Astro 500

Techniques of Modern Observational Astrophysics

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Lecture Outline

- Random vs systematic error
- Modeling data uncertainties: distributions
- Characterizing distributions: moments
- Errors, weighting and propagation
- Goodness of fit, χ^2 and robust estimation
- Regressions, error models and intrinsic scatter

Take away from last lecture:

- The notes contain a suitable reference for almost all of your future needs with optical-NIR photometry.
- Band-passes and calibration requires detailed information about filters, detector, telescope (optics), and atmosphere.
- Well-calibrated photometry is difficult to achieve.
  - 10%? You're not trying hard enough.
  - 5%? Ok.
  - 3%? Good. You are pressing the limit of the absolute calibration.
  - 1%? Don't fool yourself; you're limited by the absolute calibration.

Which brings up the topic of precision vs accuracy…

Random vs systematic error

- Same as the difference between precision vs accuracy
  - Precision: How well can you measure a quantity (what's the variance of repeat measurements)?
  - Accuracy: How well do your measurements (in the mean) reflect the value you are trying to measure?
  - *Know the difference – fundamental.*
- We're lucky when an astronomical result includes a quote of random error. Systematic errors in astronomy are rarely addressed, but this is changing; it has long been common-place in Physics.
- In error handling and reporting, be a physicist in rigor with the intuition of an astronomer.

Modeling Uncertainties: Distributions

- Binomial – coin-toss
- Poisson – generalized counting statistics ($\sqrt{N}$)
- Gaussian – "normal" distribution, appropriate for most error distributions
- Lorentzian – suitable to describe data related to resonances

- Processes in the universe do not "obey" these distributions, they are merely human-generated, mathematical contrivances.
- Amazingly, a number of processes in the universe do appear to be well described by these distributions

Characterizing distributions

- Moments
- 1st: Mean, $\bar{x}$ (location)
  - Other 1st-moment indicators:
    - *median* (robust estimator)
    - *mode*
- 2nd: Standard deviation, σ (width)
  - Other 2nd-moment indicators:
    - *Average deviation* (robust estimator): $AD = \frac{1}{N}\sum_{i=1}^{N}\left|x_i - \bar{x}\right|$
    - *full-width half-maximum (FWHM)*
- 3rd: Skew, s (symmetry)
- 4th: Kurtosis, k (shape)

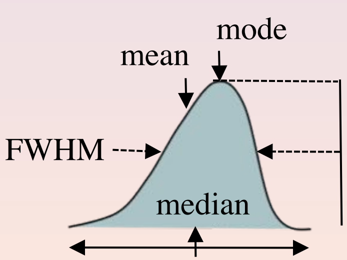
$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\sigma^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(x_i - \bar{x}\right)^2$$

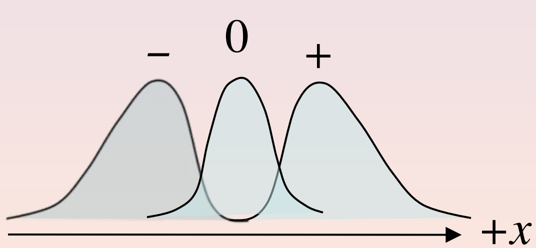
$$s = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_i - \bar{x}}{\sigma}\right)^3$$

$$k = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_i - \bar{x}}{\sigma}\right)^4 - 3$$

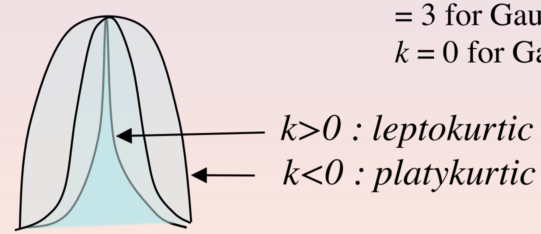
= 3 for Gaussian
$k = 0$ for Gaussian



1st & 2nd moments



skew



kurtosis

Gaussian distribution

- By adopting a distribution function you can relate moments to distribution function parameters
- You can also invert the process, compare moments and determine the suitability of model distribution choice
- For a Gaussian distribution the following holds:

  - 1st: mean=mode=median
  - 2nd: $2.354\,\sigma = FWHM$
  - 3rd: Skew, $s = 0$ *(symmetric)*
  - 4th: Kurtosis, $k = 0$ *(normal)*

- This is true strictly *only* for a Gaussian.

Standard deviation vs standard error

- σ is the *standard deviation*. It describes the width of a distribution, but is only proportional to the error in the estimate of the mean.
- $\sigma_{\bar{x}}$ is the *standard error in the mean*, $\bar{x}$. It depends on the distribution width and how well it is sampled, i.e., N.
- In general:

$$\sigma_{\bar{x}} = \sigma / \sqrt{N}$$

regardless of the distribution shape.

