# STSCI 4780
# Relationships between variables: Regression, 2

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# Agenda

- Recap of linear regression setup
- Connection to least squares
- Posterior normality
- Nonlinear curve fitting
  - Separable nonlinear models & Jaynes-Bretthorst algorithm
  - (Spectrum analysis)

# Simple normal linear regression

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

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

- Parameters are $M$ coefficients/amplitudes: $\theta = \{A_\alpha\}$, $\alpha = 1$ to $M$
- Regression function is *linear wrt $A_\alpha$* (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 $\omega$ *fixed/known*)
- PDFs for errors are *normal*, with *known* $\sigma$

# Likelihood function

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

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

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

## *Vector notation*

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

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 (the MAP estimate—"maximum a posteriori") is then the maximum likelihood estimate (MLE), which satisfies (for $\gamma = 1$ to $M$)

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

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

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

*The modal model is the one whose projection on each basis function matches the data's projection on each basis function*

In terms of the $M \times M$ *model metric matrix*, $\eta_{\alpha\beta} \equiv \vec{g}_\alpha \cdot \vec{g}_\beta$,

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

# *Regression geometry*

Sums of squares in normal-based likelihood exponents makes normal linear regression look like Euclidean geometry in $N$-D space, with projections into the $M$-D subspace spanned by the model basis

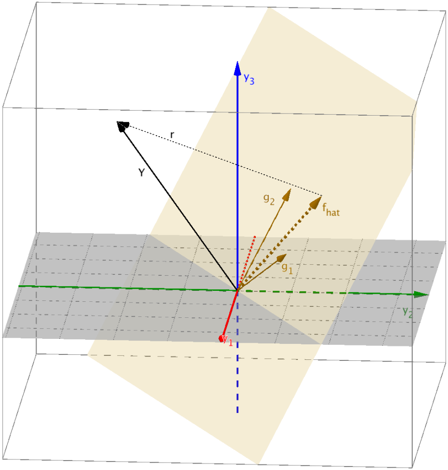
The metric generalizes the Pythagorean theorem to non-orthonormal coordinates

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"

# Connections to least squares estimation

For a flat prior and fixed $\sigma$, 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 $x_i$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 *Gram matrix* or *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

# Posterior is multivariate normal

Write $A_\alpha = \hat{A}_\alpha(\vec{x}, \vec{y}) + \delta A_\alpha$ (expressing $A_\alpha$'s in terms of $\delta A_\alpha$'s); then

$$
\begin{aligned}
Q(\{A_\alpha\}) = (\vec{y} - \vec{f})^2 &= \left(\vec{y} - \sum_\alpha \hat{A}_\alpha \vec{g}_\alpha - \sum_\beta \delta A_\beta \vec{g}_\beta\right)^2 \\
&= \left(\vec{y} - \sum_\alpha \hat{A}_\alpha \vec{g}_\alpha\right)^2 + \left(\sum_\alpha \delta A_\alpha \vec{g}_\alpha\right)^2 \\
&\quad - 2\left(\sum_\beta \delta A_\beta \vec{g}_\beta\right) \cdot \left(\vec{y} - \sum_\alpha \hat{A}_\alpha \vec{g}_\alpha\right) \\
&= Q_{\min} + \left(\sum_\alpha \delta A_\alpha \vec{g}_\alpha\right) \cdot \left(\sum_\beta \delta A_\beta \vec{g}_\beta\right) \\
&\quad - 2 \sum_\beta \delta A_\beta \left(\vec{g}_\beta \cdot \vec{y} - \sum_\alpha \hat{A}_\alpha \eta_{\alpha\beta}\right) \quad \leftarrow \text{ mode cond'n}
\end{aligned}
$$

$$
\begin{aligned}
Q(\{A_\alpha\}) &= Q_{\min} + \sum_\alpha \sum_\beta \delta A_\alpha \delta A_\beta \eta_{\alpha\beta} \\
&= r^2 + \sum_\alpha \sum_\beta (A_\alpha - \hat{A}_\alpha)\eta_{\alpha\beta}(A_\beta - \hat{A}_\beta)
\end{aligned}
$$

where $\vec{r} \equiv \vec{y} - \hat{\vec{f}}$ is the *residual vector* between the data and the best-fit model

