Data Mining
Graphical Models for Discrete Data
Undirected Graphs (Markov Random Fields)

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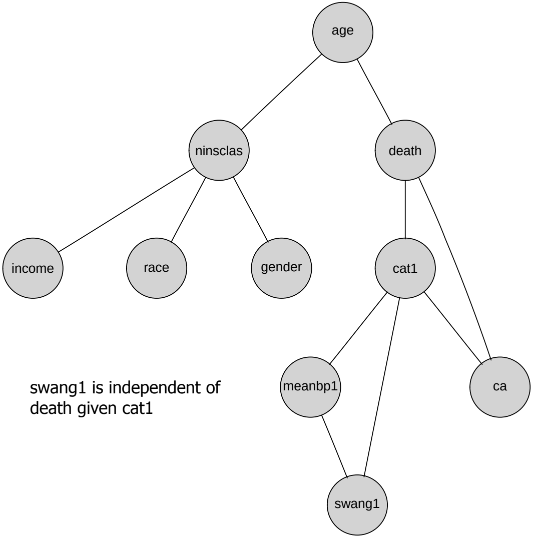
Overview of Coming Two Lectures

- Introduction
- Independence and Conditional Independence
- Graphical Representation of Conditional Independence
- Log-linear Models
  - Hierarchical
  - Graphical
  - Decomposable
- Maximum Likelihood Estimation
- Model Testing
- Model Selection

Graphical Models for Discrete Data

- Task: model the associations (dependencies) between a collection of discrete variables.
- There is no designated *target* variable to be predicted: all variables are treated equal.
- This doesn't mean these models can't be used for prediction. They can!

Graphical Model for Right Heart Catheterization Data



swang1 is independent of
death given cat1

An example

Consider the following table of counts on X and Y:

$n(x,y)$	y			
x	q	r	s	$n(x)$
a	2	5	3	10
b	10	20	10	40
c	8	35	7	50
$n(y)$	20	60	20	100

Suppose we want to estimate the joint distribution of X and Y.

The Saturated Model

Saturated (unconstrained) model

$$\hat{P}(x,y) = \frac{n(x,y)}{n}$$

requires the estimation of 8 probabilities.

The fitted counts $\hat{n}(x,y) = n\hat{P}(x,y)$ are the same as the observed counts.

$\hat{P}(x,y)$	y			
x	q	r	s	$\hat{P}(x)$
a	0.02	0.05	0.03	0.1
b	0.10	0.20	0.10	0.4
c	0.08	0.35	0.07	0.5
$\hat{P}(y)$	0.2	0.6	0.2	1

$\hat{n}(x,y)$	y			
x	q	r	s	$\hat{n}(x)$
a	2	5	3	10
b	10	20	10	40
c	8	35	7	50
$\hat{n}(y)$	20	60	20	100

The Saturated Model and the Curse of Dimensionality

The saturated model estimates cell probabilities by dividing the cell count by the total number of observations. It makes no simplifying assumptions. This approach doesn't scale very well!

Suppose we have k categorical variables with m possible values each.

To estimate the probability of each possible combination of values would require the estimation of m^k probabilities. For $k = 10$ and $m = 5$, this is

$$5^{10} \approx 10 \text{ million probabilities}$$

This is a manifestation of the *curse of dimensionality*: we have fewer data points than probabilities to estimate. Estimates will become unreliable.

How to avoid this curse

Make independence assumptions to obtain a simpler model that still gives a good fit.

Independence Model

$$\hat{P}(x,y) = \hat{P}(x)\hat{P}(y) = \frac{n(x)}{n}\frac{n(y)}{n} = \frac{n(x)n(y)}{n^2}$$

requires the estimation of just 4 probabilities instead of 8.