Weighting your data

- Moment estimates of a distribution can be dramatically improved in *precision* by weighting the data according to the uncertainties specific to each datum (heteroscedastic errors)
- $w_i \equiv 1/\sigma_i^2$
- σ_i is the variance on each datum x_i
- Similar generalizations for s and k.
- And it is still true:

$$\sigma_{\bar{x}_w} = \sigma_w / \sqrt{N}$$

$$\bar{x}_w = \frac{\sum_{i=1}^{N} (w_i x_i)}{\sum_{i=1}^{N} w_i}$$

$$\sigma_w^2 = \frac{N}{N-1} \frac{\sum_{i=1}^{N} \left[w_i (x_i - \bar{x})^2 \right]}{\sum_{i=1}^{N} w_i}$$

- Look familiar?

$$\lambda_{\text{eff}} \equiv \frac{\int \lambda S_\lambda f_\lambda \, d\lambda}{\int S_\lambda f_\lambda \, d\lambda},$$

Error propagation

- Gaussian quadrature or N-dimensional hypotenuse

$$f = f(x_i, \ldots x_n)$$

$$df = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i} dx_i \right)^2}$$

$$dx_i = \sigma_{x_i}$$

- When errors on individual parameters, or components, x_i, of your observable, f, are uncorrelated (orthongonal):
- With covariance:

$$df = \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i} dx_i \right)^2 + 2 \sum_{j \neq i} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} dx_{ij}}$$

$$dx_{ij} = \sigma_{ij}$$

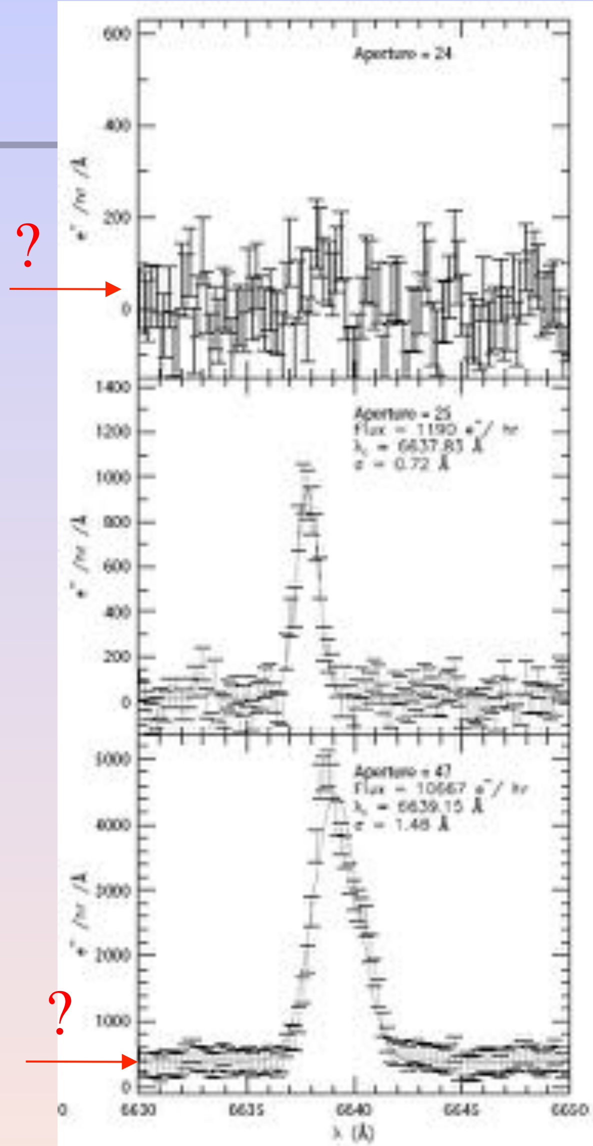
- Best to work in terms of covariance matrix

