Deep Learning - Foundations and Concepts

Chapter 11. Structured Distributions

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Outline

Graphical models

The framework of probabilistic graphical models allows structured probability distributions to be expressed in graphical form:

- They provide a simple way to visualize the structure of a probabilistic model and can be used to design and motivate new models.
- Insights into the properties of the model, including conditional independence properties, can be obtained by inspecting the graph.
- The complex computations required to perform inference and learning in sophisticated models can be expressed in terms of graphical operations.

Directed graphs

- In a probabilistic graphical model, each node represents a random variable, and the links express probabilistic relationships between these variables.
- Directed graphical models (Bayesian networks, or Bayes nets): The graphs have a particular direction indicated by arrows, useful for expressing causal relationships between random variables (the focus of this chapter).
- Undirected graphical models (Markov random fields): The links do not carry arrows and have no directional significance, useful for expressing soft constraints between random variables.

Factorization

Consider a joint distribution $p(a, b, c)$ over three variables a, b and c. We can write the joint distribution in the form:

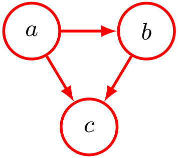
$$p(a, b, c) = p(c|a, b)p(b|a)p(a)$$

which can be represented in terms of a simple graphical model as follows:

- Introduce a node for each of the random variables a, b and c.
- If a random variable y is conditioned on another random variable x, then add a directed link from x to y. We say that x is the parent of y, and y is the child of x.

Factorization

Figure: A directed graphical model representing the decomposition $p(a, b, c) = p(c|a, b)p(b|a)p(a)$



Factorization

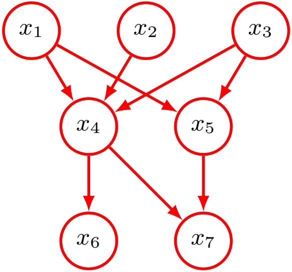
A directed graph also defines a joint distribution given by the product, over all of the nodes of the graph, of a conditional distribution for each node conditioned on the variables corresponding to the parents of that node in the graph. Thus for a graph with K nodes, the joint distribution is given by:

$$p(x_1, \ldots, x_K) = \prod_{k=1}^{K} p(x_k | \mathrm{pa}(k))$$

where $\mathrm{pa}(k)$ denotes the set of parents of x_k.

Factorization

Figure: This directed graph represents the joint distribution $p(x_1)p(x_2)p(x_3)p(x_4|x_1,x_2,x_3)p(x_5|x_1,x_3)p(x_6|x_4)p(x_7|x_4,x_5)$



Discrete variables

Dropping links in the graph reduces the number of independent parameters in a model. Consider two discrete variables x^1 and x^2, each of which has K states. The joint distribution can be written:

$$p(x_1, x_2; \mu) = \prod_{k=1}^{K} \prod_{k'=1}^{K} \mu_{kk'}^{x_k^1 x_{k'}^2}$$

- If there is a link from x^1 to x^2, we need $K^2 - 1$ parameters.
- If x^1 and x^2 are independent, we only need $2(K-1)$ paramters.
- In general, when there are M variables:
  - If their joint distribution is fully connected, we need $K^M - 1$ parameters.
  - If they are independent, we only need $M(K-1)$ parameters.

Discrete variables

Figure: By dropping the link from x^1 to x^2, the number of parameters needed dropped from $K^2 - 1$ to $2(K - 1)$

Discrete variables

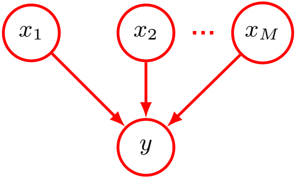
An alternative way to reduce the number of independent parameters in a model is by sharing parameters:

- For the graphical model on the left, we need $K-1+(M-1)K(K-1)$ parameters.
- For the graphical model on the right, we only need $K-1+K(K-1)=K^2-1$ paramters.

Discrete variables

Another way to reduce the number of independent parameters in a model is by using parameterized representations for the conditional distributions instead of complete tables of conditional probability values. For the example graph, assuming x_m are binary variables:

- If using complete tables, we need 2^M parameters.
- If using parameterized representation $p(y = 1|x_1, \ldots, x_M) = \sigma(w_0 + \sum_{m=1}^{M} w_m x_m)$, we only need $M + 1$ parameters.



