Linear Algebra Solution to Straight line fit

As an example of a more realistic data-driven analysis, let's consider a simple three-parameter linear model which fits a straight-line to data with unknown errors. The parameters will be the y-intercept α , the slope β , and the (unknown) normal scatter σ about the line.

For data $D = \{x_i, y_i\}$, the model is

$$\hat{y}(x_i|\alpha,\beta)=\alpha+\beta x_i,$$

and the likelihood is the product of the Gaussian distribution for each point:

$$\mathscr{L}(D|\alpha,\beta,\sigma) = (2\pi\sigma^2)^{-N/2} \prod_{i=1}^{N} \exp\left[\frac{-[y_i - \hat{y}(x_i|\alpha,\beta)]^2}{2\sigma^2}\right].$$

arXiv:1411.5018

Jake Van Der Plas

Frequentism and Bayesianism:

A Python Driven Primer

algebra. If we define the *parameter vector*, $\theta = [\alpha \ \beta]^T$; the response vector, $Y = [y_1 \ y_2 \ y_3 \ \cdots \ y_N]^T$; and the design matrix,

$$X = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_N \end{bmatrix}^T,$$

it can be shown that the maximum likelihood solution is

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} (\boldsymbol{X}^T \boldsymbol{Y}).$$

The confidence interval around this value is an ellipse in parameter space defined by the following matrix:

$$\Sigma_{\hat{ heta}} \equiv \left[egin{array}{ccc} \sigma_{lpha}^2 & \sigma_{lphaeta} \ \sigma_{lphaeta} & \sigma_{eta}^2 \end{array}
ight] = \sigma^2 (M^T M)^{-1}.$$

Here σ is our unknown error term; it can be estimated based on the variance of the residuals about the fit. The off-diagonal elements of $\Sigma_{\hat{\theta}}$ are the correlated uncertainty between the estimates. In code, the computation looks like this:

```
import numpy as np
import matplotlib.pyplot as plt
from scipy import stats
from scipy import ndimage
np.random.seed(42)
theta true = (25. 0.5)
xdata = 100 * np.random.random(20)
vdata = theta true[0] + theta true[1] * xdata
vdata = np.random.normal(ydata, 10)
# Compute the frequentist version
X = np.vstack([np.ones like(xdata), xdata]).T
theta freg = np.linalg.solve(np.dot(X.T, X),
                             np.dot(X.T, vdata))
y model = np.dot(X, theta freq)
sigma y = np.std(ydata - y model)
Sigma freq = sigma y ** 2 *
np.linalg.inv(np.dot(X.T, X))
```

Code by Jake Van der Plas

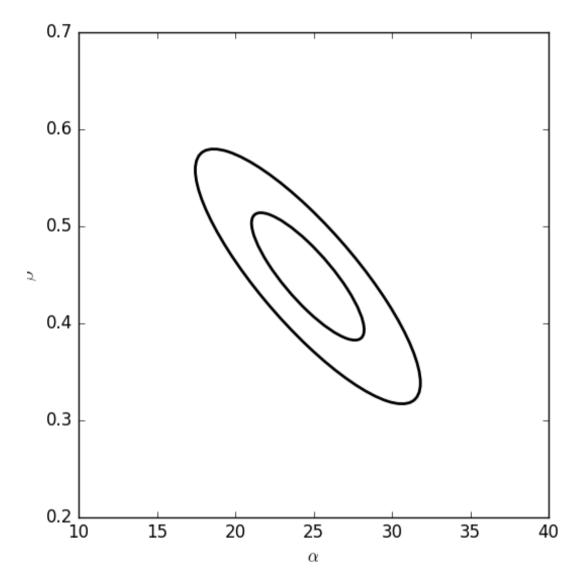
Full source code available at https://tinyurl.com/y9hhded4

```
def get_principal(Sigma):
    # See Ivezic, Connolly, VanderPlas, and Gray, section 3.5.2
    sigma_x2 = Sigma[0, 0]
    sigma_y2 = Sigma[1, 1]
    sigma_xy = Sigma[0, 1]

alpha = 0.5 * np.arctan2(2 * sigma_xy, sigma_x2 - sigma_y2)
    tmp1 = 0.5 * (sigma_x2 + sigma_y2)
    tmp2 = np.sqrt(0.25 * (sigma_x2 - sigma_y2) ** 2 + sigma_xy ** 2)

return np.sqrt(tmp1 + tmp2), np.sqrt(tmp1 - tmp2), alpha
```

```
print("Frequentist Version")
print(" theta = {0}".format(theta_freq))
print(" sigma_y = {0}".format(sigma_y))
print(" Sigma = {0}".format(Sigma_freq))
from matplotlib.patches import Ellipse
fig, ax = plt.subplots(figsize=(6, 6))
sigma1, sigma2, alpha = get principal(Sigma freg)
for nsigma in [1, 2]:
    ax.add patch(Ellipse(theta_freq,
                           2 * nsigma * sigma1, 2 *
nsigma * sigma2,
                           angle=np.degrees(alpha),
                           lw=2. ec='k'. fc='none'))
ax.plot([0, 0], [0, 0], '-k', lw=2)
ax.set xlim(10, 40)
ax.set_ylim(0.2, 0.7)
ax.set xlabel(r'$\alpha$')
ax.set ylabel(r'$\beta$')
plt.show()
```



