Some basic statistics and curve fitting techniques

Some important concepts:

- Data
- Statistical description of data (data reduction, independence)
- The use of statistics to make a point:
  1. Statistics never proves a point.
  2. If you need fancy statistic to support a point, your point is, at best, weak…

Statistical description of data

Statistical moments (1st and 2nd):

- Mean: $$\bar{x} = \frac{1}{N}\sum_{j=1}^{N} x_j$$
- variance: $$Var = \frac{1}{N-1}\sum_{j=1}^{N}\left(x_j - \bar{x}\right)^2$$
- Standard deviation: $$\sigma = \sqrt{Var}$$
- Average deviation: $$Adev = \frac{1}{N}\sum_{j=1}^{N}\left|x_j - \bar{x}\right|$$
- Standard error: $$s_{error} = \sigma / \sqrt{N}$$

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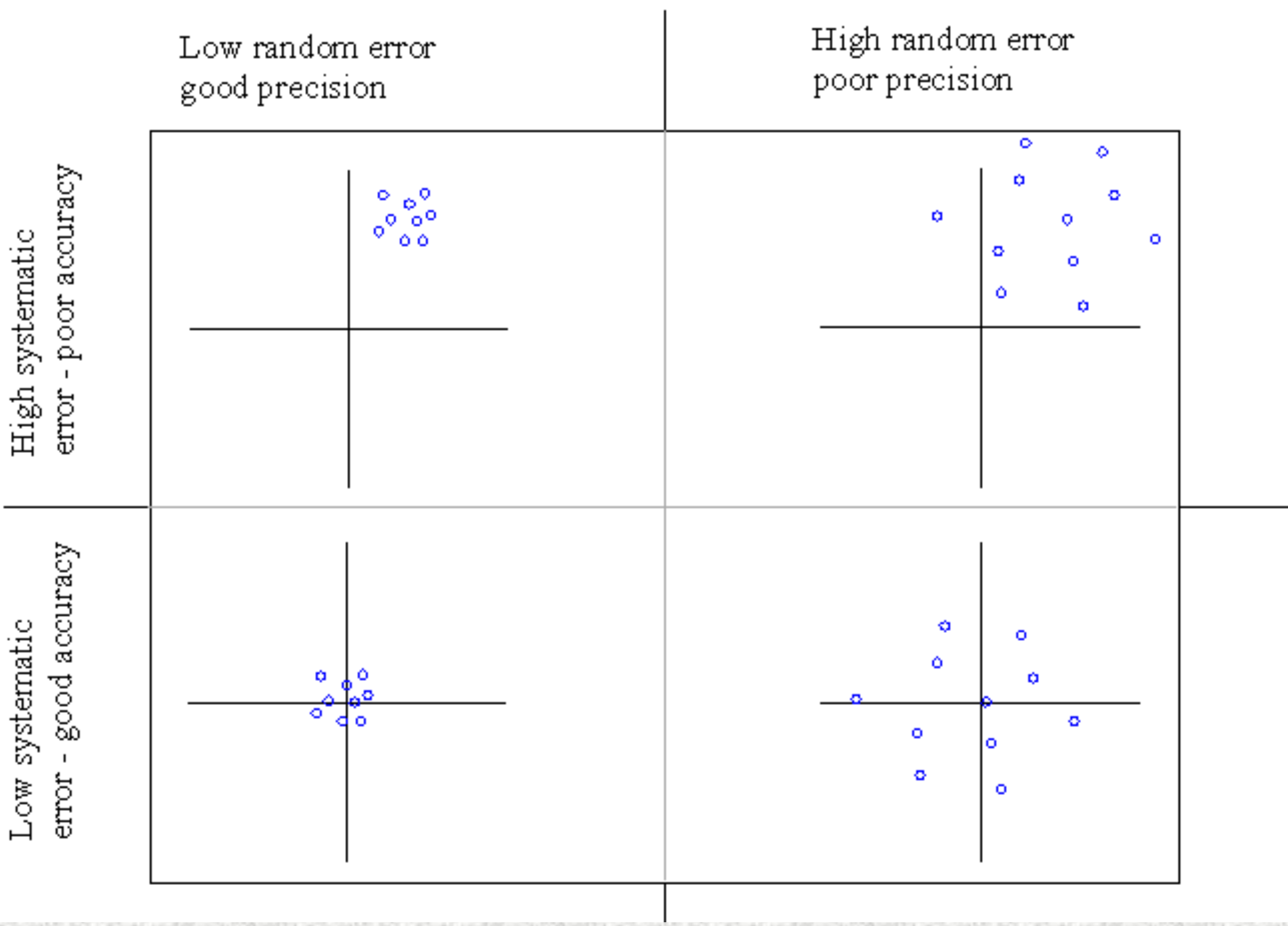
When is the uncertainty not reduced by sampling more?



