Uncertainty and Error Propagation

(From before:)
Error in Measurement

Research Group	Reported value
Yale	15 ± 7 g/cm^3
Waterloo	15 ± 8 g/cm^3
UNM	12 ± 2 g/cm^3
UCSB	15 ± 4 g/cm^3

Density of gold = 19.3 g/cm^3
Density of lead = 11.4 g/cm^3

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Conclusion: It is very important to understand the reported errors on the UNM measurement.

Uncertainty is Necessary

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- **“Error” does not mean mistake**
- Important related ideas:
  - Error and Uncertainty
  - Accuracy vs. Precision
  - Statistical vs. Systematic Uncertainty
  - Significant Figures
  - Resolution
  - Uncertainty in fitted data: errors on parameters vs. goodness of fit

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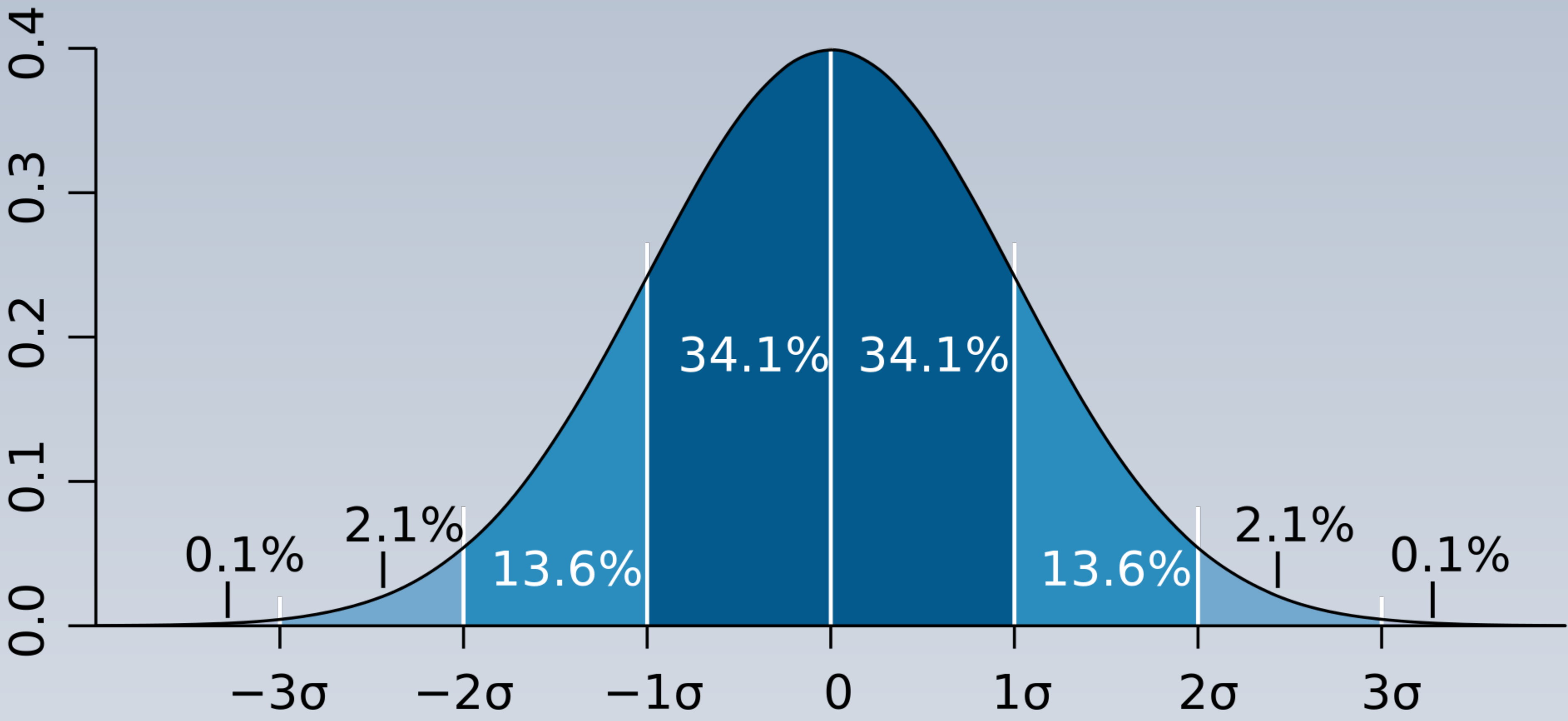
Topics covered

