Lecture 5: Fitting Observed Data 1

Outline

- Errors
- Distributions
- Computing Distributions
- Error Propagation
- Errors with Gaussian Distributions
- Fitting a Straight Line
- Fitting a Linear Model

Overview

- fitting: compare measurements with model predictions
- fitting method depends on
 - errors in observations
 - how model depends on free parameters
 - definition of best fit
- to determine errors in observations, need to propagate errors through data acquisition and reduction
- need to define what

Errors

Accuracy and Precision

- accuracy of observation measures correctness of result,
 measures of how close observational result comes to true value
- precision of observation measures how reproducible result is, measures how exactly the result is determined without reference to what that result means
- absolute precision: magnitude of uncertainty in result in same units as result
- relative precision: uncertainty in terms of fraction of value of result
- both accuracy and precision need to be considered simultaneously
- useless to determine something with high precision but highly inaccurately
- observation cannot be considered accurate if precision is low

Random and Systematic Errors

- systematic error: reproducible inaccuracy introduced by faulty equipment, calibration, or technique
- accuracy generally depends on how well one can control or compensate for systematic errors
- random error: Indefiniteness of result due to a priori finite precision of observation, measures fluctuation in repeated observations
- precision depends on how well one can overcome or analyse random errors
- random errors require repeated trials to yield precise results
- given accuracy implies a precision at least as good ⇒ depends somewhat on random errors

Distributions

Characterizing Distributions

- parent distribution: infinite number of measurements ⇒
 observations distributed according to true probability distribution
- actual observations are sample of infinite number of possible measurements
- observations estimate parameters of parent distribution
- average:

$$\mu \simeq \overline{X} \equiv \frac{1}{N} \sum_{i=1}^{N} X_i$$

variance:

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

Independent Measurements

- estimate of average assumes that all measurements x_i are independent
- for variance, already used x_i values to estimate average $\Rightarrow N-1$ independent measurements left
- reason that sum of $(x_i \overline{x})^2$ is divided by N 1
- single measurement (N = 1)
 - best value for average given by single measurement
 - no measure for variance

Sample Average

- consider \overline{x} as variable in definition of variance
- try to find value of \overline{x} for which s^2 is minimal
- set derivative of s^2 with respect to \overline{x} to zero:

$$\frac{\partial s^2}{\partial \overline{x}} = \frac{-2}{N-1} \sum_{i=1}^{N} (x_i - \overline{x}) = \frac{-2}{N-1} \left(\sum_{i=1}^{N} x_i - N \overline{x} \right) = 0$$

therefore

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

definition for sample average minimizes sample variance

Average and Variance for Binned Data

- astronomical data often binned or discrete
- all digital data is binned
- definitions

B number of bins, $b = 1, \ldots, B$

 x_b value of x in bin b

 N_b number of measurements in bin b

- normalize N_b by total number of measurements
- ullet probability that measurement falls into bin b is $P_b \equiv N_b/\sum_{b=1}^B N_b$
- average:

$$\overline{x} = \sum_{b=1}^{B} P_b x_b$$

variance:

$$s^2 = \frac{N}{N-1} \left(\sum_{b=1}^{B} P_b x_b^2 - \overline{x}^2 \right)$$

Higher-Order Moments of Distributions

- higher-order moments of distributions very sensitive to outliers
- large $x_i \overline{x}$ value dominates much more in distribution of $(x_i \overline{x})^2$ than in distribution of $|x_i \overline{x}|$
- therefore do not use even higher moments such as
 - Skewness:

$$\equiv \frac{1}{N\sigma^3} \sum (x_i - \overline{x})^3$$

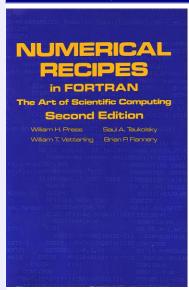
Kurtosis

$$\equiv \frac{1}{N\sigma^4} \sum (x_i - \overline{x})^4 - 3$$

- σ is standard deviation
- subtraction of 3 in kurtosis makes kurtosis of Gaussian zero

