Data Analysis and Fitting: Errors and Goodness of Fit

Ashton S. Reimer

[1]Center for Geospace Studies
SRI International

July 2021

Topics

1. Errors
2. Goodness of Fit

Chi-Squared

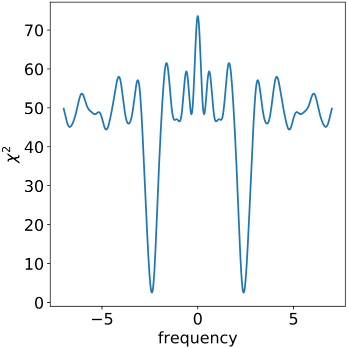
We can use least-squares to solve inverse problems:

$$\chi^2(\mathrm{p}) = [\mathrm{y} - f(\mathrm{p})]^T \, \Sigma_{\mathrm{e}}{}^{-1} \, [\mathrm{y} - f(\mathrm{p})]$$

where $\hat{\mathrm{p}}_{LS}$ are the "best-fit" model parameters, those that minimizes $\chi^2(\mathrm{p})$

Great! But:

- What are the errors in the fitted parameters $\hat{\mathrm{p}}_{LS}$?
- Is the fit meaningful? Does the model accurately reproduce the measurements?



Error Propagation (e.g. Linear Least-Squares)

For a linear forward model:

$$\mathrm{y} = f(\mathrm{p}) + \mathrm{e} \qquad f(\mathrm{p}) = H\mathrm{p}$$

The Least-Squares solution is:

$$\hat{\mathrm{p}}_{LS} = \left[H^T \Sigma_e^{-1} H\right]^{-1} H^T \Sigma_e^{-1} \mathrm{y}$$

Given that jointly Gaussian random variables have the following property:

$$\mathrm{Y} = A\mathrm{X} \quad \Rightarrow \quad \Sigma_{\mathrm{Y}} = A \Sigma_{\mathrm{X}} A^T$$

it can be shown that:

$$\Sigma_{\hat{\mathrm{p}}_{\mathrm{LS}}} = \left[H^T \Sigma_e^{-1} H\right]^{-1}$$

Error Propagation (e.g. Nonlinear Least Squares)

For a non-linear forward model, guess a p_i, linearize, and step towards minimum:

$$\mathrm{y} = f(\mathrm{p}) + \mathrm{e} \qquad f(\mathrm{p}_i + \Delta\mathrm{p}) \approx f(\mathrm{p}_i) + \mathrm{J}_i \Delta\mathrm{p} \qquad \mathrm{J}_i = \frac{\partial f}{\partial \mathrm{p}_i}$$

J is known as the Jacobian:

$$\mathrm{J} = \begin{pmatrix} \frac{\partial f_0}{\partial p_0} & \frac{\partial f_0}{\partial p_1} & \cdots & \frac{\partial f_0}{\partial p_{N-1}} \\ \frac{\partial f_1}{\partial p_0} & \frac{\partial f_1}{\partial p_1} & \cdots & \frac{\partial f_1}{\partial p_{N-1}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_{M-1}}{\partial p_0} & \frac{\partial f_{M-1}}{\partial p_1} & \cdots & \frac{\partial f_{M-1}}{\partial p_{N-1}} \end{pmatrix}$$

J is $M \times N$ (tall and skinny)

Non-linear fitting process:

- iterate until $\mathrm{p}_{i+1} = \hat{\mathrm{p}}_{\mathrm{LS}}$: that which minimizes χ^2
- The covariance of $\hat{\mathrm{p}}_{\mathrm{LS}}$ is:

$$\Sigma_{\hat{\mathrm{p}}_{\mathrm{LS}}} = \left[\mathrm{J}^T \Sigma_e^{-1} \mathrm{J}\right]^{-1}$$

Note the similarity to the linear case!