An aside: logarithmic derivatives

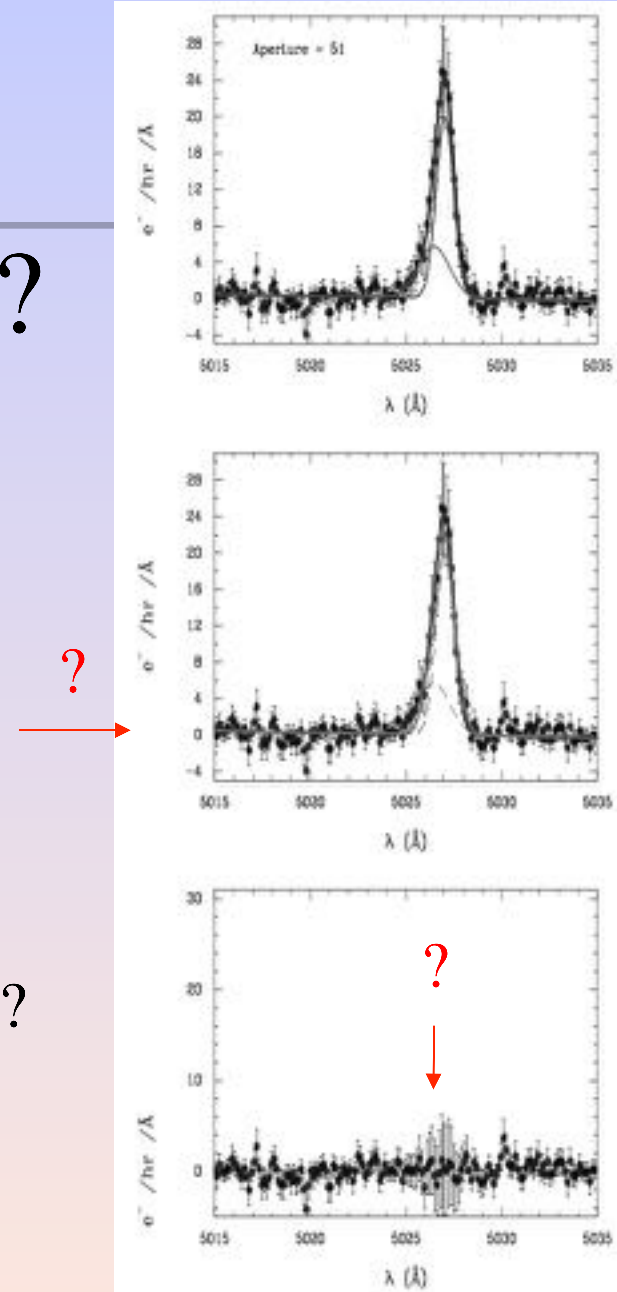
- The best way to present errors or to examine covariance:
- $d\log x = \frac{dx}{x}$ is scale free and gives the fractional error
- $\frac{d\ln x}{d\ln y} = \frac{y}{x}\frac{dx}{dy}$
- “neper-esque”

Are your errors any good?

- Look at your data and think about what it means.
- Think in terms of probability, specifically the probability distribution suitable for your adopted data model (typically Gaussian).
- For a Gaussian distribution of errors you expect
  - 68% of data lie within $\pm 1\sigma$
  - 95% of data lie within $\pm 2\sigma$
  - 99.7% of data lie within $\pm 3\sigma$



How do these look?



What assumptions do you make in your assessment?

Goodness of fit: χ^2

$$\chi^2 = \sum_{i=1}^{N} \left\{ \left[y_i - y(x_j,\ldots,x_n) \right]^2 / \sigma_i^2 \right\}$$

a 2nd moment, error-weighted

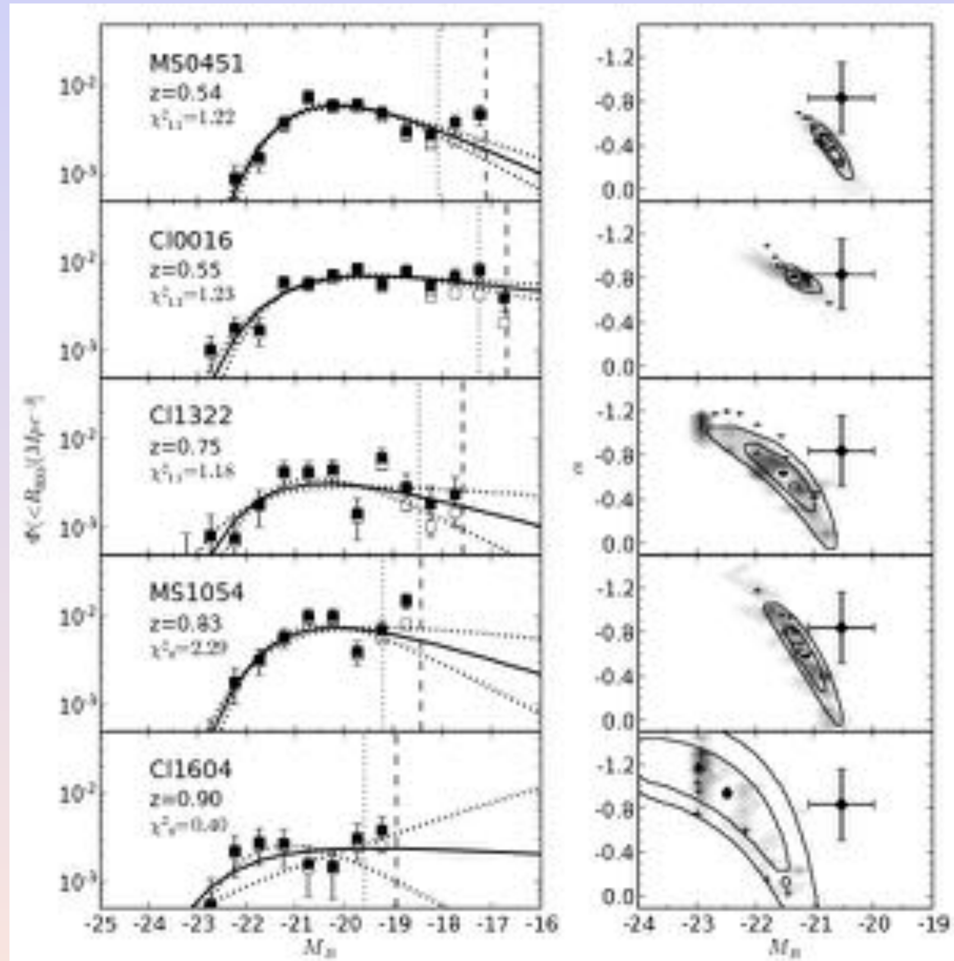
- Formal definition:
- Reduced-χ^2: $= \chi_\nu^2 = \chi^2/\nu$
  - y_i = data
  - σ_i = errors on data
  - $y(x_1,\ldots,x_n)$ = model as function of parameters $(x_1,\ldots,x_n)$
  - $\nu = N - n - 1$, where n are the number of model parameters
- What does it mean? For a good model and well defined errors you expect: $\chi_\nu^2 = 1$.
- χ^2, χ_ν^2 useful to estimate goodness of fit of model as well as for defining *confidence intervals* on model parameters by using probability distribution.
  - Some assumptions and limitations apply. See Bevington and Press et al. (Num.Rec.) for discussion.
- Must have good error estimates.