Fit of independence model

The fitted counts of the independence model are given by

$$\hat{n}(x,y) = n\hat{P}(x,y) = n\,\frac{n(x)n(y)}{n^2} = \frac{n(x)n(y)}{n}$$

For example

$$\hat{n}(x=b, y=s) = \frac{n(x=b)n(y=s)}{n} = \frac{40 \times 20}{100} = 8$$

Compare the fitted counts (left) with the observed counts (right):

$\hat{n}(x,y)$	y			
x	q	r	s	$\hat{n}(x)$
a	2	6	2	10
b	8	24	8	40
c	10	30	10	50
$\hat{n}(y)$	20	60	20	100

$n(x,y)$	y			
x	q	r	s	$n(x)$
a	2	5	3	10
b	10	20	10	40
c	8	35	7	50
$n(y)$	20	60	20	100

Fit of independence model

- The fitted counts of the independence model are quite close to the observed counts.
- We could conclude that the independence model gives a satisfactory fit of the data.
- Use a statistical test to make this more precise (discussed later).

Independence Model

- The saturated model requires the estimation of $m^k - 1$ probabilities.
- The mutual independence model requires just $k(m - 1)$ probability estimates.
- Mutual independence model is usually not appropriate (all variables are independent of one another).
- Interesting models are somewhere in between saturated and mutual independence: this requires the notion of *conditional* independence.

Rules of Probability

1. Sum Rule:

$$\boxed{P(X) = \sum_Y P(X, Y)}$$

2. Product Rule:

$$\boxed{P(X, Y) = P(X)P(Y|X)}$$

3. If X and Y are independent, then

$$\boxed{P(X, Y) = P(X)P(Y)}$$

Independence of (sets of) random variables

Let X and Y be (sets of) random variables.
X and Y are independent if and only if:

$$P(x, y) = P(x)P(y) \text{ for all values } (x, y).$$

Equivalently:

$$P(x \mid y) = P(x), \text{ and } P(y \mid x) = P(y)$$

Y doesn't provide any information about X (and vice versa)

We also write $X \perp\!\!\!\perp Y$.

For example: gender is independent of eye color.

Factorisation criterion for independence

We can relax our burden of proof a little bit:

X and Y are independent iff there are functions $g(x)$ and $h(y)$ (not necessarily the marginal distributions of X and Y) such that

$$P(x, y) = g(x)h(y)$$

In logarithmic form this becomes (since $\log ab = \log a + \log b$):

$$\boxed{\log P(x, y) = g^*(x) + h^*(y),}$$

where $g^*(x) = \log g(x)$.

Factorisation criterion for independence: proof

Suppose that for all x and y:

$$P(x, y) = g(x)h(y)$$

Then

$$P(x) = \sum_y P(x, y) = \sum_y g(x)h(y) = g(x) \sum_y h(y) = c_1 \; g(x)$$

So $g(x)$ is proportional to $P(x)$. Likewise, $h(y)$ is proportional to $P(y)$. Therefore

$$P(x, y) = g(x)h(y) = \frac{1}{c_1} P(x) \frac{1}{c_2} P(y) = c_3 P(x)P(y)$$

Summing over both x and y establishes that $c_3 = 1$, so X and Y are independent.

Conditional Independence

X and Y are *conditionally* independent given Z iff

$$P(x, y \mid z) = P(x \mid z)P(y \mid z) \tag{1}$$

for all values (x, y) and for all values z for which $P(z) > 0$. Equivalently:

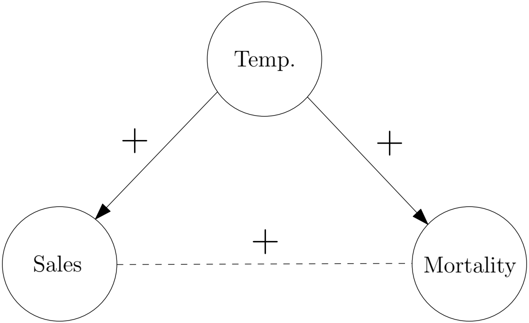
$$P(x \mid y, z) = P(x \mid z)$$

If I already know the value of Z, then Y doesn't provide any additional information about X.

We also write $X \perp\!\!\!\perp Y \mid Z$.

For example: ice cream sales is independent of mortality among the elderly given the weather.