The posterior is thus a multivariate normal (MVN) distribution for $A = \{A_\alpha\}$:

$$
\begin{aligned}
p(\{A_\alpha\}|\vec{y}, \sigma) &\propto \frac{1}{\sigma^N} \exp\left[-\frac{Q(\{A_\alpha\})}{2\sigma^2}\right] \\
&\propto \frac{1}{\sigma^N} \exp\left[-\frac{r^2}{2\sigma^2}\right] \exp\left[-\frac{1}{2}(A - \hat{A}) \cdot \mathbf{V}^{-1} \cdot (A - \hat{A})\right]
\end{aligned}
$$

MVN for the $A$'s with (marginal) means $\hat{A}_\alpha$, inverse covariance matrix $\mathbf{V}^{-1} = \boldsymbol{\eta}/\sigma^2$, and covariance matrix

$$
\mathbf{V} = \sigma^2 \boldsymbol{\eta}^{-1}
$$

# Consequences of posterior normality

## *Joint HPD regions for coefficients*

Write $p(A|\vec{y},\sigma) = Ce^{-\chi^2/2}$ with

$$\chi^2(A) = \frac{Q(A)}{\sigma^2} = \frac{r^2}{\sigma^2} + \Delta\chi^2(A),$$

$$\text{with} \quad \Delta\chi^2(A) \equiv (A - \hat{A}) \cdot \mathbf{V}^{-1} \cdot (A - \hat{A})$$

$$\Rightarrow \quad p(A|\vec{y},\sigma) \propto e^{-\Delta\chi(A)^2/2}$$

An HPD region with probability $C$ is bounded by a surface of constant density, i.e., a surface of constant $\Delta\chi^2(A) = \Delta\chi^2_{\rm crit}$, chosen so

$$C = \int_{\Delta\chi^2 < \Delta\chi^2_{\rm crit}} \mathrm{d}^M A \; p(A|\vec{y},\sigma)$$

Normality $\rightarrow$ choose $\Delta\chi^2_{\rm crit}$ so that $C$ is the probability that $\chi^2 < \Delta\chi^2_{\rm crit}$ in the $\chi^2$ distribution with $M$ degrees of freedom

## *Uncertain $\sigma$*

Adopt a log-flat prior for $\sigma$, i.e., $p(\sigma) \propto 1/\sigma$; then as a function of $\sigma$, the posterior is

$$p(\sigma, A|\vec{y}) \propto \frac{1}{\sigma^{N+1}}\; e^{-Q(A)/2\sigma^2}$$

Marginalize over $\sigma$ just as we did for normal $(\mu, \sigma)$ inference; this gives

$$p(\sigma, A|\vec{y}) \propto \left[1 + \frac{\Delta Q(A)}{r^2}\right]^{-N/2},$$

where $\Delta Q(A) \equiv (A - \hat{A}) \cdot \boldsymbol{\eta} \cdot (A - \hat{A})$

This is a *multivariate Student's t distribution*

## *Marginalizing over coefficients*

- Marginalizing over a *subset* of coefficients is straightforward using the fact that MVN conditional distributions are normal with fixed variance; can show the marginal is proportional to the *profile likelihood*
- Marginalizing over *all* coefficients can be done analytically by *diagonalizing the metric* $\rightarrow$ the MVN normalization constant is $\sqrt{\det \mathbf{V}}$

## *Conjugate priors*

Since the likelihood function is MVN with respect to $A$, a MVN prior for $A$ is a *conjugate prior*, resulting in a posterior that remains MVN

