

STSCI 4780/5780

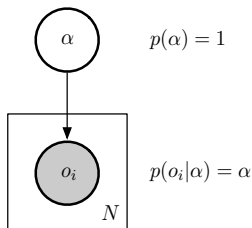
Relationships between variables: Regression

Tom Lored, CCAPS & SDS, Cornell University

© 2022-03-29

Recap via DAGs

Univariate data DAGs — Bernoulli trials



Read *generic* structure of the joint dist'n off the DAG:

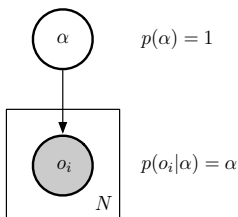
$$p(\alpha, \{o_i\}) = p(\alpha) \prod_{i=1}^N p(o_i | \alpha)$$

Plug in distributions for the specific problem:

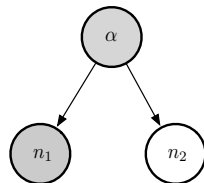
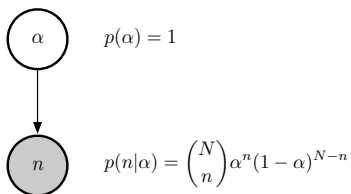
$$\begin{aligned} p(\alpha, \{o_i\}) &= 1 \times \prod_{i=1}^N \alpha^{o_i} (1 - \alpha)^{1-o_i} \\ &= \alpha^n (1 - \alpha)^{N-n} \end{aligned}$$

Univariate data DAGs

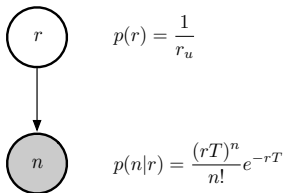
Bernoulli outcomes



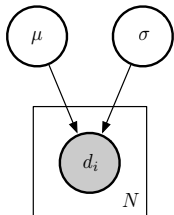
Binomial counts — estimation, prediction



Poisson counts



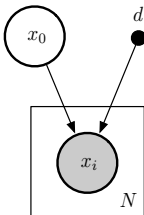
Normal mean and standard deviation



$$p(\mu) = C$$
$$p(\sigma) \propto \frac{1}{\sigma}$$

$$p(d_i|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(d_i - \mu)^2}{2\sigma^2}}$$

Cauchy location estimation



$$p(x_0) = C$$

$$p(x_i|x_0, d) = \frac{1}{\pi d} \frac{1}{1 + \left(\frac{x_i - x_0}{d}\right)^2}$$

Common features

- *Univariate data*—binary, integer or real *scalar* samples
- *Conditionally independent* data

Most problems also univariate in parameter space

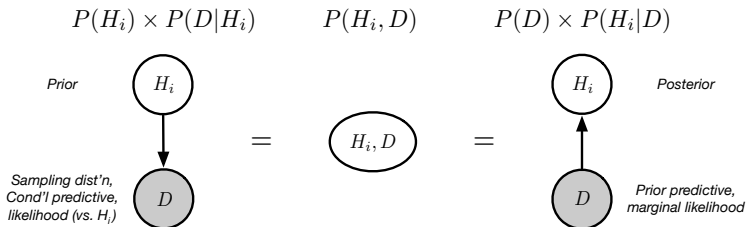
Repeated sampling problems were (conditionally) IID

These were all univariate parametric distribution estimation problems:

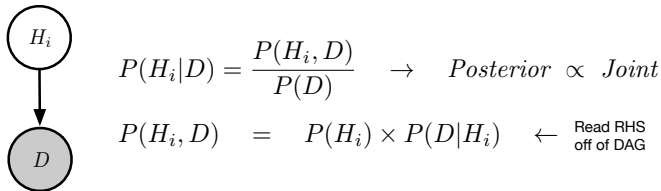
- Discrete data: Parametric PMF estimation
- Continuous data: Parametric density (PDF) estimation

Bayes's theorem and DAGs

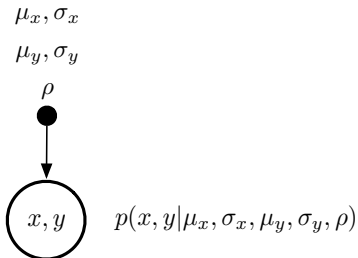
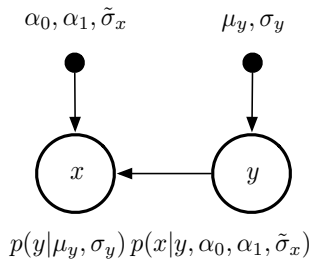
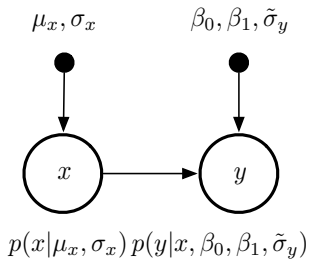
Joint distribution ("AND" rule) as a "DAG equation":