The Causal Picture



$$P(\text{Mortality} = \text{hi} \mid \text{Sales} = \text{hi}) \neq P(\text{Mortality} = \text{hi})$$

$$P(\text{Mortality} = \text{hi} \mid \text{Temp.} = \text{hi}, \text{Sales} = \text{hi}) = P(\text{Mortality} = \text{hi} \mid \text{Temp.} = \text{hi})$$

Factorisation Criterion for Conditional Independence

An equivalent formulation is (multiply equation (1) by $P(z)$):

$$P(x, y, z) = P(x, z)\frac{P(y, z)}{P(z)}$$

Factorisation criterion: $X \perp\!\!\!\perp Y \mid Z$ iff there exist functions g and h such that

$$P(x, y, z) = g(x, z)h(y, z)$$

or alternatively

$$\boxed{\log P(x, y, z) = g^*(x, z) + h^*(y, z)}$$

for all (x, y) and for all z for which $P(z) > 0$.

Conditional Independence Graph

Random Vector $X = (X_1, X_2, \ldots, X_k)$ with probability distribution $P(X)$.
Graph $G = (K, E)$, with $K = \{1, 2, \ldots, k\}$.

The conditional independence graph of X is the undirected graph $G = (K, E)$ where $\{i, j\}$ is *not* in the edge set E if and only if:

$$X_i \perp\!\!\!\perp X_j \mid \text{rest}$$

Conditional Independence Graph: Example

$X = (X_1, X_2, X_3, X_4), 0 < x_i < 1$ with probability density

$$P(x) = e^{c+x_1+x_1x_2+x_2x_3x_4}$$

Now

$$\log P(x) = c + x_1 + x_1x_2 + x_2x_3x_4$$

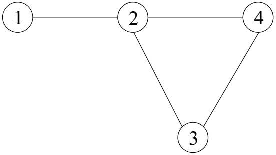
Application of the factorisation criterion gives

$$X_1 \perp\!\!\!\perp X_4 \mid (X_2, X_3) \text{ and } X_1 \perp\!\!\!\perp X_3 \mid (X_2, X_4),$$

For example

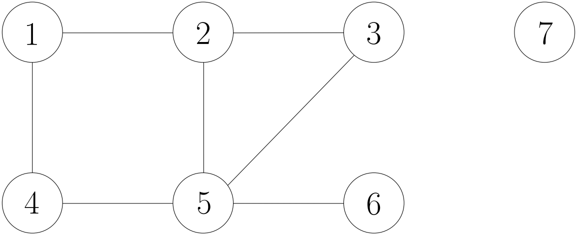
$$\log P(x) = \underbrace{c + x_1 + x_1x_2}_{g(x_1,x_2,x_3)} + \underbrace{x_2x_3x_4}_{h(x_2,x_3,x_4)}$$

Hence, the conditional independence graph is:



Separation and Conditional Independence

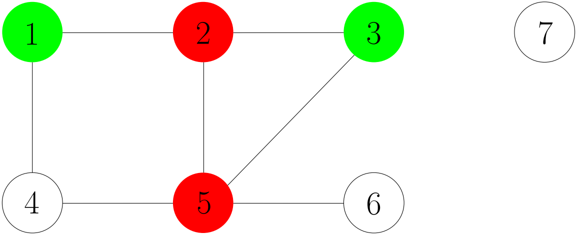
Consider the following conditional independence graph:



- $X_1 \perp\!\!\!\perp X_3 \mid (X_2, X_4, X_5, X_6, X_7)$

$\{2,5\}$ separates 1 from 3

Consider the following conditional independence graph:



- $X_1 \perp\!\!\!\perp X_3 \mid (X_2, X_4, X_5, X_6, X_7)$
- $\{2,5\}$ separates 1 from 3 $\Rightarrow X_1 \perp\!\!\!\perp X_3 \mid (X_2, X_5)$

Separation and Conditional Independence

Notation:

$$X_a = (X_i \ : \ i \in a)$$

where a is a subset of $\{1, 2, \ldots, k\}$.

For example, if $a = \{1, 3, 6\}$ then $X_a = (X_1, X_3, X_6)$.

The set a separates node i from node j iff every path from node i to node j contains one or more nodes in a (every path "goes through" a).

a separates b from c (a, b, c disjoint):

$$\text{For every } i \in b \text{ and } j \in c : a \text{ separates } i \text{ from } j$$

Equivalent Independence (Markov) Properties

1. Pairwise: for all non-adjacent vertices i and j

$$X_i \perp\!\!\!\perp X_j \mid \text{rest}$$

   This is how we defined the graph.

