability distribution over X for each value of Y:

$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)}$$

In **Example 0.2**, $P(X | Y = A) = \begin{bmatrix} 0.5 & 0.5 & 0 \end{bmatrix}$.

The chain rule:

$$P(X_1, \dots, X_k) = P(X_1)P(X_2 \mid X_1) \cdots P(X_k \mid X_1, \dots, X_{k-1})$$

Bayes rule:

$$P(X \mid Y) = \frac{P(Y \mid X)P(X)}{P(Y)}$$

0.1.4 Conditional Probability Distributions and Noisy Or

In some cases (as we will see extensively in this course), instead of defining the *joint probability distribution*, we decompose it and use *conditional probability distributions* (CPDs). For example, a joint probability distribution over three RV's can be decomposed per the chain rule to P(X, Y, Z) = P(X)P(Y|X)P(Z|X, Y), and if we know that $P \models X \perp Y$, we have: P(X, Y, Z) = P(X)P(Y)P(Z|X, Y).

In the case of discrete RVs, the CPD P(Z | X, Y) can be defined explicitly by a table. Notice that each row sums to 1 (so there are 4 free parameters). Notice the notation $P(z^0) = P(Z = 0) = P_Z(0)$.

X	Y	$P(z^0 \mid X, Y)$	$P(z^1 \mid X, Y)$
0	0	1	0
0	1	0.5	0.5
1	0	0.2	0.8
1	1	0.1	0.9

The explicit CPD table grows exponentially with the number of parameters conditioned-on.

In many cases, we don't need to model a complex interaction between the different causes (combinations of parent values) – we might want the CPD to represent some sort of a probabilistic OR model that scales linearly with additional variables. The Noisy Or model provides this kind of independence of causal influence:

Definition 0.3 Noisy Or

A binary RVY depends on k binary variables X_1, \ldots, X_k in a noisy-or model if:

$$P(Y = 0 \mid x_1, \dots, x_k) = (1 - \lambda_0) \prod_{i=1}^k (1 - \lambda_i)^{x_i}$$

 λ_0 is the *leak* parameter, allowing a positive probability for Y = 1 even of all X_i are 0. λ_i are the *noise parameters* defining the amount by which $X_i = 1$ reduces the probability that Y = 0. When $\lambda_0 = 0$ and all noise parameters λ_i equal 1, the model behaves like a deterministic OR.

The CPD we defined above actually matches a Noisy-Or model with parameters $\lambda_0 = 0$, $\lambda_Y = 0.5$, $\lambda_X = 0.8$.

Example 0.4 Noisy-or and explaining away

We have a joint distribution of three binary RVs defined by $P(X, Y, Z) = P(X)P(Y)P(Z \mid X, Y)$, where $P(Z \mid X, Y)$ is defined by a noisy-or model. We need to show that the model satisfies the explaining away property: $P(x^1|z^1) \ge P(x^1|y^1, z^1)$.

Proof: We will prove for the case of $\lambda_0 = 0$ (although the claim is true in the general case)

$$P(x^{0} | y^{1}, z^{1}) = \frac{P(y^{1} | x^{0}, z^{1})P(x^{0} | z^{1})}{P(y^{1} | z^{1})}$$

(this is an extension of the Bayes rule, we will prove later)

$$P(y^{1} | x^{0}, z^{1}) = 1 - P(y^{0} | x^{0}, z^{1})$$

= $1 - \frac{P(z^{1} | x^{0}, y^{0}) P(y^{0} | x^{0})}{P(z^{1} | x^{0})}$
= 1 since $P(z^{1} | x^{0}, y^{0}) = 0$

Substituting this into the first expression we get, $P(x^0 \mid y^1, z^1) = \frac{P(x^0 \mid z^1)}{P(y^1 \mid z^1)} \ge P(x^0 \mid z^1)$ (since $P(y^1 \mid z^1) \le 1$). Thus $P(x^1 \mid y^1, z^1) = 1 - P(x^0 \mid y^1, z^1) \le 1 - P(x^0 \mid z^1) = P(x^1 \mid z^1)$.

Note that we did not use the fact that the CPD is a noisy-or, but only that $P(z^1|x^0, y^0) = 0$.

Claim 0.5

$$P(X \mid Y, Z) = \frac{P(Y \mid X, Z)P(X \mid Z)}{P(Y \mid Z)}$$

Proof: Per the chain rule:

$$P(X, Y, Z) = P(X | Y, Z)P(Y | Z)P(Z) = P(Y | X, Z)P(X | Z)P(Z)$$

0.1.5 Independence in Random Variables

 \mathbf{X}, \mathbf{Y} and \mathbf{Z} (in bold) are <u>sets</u> of random variables.