Goodness of fit: example

- Schecter luminosity function fitting

$$\phi(M)\,\mathrm{d}M = 0.4 \ln 10 \times \phi^* 10^{-0.4(M-M^*)(\alpha+1)} \times \exp\left[-10^{-0.4(M-M^*)}\right] \mathrm{d}M.$$

- *lhs*:
  - o best fit (solid curve)
  - o 68% CL fits (dotted curves)
- *rhs*
  - o 65, 95% joint confidence intervals on α-M* (contours)
  - o Jack-knife errors (greyscale)



Crawford et al. ’09 (ApJ, 690, 1158)

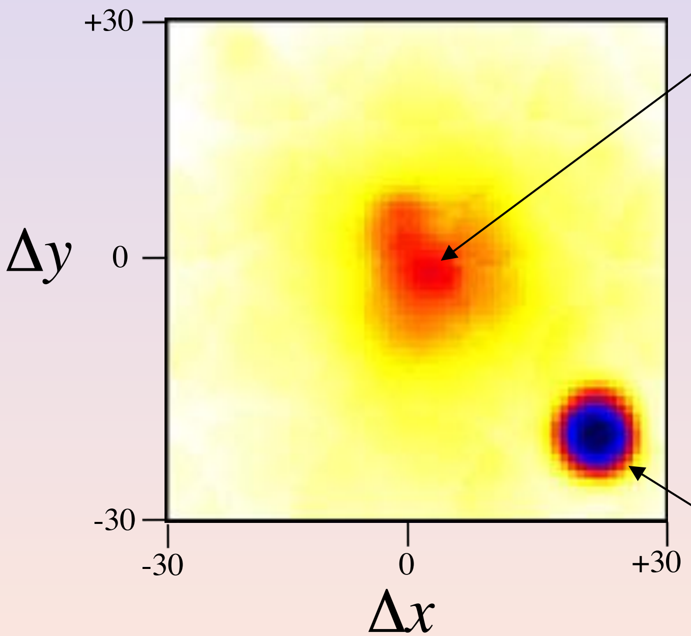
Minimization: χ^2

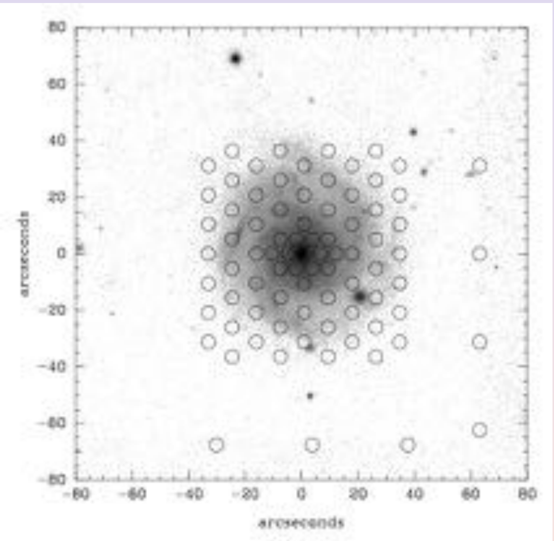
- Several methods for finding the model parameters yielding the minimum χ^2 for your data (the “best fit”).
  - See Press et al. (Num.Rec.)
- Brute force – just map it out over N-dimensional parameter space
- Downhill simplex: N+1 dimensional “amoeba” steps toward minimum
  - Requires no function derivatives
  - Easy to implement
  - slow
- Levenberg-Marquardt: smooth variation from inverse-Hessian to steepest-descent methods
  - Standard non-linear least-squares routine
  - Computationally fast
