STSCI 4780/5780
Relationships between variables: Preliminaries
(Conditional dependence & independence, graphical models, regression)

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Agenda

1. **Relationships between variables**
2. **Joint distributions and graphical models**
3. **Example: Binomial prediction**

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Relationships between variables

We're interested in settings where each case/item/object has *two or more properties* $(x, y, \ldots)$; we want to learn how they are related

Goals

- **Explanatory:** Seek to understand the processes/mechanisms linking x and y...
- **Predictive:** Seek to predict a future y value from observing or controlling a future x value

We will develop tools and terminology for building and describing explanatory and predictive models for multivariate data

For more on explanatory vs. predictive goals: "To explain or to predict?" (Galit Shmueli 2010)

Terminology

Types of studies

- **Correlation/dependence:** Learn about the *joint distribution*, $p(x, y)$, in settings where x and y are both potentially uncertain/random
- **Regression/conditional density estim'n:** Learn about the *conditional distribution*, $p(y|x)$, in either of two settings:
  - x is controllable/deterministic
  - x is "random" (uncertain a priori, described via probability)

Names of variables (conditional/regression setting)

- x: covariate, regressor, predictor, explanatory variable, input, independent variable
- y: response, prediction, output, dependent variable
- Either/both may be vectors

Conditional distribution properties

- **Regression function:** The *conditional expectation value* (conditional mean) of y *given* x is the regression function

$$f(x) = \mathbb{E}(y|x) \equiv \int dy\; y\, p(y|x)$$

- **Variance:**
  - $\mathrm{Var}(y|x) = \text{Const}$: *homoskedastic*
  - $\mathrm{Var}(y|x) \neq \text{Const}$: *heteroskedastic*

Regression = Learning a conditional *expectation*

Conditional density estimation = Learning a conditional *distribution*, $p(y|x, \cdots)$

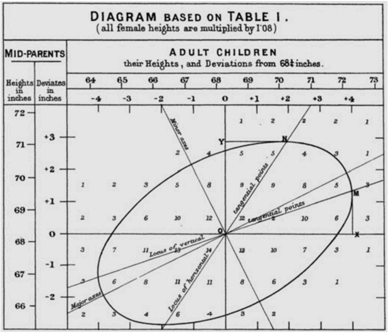
(Joint) Density estimation = Learning $p(x, y)$ (when x is also uncertain/random)

Examples with random x

Population studies

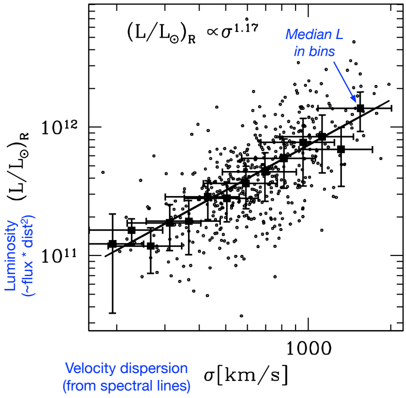
Heights of parents ("midparent") and children

Contour of counts in cells



Galton (1885) "Regression Towards Mediocrity in Hereditary Stature"

Faber-Jackson relation for elliptical galaxies



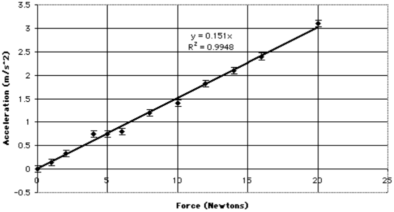
Bernardi+ (2002)

Examples with deterministic x

Curve fitting

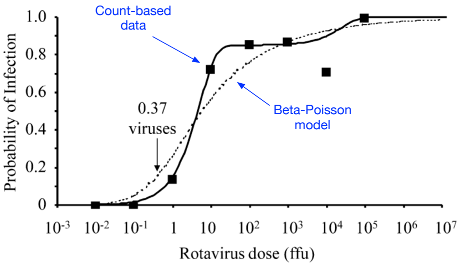
Newton's 2nd law: $a = \frac{F}{m}$

Apply different forces to a fixed mass



Batesville HS AP Physics Class

Dose-response curve



Gale (2003), "Developing risk assessments of waterborne microbial contaminations"

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Joint, conditional, and marginal distributions

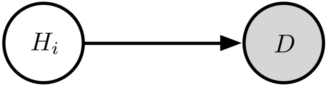
Bayesian inference is largely about the interplay between *joint*, *conditional*, and *marginal* distributions for related quantities