 $(\mathbf{X} \perp \mathbf{Y}) \iff P(\mathbf{X}, \mathbf{Y}) = P(\mathbf{X})P(\mathbf{Y}) : \mathbf{X} \text{ and } \mathbf{Y} \text{ are (marginally) independent.}$

In Example 0.2, $P(X = 1, Y = A) = 0.3 \neq 0.4 \times 0.6 = P(X = 1)P(Y = A) \Rightarrow \text{not independent.}$

 $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) \iff P(\mathbf{X}, \mathbf{Y} \mid Z) = P(\mathbf{X} \mid \mathbf{Z})P(\mathbf{Y} \mid \mathbf{Z}) : \mathbf{X} \text{ and } \mathbf{Y} \text{ are conditionally independent given } \mathbf{Z}.$ Additional properties:

- Symmetry: $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) \implies (\mathbf{Y} \perp \mathbf{X} \mid \mathbf{Z})$
- Decomposition: $(\mathbf{X} \perp \mathbf{Y}, \mathbf{W} \mid \mathbf{Z}) \implies (\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z})$
- Weak union: $(\mathbf{X} \perp \mathbf{Y}, \mathbf{W} \mid \mathbf{Z}) \implies (\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}, \mathbf{W})$
- Contraction: $(\mathbf{X} \perp \mathbf{W} \mid \mathbf{Z}, \mathbf{Y})$ and $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) \implies (\mathbf{X} \perp \mathbf{Y}, \mathbf{W} \mid \mathbf{Z})$

Proof: (Decomposition)

By the definition of conditional independence we have: $P(X, Y, W \mid Z) = P(X \mid Z) \cdot P(Y, W \mid Z)$

$$P(X, Y \mid Z) = \sum_{w} P(X, Y, w \mid Z)$$
$$= P(X \mid Z) \sum_{w} P(Y, w \mid Z)$$
$$= P(X \mid Z) P(Y \mid Z)$$

0.1.6 Queries

Once we built a probability distribution, we can use it to answer some questions.

The posterior distribution given some evidence: $P(\mathbf{Y} | \mathbf{E} = e)$

Let χ be the set of all random variables, **E** the observed variables (evidence), **Y** the set of variables we are interested in and $\mathbf{Z} = \chi - \mathbf{Y} - \mathbf{E}$, all other variables.

The marginal MAP query of \mathbf{Y} given \mathbf{E} is:

$$MAP(\mathbf{Y} \mid \mathbf{E} = e) = \operatorname*{arg\,max}_{y} \sum_{z} P(Y = y, Z = z \mid E = e)$$

0.2 Graphs

0.2.1 Paths, Trails, Cycles and Loops

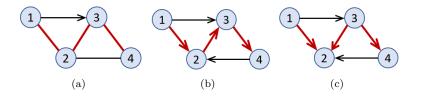


Figure 0.1: (a) undirected path (b) directed path (c) trail

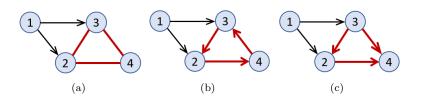


Figure 0.2: (a) undirected cycle (b) directed cycle (c) loop

0.2.2 Trees and Forests

Some definitions:

- DAG directed graph that contains no cycles
- *Singly-connected* contains no cycles or loops
- Singly-connected undirected graph = forest
- Singly-connected undirected graph that is also connected = tree
- Singly-connected directed graph = *polytree*
- Directed graph with at most one *parent* per node = *forest*
- A connected directed forest = tree

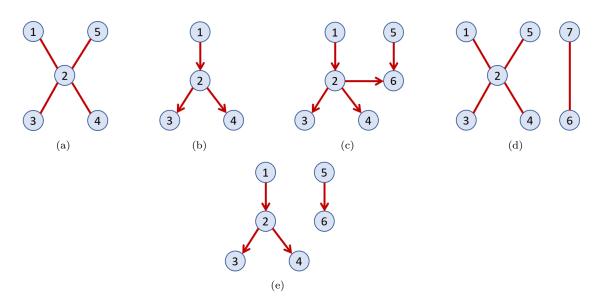


Figure 0.3: (a) undirected tree (b) directed tree (c) polytree (single-connected directed graph) (d) undirected forest (e) directed forest

0.2.3 Topological Ordering

Definition 0.6 Topological Ordering

An ordering of the nodes X_1, \ldots, X_n in a graph $\mathcal{G} = (\chi, \mathcal{E})$ is a topological ordering if whenever $X_i \to X_j \in \mathcal{E}$ than i < j.

Given a directed graph, there might be several valid topological ordering of the nodes. For example:

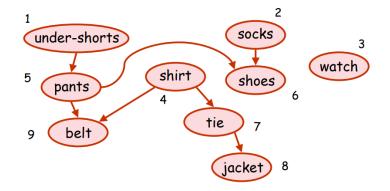


Figure 0.4: Directed graph and a valid topological ordering

Claim 0.7 A DAG has at least one topological order.

There are several algorithms for finding a topological order (for example, using DFS). We will discuss the following algorithm:

Algorithm 1 Topological Sort
1: procedure TopologicalSort(DAG \mathcal{G})
2: $res \leftarrow \emptyset$
3: while \mathcal{G} is not empty do
4: $v \leftarrow \text{any node in } \mathcal{G} \text{ with zero in-degree (no parents)}$
5: Add v to res
6: Remove v and its edges from \mathcal{G}
7: return res

Proof: Correctness of Algorithm 1

We need to show that whenever we add a node v to *res*, we do not break the topological order i.e. there is no edge in \mathcal{G} from a node not in *res* yet to v.

This is true since:

- If v had no parents originally, there cannot be such an edge.
- If v has parents that were removed, they are already in res.

The algorithm cannot get stuck since every DAG has at least one node with zero in-degree (if every node has a parent, we can continue traveling upwards until we reach a visited node).

References

- Gal Chechnik. Background on probability theory. https://moodle.cs.huji.ac.il/cs12/file.php/67800/chap1.pdf.
- [2] Daphne Koller and Nir Friedman. Probabilistic graphical models: principles and techniques. MIT press, 2009.
- [3] Andrew Ng. CS 229 machine learning course materials. *Stanford University*, 2016. http://cs229.stanford.edu/section/cs229-prob.pdf.