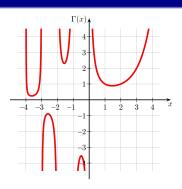
Computing Distributions

Numerical Recipes



- funamental book on numerical algorithms
- exists for different programming languages
- 2nd edition available online at www.nr.com/oldverswitcher.html
- Chapter 6 contains algorithms to calculate special functions

Gamma Function



commons.wikimedia.org/wiki/File:Gamma-function.svg

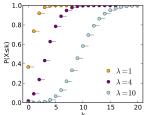
- $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$
- integer z: gamma function equals factorial with offset of one

$$n! = \Gamma(n+1)$$

Factorial

- small $n \Rightarrow$ compute factorial directly as $n \times (n-1) \times (n-2) \dots$
- large values ⇒ gamma-function
- large n, factorial larger than largest number allowed by computer
 - single precision (IEEE 754 32-bit decimal) has maximum exponents of -126, +127
 - double precision (EEE 754 64-bit declimal) has maximum exponents of -1022, 1023
 - calculate logarithm of factorial or logarithm of gamma function
- useful function routines from Numerical Recipes:
 - function gammln(x) returns $\ln \Gamma(x)$ for input x
 - function factrl(n) returns real n! for input integer n
 - function factln(n) returns real $\ln n!$ for input integer n
 - function bico(n,k) returns real $\binom{n}{k}$ for integer inputs n, k
- useful to compute large number of frequently used distributions

Cummulative Poisson Distribution



en.wikipedia.org/wiki/Poisson distribution

• cumulative Poisson probability describes probability that Poisson process will lead to result between 0 and k-1 inclusive:

$$P_{x}(< k) \equiv \sum_{n=0}^{k-1} P_{P}(k, x)$$

• incomplete gamma function:

$$P(a,x) \equiv \frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t} dt$$

Cummulative Poisson Distribution (continued)

complement also called incomplete gamma function

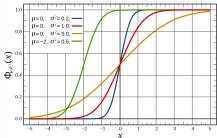
$$Q(a,x) \equiv 1 - P(a,x) \equiv \frac{1}{\Gamma(a)} \int_{x}^{\infty} t^{a-1} e^{-t} dt$$

cumulative Poisson probability:

$$P_X(\langle k \rangle) = Q(k, x)$$

- corresponding routines in Numerical Recipes are:
 - function gammp (a, x) returns P(a, x) for input a, x
 - function gammq(a,x) returns Q(a,x) for input a,x

Cummulative Gauss Distribution



en.wikipedia.org/wiki/Normal_distribution

integral probability of Gauss function from error function:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

complementary error function:

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^2} dt$$

Cummulative Gauss Distribution (continued)

error functions given by incomplete gamma functions:

$$\operatorname{erf}(x) = P(1/2, x^2) \qquad (x \ge 0)$$

 $\operatorname{erfc}(x) = Q(1/2, x^2) \qquad (x \ge 0)$

- corresponding routines in Numerical Recipes are:
 - function erf(x) returns erf(x) for input x, using gammp
 - function erfc(x) returns erfc(x) for input x, using gammq
 - function erfcc(x) returns erfc(x) based on direct series development

Error Propagation

Basics

• function *f* depends on variables *u*, *v*, . . .:

$$f \equiv f(u, v, \ldots)$$

estimate variance of f

$$\sigma_f^2 \equiv \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N (f_i - \bar{f})^2$$

knowing variances $\sigma_u, \sigma_v, \dots$ of variables u, v, \dots

assumption, usually only approximately correct, that average of f
is well approximated by value of f for averages of variables:

$$\overline{f} = f(\overline{u}, \overline{v}, \ldots)$$

Basics (continued)

• Taylor expansion of *f* around average:

$$f_i - \overline{f} \simeq (u_i - \overline{u}) \frac{\partial f}{\partial u} + (v_i - \overline{v}) \frac{\partial f}{\partial v} + \dots$$

variance in f:

$$\sigma_f^2 \simeq \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N \left[(u_i - \overline{u}) \frac{\partial f}{\partial u} + (v_i - \overline{v}) \frac{\partial f}{\partial v} + \ldots \right]^2$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \left[(u_i - \overline{u})^2 \left(\frac{\partial f}{\partial u} \right)^2 + (v_i - \overline{v})^2 \left(\frac{\partial f}{\partial v} \right)^2 + 2(u_i - \overline{u})(v_i - \overline{v}) \frac{\partial f}{\partial u} \frac{\partial f}{\partial v} + \ldots \right]$$