Gaussian variables

For graphical models in which the nodes represent continuous variables having Gaussian distributions, we consider linear Gaussian models:

$$p(x_i|\mathrm{pa}(i)) = \mathcal{N}(x_i; \sum_{j\in\mathrm{pa}(i)} w_{ij}x_j + b_i, v_i)$$

where w_{ij} and b_i are parameters governing the mean and v_i is the variance of the conditional distribution for x_i. It's easy to see that the joint distribution is a multivariate Gaussian:

$$-\log p(x_1, \ldots, x_D) = -\log \prod_{i=1}^{D} p(x_i|\mathrm{pa}(i))$$

$$= \frac{1}{2}\sum_{i=1}^{D} \frac{1}{v_i}(x_i - \sum_{j\in\mathrm{pa}(i)} w_{ij}x_j - b_i)^2 + \frac{1}{2}\sum_{i=1}^{D} \log v_i + \frac{D}{2}\log 2\pi$$

Gaussian variables

Let's calculate $E(x_i)$ and $\mathrm{cov}(x_i, x_j)$:

$$
\begin{aligned}
E(x_i) = \int x_i p(x) \mathrm{d}x &= \int x_i \prod_{k=1}^{D} p(x_k|\mathrm{pa}(k)) \mathrm{d}x \\
&= \int \prod_{k=1}^{i-1} p(x_k|\mathrm{pa}(k)) (\int x_i p(x_i|\mathrm{pa}(i)) \mathrm{d}x_i) \mathrm{d}x_1 \cdots \mathrm{d}x_{i-1} \\
&= \int (\sum_{j \in \mathrm{pa}(i)} w_{ij} x_j + b_i) \prod_{k=1}^{i-1} p(x_k|\mathrm{pa}(k)) \mathrm{d}x_1 \cdots \mathrm{d}x_{i-1} \\
&= \int (\sum_{j \in \mathrm{pa}(i)} w_{ij} x_j + b_i) p(x) \mathrm{d}x \\
&= \sum_{j \in \mathrm{pa}(i)} w_{ij} E(x_j) + b_i
\end{aligned}
$$

Gaussian variables

For $i < j$:

$$
\begin{aligned}
E(x_i x_j) &= \int x_i x_j p(x) \mathrm{d}x = \int x_i x_j \prod_{l=1}^{D} p(x_l|\mathrm{pa}(l)) \mathrm{d}x \\
&= \int x_i \prod_{l=1}^{j-1} p(x_l|\mathrm{pa}(l)) (\int x_j p(x_j|\mathrm{pa}(j)) \mathrm{d}x_j) \mathrm{d}x_1 \cdots \mathrm{d}x_{j-1} \\
&= \int (\sum_{k \in \mathrm{pa}(j)} w_{jk} x_k + b_j) x_i \prod_{l=1}^{j-1} p(x_l|\mathrm{pa}(l)) \mathrm{d}x_1 \cdots \mathrm{d}x_{j-1} \\
&= \int (\sum_{k \in \mathrm{pa}(j)} w_{jk} x_k + b_j) x_i p(x) \mathrm{d}x \\
&= \sum_{k \in \mathrm{pa}(j)} w_{jk} E(x_i x_k) + b_j E(x_i)
\end{aligned}
$$

Gaussian variables

$$
\begin{aligned}
E(x_i^2) &= \int x_i^2 p(x)\mathrm{d}x = \int x_i^2 \prod_{l=1}^{D} p(x_l|\mathrm{pa}(l))\mathrm{d}x \\
&= \int \prod_{l=1}^{i-1} p(x_l|\mathrm{pa}(l))(\int x_i^2 p(x_i|\mathrm{pa}(i))\mathrm{d}x_i)\mathrm{d}x_1 \cdots \mathrm{d}x_{i-1} \\
&= \int ((\sum_{k\in\mathrm{pa}(i)} w_{ik}x_k + b_i)^2 + v_i)\prod_{l=1}^{i-1} p(x_l|\mathrm{pa}(l))\mathrm{d}x_1 \cdots \mathrm{d}x_{i-1} \\
&= \int ((\sum_{k\in\mathrm{pa}(i)} w_{ik}x_k + b_i)^2 + v_i)p(x)\mathrm{d}x \\
&= \sum_{j,k\in\mathrm{pa}(i)} w_{ij}w_{ik}E(x_j x_k) + 2b_i \sum_{k\in\mathrm{pa}(i)} w_{ik}E(x_k) + b_i^2 + v_i
\end{aligned}
$$