Statistical description of data

Probability distribution:

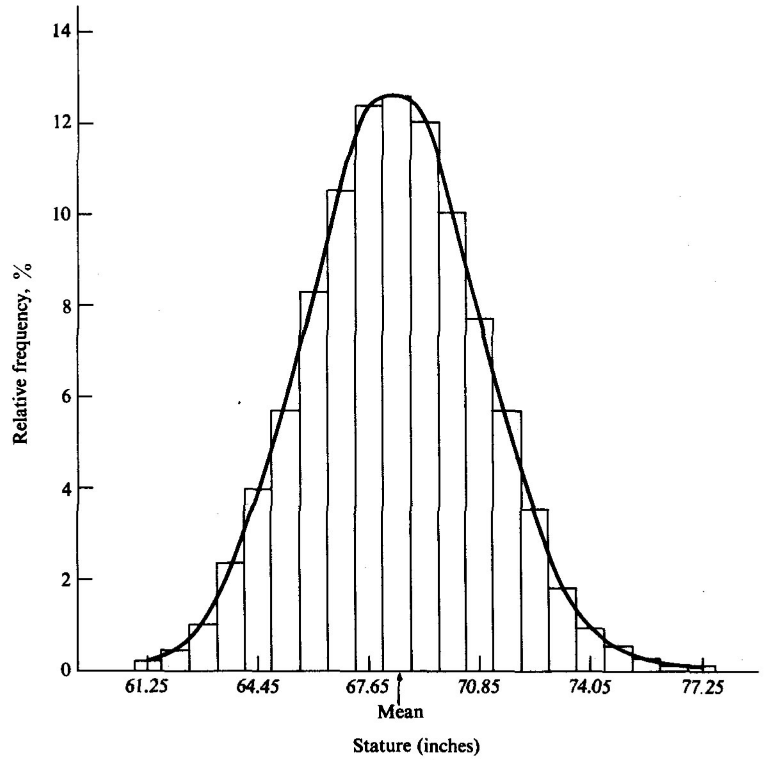


Fig. 1-2 Histogram of frequency distribution of stature of 24,404 U.S. Army males. Adapted from data of Newman and White.

Non-normal probability distribution:

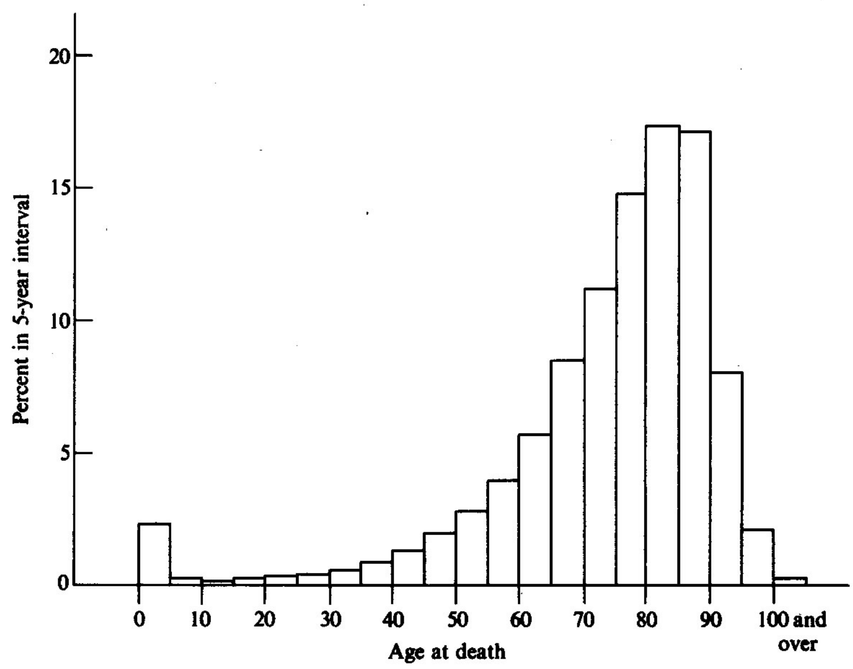


Fig. 1–3 U.S., female, 1965: percent dying in each 5-year age interval (the 100–105 interval includes all deaths after 100 rather than only those occurring in the interval). Data from N. Keyfitz and W. Flieger, *World Population: An Analysis of Vital Data.* Chicago: University of Chicago Press, 1968, p. 45.