  - Yields covariance matrix for parameter error estimation
  - Requires function derivatives
- All methods suffer from trapping in false (local) minima.
- Must looking at χ^2 maps to assess parameter covariance and uniqueness

χ^2 : False minima

- Example: Spatial registration of SparsePak (sparsely-sampled IFU) spectral-continuum data to 2D broad-band images
- Which minima correctly identifies the centering?

χ^2 map





Deeper minimum due to star in image not in IFU spectra at offset co-incident with galaxy center.

Outside the box

- What does it mean if $\chi_\nu^2 > 1$ or $\chi_\nu^2 < 1$?
  - Under or over estimated your errors
  - Bad model
  - Can't use χ^2 for confidence-interval estimation on model parameters.
- What *can* you do?
- Force $\chi_\nu^2 = 1$ by adjusting errors in an "unbiased" way

added term

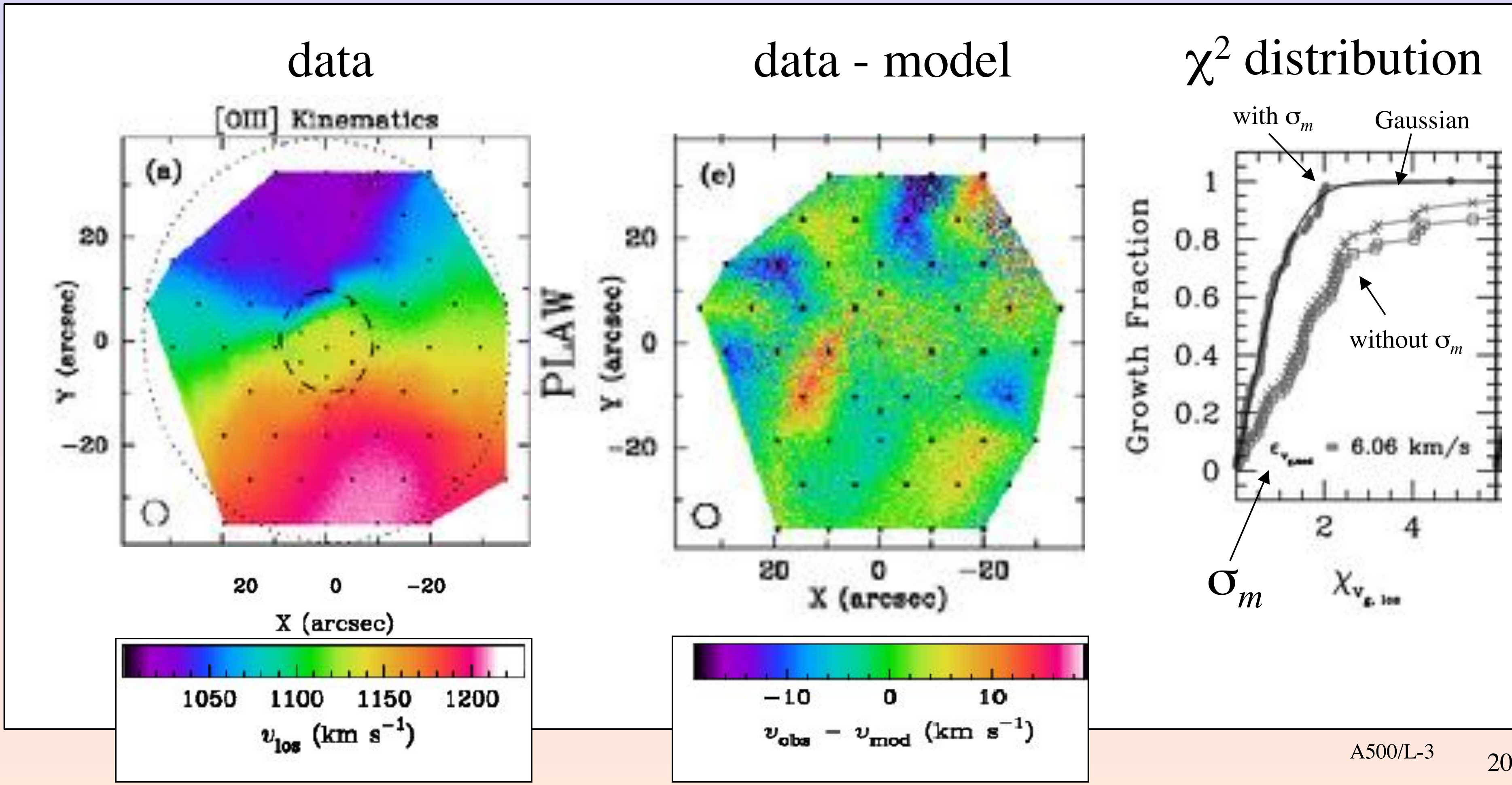
$$\chi^2 = \sum_{i=1}^{N} \left\{ \left[y_i - y(x_j, \ldots, x_n) \right]^2 / \left(\sigma_i^2 + \sigma_m^2 \right) \right\}$$