Gaussian variables

Finally, for $i \neq j$ we have:

$$\begin{aligned}
\mathrm{cov}(x_i, x_j) &= E(x_i x_j) - E(x_i)E(x_j) = \sum_{k \in \mathrm{pa}(j)} w_{jk} \mathrm{cov}(x_i, x_k) \\
\mathrm{cov}(x_i, x_i) &= E(x_i^2) - (E(x_i))^2 \\
&= \sum_{j,k \in \mathrm{pa}(i)} w_{ij} w_{ik} \mathrm{cov}(x_j, x_k) + v_i \\
&= \sum_{k \in \mathrm{pa}(i)} w_{ik} \mathrm{cov}(x_i, x_k) + v_i
\end{aligned}$$

We can calculate $E(x_i)$ and $\mathrm{cov}(x_i, x_j)$ by starting at the lowest numbered node and working recursively through the graph.

Binary classifier

Suppose a binary classifier model has probability distributions of the form:

$$p(t_1, \ldots, t_N, w | x^1, \ldots, x^N; \lambda) = p(w; \lambda) \prod_{n=1}^{N} p(t_n | x^n; w)$$

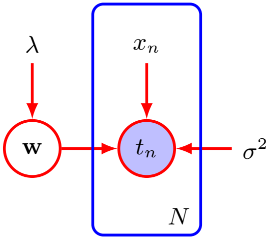
$$p(w; \lambda) = \mathcal{N}(w; 0, \lambda I)$$

Figure: Directed graphical model representing the binary classifier model and its more compact version

Parameters and observations

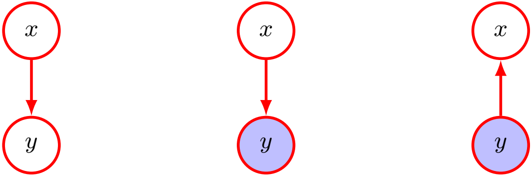
There are three kinds of variables in a directed graphical model:

- Unobserved (also called latent, or hidden) stochastic variables are denoted by open red circles.
- When stochastic variables are observed, so that they are set to specific values, they are denoted by red circles shaded with blue.
- Non-stochastic parameters are denoted by floating variables.



Bayes' theorem

Figure: A graphical representation of Bayes' theorem



Conditional independence

Consider three variables a, b and c, we say that a is conditionally independent of b given c if

$$p(a|b,c) = p(a|c)$$

holds for every possible value of c. Equivalently, this can be written as:

$$p(a,b|c) = p(a|b,c)p(b|c) = p(a|c)p(b|c)$$

We will sometimes use a shorthand notation for conditional independence in which

$$a \perp\!\!\!\perp b|c$$

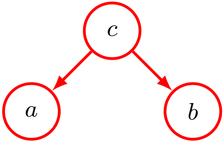
denotes that a is conditionally independent of b given c. In particular, the notation $a \perp\!\!\!\perp b|\emptyset$ denotes that a is independent of b.

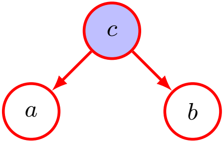
Conditional independence

- An important and elegant feature of graphical models is that conditional independence properties of the joint distribution can be read directly from the graph without having to perform any analytical manipulations.
- The general framework for achieving this is called d-separation, where the “d” stands for “directed”.

Three example graphs

Figure: The first of three examples





Three example graphs

- The joint distribution is given by: $p(a,b,c) = p(a|c)p(b|c)p(c)$.
  - Question: Is $a \perp\!\!\!\perp b|\emptyset$ true?
  - Answer: No, because $p(a,b) = \sum_c p(a,b,c) = \sum_c p(a|c)p(b|c)p(c) \neq p(a)p(b)$.
  - Question: Is $a \perp\!\!\!\perp b|c$ true?
  - Answer: Yes, because $p(a,b|c) = \frac{p(a,b,c)}{p(c)} = p(a|c)p(b|c)$.
- Consider the path from node a to node b via c:
  - The node c is said to be tail-to-tail with respect to this path.
  - The presence of such a path connecting nodes a and b causes these nodes to be dependent.
  - The conditioned node blocks the path from a to b and causes a and b to become conditionally independent.