Ex: Bayes's theorem relating hypotheses and data ($||\mathcal{C}$):

$$P(H_i|D) = \frac{P(H_i)P(D|H_i)}{P(D)} = \frac{P(H_i, D)}{P(D)} = \frac{\text{joint for everything}}{\text{marginal for knowns}}$$

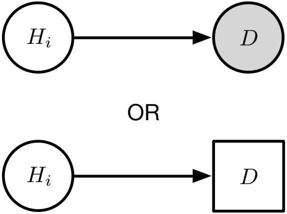
The usual form ($\propto$ prior $\times$ likelihood) focuses on an *available factorization* of the joint

Express this factorization via a *directed acyclic graph* (DAG):



Joint distribution structure as a graph

- Graph = *nodes/vertices* connected by *edges/links*
- Circular/square nodes/vertices = a priori uncertain/random quantities
  - Gray or square = quantity becomes known as data
- Directed edges specify conditional dependence
- Absence of an edge indicates conditional *in*dependence
  → a variable can be *dropped* in a factor in the joint
  → *the most important edges are the missing ones*



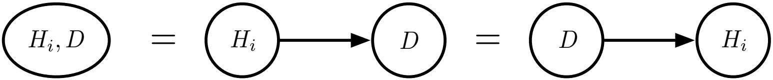
$$P(H_i, D) = P(H_i) \times P(D|H_i)$$

A DAG tells you what factorization is *available* or *of interest*

Other factorizations—or the full joint probability for *all* nodes—exist and may be found via probability theory

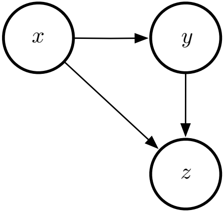
E.g., the product rule (for conjunctions) as a "graphical equation":

$$P(H_i, D) \quad = \quad P(H_i) \times P(D|H_i) \quad = \quad P(D) \times P(H_i|D)$$

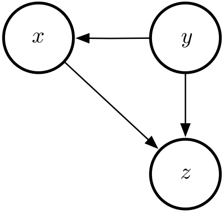


$p(x, y, z)$

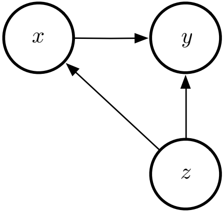
$p(x)p(y|x)p(z|x, y)$



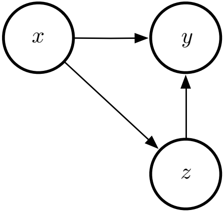
$p(y)p(x|y)p(z|y, x)$



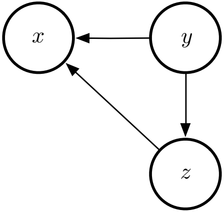
$p(z)p(x|z)p(y|z, x)$



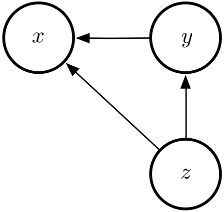
$p(x)p(z|x)p(y|x, z)$



$p(y)p(z|y)p(x|y, z)$

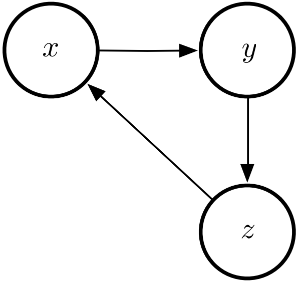


$p(z)p(y|z)p(x|z, y)$



Cycles not allowed

$$p(x|z) \times p(y|x) \times p(z|y)?$$



We can focus on *directed acyclic graphs* (DAGs)

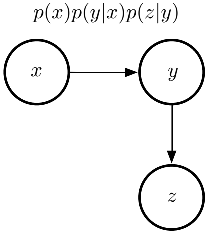
Conditional independence

Suppose for the problem at hand z is independent of of x when y is known:

$$p(z|x, y) = p(z|y)$$

We say: "z is *conditionally independent* of x, given y"

$$z \perp\!\!\!\perp x \mid y$$



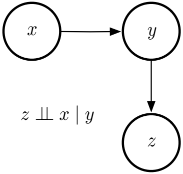
Absence of an edge indicates conditional *in*dependence
Missing edges indicate simplification in structure
(there is no 3-argument function above)

$\rightarrow$ *the most important edges are the missing ones* (see CI on SE)

