Gould 2003 χ^2 & linear fits, & how uncertainties in slope parameters (& quadratic parameters) scale with baseline

2020/01/28.0

Recall

$$\boxed{\mathrm{cov}(y_1, y_2) \equiv \langle (y_1 - \langle y_1\rangle)(y_2 - \langle y_2\rangle)\rangle = \langle y_1 y_2\rangle - \langle y_1\rangle\langle y_2\rangle},$$

where

$$\langle y\rangle \equiv \frac{\int y\, g(y)\, dy}{\int g(y)\, dy},$$

y is a random variable drawn from distribution $g(y)$.

$$\mathrm{var}(y) \equiv \mathrm{cov}(y,y) = \langle y^2\rangle - \langle y\rangle^2, \quad \sigma_y \equiv (\mathrm{var}(y))^{1/2}$$

Given N data points y_k with errors σ_k, recall

$$\chi^2 \equiv \sum_{k=1}^{N} \frac{(y_k - y_{k,\mathrm{mod}})^2}{\sigma_k^2}.$$

If $\sigma_k \sim \mathcal{N}(\mu,\sigma)$, then $\mathcal{L} = \exp(-\chi^2/2)$.

The covariance matrix $\boxed{C_{kl} \equiv \mathrm{cov}(y_k, y_l)}$ is symmetric, $C = C^T$.

Recall a linear model with n parameters is given by

$$y_{\mathrm{mod}} \equiv \sum_{i=1}^{n} a_i f_i(x)$$

where $f_i(x)$ are n arbitrary functions of x, the independent variable.

χ^2 for linear models, & minization

Set $\boxed{B \equiv C^{-1}}$, the inverse of the covariance matrix (also symmetric).

$$\chi^2 = \sum_{k=1}^{N}\sum_{l=1}^{N} (y_k - y_{k,\mathrm{mod}})\, B_{kl}\, (y_l - y_{l,\mathrm{mod}})$$

$\Updownarrow$ " $\frac{1}{\sigma^2}$ ".

Substituting the linear model, and hiding sums over $k, l, i, j \ldots$

$$\chi^2 = [y_k - a_i f_i(x_k)]\, B_{kl}\, [y_l - a_j f_j(x_l)].$$

Σ_{kl} over N data pt.

$\Sigma_{i,j}$ over n parameters.

Minimizing χ^2

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$$\chi^2 = y_k B_{kl} y_l - 2a_i d_i + a_i b_{ij} a_j,$$ where define

$$\boxed{d_i \equiv y_k B_{kl} f_i(x_l)} \; ; \; \boxed{b_{ij} \equiv f_i(x_k) B_{kl} f_j(x_l).}$$

To minimize, set derivatives of χ^2 wrt. all the parameters to be 0:

$$0 = \frac{\partial \chi^2}{\partial a_m} \overset{\text{take derivative}}{=} -2\delta_{im} d_i + \delta_{im} b_{ij} a_j + a_i b_{ij} \delta_{jm}$$

[because $\frac{\partial a_i}{\partial a_m} = \delta_{im}$

$$\overset{\text{sum over } i}{=} -2d_m + b_{mj} a_j + a_i b_{im}$$

$$\overset{\text{join}}{=} 2(b_{mj} a_j - d_m)$$

$$\Rightarrow d_m = b_{mj} a_j \Rightarrow \boxed{a_i = c_{ij} d_j}, \text{ for } \boxed{c_{ij} \overset{\text{nah... this is only true at the matrix level}}{=} b_{ij}^{-1}}.$$

Note d_i are random variables, but c_{ij} & b_{ij} are combinations of constants

Covariances:

To get covariances of a_i, $\mathrm{cov}(a_i, a_j)$, and the associated errors, $\sqrt{\mathrm{cov}(a_i, a_i)}$, you need to calculate covariances of d_i,

$$\mathrm{cov}(d_i, d_j) = \mathrm{cov}(y_k B_{kl} f_i(x_l), y_p B_{pq} f_j(x_q))$$

$$= y_k B_{kl} y_p B_{pq} \,\mathrm{cov}(f_i(x_l), f_j(x_q))$$

$$\overset{\text{linear alg.}}{=} f_i(x_l) B_{kl} f_j(x_k).$$

$$\boxed{\mathrm{cov}(d_i, d_j) = b_{ij}}$$

Example: a linear

$$y_{mod} = a_1 f_1(x) + a_2 f_2(x) = a_1 + a_2 x.$$

$f_1(x) = 1, \quad f_2(x) = x.$ Take uncorrelated measurements, $\sigma_k = \sigma$ equal.