  - σ_m is a constant "model error" for all data y_i, chosen to make $\chi_\nu^2 = 1$.
- χ^2 can once again be used for confidence-interval estimation on model parameters.
- When can you do this, i.e., when is it ok to "fudge it?"
- Is this voodoo statistics or are we ahead of the statisticians?

WARNING: no commonly accepted norm

Outside the box: example

- Ionized-gas velocity fields of galaxy disks
  - Andersen (2001, Ph.D.), Westfall (2009, Ph.D.)

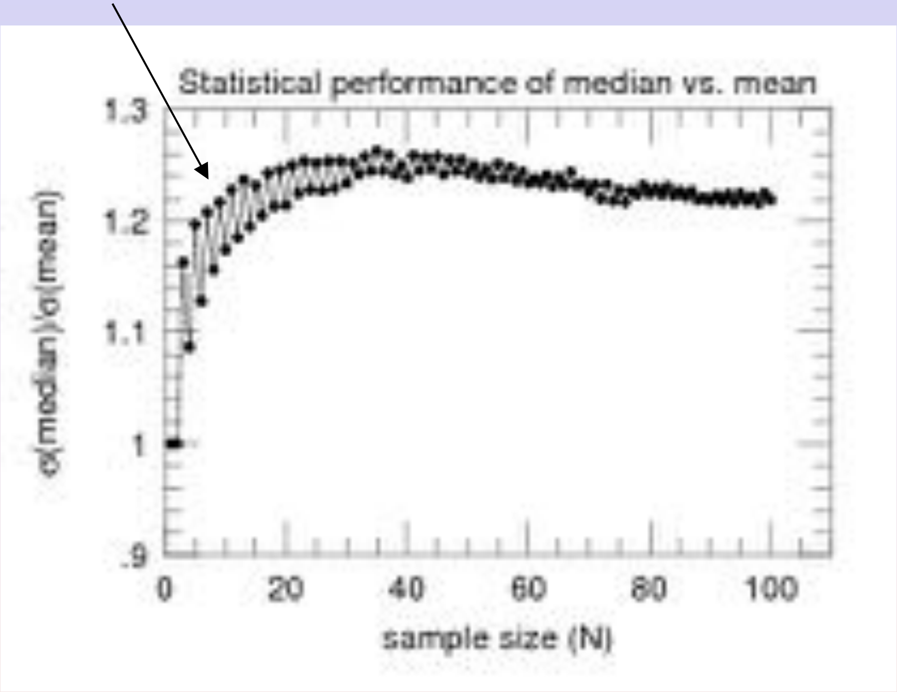


Robust estimation

- Usually trade-offs between precision and accuracy
- Robust estimators typically improve accuracy at the sacrifice of precision.
- When to make this trade is a judgment call based on the quality and "issues" associated with your data.
- You should understand (i.e., model) the amplitude of the trade-off.
- Two examples:
  - (1) median vs. mean
  - (2) σ-clipping

Robust estimation: median

Why fluctuations?