Model Comparison

Week 4+5

Introduction to Model Comparison

Qt : Given a dataset:

- 1) how do we decide which among (two or more) models fit the data best
- 2) How do we quantify the significance of goodness of fit of the best model compared to disfavored model?

Multiple methods to address the above questions:

- Frequentist model comparison tests (based on difference in chi-square or log-likelihood ratio)
- Bayesian methods (to be discussed later)
- Information criterion based methods

Frequentist Model Comparison

http://jakevdp.github.io/blog/2015/08/07/frequentism-and-bayesianism-5-model-selection/

arXiv:1607.03549 by Louis Lyons (Sect 13)

Astro-ph/0701113

arXiv:1901.07726 Kerscher & Weller

arXiv:1607.03845 (SD)

A simple application to test if measurements of Newton's Constant show sinusoidal dependence with time as proposed by some authors.

arXiv: 1706.01202 (Shalini Ganguly + SD)

Statistical Significance of spectral lag transition in GRB160625B

arXiv:1906.05726 Aditi Krishak, Aisha Dantuluri, SD model comparison of annual modulation in DM experiments

arXiv:2003.10127 Aditi Krishak, SD model comparison for modified gravity in Eot-wash

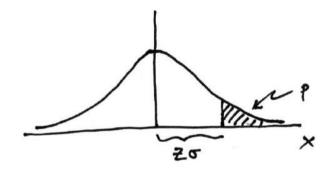
Frequentist Model Comparison Summary

- Calculate best fit χ 2 for each model
- Calculate χ^2 for each model and the one with larger value of χ^2 GOF (or χ^2 pdf) is the preferred value.
- Use the fact that if the two models are nested $\Delta \chi 2$ between the two models has a $\chi 2$ distribution with DOF = difference in number of free parameters between model 2 and model 1.
- Consider the model with fewer free parameters as the null hypothesis calculate the p-value that simply by chance we would see the more complicated model.
- p-value = 1-chi-square CDF for DOF=difference in no of free parameters and $\chi 2 = \Delta \chi 2$ (between the two models)

In Python use p-value = 1-stats.chi2(ν).cdf($\Delta \chi^2$)

Significance from *p*-value

Often define significance Z as the number of standard deviations that a Gaussian variable would fluctuate in one direction to give the same p-value.



$$p = \int_{Z}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^{2}/2} dx = 1 - \Phi(Z)$$

$$Z = \Phi^{-1}(1 - p)$$

Significance also known as Z-score

Glenn Cowan lecture

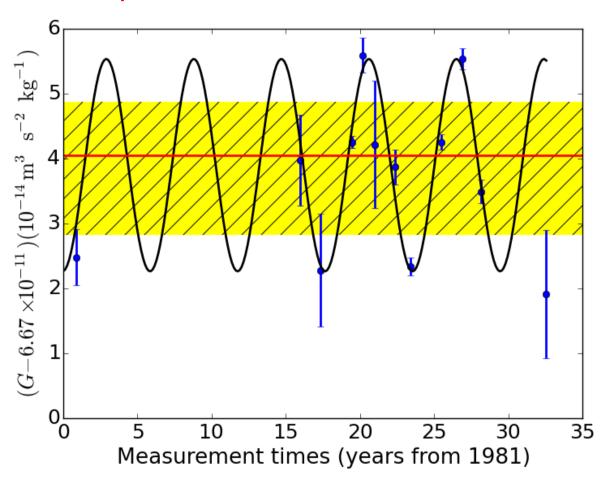
Notes

TMath::Prob

TMath::NormQuantile

In Python: Use stats.norm.isf(p-value)

Model Comparison Tests of G variation



arXiv:1607.03845

Model Comparison Tests of G variation

$$y_i = A \sin[\phi_0 + 2\pi(t_i/P)] + \mu_G,$$

- H1. Data is consistent with a constant offset + measured uncertainties
- H2. Same as H1, but an additional unknown systematic offset.
- H3. Data is described by above equation (showing sinusoidal variation)
- H4. Same as H3, but an additional unknown systematic offset.