Statistical description of data

Nonparametric statistics (when the distribution is unknown):

- rank statistics

$$x_1, x_2, \ldots.., x_N \rightarrow 1, 2, \ldots.., N$$

- Median
- percentile
- Deviation estimate
- The mode

Issue: *robustness*

Statistical description of data

Robust: "insensitive to small departures form the idealized assumptions for which the estimator is optimized."

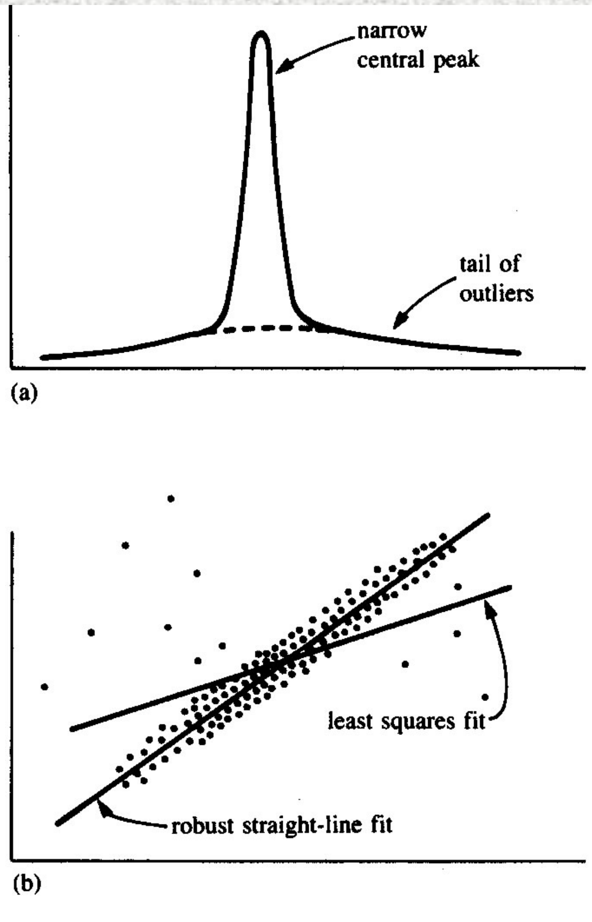
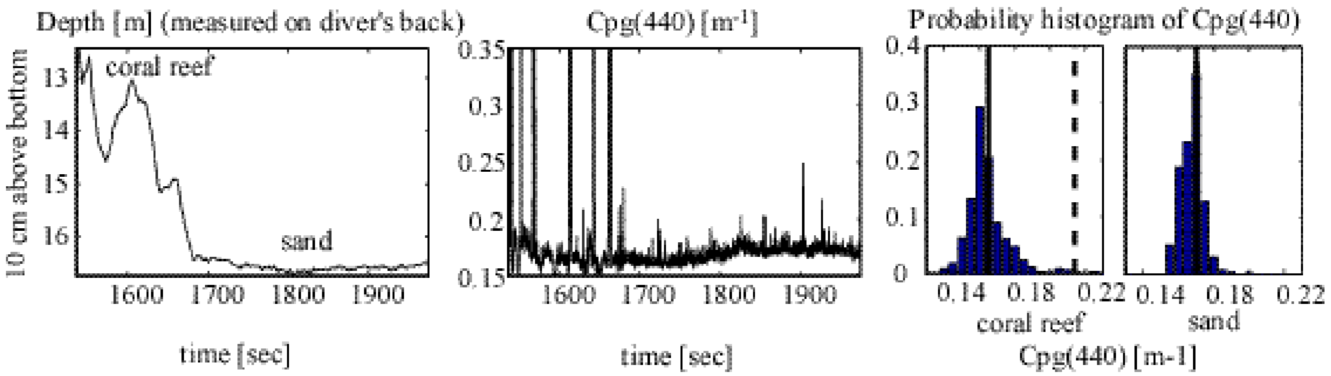
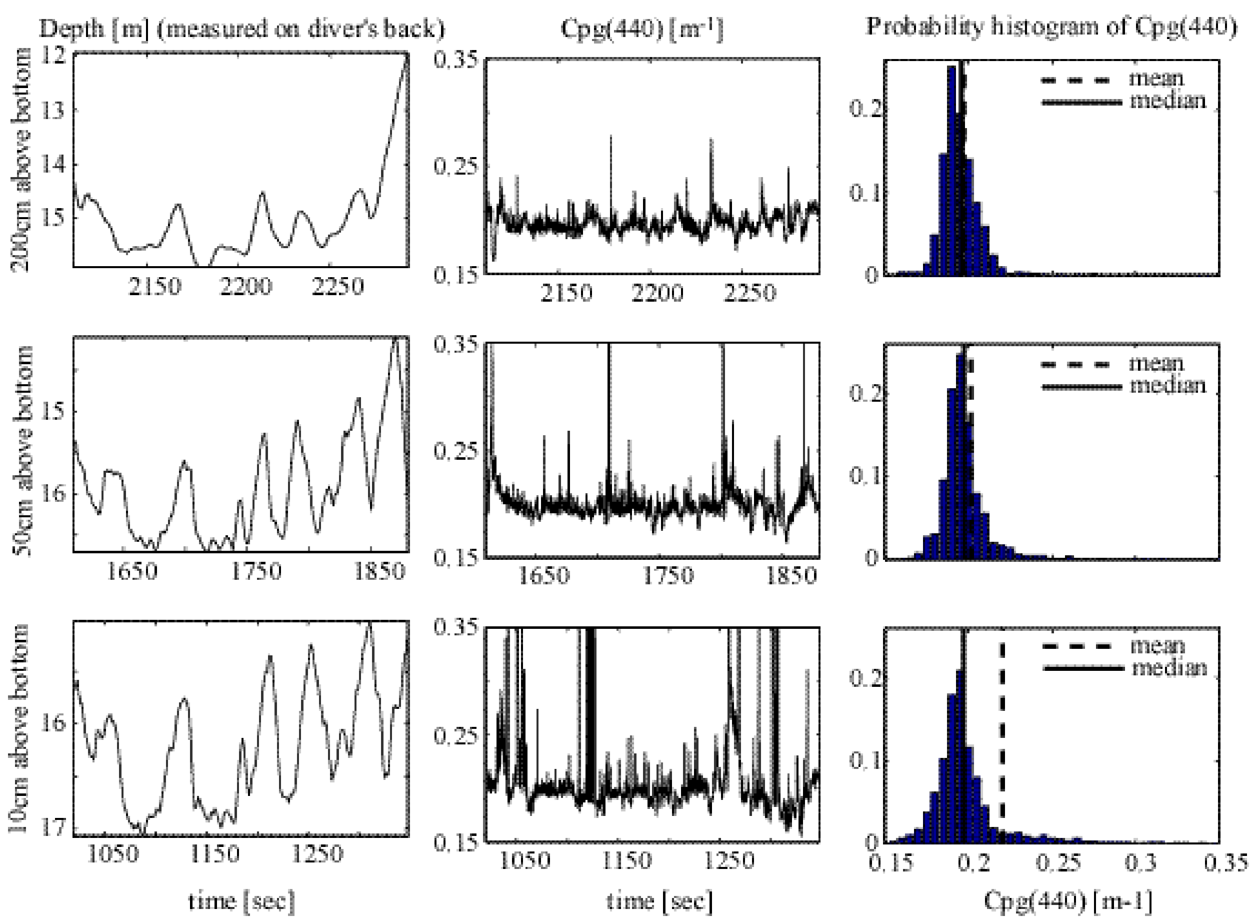