- Reporting uncertainty in measurements
- Significant figures
- Error propagation for specific and general calculations
- Mean and standard deviation
- Today:
  - Standard error and the normal distribution
  - Errors on fit parameters
  - Weighted fits
  - Chi square and goodness of fit

Review: Normal/Gaussian distribution and standard deviation



Mean and standard deviation

Mean:

$$\mu = \frac{x_1 + x_2 + \cdots + x_N}{N}$$

Standard Deviation:

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N}(x_i - \mu)^2}{N}}$$

Standard deviation vs. standard error: the normal distribution

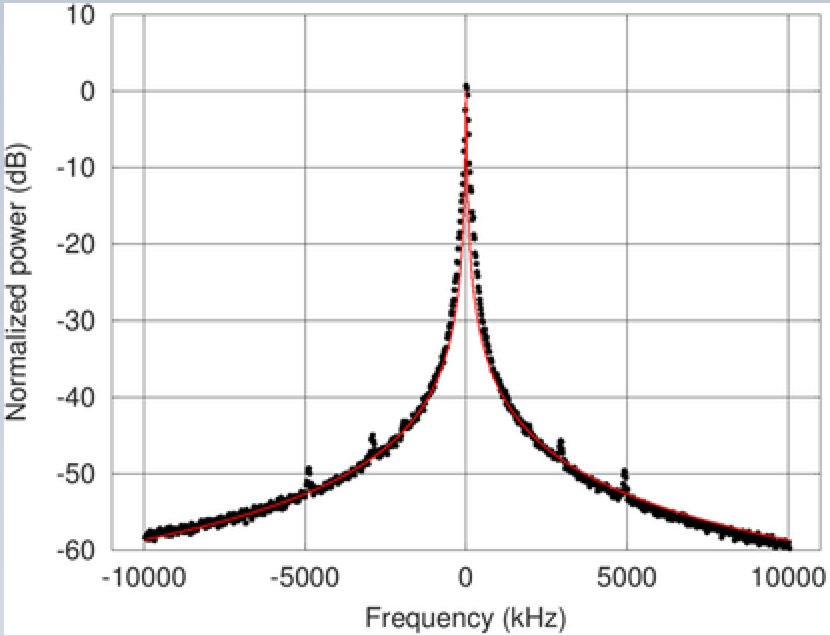
The error on the fitted/calculated mean of a dataset is <u>not the same as</u> the standard deviation.