Bayes's theorem via the joint for hypothesis & data:



Bivariate normal sampling dist'n DAGs

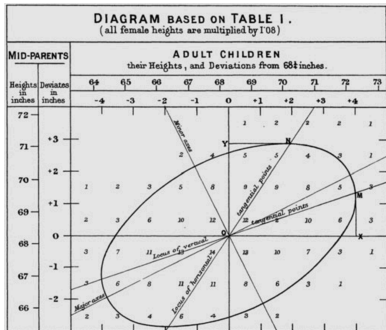


Lec16 recap: Examples with random \times

Population studies

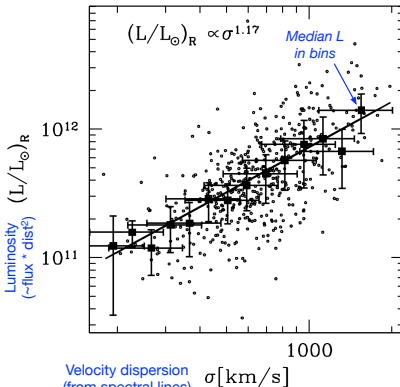
Heights of parents (“midparent”) and children

Contour of counts in cells



Galton (1885) “Regression Towards Mediocrity in Hereditary Stature”

Faber-Jackson relation for elliptical galaxies



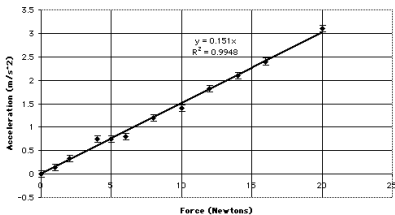
Bernardi+ (2002)

Lec16 recap: Examples with deterministic \times

Curve fitting

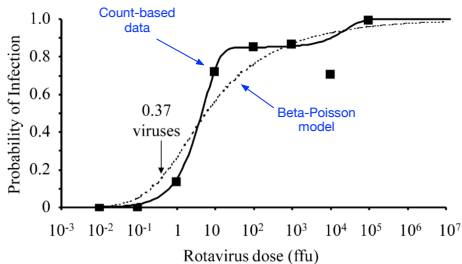
Newton's 2nd law: $a = \frac{F}{m}$

Apply different forces to a fixed mass



Batesville HS AP Physics Class

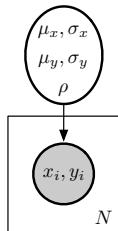
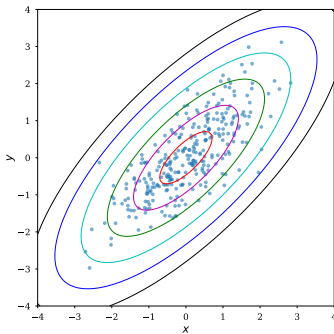
Dose-response curve



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

Bivariate normal inference problems

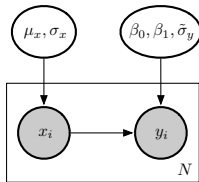
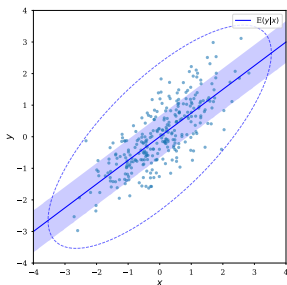
BMN density estimation



$$\text{Joint: } p(\mu_x, \sigma_x, \mu_y, \sigma_y, \rho) \prod_{i=1}^N p(x_i, y_i | \mu_x, \sigma_x, \mu_y, \sigma_y, \rho)$$

$$\text{Inference: } p(\mu_x, \sigma_x, \mu_y, \sigma_y, \rho | \{x_i, y_i\}) \propto \text{Joint}$$

BVN regression



$$\text{Joint: } p(\mu_x, \sigma_x) p(\beta_0, \beta_1, \tilde{\sigma}_y) \prod_{i=1}^N p(x_i | \mu_x, \sigma_x) p(y_i | x_i, \beta_0, \beta_1, \tilde{\sigma}_y)$$

$$\begin{aligned} \text{Inference: } p(\beta_0, \beta_1, \tilde{\sigma}_y | \{x_i, y_i\}) &= \int d\mu_x \int d\sigma_x p(\mu_x, \sigma_x, \beta_0, \beta_1, \tilde{\sigma}_y | \{x_i, y_i\}) \\ &\propto p(\beta_0, \beta_1, \tilde{\sigma}_y) \prod_{i=1}^N p(y_i | x_i, \beta_0, \beta_1, \tilde{\sigma}_y) \end{aligned}$$