Basics (continued)

variances of u and v

$$\sigma_u^2 \equiv \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N (u_i - \overline{u})^2; \qquad \sigma_v^2 \equiv \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N (v_i - \overline{v})^2$$

covariance of u and v

$$\sigma_{uv}^2 \equiv \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^N (u_i - \overline{u})(v_i - \overline{v})$$

use these defintions to obtain

$$\sigma_f^2 = \sigma_u^2 \left(\frac{\partial f}{\partial u}\right)^2 + \sigma_v^2 \left(\frac{\partial f}{\partial v}\right)^2 + 2\sigma_{uv}^2 \frac{\partial f}{\partial u} \frac{\partial f}{\partial v} + \dots$$

Basics (continued)

from before

$$\sigma_f^2 = \sigma_u^2 \left(\frac{\partial f}{\partial u}\right)^2 + \sigma_v^2 \left(\frac{\partial f}{\partial v}\right)^2 + 2\sigma_{uv}^2 \frac{\partial f}{\partial u} \frac{\partial f}{\partial v} + \dots$$

- if differences $u_i \overline{u}$ and $v_i \overline{v}$ not correlated \Rightarrow sign of product as often positive as negative \Rightarrow covariance small compared to other terms
- if differences are correlated \Rightarrow most products $(u_i \overline{u})(v_i \overline{v})$ positive \Rightarrow cross-correlation term can be large

Examples of Error Propagation

Weighted Sum: f = au + bv

partial derivatives

$$\frac{\partial f}{\partial u} = a, \qquad \frac{\partial f}{\partial v} = b$$

variance

$$\sigma_f^2 = a^2 \sigma_u^2 + b^2 \sigma_v^2 + 2ab \sigma_{uv}^2$$

- a and b can be positive or negative
- signs only affect cross-correlation term
- cross-correlation term can be negative ⇒ makes variance smaller
- example: if each u_i is accompanied by a v_i such that $v_i \overline{v} = -(b/a)(u_u \overline{u})$, then $f = a\overline{u} + b\overline{v}$ for all u_i, v_i pairs, and $\sigma_f^2 = 0$

Product: f = auv

partial derivative

$$\frac{\partial f}{\partial u} = av, \qquad \frac{\partial f}{\partial v} = au$$

variance

$$\frac{{\sigma_f}^2}{f^2} = \frac{{\sigma_u}^2}{u^2} + \frac{{\sigma_v}^2}{v^2} + \frac{2{\sigma_{uv}}^2}{uv}$$

Division: f = au/v

partial derivatives

$$\frac{\partial f}{\partial u} = \frac{a}{v}, \qquad \frac{\partial f}{\partial v} = -\frac{au}{v^2}$$

variance

$$\frac{{\sigma_f}^2}{f^2} = \frac{{\sigma_u}^2}{u^2} + \frac{{\sigma_v}^2}{v^2} - \frac{2{\sigma_{uv}}^2}{uv}$$

Exponent: $f = ae^{bu}$

partial derivatives

$$\frac{\partial f}{\partial u} = bf$$

variance

$$\frac{\sigma_f}{f} = b\sigma_u$$

Power: $f = au^b$

partial derivatives

$$\frac{\partial f}{\partial u} = \frac{bf}{u}$$

variance

$$\frac{\sigma_f}{f} = b \frac{\sigma_u}{u}$$

Fitting Observations with Gaussian Error Distributions

Least Squares Method

- series of measurements y_i with associated errors distributed according to Gaussian with width σ_i
- same as each measurement drawn from Gaussian with width σ_i around model value y_m
- probability $P(y_i) \equiv P_i$ of obtaining a single measurement y_i in interval Δy given by

$$P_{i}\Delta y = \frac{1}{\sqrt{2\pi}\sigma_{i}}e^{\frac{-(y_{i}-y_{m})^{2}}{2\sigma_{i}^{2}}}\Delta y$$