2. Global: if a separates b from c (a, b, c disjoint), then

$$X_b \perp\!\!\!\perp X_c \mid X_a$$

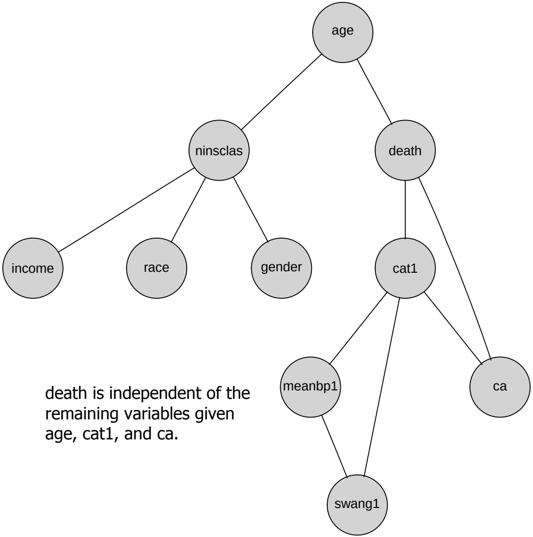
3. Local:

$$X_i \perp\!\!\!\perp \ \text{rest} \mid \text{boundary}(i),$$

   where boundary(i) is the set of nodes adjacent (directly connected) to node i.

These properties are equivalent in the following sense: if all pairwise independencies corresponding to graph G hold for a given probability distribution, then all the global independencies corresponding to G also hold for that distribution (and vice versa).

Graphical Model for Right Heart Catheterization Data



death is independent of the remaining variables given age, cat1, and ca.

Bernoulli random variable

Let X be a Bernoulli random variable with $P(X = 1) = p(1)$ and $P(X = 0) = p(0)$.

We can write the probability function in a single formula as follows:

$$P(X = x) = p(1)^x p(0)^{1-x} \qquad \text{for } x \in \{0, 1\}$$

Check that filling in $x = 1$ gives $p(1)$, and filling in $x = 0$ gives $p(0)$ as required.

Taking logarithms we get:

$$\begin{aligned} \log P(X = x) &= \log \left(p(1)^x p(0)^{1-x} \right) \\ &= \log p(1)^x + \log p(0)^{1-x} \\ &= x \log p(1) + (1 - x) \log p(0) \\ &= \log p(0) + \log \frac{p(1)}{p(0)}\, x \end{aligned}$$

2×2 Table

The probability function P_{12} of bivariate Bernoulli random vector (X_1, X_2) is determined by

$$P(x_1, x_2) = p(x_1, x_2)$$

where $p(x_1, x_2)$ is the table of probabilities:

$p(x_1, x_2)$	$x_2 = 0$	$x_2 = 1$	Total
$x_1 = 0$	$p(0,0)$	$p(0,1)$	$p_1(0)$
$x_1 = 1$	$p(1,0)$	$p(1,1)$	$p_1(1)$
Total	$p_2(0)$	$p_2(1)$	1

Probability function for 2 × 2 Table

Again we can write this as a single formula:

$$P(x_1, x_2) = p(0,0)^{(1-x_1)(1-x_2)} p(0,1)^{(1-x_1)x_2} p(1,0)^{x_1(1-x_2)} p(1,1)^{x_1 x_2}$$

Taking logarithms and collecting terms in x_1, x_2, and x_1x_2 gives:

$$\begin{aligned} \log P(x_1, x_2) &= \log p(0,0) + \log \frac{p(1,0)}{p(0,0)}\, x_1 + \\ &\quad \log \frac{p(0,1)}{p(0,0)}\, x_2 + \log \frac{p(1,1)p(0,0)}{p(0,1)p(1,0)}\, x_1 x_2 \end{aligned}$$

Verify this using elementary properties of logarithms:

1. $\log a^b = b \log a$,
2. $\log \frac{a}{b} = \log a - \log b$, and
3. $\log ab = \log a + \log b$.