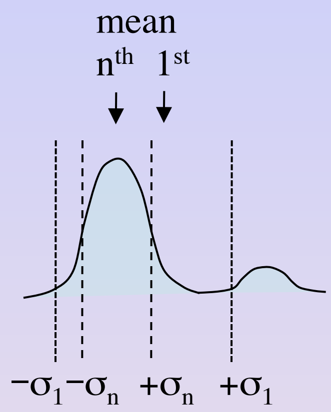


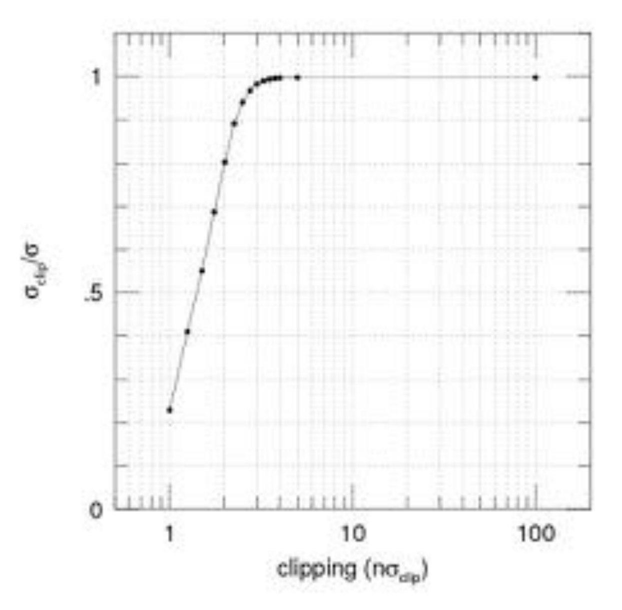
Experiment: compute variance (σ) in mean and median estimated for N data points sampling the same intrinsic Gaussian distribution (same parent mean and σ).

- The median is the 50^{th}-percentile of a sorted list.
- The median is a robust estimator of the mean because it is relatively impervious to outlier data, e.g., a non-Gaussian tail.
- As long as the majority of data cluster around the true mean, then the median is more reliable (i.e., *more accurate*) than the mean.
- However, the median is 20-25% noiser than the mean when the distribution is close to Gaussian, i.e., it is *less precise*.

Robust estimation: σ-clipping

- Iterative-clipping of moments: good for mean and σ
  - ➢ Also applies to χ^2
- Choose a clipping level
- Define a convergence criterion
- Skew is good choice for assumption of normal distribution (s=0)
  - ➢ Can check assumption by calculating kurtosis
- Note correction factor needed to complete integral for both σ and k (even moments)



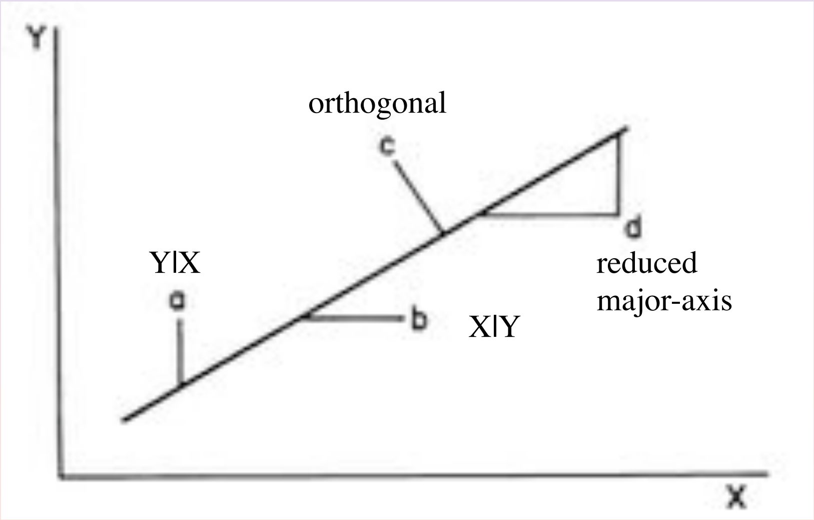


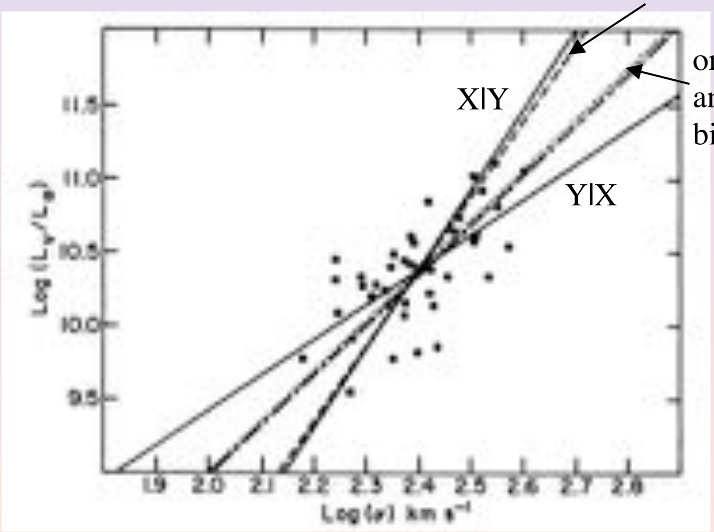
Linear Regressions

- Regressions are based on solving a set of linear equations based on different moments of the data and weighted by errors or priors.
- There are difference kinds of regression models (moments)
  - X|Y, Y|X, bisector, orthogonal
  - There are different assumptions to be made about errors that also lead to different moments and regressions
  - Is there an independent variable? (one variable with no errors)
  - Are the errors heteroscedastic or homoscedastic? (different or the same for all data)
  - Is there intrinsic scatter (usually other dimensions not known)?
- There is *no right regression model* (it depends what you want to learn), but there are correct and incorrect errors models and assumptions.
  - Social science analysis is plagued by systematic errors due to inaccurate models, but we're not free of such pitfalls because the universe is complicated.