$$d_1 = y_k B_{kl} f_1(x_l)$$
$$= y_k \delta_{kl} \sigma_k^{-2} f_1(x_l)$$
$$= y_k \sigma_k^{-2} f_1(x_k)$$
$$= \sum_{k=1}^{N} y_k \sigma_k^{-2}$$

$$d_2 = y_k B_{kl} f_2(x_l)$$
$$= y_k \delta_{kl} \sigma_k^{-2} f_2(x_l)$$
$$= y_k \sigma_k^{-2} f_2(x_k)$$
$$= \sum_{k=1}^{N} y_k \sigma_k^{-2} x_k$$

$$\langle x \rangle = \int x f(x)\, dx \Big/ \int f(x)\, dx$$

$$\langle x_k \rangle = \frac{\sum_{k=1}^{N} x_k}{N} \quad \text{e.g. } \{1,2,3\}$$

$$\langle x_k^2 \rangle \stackrel{?}{=} \frac{\sum x_k^2}{N} \quad \{1,4,9\}$$

Now $b_{ij} = \mathrm{cov}(d_i, d_j)$, so

$$b_{11} \stackrel{!}{=} \mathrm{cov}(d_1, d_1) = c_{11}^{-1}$$
$$= \langle d_1^2 \rangle - \langle d_1 \rangle \langle d_1 \rangle$$

using $b = c^{-1}$

$$= c_{11}^{-1}$$

$$= \sum_{k=1}^{N} \frac{1}{\sigma_k^2}; \quad b_{12} = b_{21} = \sum_{k=1}^{N} \frac{x_k}{\sigma_k^2}; \quad b_{22} = \sum_{k=1}^{N} \frac{x_k^2}{\sigma_k^2}$$

Claim

then for $\sigma_k = \sigma$,

$$b = \frac{N}{\sigma^2} \begin{pmatrix} 1 & \langle x \rangle \\ \langle x \rangle & \langle x^2 \rangle \end{pmatrix} \stackrel{???}{=} \begin{pmatrix} \sum_{k=1}^{N} \frac{1}{\sigma_k^2} & \sum_{k=1}^{N} \frac{x_k}{\sigma_k^2} \\ \sum_{k=1}^{N} \frac{x_k}{\sigma_k^2} & \sum_{k=1}^{N} \frac{x_k^2}{\sigma_k^2} \end{pmatrix}$$

$$\stackrel{?}{=} \frac{N}{\sigma^2} \begin{pmatrix} 1 & \sum_k x_k \\ \sum_k x_k & \sum x_k^2 \end{pmatrix}$$

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$$b_{11} \equiv f_1(x_k)\, B_{kl}\, f_1(x_l)$$
$$= 1 \cdot B_{kl} \cdot 1$$
$$\equiv \delta_{kl}\, \sigma_k^{-2}$$
$$= \sum_{k=1}^{N} \sigma_k^{-2}$$

$$b_{12} = b_{21}$$
$$= f_1(x_k)\, B_{kl}\, f_2(x_l)$$
$$= 1 \cdot B_{kl} \cdot x_l$$
$$= \delta_{kl}\, \sigma_k^{-2}\, x_l$$
$$= \sum_{k=1}^{N} \sigma_k^{-2}\, x_k$$

