STSCI 4780
Relationships between variables: Regression, 2

Tom Loredo, CCAPS & SDS, Cornell University

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_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*

Likelihood function

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

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

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

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

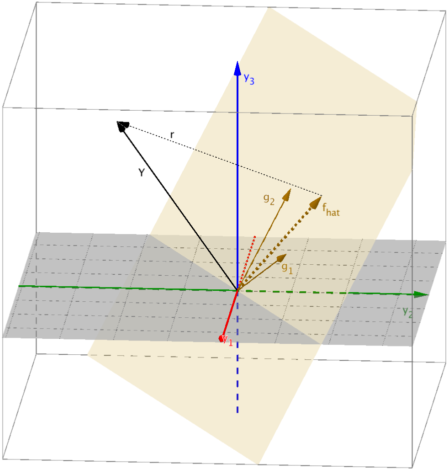
The metric generalizes the Pythagorean theorem to non-orthonormal coordinates

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 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 *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 $A_\alpha = \hat{A}_\alpha + \delta A_\alpha$ (expressing A_α's in terms of δA_α's); then

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

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

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 χ^2 distribution with M degrees of freedom

Uncertain σ

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

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

Marginalize over σ just as we did for normal (μ, σ) 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 χ^2* fitting of linear models (with full **E** it's *generalized* LS)

These generalizations can be easily accommodated simply by (1) removing σ^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 σ 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 θ, 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 χ^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 σ_i by a parameter, α)
- 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 ψ

$f(x; \theta)$ 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 ψ
- Estimate amplitudes
- Compare rival models

The log-likelihood is a quadratic form in A_α,

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

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 η via Cholesky/eigen/QR decomposition.

Now write the quadratic form in terms of the Bs instead of the As:

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

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 Bs 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 As to Bs

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

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

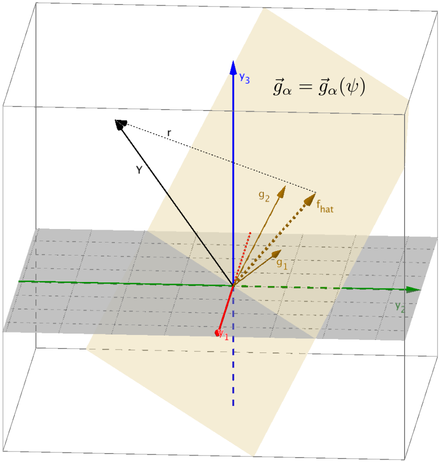
For given ψ, r^2 is just the residual sum of squares from a least squares fit to the basis functions. We can write

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

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 ω:

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

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