DAGs with missing edges

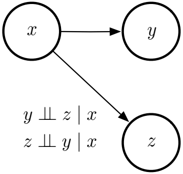
Conditional independence

$p(x)\,p(y|x)\,p(z|y)$



"Causal chain"

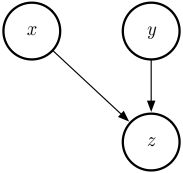
$p(x)\,p(y|x)\,p(z|x)$



"Common cause"

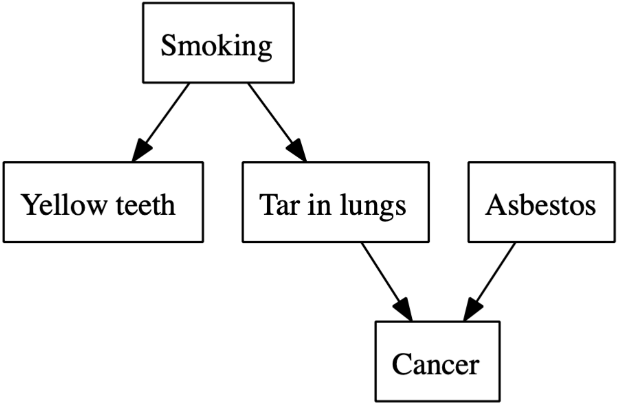
Conditional dependence

$p(x)\,p(y)\,p(z|x,y)$

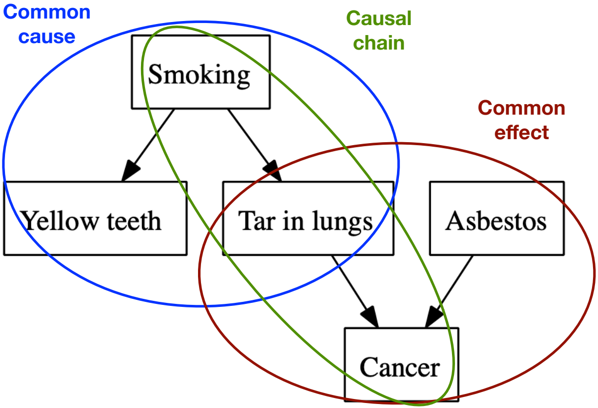


"Multiple causes
or common effect"

Example graphical model — Smoking and cancer



DAG model indicating (hypothetical) relationships between smoking, cancer, and other covariates (Shalizi 2016).



DAG model indicating (hypothetical) relationships between smoking, cancer, and other covariates (Shalizi 2016).

Conditional vs. complete independence

"z is *conditionally* independent of x, given y"

$$\neq$$

"z is independent of x"

(Complete) independence would imply:

$$p(z|x) = p(z) \quad \text{(i.e., not a function of } x\text{)}$$

Conditional independence is weaker:

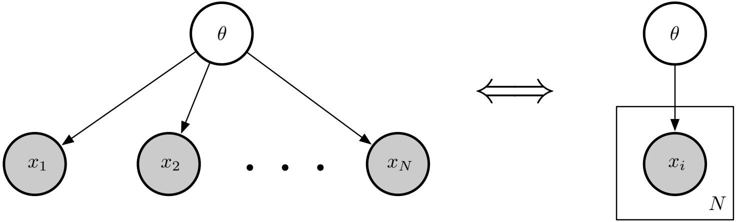
$$\begin{aligned} p(z|x) &= \int dy\ p(z, y|x) \\ &= \int dy\ p(y|x)\, p(z|x, y) \\ &= \int dy\ p(y|x)\, p(z|y) \quad \text{since } z \perp\!\!\!\perp x \mid y \end{aligned}$$

Although x drops out of the last factor, x dependence remains in $p(y|x)$

x *does* provide information about z, but it only does so through the information it provides about y (which directly influences z)

Bayes's theorem with IID samples

For model with parameters θ predicting data $D = \{x_i\}$ that are IID given θ:



$$p(\theta, D) = p(\theta)p(\{x_i\}|\theta) \;=\; p(\theta)\prod_{i=1}^{N} p(x_i|\theta)$$

"IID" means each datum is *conditionally independent* of others, *given* θ

To find the posterior for the unknowns (θ), divide the joint by the marginal for the knowns ($\{x_i\}$):

$$p(\theta|\{x_i\}) = \frac{p(\theta)\prod_{i=1}^{N} p(x_i|\theta)}{p(\{x_i\})} \quad \text{with} \quad p(\{x_i\}) = \int d\theta\, p(\theta)\prod_{i=1}^{N} p(x_i|\theta)$$