And similarly for b_{22}, $b_{22} = \sum_{k=1}^{N} x_k^2\, \sigma_k^{-2}$

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so

$$b = \begin{pmatrix} \sum_{k=1}^{N} \sigma_k^{-2} & \sum_{k=1}^{N} x_k\, \sigma_k^{-2} \\ \sum_{k=1}^{N} x_k \sigma_k^{-2} & \sum_{k=1}^{N} x_k^2\, \sigma_k^{-2} \end{pmatrix}$$

note

$N\langle x_k\rangle = \sum_k x_k$

$N\langle x_k^2\rangle = \sum x_k^2$

$$= \frac{1}{\sigma^2} \begin{pmatrix} \sum_{k=1}^{N} 1 & \sum_{k=1}^{N} x_k \\ \sum_{k=1}^{N} x_k & \sum_{k=1}^{N} x_k^2 \end{pmatrix}$$

$$b = \frac{N}{\sigma^2} \begin{pmatrix} 1 & \langle x\rangle \\ \langle x\rangle & \langle x^2\rangle \end{pmatrix}$$

Now $c \equiv b^{-1}$.

For 2×2 $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$

$$A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \frac{1}{ad-bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

For 3×3 $A = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$

$$A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} & \cdots & \cdots \\ \cdots & \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix} & \\ \cdots & \cdots & \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} \end{pmatrix}$$

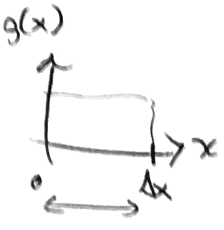
where

$$\det(A) = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

so

$$c = b^{-1} = \frac{\sigma^2}{N} \frac{1}{\langle x^2\rangle - \langle x\rangle^2} \begin{pmatrix} \langle x^2\rangle & -\langle x\rangle \\ -\langle x\rangle & 1 \end{pmatrix}$$

and the error on the slope is given by



$$\mathrm{var}(a_2) = (\sigma(a_2))^2 = c_{22} = \frac{\sigma^2}{N\,\mathrm{var}(x)}.$$

If x is uniformly distributed over an interval Δx,
then $\mathrm{var}(x) = (\Delta x)^2/12$.

In this case,

$$\mathrm{var}(a_2) = c_{22} = (\sigma(a_2))^2 = \frac{12\sigma^2}{N(\Delta x)^2}$$

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Example #2, quadratic case

$$y_{mod} = a_1 f_1(x) + a_2 f_2(x) + a_3 f_3(x) = a_1 + a_2 x + a_3 x^2.$$

i.e., $f_1(x) = 1$, $f_2(x) = x$, $f_3(x) = x^2$.

$$d_1 \equiv y_k B_{kl} f_1(x_l)$$
$$= y_k \sigma_k^{-2} \delta_{kl} \cdot 1$$
$$d_1 = \sum_k y_k \sigma_k^{-2}$$

$$d_3 = y_k B_{kl} f_3(x_l)$$
$$d_3 = \sum_k y_k \sigma_k^{-2} x_k^2$$

similarly, as before

$$d_2 = \sum_k y_k \sigma_k^{-2} x_k.$$

Also like before,

$$b_{11} = \sum_k \sigma_k^{-2}; \quad b_{22} = \sum_k x_k^2 \sigma_k^{-2}; \quad b_{33} = \sum x_k^4 \sigma_k^{-2}$$

$$b_{12} = b_{21} = \sum_k \sigma_k^{-2} x_k \quad \text{as before.}$$

Now

$$b_{13} = b_{31} = \sum_k \sigma_k^{-2} x_k^2, \quad \text{and} \quad b_{23} = b_{32} = \sum_k \sigma_k^{-2} x_k^3.$$

Good. So

$$b = \frac{N}{\sigma^2} \begin{pmatrix} 1 & \langle x \rangle & \langle x^2 \rangle \\ \langle x \rangle & \langle x^2 \rangle & \langle x^3 \rangle \\ \langle x^2 \rangle & \langle x^3 \rangle & \langle x^4 \rangle \end{pmatrix}$$

And the element of the covariance matrix we care about is C_{33}. This can be evaluated by taking many determinants!

