# STSCI 4780
# 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

# 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:** Learn about the *conditional distribution*, $p(y|x)$, in settings where $x$ is controllable/deterministic, or in settings where $x$ is random but becomes known

## *Names of variables*

- $x$: covariate, regressor, predictor, explanatory variable, input, independent variable
- $y$: response, prediction, output, dependent variable

## *Conditional distribution properties*

- **Regression function:** The 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)

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# Joint, conditional, and marginal distributions

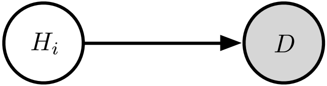
Bayesian inference is largely about the interplay between *joint*, *conditional*, and *marginal* distributions for related quantities

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

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

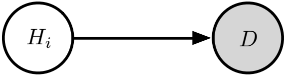
The usual form identifies an *available factorization* of the joint

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

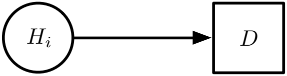


# Joint distribution structure as a graph

- 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*



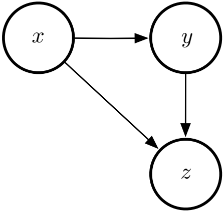

OR



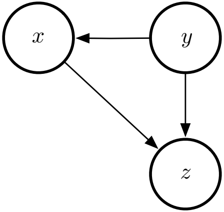

$$P(H_i, D) = P(H_i) \times P(D|H_i)$$

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

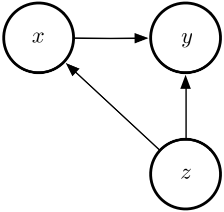
$p(x)p(y|x)p(z|x, y)$



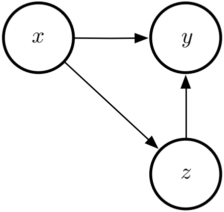

$p(y)p(x|y)p(z|y, x)$



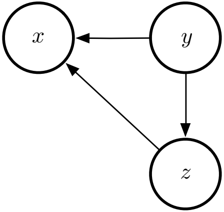

$p(z)p(x|z)p(y|z, x)$



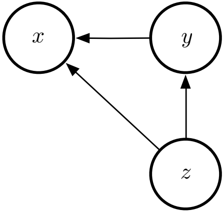

$p(x)p(z|x)p(y|x, z)$




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

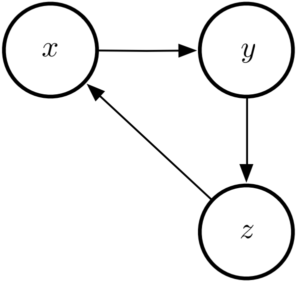



$p(z)p(y|z)p(x|z, y)$



# Cycles not allowed

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




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

# Conditional independence

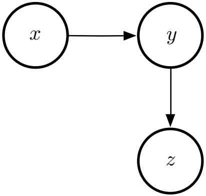
Suppose for the problem at hand $z$ is independent of of $x$ when $y$ is known:

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

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

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

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




Absence of an edge indicates conditional *in*dependence

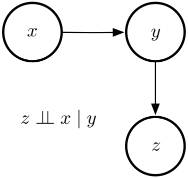
Missing edges indicate simplification in structure

$\rightarrow$ *the most important edges are the missing ones*

# DAGs with missing edges

## Conditional independence

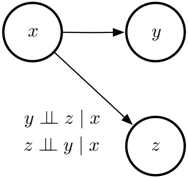
$p(x)\,p(y|x)\,p(z|y)$




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

"Causal chain"

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



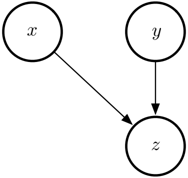

$y \perp\!\!\!\perp z \mid x$

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

"Common cause"

## Conditional dependence

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




"Common effects"