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Binomial counts

   . . . n_1 heads in N flips

   . . . n_2 heads in N flips

Suppose we know n_1 and want to predict n_2

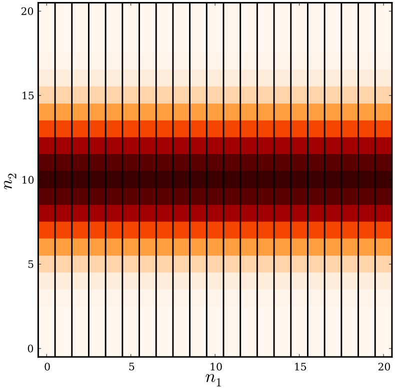
Predicting binomial counts — known α

Success probability $\alpha \to p(n|\alpha) = \frac{N!}{n!(N-n)!}\alpha^n(1-\alpha)^{N-n} \qquad || \, N$

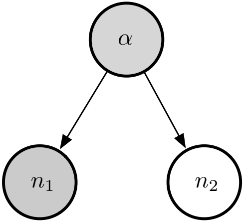
Consider two successive runs of $N = 20$ trials, *known* $\alpha = 0.5$

$$p(n_2|n_1, \alpha) = p(n_2|\alpha) \qquad || \, \mathcal{C}$$

n_1 and n_2 are *conditionally independent*



DAG for binomial prediction — known α



$$p(\alpha, n_1, n_2) = p(\alpha)p(n_1|\alpha)p(n_2|\alpha)$$

$$\begin{aligned} p(n_2|\alpha, n_1) &= \frac{p(\alpha, n_1, n_2)}{p(\alpha, n_1)} \\ &= \frac{p(\alpha)p(n_1|\alpha)p(n_2|\alpha)}{p(\alpha)p(n_1|\alpha)} \\ &= p(n_2|\alpha) \end{aligned}$$

Knowing α lets you predict each n_i, independently

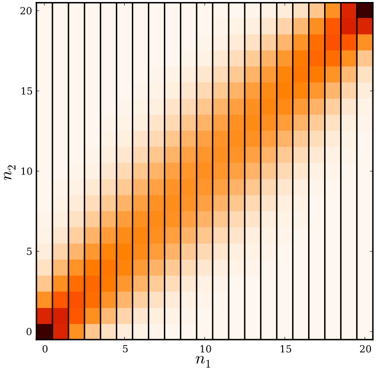
Predicting binomial counts — uncertain α

Consider the same setting, but with α *uncertain*

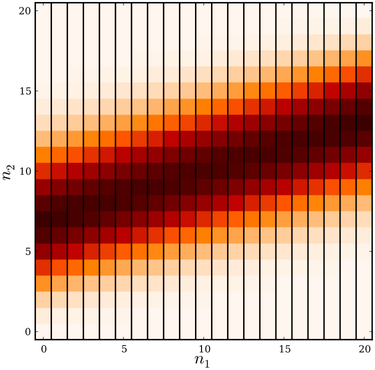
Outcomes are *physically* independent, but n_1 tells us about $\alpha \rightarrow$ outcomes are *marginally dependent* (see Lec 09 for calculation):

$$p(n_2|n_1) = \int d\alpha \; p(\alpha, n_2|n_1) \; = \; \int d\alpha \; p(\alpha|n_1)\, p(n_2|\alpha) \qquad || \, \mathcal{C}$$

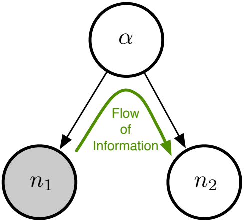
Flat prior on α



Prior: $\alpha = 0.5 \pm 0.1$



DAG for binomial prediction



$$p(\alpha, n_1, n_2) = p(\alpha)p(n_1|\alpha)p(n_2|\alpha)$$

From joint to conditionals:

$$p(\alpha|n_1, n_2) = \frac{p(\alpha, n_1, n_2)}{p(n_1, n_2)} = \frac{p(\alpha)p(n_1|\alpha)p(n_2|\alpha)}{\int d\alpha\ p(\alpha)p(n_1|\alpha)p(n_2|\alpha)}$$

$$p(n_2|n_1) = \frac{\int d\alpha\, p(\alpha, n_1, n_2)}{p(n_1)}$$

Observing n_1 lets you learn about α
Knowledge of α affects predictions for n_2 $\rightarrow$ dependence on n_1