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The ~~element~~ entry is

$$c_{33}^{element} = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

$$c_{33}^{element} = 1 \cdot \langle x^2\rangle - \langle x\rangle\langle x\rangle$$

$$= \langle x^2\rangle - \langle x\rangle^2 = \mathrm{var}(x)$$

The prefactor will be (one over ...)

$$\det(b) = 1 \cdot \begin{vmatrix} \langle x^2\rangle & \langle x^3\rangle \\ \langle x^3\rangle & \langle x^4\rangle \end{vmatrix} - \langle x\rangle \begin{vmatrix} \langle x\rangle & \langle x^3\rangle \\ \langle x^2\rangle & \langle x^4\rangle \end{vmatrix} + \langle x^2\rangle \begin{vmatrix} \langle x\rangle & \langle x^2\rangle \\ \langle x^2\rangle & \langle x^3\rangle \end{vmatrix}$$

$$= \langle x^2\rangle\langle x^4\rangle - \langle x^3\rangle^2 - \langle x\rangle^2\langle x^4\rangle + \langle x\rangle\langle x^2\rangle\langle x^3\rangle$$
$$+ \langle x^2\rangle\langle x\rangle\langle x^3\rangle - \langle x^2\rangle^3$$

$$\det(b) = \langle x^2\rangle\langle x^4\rangle - \langle x^3\rangle^2 - \langle x\rangle^2\langle x^4\rangle - \langle x^2\rangle^3 + 2\langle x\rangle\langle x^2\rangle\langle x^3\rangle \quad (*)$$

So

$$c_{33} = \frac{1}{\det(b)} \cdot c_{33}^{element} = \frac{\sigma^2\,\mathrm{var}(x)}{N\,\det(b)} = \frac{12\sigma^2}{N(\Delta x)^2} \cdot \frac{1}{\det(b)}$$

If $x \sim U[0, \Delta x]$, then take as fact that

$$\mathrm{mean}(x) = \frac{1}{2}\Delta x = \langle x\rangle$$

$$\mathrm{var}(x) = \frac{1}{12}(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$$

$$\mathrm{skewness}(x) = 0 = \langle x^3\rangle - 3\langle x\rangle\left(\langle x^2\rangle - \langle x\rangle^2\right) - \langle x\rangle^3$$

and

$$f(x) = \begin{cases} 1/\Delta x & \text{for } 0 < x < \Delta x \\ 0 & \text{else} \end{cases}$$

which yields b/c $\langle x^n \rangle \equiv \int f(x)\, x^n\, dx = \frac{1}{\Delta x}\int x^n\, dx$

$$\langle x \rangle = \frac{1}{\Delta x}\int_0^{\Delta x} x\, dx = \frac{1}{\Delta x}\left(\frac{1}{2}x^2\Big|_0^{\Delta x}\right) = \frac{1}{2}(\Delta x)$$

$$\langle x^2 \rangle = \frac{1}{\Delta x}\int_0^{\Delta x} x^2\, dx = \frac{1}{\Delta x}\left(\frac{1}{3}x^3\Big|_0^{\Delta x}\right) = \frac{1}{3}(\Delta x)^2$$

$$\langle x^3 \rangle = \frac{1}{4}(\Delta x)^3$$

$$\langle x^4 \rangle = \frac{1}{5}(\Delta x)^4$$

Therefore

$$\det(B) = \frac{1}{3}(\Delta x)^2\, \frac{1}{5}(\Delta x)^4 - \left(\frac{1}{4}(\Delta x)^3\right)^2 - \left(\frac{1}{2}\Delta x\right)^2 \frac{1}{5}(\Delta x)^4 - \left(\frac{1}{3}(\Delta x)^2\right)^3 + 2\,\frac{1}{24}(\Delta x)(\Delta x)^2(\Delta x)^3$$

$$= (\Delta x)^6\left(\frac{1}{15} - \frac{1}{16} - \frac{1}{20} - \frac{1}{27} + \frac{1}{12}\right)$$

$$= \frac{(\Delta x)^6}{2160}$$

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and we get

$$C_{33} = \mathrm{var}(a_3) = (\sigma(a_3))^2 = \frac{(12 \cdot 2160)\,\sigma^2}{N}\,\frac{1}{(\Delta x)^8}$$

$$(\sigma(a_3))^2 = \frac{25{,}920\,\sigma^2}{N}\,\frac{1}{(\Delta x)^8}$$

and $\sigma(a_3) = \frac{(25{,}920)^{1/2}\,\sigma}{N^{1/2}}\,\frac{1}{(\Delta x)^4}$ $\boxed{**}$.