Hypothesis	μ	σ_{sys}	A	P(yrs)	ϕ_0	DOF	χ^2/DOF	$P(\chi^2,\nu)$
H1 H2 H3 H4	6.766×10^{-11} 6.674×10^{-11} 6.674×10^{-11} 6.571×10^{-11}	-	$\begin{array}{c} - \\ - \\ 1.64 \times 10^{-14} \\ 1.9 \times 10^{-14} \end{array}$	- 5.9 7.57	- -0.07 0.0011	11 10 8 7	28.04 1.27 2.93 1.71	6.8×10^{-60} 0.059 0.0011 0.032

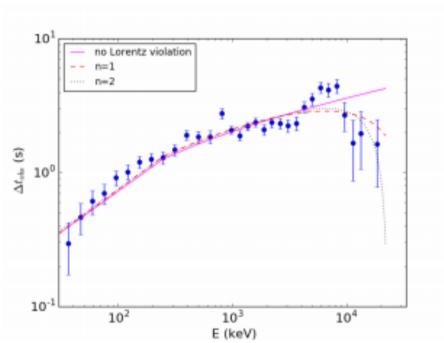


Figure 1: Summary of the best fit LIV models for n=1 and n=2 along with no Lorentz violation superposed on top of the spectral lag data from GRB 160625B. We note that one data point at $(E, \Delta t) = (15708 \text{ keV}, -0.223 \text{ sec})$ has been omitted for brevity. All the spectral lag data points have been obtained from Table 1 of W17.

Shalini Ganguly, SD (arXiv:1706.01202)

	No LIVª	(n=1)b	(n=2)°
Frequentist			
DOF	35	34	34
$\chi^2/{\rm DOF}$	2.6	2.37	2.23
χ^2 GOF	2.2×10^{-7}	3.7×10^{-6}	1.5×10^{-5}
p-value		0.0014	9.2×10^{-5}
significance		3.05σ	3.74σ
Δ AIC		8.2	12.9
Δ BIC		6.9	11.7

^aNo Lorentz Invariance ^bLorentz Invariance up to linear (n=1) order ^cLorentz Invariance up to quadratic (n=2) order

Information Criterion based tests

Akaike Information Criterion: based on Kullbeck-Leibler information entropy Bayesian Information Criterion: based on Bayesian evidence

arXiv:1207.5875 Shi, Huang and Lu astro-ph/0701113 Liddle

$$BIC \equiv -2 \ln \mathcal{L}_{max} + k \ln N,$$

$$AIC \equiv -2 \ln \mathcal{L}_{\text{max}} + 2k,$$

$$AIC_{c} = AIC + \frac{2k(k+1)}{N-k-1}.$$

N = no of data points K = no of free parameters

Strength of Evidence Tests for AIC/BIC

For the AIC, Burnham & Anderson (2003) featured the following "strength of evidence" in the form of $\Delta AIC = AIC_i - AIC_{min}$:

```
\Delta AIC Level of Empirical Support For Model i 0-2 Substantial 4-7 Considerably Less > 10 Essentially None
```

arXiv:1207. 5875 by Shi et al

For the BIC, Robert & Adrian (1995) featured the following "strength of evidence", where $\Delta BIC = BIC_i - BIC_{min}$:

$\Delta \mathrm{BIC}$	Evidence against Model i
0 - 2	Not Worth More Than A Bare Mention
2 - 6	Positive
6 - 10	Strong
> 10	Very Strong

Other Advanced Model-Comparison Tests

- Deviance Information Criterion
- Takeuchi Information Criterion
- WAIC
- F-test
- Likelihood ratio tests
- · Cross-validation
- Bayesian Methods: Bayes Factor, Posterior Odds Ratio

For more advanced details see the following note by Louis Lyons https://www-cdf.fnal.gov/physics/statistics/notes/H0H1.pdf

For more examples of model comparison in Cosmology/Astrophysics, see

Liddle: astro-ph/0701113

Liddle, Mukherjee, Parkinson: astro-ph/0608184

Kerscher and Weller arXiv:1901.07726