• different measurements have different associated errors σ_i

Least Squares Method (continued)

probability P of obtaining series of N measurements

$$P(\Delta y)^{N} \equiv \prod_{i=1}^{N} (P_{i} \Delta y) = \frac{1}{(2\pi)^{N/2} \prod_{i} \sigma_{i}} \exp \left[-\frac{1}{2} \sum_{i=1}^{N} \frac{(y_{i} - y_{m})^{2}}{\sigma_{i}^{2}} \right] \Delta y^{N}$$

highest probability P for smallest

$$\chi^{2} \equiv \sum_{i=1}^{N} \chi_{i}^{2} \equiv \sum_{i=1}^{N} \frac{(y_{i} - y_{m})^{2}}{\sigma_{i}^{2}}$$

- determine most probable model value for y_m for series of measurements y_i by finding value(s) for y_m for which sum of squares $(y_i y_m)^2/\sigma_i^2$ is minimal
- method of least squares, first described by Gauss

Chi-Squared Distribution

- if errors are gaussian, each χ_i is random draw from normal distribution
- sum of χ_i^2 is called *chi-square*
- N measurements fit by model with M parameters: N M independent measurements
- probability distribution for χ^2 is *chi-square distribution* for N-M degrees of freedom
- distribution obtained by drawing N M random samples from normal distribution and add squares
- probability of given χ^2 from gammq-function
- probability that observed χ^2_{obs} or greater is reached for N-M degrees of freedom is $P(\chi^2_{obs}) = \text{gammq}(0.5(N-M), 0.5\chi^2_{obs})$

Chi-Squared Distribution (continued)

- if probability is very small ⇒ something is wrong
 - wrong model
 - errors underestimated
 - errors not distributed as Gaussians
- probability of 0.05 is often acceptable
- wrong models produce much smaller probabilities (< 0.000001)
- probability of 5% occurs, on average, once every 20 trials
- finding 0.05 probability due to chance quite common
- consistently low probabilities must be investigated

Negative Results

- apparently significant results can arise from ignoring negative results
- lottery winner is person with correct six-digit number
- probability for one person to have winning number is one in a million
- if several million people participate we expect several to have guessed the correct number
- less obvious: repeated experiment, i.e. stock broker
- ten million people predict how stocks change in value
- after one year, select top 10% predictors
- repeat for total of six rounds ⇒ (on average) ten brokers will have predicted among top 10% for six years in a row, even if prediction process is purely random!
- must know total number of brokers to decide wether they are better than random

Model Fitting

- fit model to data set, present 3 parts:
 - **1** best-fit values of parameters a_1, a_2, \ldots
 - errors in these parameters
 - \odot probability that measured χ^2 is obtained by chance; i.e. the probability that model adequately describes measurements
- 5 cases for y_m
 - \bigcirc constant (y_m same for all i)
 - 2 straight line $y_m = a + bx$ where y_m depends on variable x and model parameters a, b
 - 3 straight line $y_m = a + bx$ where y_m depends on variables x, y, model parameters a, b
 - Iinear function $y_m = f(x, a, b, c, ...$ where y_m depends on variable x and linearly on model parameters a, b, ...
 - **5** general (non-linear) case where y_m depends on variable x and parameters $a_1, a_2, \ldots; y_m = y_m(x; \vec{a})$

Weighted Averages

- constant model $y_m = a \Rightarrow a$ best estimate for average \overline{y} of y_i
- most probable value of a by minimizing χ^2 with respect to a

$$\frac{\partial}{\partial a} \left[\sum_{i=1}^{N} \frac{(y_i - a)^2}{{\sigma_i}^2} \right] = 0 \Rightarrow \sum_{i=1}^{N} \frac{y_i - a}{{\sigma_i}^2} = 0$$

least squares found for

$$\overline{y} \equiv a_{min} = rac{\sum_{i=1}^{N} rac{y_i}{\sigma_i^2}}{\sum_{i=1}^{N} rac{1}{\sigma_i^2}}$$

