STSCI 4780
Relationships between variables: Regression

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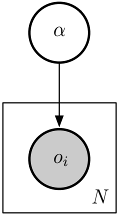
Recap via DAGs

Univariate data DAGs

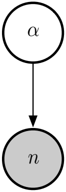
Bernoulli outcomes



$p(\alpha) = 1$

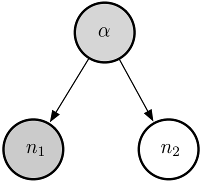
$p(o_i|\alpha) = \alpha$

Binomial counts — estimation, prediction

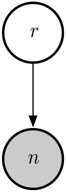


$p(\alpha) = 1$

$p(n|\alpha) = \binom{N}{n} \alpha^n (1-\alpha)^{N-n}$



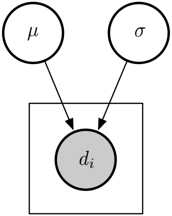
Poisson counts



$p(r) = \dfrac{1}{r_u}$

$p(n|r) = \dfrac{(rT)^n}{n!} e^{-rT}$

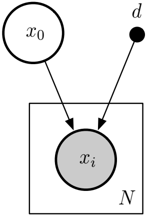
Normal mean and standard deviation



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

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

Cauchy location estimation



$$p(x_0) = C$$

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

Common features

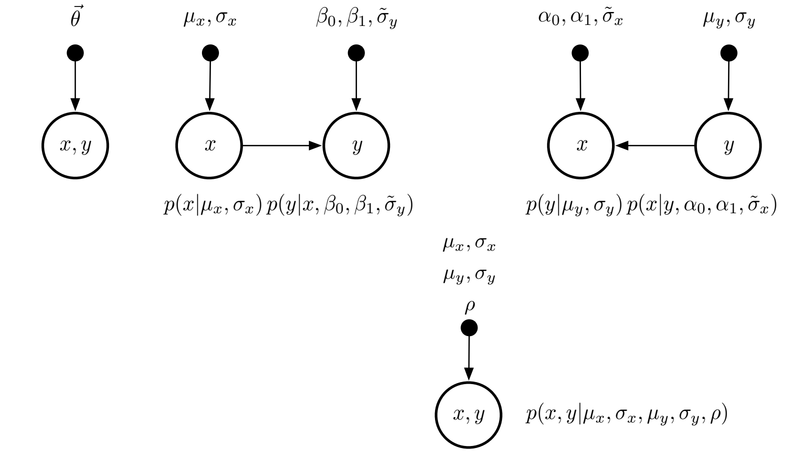
- *Univariate data*—binary, integer or real *scalar* samples
- *Conditionally independent* data

Most problems also univariate in parameter space
Repeated sampling problems were IID

These were all univariate parametric distribution estimation problems:

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

Bivariate normal sampling dist'n DAGs

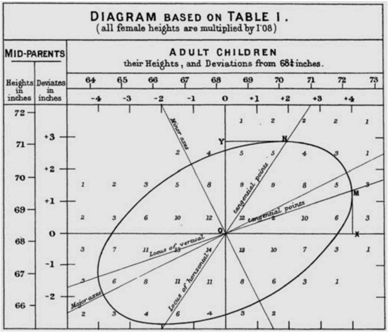


Lec16 recap: Examples with random x

Population studies

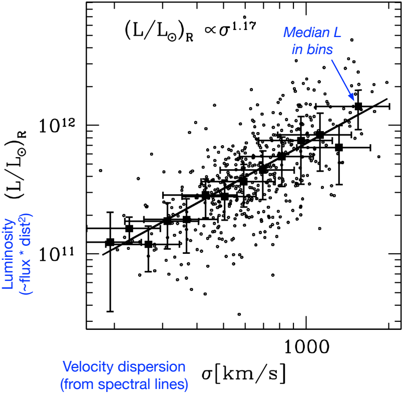
Heights of parents ("midparent") and children

Contour of counts in cells



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

Faber-Jackson relation for elliptical galaxies

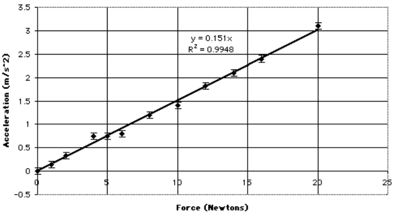


Bernardi+ (2002)

Lec16 recap: Examples with deterministic x
Curve fitting

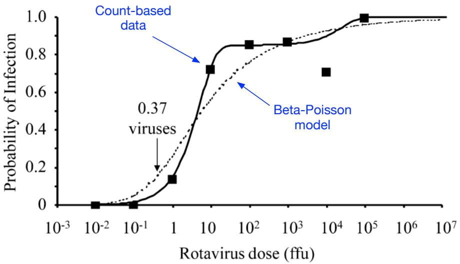
Newton's 2nd law: $a = \frac{F}{m}$

Apply different forces to a fixed mass



Batesville HS AP Physics Class

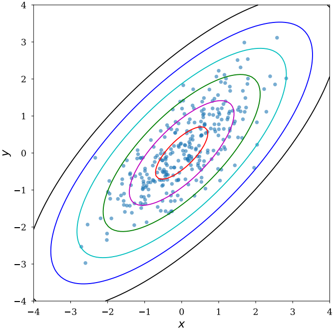
Dose-response curve

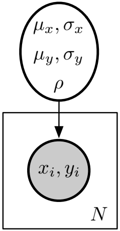


Gale (2003), "Developing risk assessments of waterborne microbial contaminations"