Error Propagation

The covariance of the fitted parameters is the covariance of the input data propagated through the least-squares operation:

$$\Sigma_{\hat{\mathsf{p}}_{\mathrm{LS}}} = \left[\mathsf{J}^T \Sigma_e^{-1} \mathsf{J} \right]^{-1}$$

“Error bars” for fitted parameters:

- Assumption: measurement errors are **Gaussian** distributed with covariance Σ_e, denoted $\mathcal{N}(0, \Sigma_e)$
- The “errors” in the fitted parameters are related to confidence intervals
- Confidence intervals are constructed from $\Sigma_{\hat{\mathsf{p}}_{\mathrm{LS}}}$
- $\Sigma_{\hat{\mathsf{p}}_{\mathrm{LS}}}$ may look reasonable, even if the fit is meaningless

Constructing Confidence Intervals: From Fitted Covariance

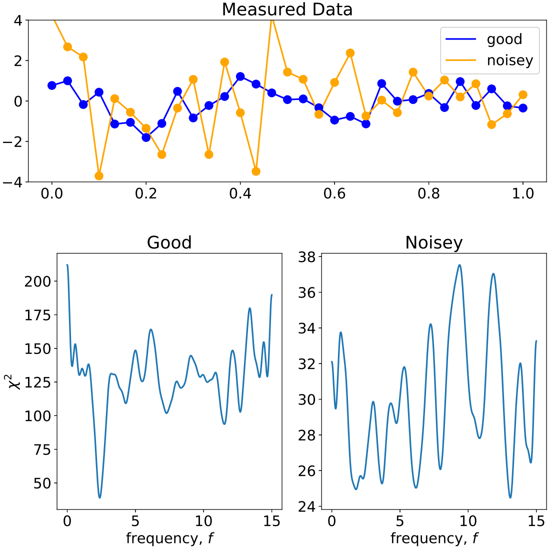
Error bars, δp_m, for a fitted parameter can be constructed from the covariance $\Sigma_{\hat{\mathrm{p}}_{\mathrm{LS}}}$ and a $\Delta\chi^2$:

$$\delta p_m = \pm\sqrt{\Delta\chi^2}\sqrt{\Sigma_{mm}}$$

The value of $\Delta\chi^2$ selects the "significance level":

- $\Delta\chi^2$ is found in lookup tables calculated from the CDF of the χ^2 distribution
- Single parameter fit, $N = 1$:
  - a 68% significance: $\Delta\chi^2 = 1$
  - a 95.4% significance: $\Delta\chi^2 = 4$
- Two parameter fit, $N = 2$:
  - a 68% significance: $\Delta\chi^2 = 2.3$

Challenges With Constructing Confidence Intervals



Validity of Confidence Intervals

Only quantitatively valid when:

- measurement errors are Gaussian, and
  - the model $f(\mathrm{p})$ is linear in for all p, or
  - measurement errors are small enough that $f(\mathrm{p})$ can be accurate approximated by a linear model in the region around p

Otherwise, alternative fitting methods are required: Monte Carlo, Bayesian, etc.

Goodness of Fit

How do we know if the fit is even meaningful? The standard goodness of fit test involves computing the "reduced chi-squared":

$$\chi^2_\nu = \chi^2/(m - n + 1)$$

Then, typically:

- $\chi^2_\nu \approx 1$: a good fit
- $\chi^2_\nu << 1$: an "over fit"
- $\chi^2_\nu >> 1$: a poor fit

The χ^2_ν could also be slightly larger or smaller than 1 depending on how accurately one is able to estimate the input measurement errors.

Summary

Now we can answer the question: Are the fitted parameters meaningful?

- What is the uncertainty in the fitted parameters?
  - Error bars correspond to confidence intervals (CI)
  - CIs are constructed from covariance of the fitted parameters
  - For a 68% CI, interpretation is: "If we could hypothetically make and infinite set of new measurements and fit each of those, 68% of the time the 'true' value of the parameter would lie within the CI."
- Is the fit good?
  - Compute the reduced chi-squared
  - $\chi^2_\nu \approx 1$: usually means the model accurately represents the data
- All of this error analysis depends on the assumption that measurement errors are **Gaussian** distributed with covariance Σ_e such that $(y_m - f_m)/\sigma_m$ are $\mathcal{N}(0, 1)$