Figure 14.6.1. Examples where robust statistical methods are desirable: (a) A one-dimensional distribution with a tail of outliers; statistical fluctuations in these outliers can prevent accurate determination of the position of the central peak. (b) A distribution in two dimensions fitted to a straight line; non-robust techniques such as least-squares fitting can have undesired sensitivity to outlying points.

Statistical description of data

Examples from COBOP:





Relationship between 2 variables

Linear correlation:

$$r = \frac{\sum_i \left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right)}{\sqrt{\sum_i \left(x_i - \bar{x}\right)^2}\sqrt{\sum_i \left(y_i - \bar{y}\right)^2}}$$

Rank-order correlation:

$$r_s = \frac{\sum_i \left(R_i - \bar{R}\right)\left(S_i - \bar{S}\right)}{\sqrt{\sum_i \left(R_i - \bar{R}\right)^2}\sqrt{\sum_i \left(S_i - \bar{S}\right)^2}}$$

Regressions of type I and type II

Uncertainties in y only:

$$y(x) = ax + b$$

$$\chi^2 = \sum_{i=1:N} \left(\frac{y_i - a - bx_i}{\sigma_i} \right)^2$$

Minimize χ^2 by taking the derivative of χ^2 wrt *a* and *b* and equal it to zero.

What if we have errors in both x and y?

Press et al.' s approach:

$$y(x) = ax + b$$

$$\chi^2 = \sum_{i=1:N} \frac{(y_i - ax_i - b)^2}{\sigma^2{}_{yi} + a^2\sigma^2{}_{xi}}$$

$$Var(y_i - ax_i - b) = \sigma^2{}_{yi} + a^2\sigma^2{}_{xi}$$

Minimize χ^2 by taking the derivative of χ^2 wrt *a* and *b* and equal it to zero.