## *Heteroskedastic cases*

If the errors are correlated rather than IID, then the quadratic form is a double sum using the noise covariance matrix, **E**:

$$Q(A) = \sum_{i,j} [y_i - f_i(A)][\mathbf{E}^{-1}]_{ij}[y_j - f_j(A)]$$

A special case is independent but *heteroskedastic* errors, for which

$$Q(A) = \sum_i \frac{[y_i - f_i(A)]^2}{\sigma_i^2}$$

This corresponds to *weighted least squares* or *minimum* $\chi^2$ fitting of linear models (with full **E** it's *generalized* LS)

These generalizations can be easily accommodated simply by (1) removing $\sigma^2$ everywhere, and (2) *redefining vector dot products* using **E** as a metric on the $N$-D space of $y_i$ coordinates:

$$\vec{a} \cdot \vec{b} \equiv \sum_{ij} a_i [\mathbf{E}^{-1}]_{ij} b_j$$

All results are *unchanged* by this (but marginalization over $\sigma$ is no longer relevant)

# Bayesian nonlinear curve fitting & least squares

## *Setup*

Data $D = \{y_i\}$ are measurements of an underlying function $f(x;\theta)$ at $N$ sample points $\{x_i\}$. Let $f_i(\theta) \equiv f(x_i;\theta)$:

$$y_i = f_i(\theta) + \epsilon_i, \qquad \epsilon_i \sim N(0, \sigma_i^2)$$

We seek learn $\theta$, or to compare different functional forms (model choice, $M$).

## *Likelihood*

$$\begin{aligned}
p(D|\theta, M) &= \prod_{i=1}^{N} \frac{1}{\sigma_i\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{y_i - f_i(\theta)}{\sigma_i}\right)^2\right] \\
&\propto \exp\left[-\frac{1}{2}\sum_i \left(\frac{y_i - f_i(\theta)}{\sigma_i}\right)^2\right] \\
&= \exp\left[-\frac{\chi^2(\theta)}{2}\right]
\end{aligned}$$

## *Posterior*

For prior density $\pi(\theta)$,

$$p(\theta|D, M) \propto \pi(\theta) \exp\left[-\frac{\chi^2(\theta)}{2}\right]$$

If you have a least-squares or $\chi^2$ code:

- Think of $\chi^2(\theta)$ as $-2 \log \mathcal{L}(\theta)$.
- Bayesian inference amounts to exploration and numerical integration of $\pi(\theta) e^{-\chi^2(\theta)/2}$.
- If noise level is uncertain, keep the $1/\sigma_i$ factors (dropped above!) and include noise parameters in inference (e.g., scale all $\sigma_i$ by a parameter, $\alpha$)
- If any of the parameters appear *linearly*, our linear regression results show that their likelihood function—conditional on the remaining parameters—will be MVN $\rightarrow$ analytical simplifications

# Important Case: Separable Nonlinear Models

A (linearly) separable model has parameters $\theta = (A, \psi)$:

- Linear amplitudes $A = \{A_\alpha\}$
- Nonlinear parameters $\psi$

$f(x; \theta)$ is a linear superposition of $M$ nonlinear components $g_\alpha(x; \psi)$:

$$
\begin{aligned}
y_i &= \sum_{\alpha=1}^{M} A_\alpha g_\alpha(x_i; \psi) + \epsilon_i \\
\text{or} \qquad \vec{y} &= \sum_{\alpha} A_\alpha \vec{g}_\alpha(\psi) + \vec{\epsilon}.
\end{aligned}
$$

Recall: "linear/nonlinear" refers to how the predictions depend on the *parameters*, not how they depend on the sample location!