# 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:

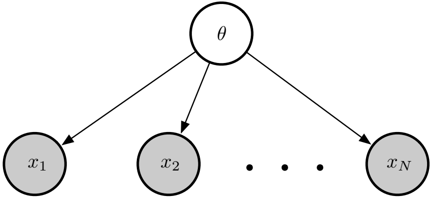
$$\begin{aligned} p(z|x) &= \int dy\ p(z, y|x) \\ &= \int dy\ p(y|x)\, p(z|x, y) \\ &= \int dy\ p(y|x)\, p(z|y) \quad \text{since } z \perp\!\!\!\perp x \mid y \end{aligned}$$

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

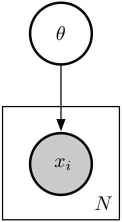
$x$ *does* provide information about $z$, but it only does so through the information it provides about $y$ (which directly influences $z$)

# Bayes's theorem with IID samples

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




$$\Longleftrightarrow$$




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

"IID" means each datum is *conditionally independent* of others, *given* $\theta$

To find the posterior for the unknowns ($\theta$), 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 $n_2$

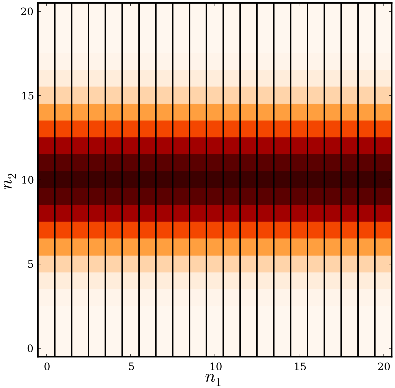
# Predicting binomial counts — known $\alpha$

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

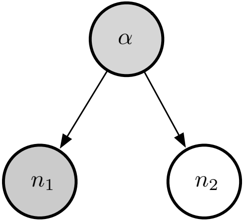
Consider two successive runs of $N = 20$ trials, *known* $\alpha = 0.5$

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

$n_1$ and $n_2$ are *conditionally independent*



# DAG for binomial prediction — known $\alpha$




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

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

Knowing $\alpha$ lets you predict each $n_i$, independently

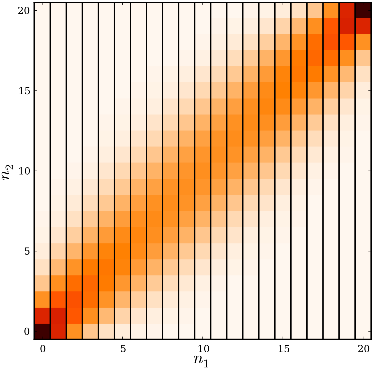
# Predicting binomial counts — uncertain $\alpha$

Consider the same setting, but with $\alpha$ *uncertain*

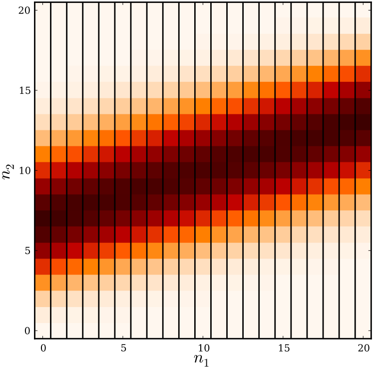
Outcomes are *physically* independent, but $n_1$ tells us about $\alpha \rightarrow$ outcomes are *marginally dependent* (see Lec 12 for calculation):

$$p(n_2|n_1, N) = \int d\alpha\; p(\alpha, n_2|n_1, N) \;=\; \int d\alpha\; p(\alpha|n_1, N)\, p(n_2|\alpha, N)$$

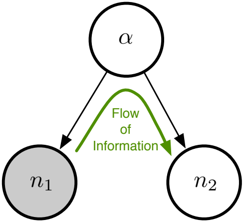
Flat prior on $\alpha$




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 $\alpha$
Knowledge of $\alpha$ affects predictions for $n_2 \rightarrow$ dependence on $n_1$