The coefficient of determination

$R^2 = 1 - MSE/Var(y)$.

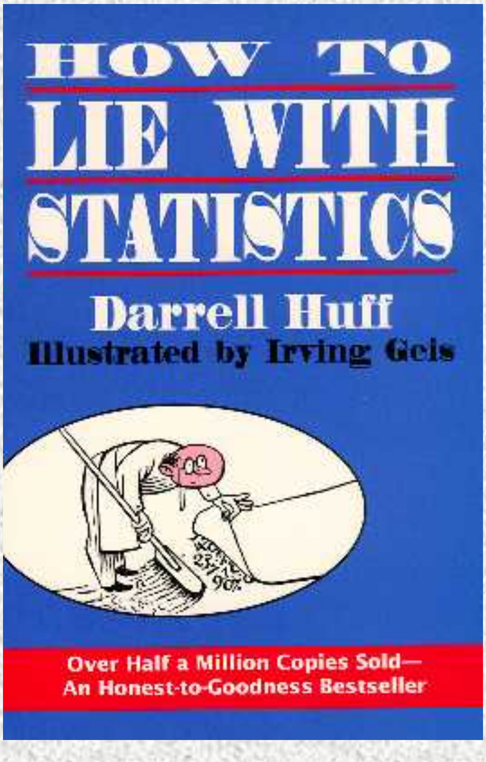
MSE=mean square error=average error of model^2/variance.

What variance does it explain?

Can it reveal cause and effect?

How is it affected by dynamic range?

R is the 'correlation coefficient'.



Regressions of type I and type II

Classic type II approach (Ricker, 1973):

The slope of the type II regression is the geometeric mean of the slope of y vs. x and the inverse of the slope of x vs. y.

$$y(x) = ax + b$$

$$x(y) = cy + d$$

$$a_{II} = \sqrt{a/c} = \pm \sigma_y / \sigma_x$$

$$\pm = sign\left\{\sum_i x_i y_i\right\}$$

Smoothing of data

Filtering noisy signals.

What is noise?

- instrumental (electronic) noise.
- Environmental ‘noise’.

“one person’s *noise* may be another person’s *signal*”

Matlab: filtfilt

Method of fluctuation

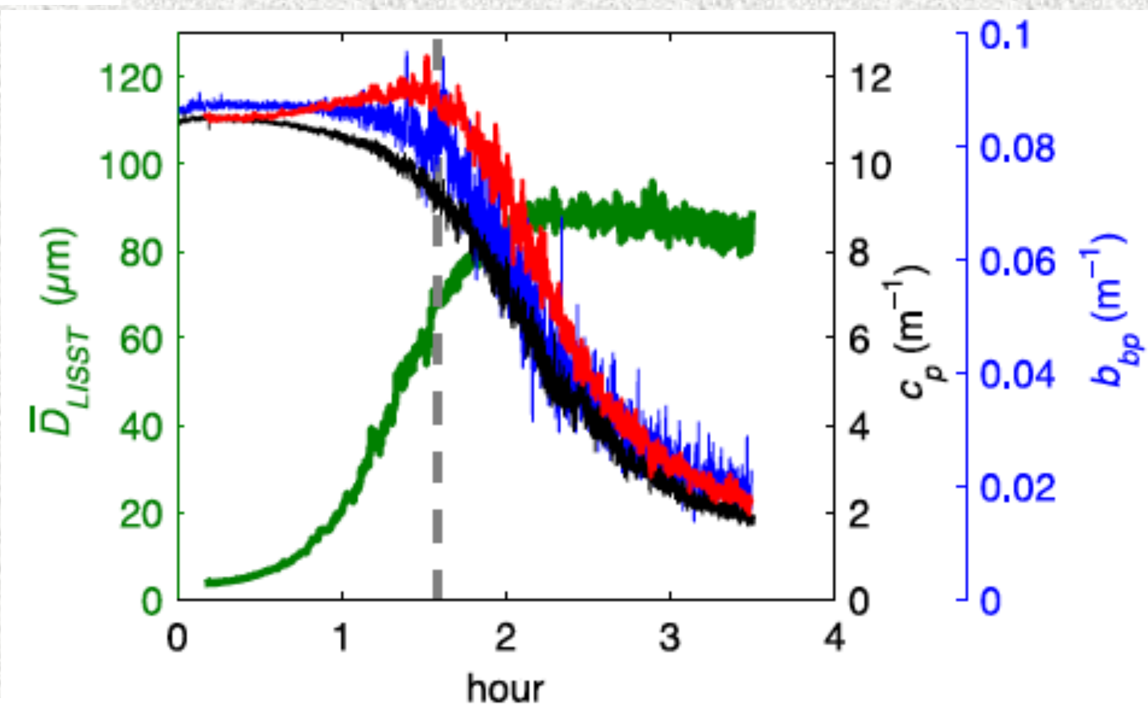
Lab aggregation exp.:

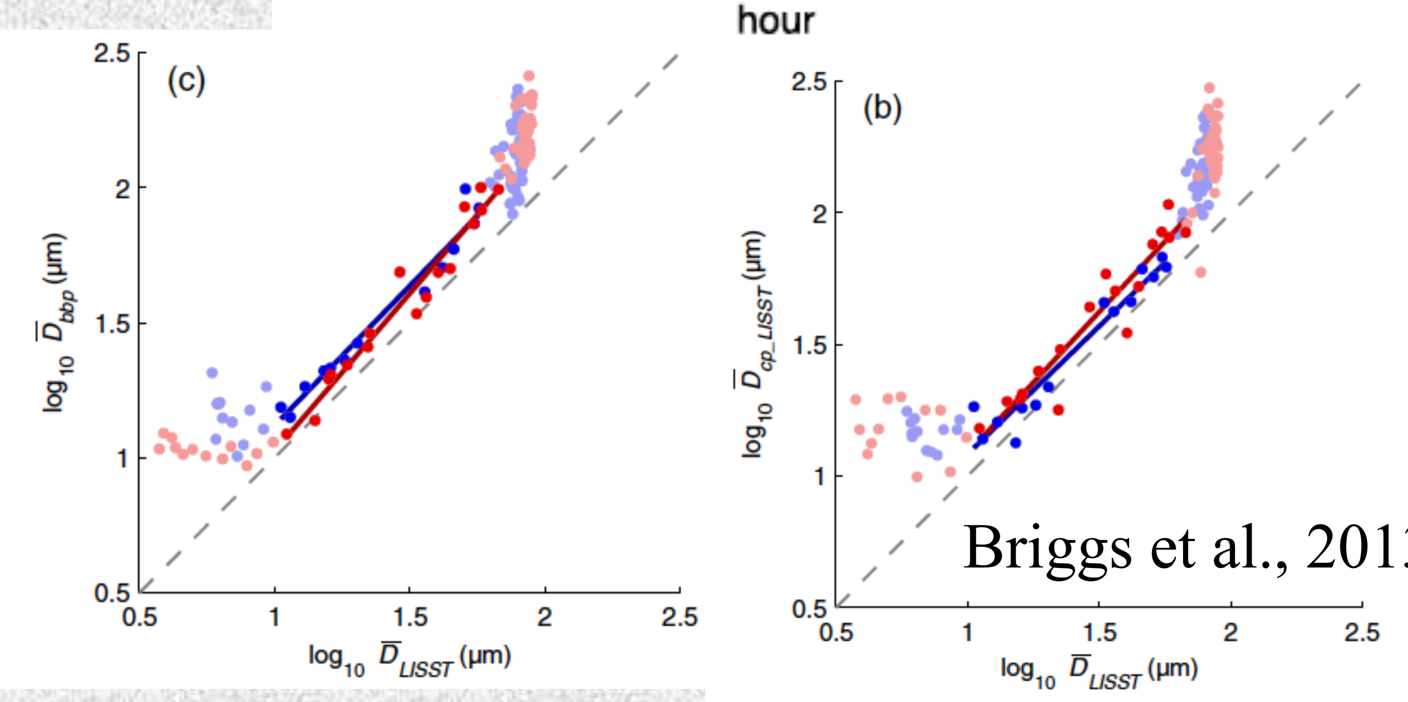
Sample volume

$$\bar{A}_{cp} = \frac{\mathrm{Var}[c_p(t)]}{E[c_p(t)]}\frac{V}{Q_c}\frac{1}{\alpha(\tau)}$$

$$\bar{D} = 2\sqrt{\bar{A}\pi^{-1}}$$

Measurement time





Briggs et al., 2013

Modeling of data

Condense/summarize data by fitting it to a model that depends on adjustable parameters.