# Examples

Polynomials (simple or orthogonal); $\psi = \emptyset$:

$$
\begin{aligned}
f(x) &= A_0 + A_1 x + A_2 x^2 + A_3 x^3 \\
&= A_0 + A_1 x + A_2'(2x^2 - 1) + A_3'(4x^3 - 3x), \quad x \in [-1, 1] \\
&= A_0 g_0(x) + A_1 g_1(x) + A_2' g_2(x) + A_3' g_3(x)
\end{aligned}
$$

Sinusoids; $\psi = \omega$:

$$
\begin{aligned}
f(x) &= A \cos(\omega x + \phi) \\
&= A_1 \cos \omega x + A_2 \sin \omega x \\
&= A_1 g_1(x, \omega) + A_2 g_2(x, \omega)
\end{aligned}
$$

Chirps; $\psi = (\omega, \alpha)$:

$$
\begin{aligned}
f(x) &= A \cos(\alpha x^2 + \omega x + \phi), \quad \text{inst. freq.} = \omega + 2\alpha x \\
&= A_1 \cos(\alpha x^2 + \omega x) + A_2 \sin(\alpha x^2 + \omega x)
\end{aligned}
$$

Exponentials; $\psi = (\tau_1, \tau_2, \ldots)$: $f(x) = A_1 e^{-x/\tau_1} + A_2 e^{-x/\tau_2} + \cdots$

# The Jaynes-Bretthorst Algorithm

Why separable structure is important: You can marginalize over $A$ *analytically* $\rightarrow$ *Jaynes-Bretthorst algorithm* ("Bayesian Spectrum Analysis & Param. Estimation" 1988)

Algorithm is closely related to linear least squares, diagonalization (eigenvectors/values), and SVD

Goals:

- Estimate the nonlinear parameters $\psi$
- Estimate amplitudes
- Compare rival models

The log-likelihood is a quadratic form in $A_\alpha$,

$$
\begin{aligned}
\mathcal{L}(A,\psi) &\propto \frac{1}{\sigma^N}\exp\left[-\frac{Q(A,\psi)}{2\sigma^2}\right] \\
\text{with}\quad Q &= \left[\vec{y}-\sum_\alpha A_\alpha \vec{g}_\alpha\right]^2 \\
&= \left[\vec{y}-\sum_\alpha A_\alpha \vec{g}_\alpha\right]\cdot\left[\vec{y}-\sum_\beta A_\beta \vec{g}_\beta\right] \\
&= y^2 - 2\sum_\alpha A_\alpha \vec{y}\cdot\vec{g}_\alpha + \sum_{\alpha,\beta} A_\alpha A_\beta \eta_{\alpha\beta}
\end{aligned}
$$

where, as before, $\quad \eta_{\alpha\beta}(\psi) = \vec{g}_\alpha(\psi)\cdot\vec{g}_\beta(\psi)$

We seek to integrate out the amplitudes, but completing the square is complicated because of the nontrivial metric $\eta_{\alpha\beta}$

Change the basis for $\vec{f}$ from $\vec{g}_\alpha$ to an *orthonormal basis* $\vec{h}_\mu$:

$$\vec{g}_\alpha = \sum_\mu a_{\alpha\mu}\vec{h}_\mu \qquad \text{with } \vec{h}_\mu \cdot \vec{h}_\nu = \delta_{\mu\nu}$$

which implies $\vec{h}_\mu = \sum_\alpha (a^{-1})_{\mu\alpha}\vec{g}_\alpha$. Note $a = a(\psi)$.

Rewriting $\vec{f}$,

$$\vec{f}(\theta) = \sum_{\alpha=1}^{M} A_\alpha \vec{g}_\alpha(\psi) = \sum_{\mu=1}^{M} B_\mu(A,\psi)\vec{h}_\mu(\psi)$$

with orthonormal amplitudes $B_\mu(A,\psi) = \sum_\alpha A_\alpha a_{\alpha\mu}(\psi)$

Some linear algebra shows that $\eta = aa^T$, so we can get $a$ from $\eta$ via Cholesky/eigen/QR decomposition.