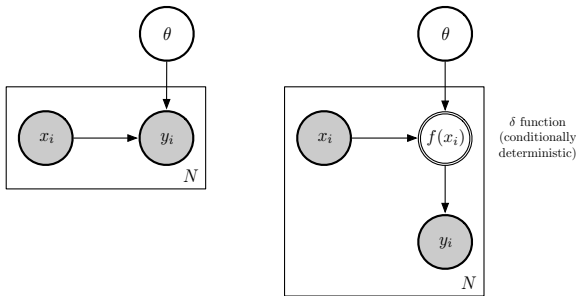
Note that the x_i marginal, $p(x_i | \mu_x, \sigma_x)$, *plays no role* in inferring the regression line (the *observed* x_i values of course play a strong role)

Parametric regression

Infer θ determining the *conditional expectation*

$$\mathbb{E}(y_i|x_i, \theta) = f(x_i; \theta)$$

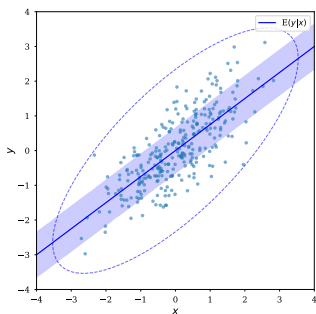
Regression function may be implicit (conditional expectation of y dist'n) or explicit ("true + error" or "typical + scatter")



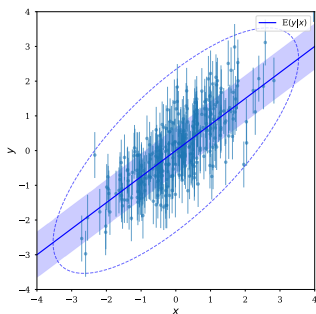
Often natural to express this via an additive error model:

$$y_i = f(x_i; \theta) + \epsilon_i; \quad \mathbb{E}(\epsilon_i) = 0$$

Population perspective



True+error perspective



Band displays the conditional prediction uncertainty for y at a given x

Error bars: *Data* do not have errors, only *inferences* have errors:

- Error bars often signify prediction uncertainty (width of the sampling dist'n)—they belong on predictions, not observations
- View as likely range of error if one naively considers each y_i as an estimate of $f(x_i)$ (disregarding other data!)

Simple normal linear regression

A function-plus-error model (interpretable either as “true value plus noise” or “typical value plus dispersion”) for scalar x and y :

$$y_i = f(x_i; \theta) + \epsilon_i; \quad \epsilon_i \sim \text{Norm}(0; \sigma^2); \quad i = 1 \text{ to } N$$

$$f(x; \theta) = \sum_{\alpha=1}^M A_{\alpha} g_{\alpha}(x)$$

for *specified* set of basis functions, $g_{\alpha}(x)$

- Parameters are M coefficients/amplitudes: $\theta = \{A_{\alpha}\}$
- Regression function is *linear wrt A_{α}* (not necessarily wrt x !)
- M *basis functions* $g_{\alpha}(x)$, e.g.:
 - Polynomials: $\{1, x, x^2, \dots\}$ (or orthogonal polynomials)
 - Sinusoids/Fourier series: $\{\sin(\omega x), \cos(\omega x), \dots\}$
(with ω *fixed/known*)
 - Splines (with fixed number & knots)
- PDFs for errors are *normal* (here IID), with *known* σ

Generalizations

- This is the *homoskedastic* case; *heteroskedastic* has variances σ_i^2 ; more generally the errors could have a *non-diagonal covariance matrix*
- *Multiple linear regression* generalizes to multiple explanatory variables; i.e., $x_i \rightarrow \mathbf{x}_i$, a vector
- *General linear models* generalize to a vector response, \mathbf{y}_i
- *Generalized linear models* assume a linear model for a *nonlinear function of the conditional expectation*:

$$\ell(\mathbb{E}(y_i | \mathbf{x}_i, \theta)) = \sum_{\alpha=1}^M A_{\alpha} g_{\alpha}(x)$$

$\ell(y)$ is the *link function*. Thus

$$\mathbb{E}(y_i | \mathbf{x}_i, \theta) = \ell^{-1} \left(\sum_{\alpha=1}^M A_{\alpha} g_{\alpha}(x) \right)$$