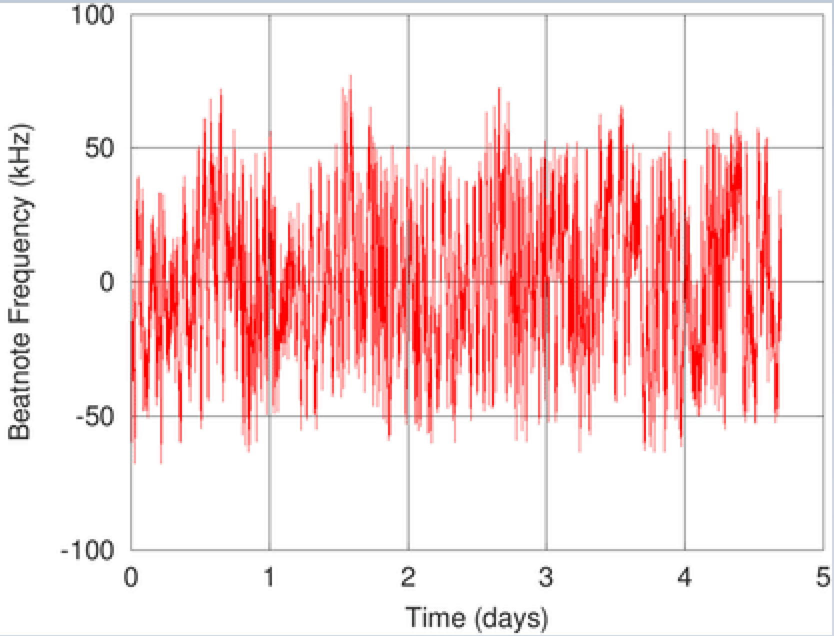
More importantly, sometimes the width (standard deviation) of a distribution has a meaning of its own.

Standard deviation vs. standard error: the normal distribution

The error on the fitted/calculated mean of a dataset is not the same as the standard deviation.

Example: laser linewidth vs. stability





Standard error

Mean:

$$\mu = \frac{x_1 + x_2 + \cdots + x_N}{N}$$

Standard Deviation:

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N}(x_i - \mu)^2}{N}}$$

Standard Error (“Standard Deviation of the Mean”):

$$\sigma_\mu = \frac{\sigma}{\sqrt{N}}$$

Standard error as a confidence interval on the mean

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Standard Deviation:

$$\sigma = \sqrt{\frac{\sum_{i=1}^{N}(x_i - \mu)^2}{N}}$$

Standard Error (“Standard Deviation of the Mean”):

$$\sigma_\mu = \frac{\sigma}{\sqrt{N}}$$

Standard deviation vs standard error

You have taken N measurements from a random population (population >> N).

What is the 68% confidence limit for the measured value of a single data point?

What is the 68% confidence limit for the value of the mean from another N data points taken in the same measurement?

--These are two different questions.

--In many cases, the spread of the data has its own meaning, separate from the mean or the uncertainty.

Gaussian (Normal) distribution:

$$y = G_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

So which do I use for error bars?

- It depends. ☺

- If you report whether your error bars come from the standard deviation or the standard error of multiple measurements, you'll be fine.

Part 2: Understanding uncertainty when fitting data to a user defined function

Caveat:

These topics could be their own course. Statistical analysis, data science, and data modeling are complex topics, and there are many ways to approach this.

I’m not trying to cover them all, nor to justify nor prove the following equations and approaches. Instead, this is just an introduction to a set of tools that can be used when fitting data.

Fitting a user defined function in MATLAB

```
modelfun = @(b,x)b(1)*exp(-b(2)*x)
mdl = fitnlm(x_data, y_data, modelfun, guess)
```

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mdl =
Nonlinear regression model:
    y ~ b1*exp( - b2*x)

Estimated Coefficients:
          Estimate       SE          tStat       pValue
          ________    ________    _______    _________
    b1     7.1492      0.91739     7.793      0.0043974
    b2    0.26977     0.046397    5.8144      0.010128

Number of observations: 5, Error degrees of freedom: 3
Root Mean Squared Error: 2.12
R-Squared: 0.927,  Adjusted R-Squared 0.902
F-statistic vs. zero model: 376, p-value = 0.000251
```

Confidence levels in fitted parameters

- Standard Error of fit parameters/coefficients are generally given by the fitting function.
- Calculated in a similar way to standard error of the mean (a.k.a. standard deviation of the mean).
- A 95% confidence limit is typically ~2 standard errors.

Weighted fits

- Can be used to account for dependent variable uncertainty when fitting data

MATLAB:

```
modelfun = @(b,x)b(1)*exp(-b(2)*x)
mdl = fitnlm(x_data, y_data, modelfun, guess,
'Weights',weights)
```

For errorbars on y_data, weights are often given by:

$$w_i = \frac{1}{\sigma_i^2}$$

Goodness of fit

Three different questions:

1. What are the best values for the fit parameters given some data and a functional form?
2. How well does this solution capture the variance in the data?
3. Is the hypothesis that the data follows the functional form correct?

Goodness of fit

Three different questions:

1. What are the best values for the fit parameters given some data and a functional form?
   → Fitted parameters and confidence levels
2. How well does this solution capture the variance in the data?
   → R^2 (coefficient of determination)
3. Is the hypothesis that the data follows the functional form correct?
   → Chi square (χ^2)

R-square

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

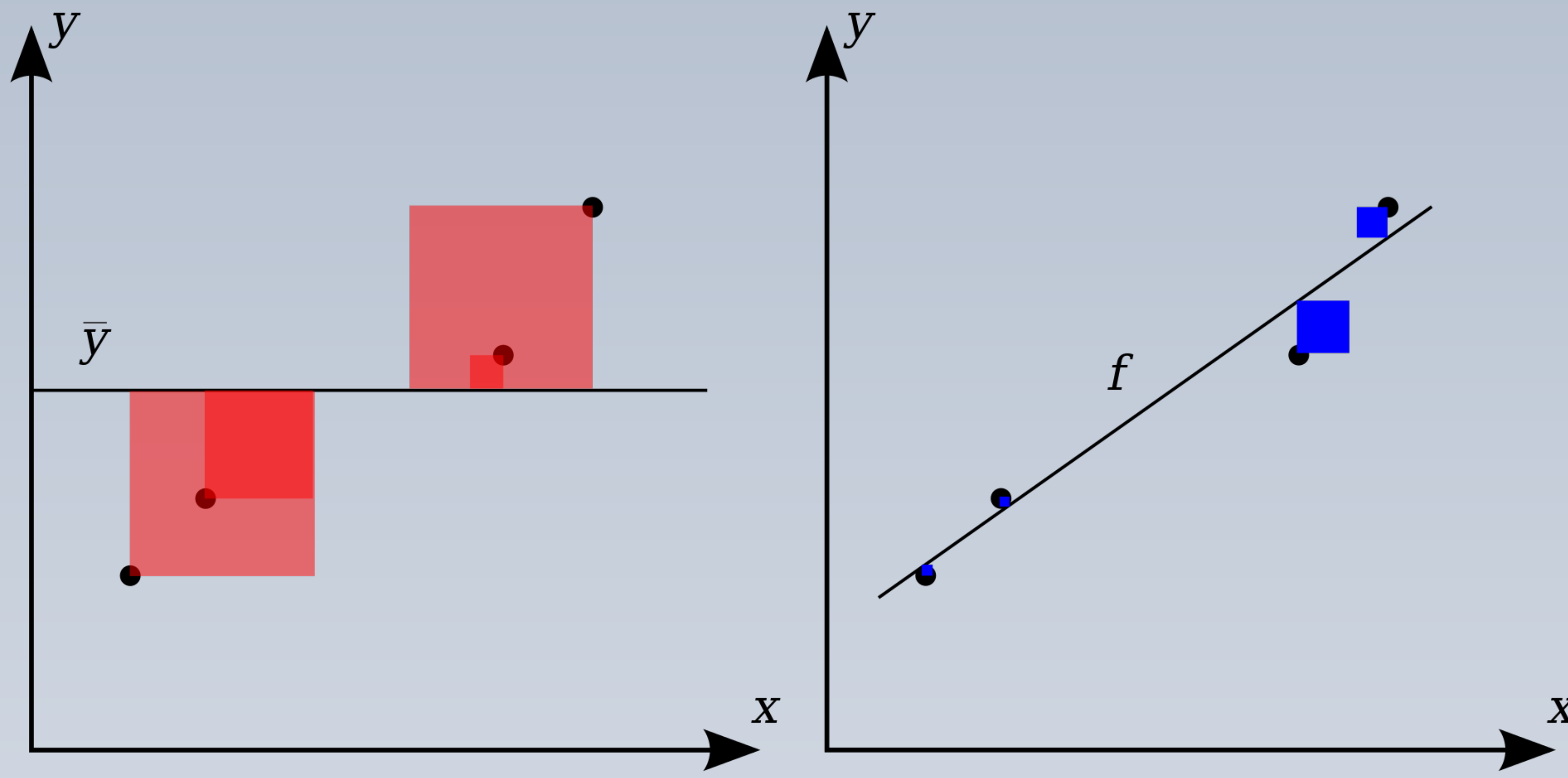
$$SS_{tot} = \sum_i (y_i - \bar{y})^2 \propto \sigma^2$$

$$SS_{res} = \sum_i (y_i - y_{fit})^2$$

(SS_{res} is the residual sum of squares from linear regression.)

R-square

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