Bivariate normal inference problems

BVN density estimation

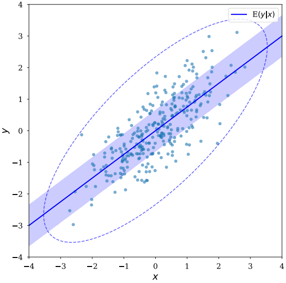


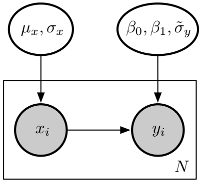


$$\text{Joint:} \quad p(\mu_x, \sigma_x, \mu_y, \sigma_y, \rho) \prod_{i=1}^{N} p(x_i, y_i | \mu_x, \sigma_x, \mu_y, \sigma_y, \rho)$$

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

BVN regression





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

Inference: $$p(\beta_0, \beta_1, \tilde{\sigma}_y|\{x_i, y_i\}) = \int d\mu_x \int d\sigma_x\, p(\mu_x, \sigma_x, \beta_0, \beta_1, \tilde{\sigma}_y|\{x_i, y_i\})$$

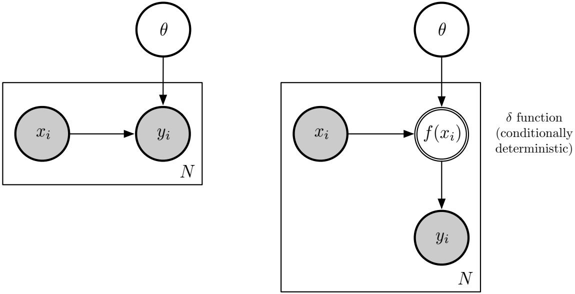
$$\propto p(\beta_0, \beta_1, \tilde{\sigma}_y) \prod_{i=1}^{N} p(y_i|x_i, \beta_0, \beta_1, \tilde{\sigma}_y)$$

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*

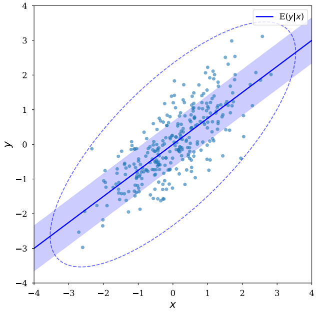
$$\mathbb{E}(y_i | x_i, \theta) = f(x_i; \theta)$$



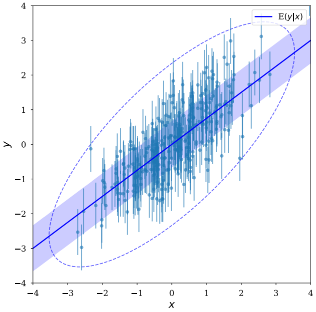
Often natural to express this via an additive error model:

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

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:

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

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

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* $g_\alpha(x)$
  - Polynomials: $\{1, x, x^2, \ldots\}$ (or orthogonal polynomials)
  - Sinusoids/Fourier series: $\{\sin(\omega x), \cos(\omega x), \ldots\}$ (with ω *fixed/known*)
- PDFs for errors are *normal* (here IID)

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., $x_i \to \boldsymbol{x}_i$, a vector
- *General linear models* generalize to a vector response, $\boldsymbol{y}_i$
- *Generalized linear models* assume a linear model for a *nonlinear function of the conditional expectation*:

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

  $\ell(y)$ is the *link function*, e.g., $\log(y)$ (Poisson regression for count data), $\log(y/(1-y))$ (logistic regression for binary responses)

Likelihood function

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

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

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

Vector notation

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

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

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

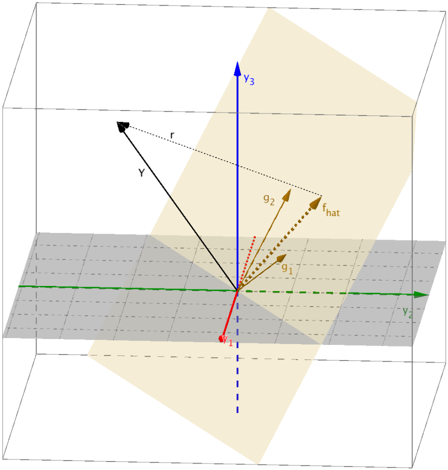
Regression geometry

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

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

$f(x) = A_1 + A_2 x$

$g_1(x) = 1 \quad \rightarrow \quad \vec{g_1} = [1, 1, 1]^T$
$g_2(x) = x \quad \rightarrow \quad \vec{g_2} = [0, 1, 2]^T$



Produced with GeoGebra Classic 5
See “LinearModelVectors.ggb”

See: GeoGebra.org

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 & 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 of 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:

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

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

$$\Rightarrow \vec{v}_1 \cdot \vec{v}_2 = \sum_{\alpha} \sum_{\beta} a_\alpha b_\beta \vec{g}_\alpha \cdot \vec{g}_\beta$$

$$= \sum_{\alpha} \sum_{\beta} a_\alpha b_\beta \eta_{\alpha\beta}$$

(If the $\vec{g}_\alpha$ 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

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

$\rightarrow$ 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_is)

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*

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