Example, CDM spectra:

$$a_g(\lambda) = \tilde{a}_g \exp\left(-s(\lambda - \lambda_0)\right)$$

particulate attenuation spectra:

$$c_p(\lambda) = \tilde{c}_p \left(\frac{\lambda}{\lambda_0}\right)^{-\gamma}$$

Modeling of data

Example: CDM spectra.

$$a_g(\lambda) = \tilde{a}_g \exp(-s(\lambda - \lambda_0))$$

$$\Rightarrow \boldsymbol{a} = \left\lfloor \tilde{a}_g , s \right\rfloor$$

Merit function:

$$\chi^2 = \sum_{i=1}^{9} \left[\frac{a_g(\lambda_i) - \tilde{a}_g \exp(-s(\lambda - \lambda_0))}{\sigma_i} \right]^2$$

- For non-linear models, there is no guarantee to have a single minimum.
- Need to provide an initial guess.

Matlab: fminsearch

Modeling of data

Lets assume that we have a model

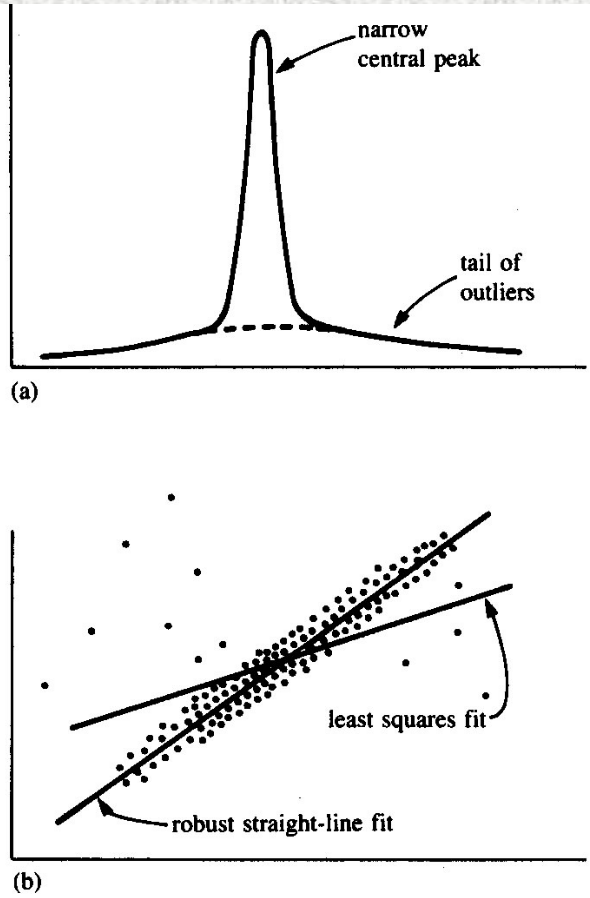
$$y = y(\lambda; \boldsymbol{a})$$

A more robust merit function:

$$\widetilde{\chi} = \sum_{i=1}^{N} \left| \frac{y(\lambda_i) - y(\lambda_i; \boldsymbol{a})}{\sigma_i} \right|$$

Problem: derivative is not continuous. Can be used to fit lines.

Statistical description of data



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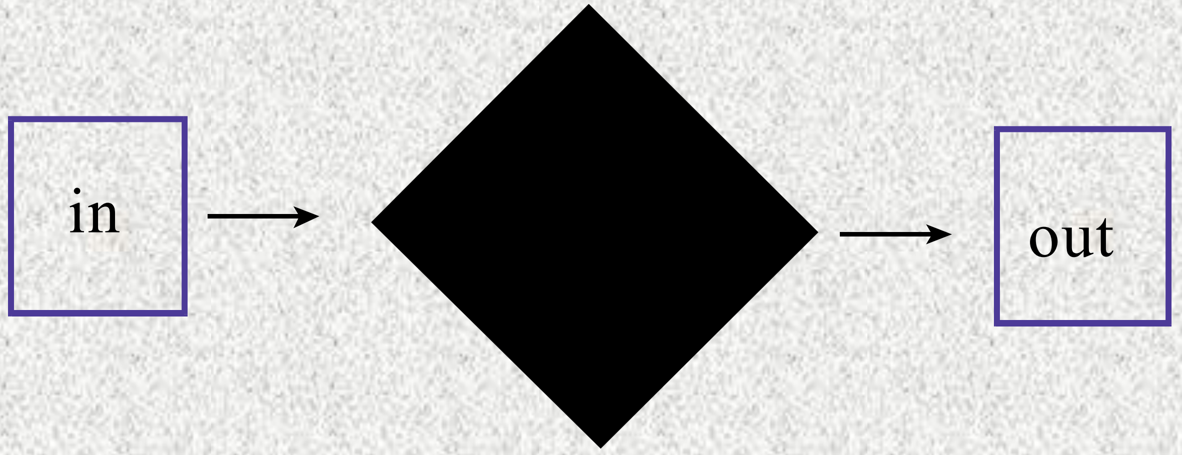
Monte-Carlo/Bootstrap methods