Log-linear expansion

Reparameterizing the right hand side leads to the so-called *log-linear expansion*

$$\log P(x_1, x_2) = u_\emptyset + u_1 x_1 + u_2 x_2 + u_{12} x_1 x_2$$

The coefficients, $u_\emptyset, u_1, u_2, u_{12}$ are known as the u-terms.

For example, the coefficient of the product $x_1 x_2$,

$$u_{12} = \log \frac{p(1,1)p(0,0)}{p(0,1)p(1,0)} = \log \mathrm{cpr}(X_1, X_2)$$

is the logarithm of the cross product ratio of X_1 and X_2.

Cross-product Ratio

The cross-product ratio between binary variables X_1 and X_2 is:

$$\text{cpr}(X_1, X_2) = \frac{p(1,1)p(0,0)}{p(0,1)p(1,0)}$$

- $\text{cpr}(X_1, X_2) > 1$: positive association between X_1 and X_2.
- $\text{cpr}(X_1, X_2) < 1$: negative association between X_1 and X_2.
- $\text{cpr}(X_1, X_2) = 1$: no association between X_1 and X_2.

Independence and u-terms

Claim:

$$X_1 \perp\!\!\!\perp X_2 \Leftrightarrow u_{12} = 0$$

Proof: the factorisation criterion states that $X_1 \perp\!\!\!\perp X_2$ iff there exist two functions g and h such that

$$\log P(x_1, x_2) = g(x_1) + h(x_2) \text{ for all } (x_1, x_2)$$

If $u_{12} = 0$, we get

$$\log P(x_1, x_2) = u_\emptyset + u_1 x_1 + u_2 x_2,$$

so

$$g(x_1) = u_\emptyset + u_1 x_1 \qquad h(x_2) = u_2 x_2$$

suffices. If $u_{12} \neq 0$, no such decomposition is possible.

Three Dimensional Bernoulli

The joint distribution of three binary variables can be written:

$$P(x_1, x_2, x_3) = p(0,0,0)^{(1-x_1)(1-x_2)(1-x_3)} \cdots p(1,1,1)^{x_1 x_2 x_3}$$

Log-linear expansion

$$\begin{aligned} \log P(x_1, x_2, x_3) &= u_\emptyset + u_1 x_1 + u_2 x_2 + u_3 x_3 + u_{12} x_1 x_2 + \\ & \quad u_{13} x_1 x_3 + u_{23} x_2 x_3 + u_{123} x_1 x_2 x_3 \end{aligned}$$

With

$$\begin{aligned} u_{123} &= \log\left(\frac{p(1,0,0)p(1,1,1)}{p(1,1,0)p(1,0,1)}\right) - \log\left(\frac{p(0,0,0)p(0,1,1)}{p(0,1,0)p(0,0,1)}\right) \\ &= \log\left(\frac{\text{cpr}(X_2, X_3 | X_1 = 1)}{\text{cpr}(X_2, X_3 | X_1 = 0)}\right) \end{aligned}$$

Independence and the *u*-terms

Observation:

$$X_2 \perp\!\!\!\perp X_3 \mid X_1 \Leftrightarrow u_{23} = 0 \text{ and } u_{123} = 0$$

Proof: use factorisation criterion.

$X_2 \perp\!\!\!\perp X_3 \mid X_1 \Leftrightarrow$ there are functions $g(x_1, x_2)$ and $h(x_1, x_3)$ such that

$$\log P(x_1, x_2, x_3) = g(x_1, x_2) + h(x_1, x_3)$$

This is only possible when $u_{23} = 0$ (so the term $x_2 x_3$ drops out), and $u_{123} = 0$ (so the term $x_1 x_2 x_3$ drops out).

Why the log-linear representation?

Why do we use the log-linear representation of the probability table?

1. We are interested in expressing conditional independence constraints.
2. There is a straightforward correspondence between such constraints being satisfied, and the elimination of certain collections of u-terms from the log-linear expansion.
3. This correspondence is established by applying the factorisation criterion: $X \perp\!\!\!\perp Y \mid Z$ if and only if there exist functions g and h such that

$$\boxed{\log P(x,y,z) = g(x,z) + h(y,z)}$$