Example $\ell(y)$ choices: $\log(y)$ (Poisson regression for count data), $\log(y/(1-y))$ (logistic regression for binary responses)

Likelihood function

Abbreviating $f_i = f(x_i; \{A_\alpha\}) = f_i(\{A_\alpha\})$,

$$\begin{aligned} p(\{y_i\}|\{x_i\}, \{A_\alpha\}) &= \frac{1}{\sigma^N (2\pi)^{N/2}} \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^N (y_i - f_i)^2 \right] \\ &= \frac{1}{\sigma^N (2\pi)^{N/2}} e^{-Q/2\sigma^2} \end{aligned}$$

$$\begin{aligned} Q(\{A_\alpha\}) &= \sum_{i=1}^N (y_i - f_i)^2 \\ &= \sum_{i=1}^N \left(y_i - \sum_{\alpha=1}^M A_\alpha g_{\alpha i} \right)^2 \quad \text{with } g_{\alpha i} \equiv g_\alpha(x_i) \\ &= \sum_{i=1}^N y_i^2 + \sum_{i=1}^N \left(\sum_{\alpha=1}^M A_\alpha g_{\alpha i} \right)^2 - 2 \sum_{i=1}^N y_i \sum_{\alpha=1}^M A_\alpha g_{\alpha i} \end{aligned}$$

Vector notation

Eliminate Roman (data) indices by denoting such quantities as N -vectors: $\vec{f} = [f_1, \dots, f_N]^T$, etc.

Let $\vec{u} \cdot \vec{v} \equiv \sum_i u_i v_i = \vec{v} \cdot \vec{u}$ (dot product, symmetric), and $u^2 \equiv \vec{u} \cdot \vec{u} = \sum_i u_i^2$ (vector squared magnitude)

Model expresses \vec{f} as a sum of M basis vectors:

$$\vec{y} = \vec{f}(\{A_\alpha\}) + \vec{\epsilon}; \quad \vec{f}(\{A_\alpha\}) = \sum_{\alpha=1}^M A_\alpha \vec{g}_\alpha$$

Quadratic form is the squared magnitude of the misfit vector:

$$\begin{aligned} Q(\{A_\alpha\}) &= \left[\vec{y} - \vec{f}(\{A_\alpha\}) \right]^2 \\ &= y^2 + f^2 - 2\vec{y} \cdot \vec{f} \\ &= y^2 + \sum_{\alpha\beta} A_\alpha A_\beta \vec{g}_\alpha \cdot \vec{g}_\beta - 2 \sum_{\alpha} A_\alpha \vec{y} \cdot \vec{g}_\alpha \end{aligned}$$

Posterior mode

Adopt a flat prior; the posterior mode is then the maximum likelihood estimate, which satisfies (for $\gamma = 1$ to M)

$$\left. \frac{\partial Q}{\partial A_\gamma} \right|_{A=\hat{A}} = 2 \sum_{\beta} \hat{A}_\beta \vec{g}_\beta \cdot \vec{g}_\gamma - 2 \vec{y} \cdot \vec{g}_\gamma = 0$$
$$\Rightarrow \sum_{\beta} \hat{A}_\beta \vec{g}_\beta \cdot \vec{g}_\gamma = \vec{y} \cdot \vec{g}_\gamma$$

Let $\hat{\vec{f}} \equiv \sum_{\beta} \hat{A}_\beta \vec{g}_\beta$ (function estimate at the mode); then

$$\hat{\vec{f}} \cdot \vec{g}_\gamma = \vec{y} \cdot \vec{g}_\gamma$$

I.e., for the *maximum a posteriori* (MAP) model,

*The model's projection on each basis function
matches the data's projection on each basis function*

Regression geometry

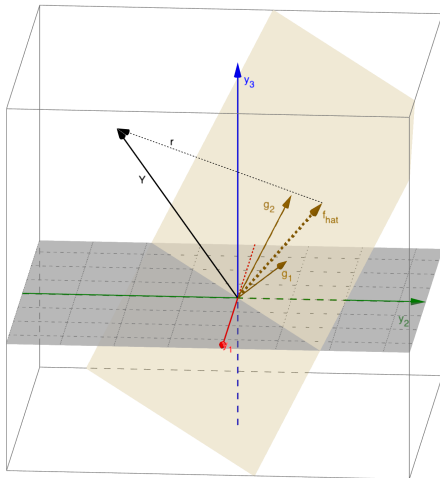
Geometry for linear regression,
 $M = 2$ bases, $N = 3$ samples

$$\vec{x} = [0, 1, 2]^T; \quad \vec{y} = [3, -2, 4]^T$$

$$f(x) = A_1 + A_2x$$

$$g_1(x) = 1 \quad \rightarrow \quad \vec{g}_1 = [1, 1, 1]^T$$

$$g_2(x) = x \quad \rightarrow \quad \vec{g}_2 = [0, 1, 2]^T$$



Produced with GeoGebra Classic 5
See "LinearModelVectors.ggb"

See: [GeoGebra.org](https://www.geogebra.org) (GeoGebra Classic app)

To be continued...