Need to establish confidence intervals in:

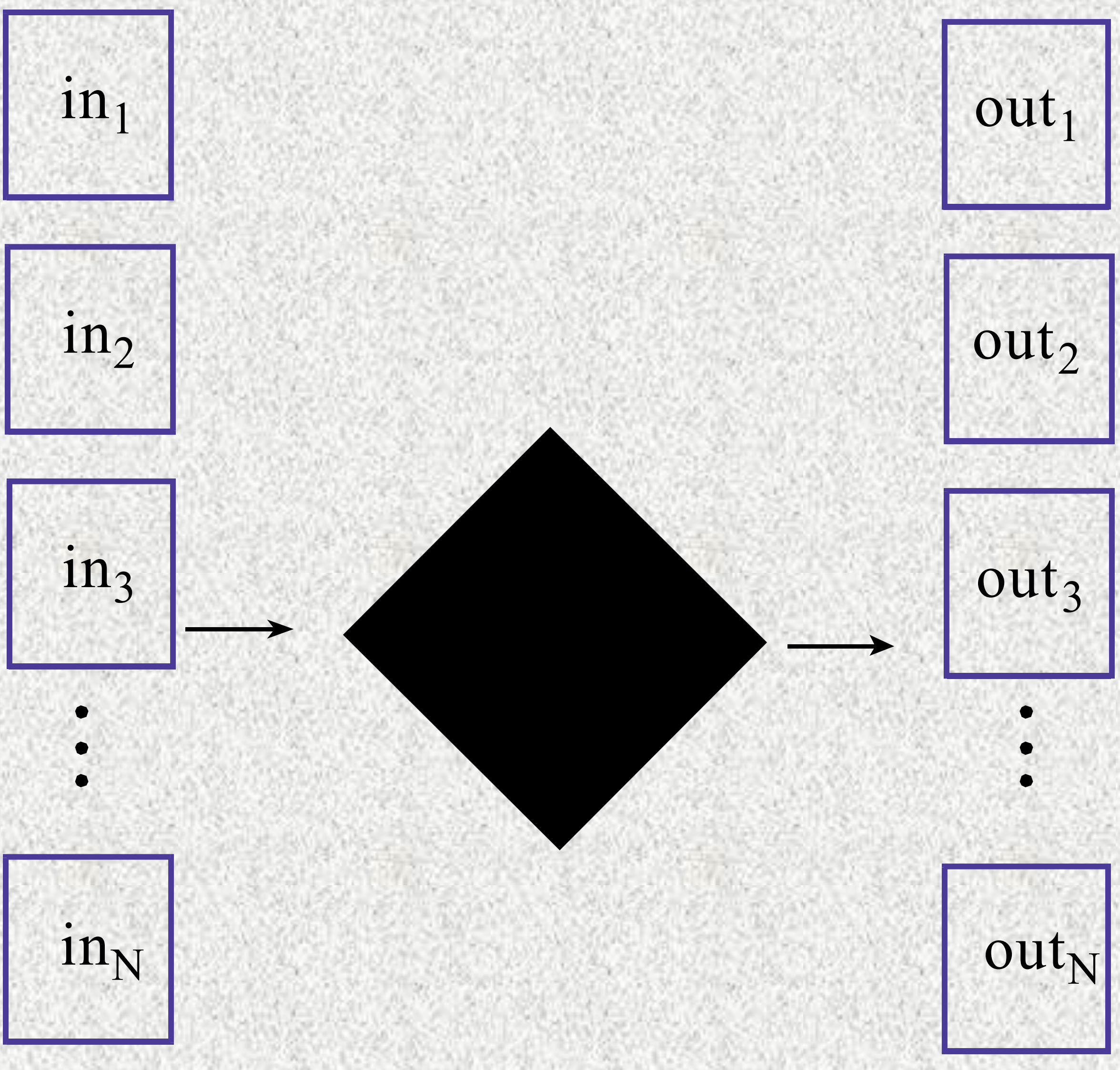
1. Fitting-model parameters (e.g. CDM fit).

2. Model output (e.g. Hydrolight).



When there is an uncertainty (or possible error) associated with the input:

Vary inputs with random errors and observe effect on output:



Example: how to assign uncertainties in derived spectral slope of CDOM.

Merit function:

$$\chi^2 = \sum_{i=1}^{9}\left(a_g(\lambda_i) \pm \Delta_i - \tilde{a}_g \exp\left(-s(\lambda - \lambda_0)\right)\right)^2$$

Randomly add uncertainties (Δ_i) to each measurement, each time performing the fit (e.g. using randn.m in Matlab, RAND in Excel).

Then do the stats for the different *s*.