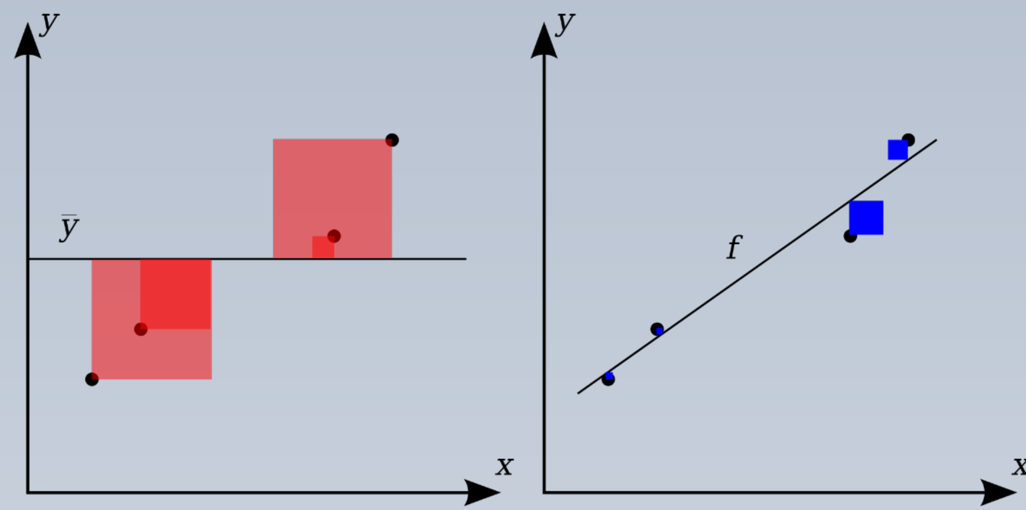


$0 \leq R^2 \leq 1$

→ Good R^2s approach 1.

R-square

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$



- Most commonly quoted g.o.f. statistic in many fields.
- Directly linked to least squares fitting.
- Doesn’t work well for nonlinear regression models.
- Does not distinguish overparameterized models.

Chi-square: goodness of fit

$$\chi^2 = \sum_i \frac{(y_{observed} - y_{expected})^2}{\sigma_i^2}$$

Reduced chi-square is divided by the degrees of freedom, ν:

$$\chi_\nu^2 = \frac{\chi^2}{\nu}$$

where ν = number of data points – constraints.

Chi-square

- Widely used in hypothesis testing
  - Can look up tables for the distribution of chi-square for specific number of degrees of freedom.
  - You compare the calculated chi-square to 95% confidence intervals.
- Reduced chi-squared
  - More common in goodness of fit; takes degrees of freedom into account
  - $\chi_\nu^2 \gg 1$ points to a function that doesn't agree with the data
  - $\chi_\nu^2 < 1$ points to a function that agrees too well with the data (overparameterization or overestimated errors)

Open homework 3 and MATLAB.

Error Analysis: an excellent reference