Now write the quadratic form in terms of the $B$s instead of the $A$s:

$$
\begin{aligned}
Q &= y^2 - 2\sum_\alpha A_\alpha \vec{y}\cdot\vec{g}_\alpha + \sum_{\alpha,\beta} A_\alpha A_\beta \eta_{\alpha\beta} \\
&= y^2 - 2\sum_\mu B_\mu \vec{y}\cdot\vec{h}_\mu + \sum_\mu B_\mu^2 \\
&= \sum_\mu \left[B_\mu - \hat{B}_\mu(\psi)\right]^2 + r^2(\psi)
\end{aligned}
$$

with $\hat{B}_\mu(\psi) \equiv \vec{y}\cdot\vec{h}_\mu(\psi)$ and the residual $\vec{r}(\psi) \equiv \vec{y} - \sum_\mu \hat{B}_\mu \vec{h}_\mu$

The posterior in terms of $B$s is

$$
p(B,\psi|D,I) \quad \propto \quad \frac{\pi(\psi)J(\psi)}{\sigma^N} \exp\left[-\frac{r^2(\psi)}{2\sigma^2}\right] \exp\left[\frac{-1}{2\sigma^2}\sum_\mu [B_\mu - \hat{B}_\mu(\psi)]^2\right]
$$

$J(\psi) = (\det\eta)^{1/2}$ comes from changing variables from $A$s to $B$s

Marginalize $B$'s analytically (*check the range!*):

$$p(\psi|D,I) \propto \frac{\pi(\psi)J(\psi)}{\sigma^{N-M}} \exp\left[-\frac{r^2(\psi)}{2\sigma^2}\right]$$

If $\sigma$ unknown, marginalize using $p(\sigma|I) \propto \frac{1}{\sigma}$.

$$p(\psi|D,I) \propto \pi(\psi)J(\psi)\left[r^2(\psi)\right]^{\frac{M-N}{2}}$$

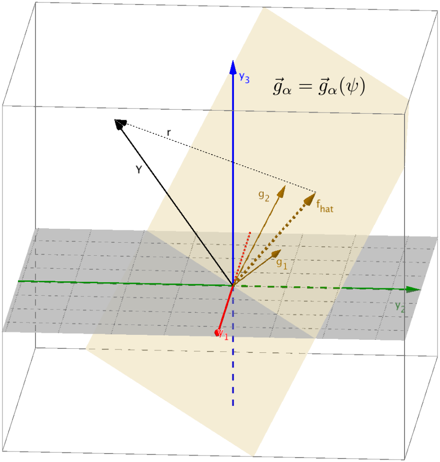
For given $\psi$, $r^2$ is just the residual sum of squares from a least squares fit to the basis functions. We can write

$$\begin{aligned} r^2(\psi) &= y^2 - \sum_\mu \hat{B}_\mu^2(\psi) \\ &= y^2 - S(\psi) \end{aligned}$$

with $S(\psi) = \sum_\mu [\vec{y} \cdot \vec{h}_\mu(\psi)]^2$, the sum of squared projections

## *Regression geometry for separable models*

The geometry is as for linear regression, but now the basis vectors (and the subspace they span) depends on the nonlinear parameters



# Application: Bayesian Spectrum Analysis

Adopt a sinusoid periodic signal model:

$$\begin{aligned} f(t) &= A\cos(\omega t - \phi) && \text{parameters } \omega, A, \phi \\ &= A_1 \cos\omega t + A_2 \sin\omega t && \text{parameters } \omega, A_1, A_2 \\ y_i &= f(t_i) + e_i && \text{Gaussian error } pdf\text{s; rms} = \sigma \end{aligned}$$

Estimate $\omega$:

$$\begin{aligned} p(\omega|D) &\propto \int dA_1 \int dA_2 \; p(\omega, A_1, A_2)\mathcal{L}(\omega, A_1, A_2) \\ &\propto p(\omega)J(\omega)\exp\left[\frac{S(\omega)}{\sigma^2}\right] \end{aligned}$$

- Equally-spaced samples: $S(\omega) \rightarrow$ *Schuster periodogram* for large $N$ (when $\eta$ is nearly diagonal) — magnitude of the discrete Fourier transform (DFT) of the time series
- Unequally-spaced samples: $S(\omega) \approx$ *Lomb-Scargle periodogram*