Metric and mode equation

To solve for the mode, define the matrix $\eta_{\alpha\beta}$:

$$\eta_{\alpha\beta} \equiv \vec{g}_\alpha \cdot \vec{g}_\beta = \eta_{\beta\alpha}$$

This is a symmetric matrix; it plays the role of a metric on the M -dimensional subspace spanned by the model functions

The mode condition is now (switch γ to α above, & use symmetry)

$$\sum_{\beta} \eta_{\alpha\beta} \hat{A}_{\beta} = \vec{y} \cdot \vec{g}_{\alpha}$$

The LHS describes the product of an $M \times M$ matrix and a column vector of M components; the RHS comprises a vector with M components—this is just a matrix equation (in the M -D model space, not the N -D sample space)

$$\Rightarrow \hat{A}_{\alpha} = \sum_{\beta} [\eta^{-1}]_{\alpha\beta} \vec{y} \cdot \vec{g}_{\beta}$$

(numerically, the most stable solvers backsolve rather than invert)

Aside on metrics

A metric defines dot products in terms of coordinates in an arbitrary (e.g., non-orthonormal) basis:

$$\vec{v}_1 = \sum_{\alpha} a_{\alpha} \vec{g}_{\alpha}$$

$$\vec{v}_2 = \sum_{\beta} b_{\beta} \vec{g}_{\beta}$$

$$\begin{aligned} \Rightarrow \vec{v}_1 \cdot \vec{v}_2 &= \sum_{\alpha} \sum_{\beta} a_{\alpha} b_{\beta} \vec{g}_{\alpha} \cdot \vec{g}_{\beta} \\ &= \sum_{\alpha} \sum_{\beta} a_{\alpha} b_{\beta} \eta_{\alpha\beta} \end{aligned}$$

(If the \vec{g}_{α} were orthogonal, only the $\alpha = \beta$ terms would be nonzero)

Key use is finding distance from coordinate differences:

$$\begin{aligned}d_{12}^2 &= |\vec{b} - \vec{a}|^2 \\&= \left[\sum_{\alpha} (b_{\alpha} - a_{\alpha}) \vec{g}_{\alpha} \right] \cdot \left[\sum_{\beta} (b_{\beta} - a_{\beta}) \vec{g}_{\beta} \right] \\&= \sum_{\alpha} \sum_{\beta} \Delta_{\alpha} \Delta_{\beta} \eta_{\alpha\beta}\end{aligned}$$

with coordinate differences $\Delta_{\alpha} \equiv b_{\alpha} - a_{\alpha}$

In an *orthonormal* basis, $\eta_{\alpha\beta} = \delta_{\alpha\beta}$, the identity matrix; in this case

$$d_{12}^2 = \sum_{\alpha} \Delta_{\alpha}^2,$$

i.e., the *Pythagorean theorem*

Metrics generalize the Pythagorean theorem to non-orthonormal coordinate systems

Connections to least squares estimation

For a flat prior and fixed σ , the posterior mode minimizes

$$Q(\{A_\alpha\}) = \sum_{i=1}^N [y_i - f_i(\{A_\alpha\})]^2$$

→ the flat-prior mode gives the *least squares estimates of the amplitudes*

The $N \times M$ matrix of model vector coordinates $[g_{\alpha i}]^T$ is the *design matrix*; it is often denoted $\mathbf{X} = X_{i\alpha}$, even though it consists of *response* values (the model basis in the y space—functions of x_i s)

The $M \times M$ metric

$$\eta_{\alpha\beta} \equiv \vec{g}_\alpha \cdot \vec{g}_\beta = \sum_i g_{\alpha i} g_{\beta i} = \mathbf{X}^T \mathbf{X}$$

is sometimes called the *Gramian matrix* (or *Gram matrix*)

The mode condition

$$\sum_\beta \eta_{\alpha\beta} \hat{A}_\beta = \vec{y} \cdot \vec{g}_\alpha$$

is a set of M equations called the *normal equations* when expressed in terms of the design matrix