Three example graphs

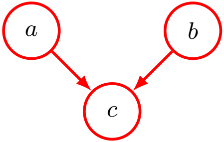
Figure: The second of three examples

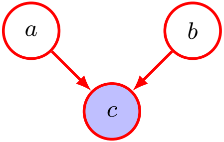
Three example graphs

- The joint distribution is given by: $p(a, b, c) = p(a)p(b|c)p(c|a)$.
  - Question: Is $a \perp\!\!\!\perp b|\emptyset$ true?
  - Answer: No, because $p(a, b) = \sum_c p(a, b, c) = \sum_c p(a)p(b|c)p(c|a) \neq p(a)p(b)$.
  - Question: Is $a \perp\!\!\!\perp b|c$ true?
  - Answer: Yes, because $p(a, b|c) = \frac{p(a,b,c)}{p(c)} = p(a|c)p(b|c)$.
- Consider the path from node a to node b via c:
  - The node c is said to be head-to-tail with respect to this path.
  - The presence of such a path connecting nodes a and b causes these nodes to be dependent.
  - The conditioned node blocks the path from a to b and causes a and b to become conditionally independent.

Three example graphs

Figure: The third of three examples





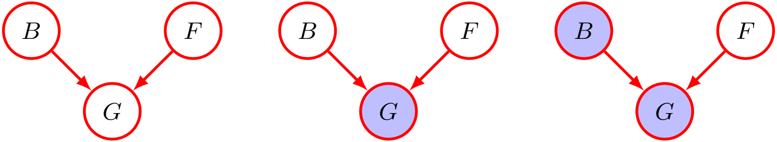
Three example graphs

- The joint distribution is given by: $p(a,b,c) = p(a)p(b)p(c|a,b)$.
  - Question: Is $a \perp\!\!\!\perp b|\emptyset$ true?
  - Answer: Yes, because $p(a,b) = \sum_c p(a,b,c) = \sum_c p(a)p(b)p(c|a,b) = p(a)p(b)$.
  - Question: Is $a \perp\!\!\!\perp b|c$ true?
  - Answer: No, because $p(a,b|c) = \frac{p(a,b,c)}{p(c)} \neq p(a|c)p(b|c)$.
- Consider the path from node a to node b via c:
  - The node c is said to be head-to-head with respect to this path.
  - When node c is unobserved, it blocks the path, and the variables a and b are independent.
  - Conditioning on c unblocks the path and renders a and b dependent. In fact, a head-to-head path will become unblocked if either the node, or any of its descendants, is observed.

Explaining away

To understand further the unusual behavior of the third example, consider three binary random variables relating to the fuel system on a car:

- B: The state of a battery that is either charged ($B = 1$) or flat ($B = 0$).
- F: The state of the fuel tank that is either full of fuel ($F = 1$) or empty ($F = 0$).
- G: The state of an electric fuel gauge and which indicates that the fuel tank is either full ($G = 1$) or empty ($G = 0$).



Explaining away

And here is the probability table:

$$p(B = 1) = 0.9$$
$$p(F = 1) = 0.9$$
$$p(G = 1|F = 1, B = 1) = 0.8$$
$$p(G = 1|F = 1, B = 0) = 0.2$$
$$p(G = 1|F = 0, B = 1) = 0.2$$
$$p(G = 1|F = 0, B = 0) = 0.1$$

Let's calculate $p(F = 0|G = 0)$ and $p(F = 0|G = 0, B = 0)$.

Explaining away

$$
\begin{aligned}
p(F=0) &= 0.1 \\
p(F=0|G=0) &= \frac{p(F=0,G=0)}{p(G=0)} \\
&= \frac{0.072+0.009}{0.162+0.072+0.072+0.009} = \frac{9}{35} \approx 0.257 \\
p(F=0|G=0,B=0) &= \frac{p(F=0,G=0,B=0)}{p(G=0,B=0)} \\
&= \frac{0.009}{0.072+0.009} = \frac{1}{9} \approx 0.111
\end{aligned}
$$

Explaining away

- We see that $p(F=0|G=0) \neq p(F=0|G=0, B=0)$, which means, when G is observed, F and B are indeed dependent.
- This accords with our intuition that finding that the battery is flat explains away the observation that the fuel gauge reads empty.
- In fact, this would also be the case if, instead of observing the fuel gauge directly, we observed the state of some descendant of G, for example a rather unreliable witness who reports seeing that the gauge was reading empty.