Different Regressions

- X|Y, Y|X, bisector, orthogonal regressions
- Isobe et al. (1990, ApJ, 364, 104):
  - ordinary least squares (OLS) – no errors
- Akritas & Bershady (1996, ApJ, 470, 706)
  - bivariate correlated errors (heteroscedastic) and intrinsic scatter (BCES)





OLS Regression formulae

TABLE 1

LINEAR REGRESSION FORMULAE FOR SLOPES

Method	Expression for Slope	Estimate of the Variance of the Slope $\widehat{\mathrm{Var}}(\beta_i)$
OLS(Y | X)	$\beta_1 = \frac{S_{xy}}{S_{xx}}$	$\frac{1}{S_{xx}^2}\left[\sum_{i=1}^{n}(x_i-\bar{x})^2(y_i-\beta_1 x_i-\bar{y}+\beta_1\bar{x})^2\right]$
OLS(X | Y)	$\beta_2 = \frac{S_{yy}}{S_{xy}}$	$\frac{1}{S_{xy}^2}\left[\sum_{i=1}^{n}(y_i-\bar{y})^2(y_i-\beta_2 x_i-\bar{y}+\beta_2\bar{x})^2\right]$
OLS bisector	$\beta_3 = (\beta_1+\beta_2)^{-1}[\beta_1\beta_2 - 1 + \sqrt{(1+\beta_1^2)(1+\beta_2^2)}]$	$\frac{\beta_3^2}{(\beta_1+\beta_2)^2(1+\beta_1^2)(1+\beta_2^2)}[(1+\beta_2^2)^2\,\widehat{\mathrm{Var}}(\beta_1) + 2(1+\beta_1^2)(1+\beta_2^2)\,\widehat{\mathrm{Cov}}(\beta_1,\beta_2) + (1+\beta_1^2)^2\,\widehat{\mathrm{Var}}(\beta_2)]$
Orthogonal regression	$\beta_4 = \frac{1}{2}[(\beta_2-\beta_1^{-1}) + \mathrm{Sign}(S_{xy})\sqrt{4+(\beta_2-\beta_1^{-1})^2}]$	$\frac{\beta_4^2}{4\beta_1^2+(\beta_1\beta_2-1)^2}[\beta_1^{-2}\,\widehat{\mathrm{Var}}(\beta_1) + 2\,\widehat{\mathrm{Cov}}(\beta_1,\beta_2) + \beta_1^2\,\widehat{\mathrm{Var}}(\beta_2)]$
Reduced major-axis	$\beta_5 = \mathrm{Sign}(S_{xy})(\beta_1\beta_2)^{1/2}$	$\frac{1}{4}\left[\frac{\beta_2}{\beta_1}\,\widehat{\mathrm{Var}}(\beta_1) + 2\,\widehat{\mathrm{Cov}}(\beta_1,\beta_2) + \frac{\beta_1}{\beta_2}\,\widehat{\mathrm{Var}}(\beta_2)\right]$

Errors on Regressions

- How do you estimate errors on slope and intercept?
- Resample your data:
  - Boot-strap – pick N data points out of sample of N, m times. Each pick is a random selection from N data points with equal probability of selecting i^{th} element.
  - Jack-knife – recalculate leaving out one datum, N times (N data)
- Monte Carlo simulation – artificial data

✧ When in doubt, “Monte Carlo” your data

✧ This applies not just to linear regressions but any modeling.

When in doubt….

- "Monte Carlo (MC) your data"
- Monte Carlo: a town in Monaco (country in SE France) famous for gambling casinos
- What you need:
    - Model of data
    - Model of errors
    - Model of data sampling (range, censorship, incompleteness, spurious source (when applicable).
    - A good random-number generator
    - A modicum of computing skill and cpu time.
- How good is it?
- Only as good as your assumptions (i.e., model)
- Test your assumptions by comparing distributions (and their characterization) generated by MC against those from the data.

Miscellaneous topics in statistics

- Items you need to explore on your own as an astronomer:
  - How do distribution- and selection-functions bias regressions?
  - Famous biases in astronomy
    - Malmquist
    - Eddington
  - What linear regression should you use? …or:
  - Should you even use a linear regression?