Weighted Averages (continued)

- determine estimate of error in \overline{y}
- \overline{y} is function of variables y_1, y_2, \dots
- if measurements y_i not correlated: variance of \overline{y} from error propagation:

$$\sigma_{\overline{y}}^2 = \sum_{i=1}^N \left[\sigma_i^2 \left(\frac{\partial \overline{y}}{\partial y_i} \right)^2 \right] = \sum_{i=1}^N \left[\sigma_i^2 \left(\frac{1/\sigma_i^2}{\sum_{k=1}^N (1/\sigma_k^2)} \right)^2 \right]$$

therefore

$$\sigma_{\overline{y}}^2 = \frac{1}{\sum_{i=1}^{N} (1/\sigma_i^2)}$$

Identical Errors

• in case where all measurement errors are identical $(\sigma_i \equiv \sigma)$

$$\overline{y} = \frac{(1/\sigma^2) \sum_{i=1}^{N} y_i}{(1/\sigma^2) \sum_{i=1}^{N} (1)} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

therefore

$$\sigma_{\overline{y}}^2 = \frac{\sigma^2}{N}$$

Fitting Straight Line

- straight line: $y_m(x, a, b) = a + bx \Rightarrow y_m(x_i, a, b) = a + bx_i$
- fit a, b by minimizing χ^2 with respect to a, b
- set corresponding derivatives χ^2 to zero:

$$\frac{\partial \sum_{i=1}^{N} [(y_i - a - bx_i)/\sigma_i]^2}{\partial a} = 0 \Rightarrow \sum_{i=1}^{N} \left(\frac{y_i - a - bx_i}{\sigma_i^2}\right) = 0 \Rightarrow$$

$$\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} - a \sum_{i=1}^{N} \frac{1}{\sigma_i^2} - b \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} = 0$$

$$\frac{\partial \sum_{i=1}^{N} [(y_i - a - bx_i)/\sigma_i]^2}{\partial b} = 0 \Rightarrow \sum_{i=1}^{N} \frac{x_i(y_i - a - bx_i)}{\sigma_i^2} = 0 \Rightarrow$$

$$\sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2} - a \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} - b \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} = 0$$

Fitting Straight Line (continued)

- all sums can be evaluated without knowing a or b
- define the following sums

$$\sum_{i=1}^{N} \frac{1}{\sigma_i^2} \equiv S; \qquad \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \equiv S_x; \qquad \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} \equiv S_{xx}$$

$$\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} \equiv S_y; \qquad \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2} \equiv S_{xy}; \qquad \Delta \equiv SS_{xx} - (S_x)^2$$

• rewrite as two equations for two unknowns a and b:

$$aS + bS_x - S_y = 0$$
$$aS_x + bS_{xx} - S_{xy} = 0$$

Fitting Straight Line (continued)

solutions

$$a = \frac{S_{xx}S_y - S_xS_{xy}}{\Delta}; \ \ b = \frac{SS_{xy} - S_xS_y}{\Delta}$$

 errors in a, b from considering a, b to depend on independent parameters y_i

$$\frac{\partial a}{\partial y_i} = \frac{S_{xx} - x_i S_x}{\sigma_i^2 \Delta}; \qquad \frac{\partial b}{\partial y_i} = \frac{x_i S - S}{\sigma_i^2 \Delta}$$

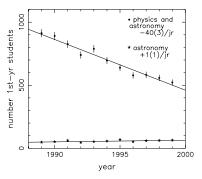
use error propagation

$$\sigma_a^2 = \frac{S_{xx}}{\Delta}; \qquad \sigma_b^2 = \frac{S}{\Delta}$$

• probability that good fit would produce observed χ^2_{obs} or bigger:

$$Q = \operatorname{gammq}\left(\frac{N-2}{2}, \frac{\chi^2_{obs}}{2}\right)$$

Straight Line Fitting Example



- number of new physics and astronomy students in Netherlands
- errors in measured integer numbers: square root of number
- actual number in year is drawn from distribution (here Poissonian) around expected value
- same in photon-counting observations

Example (continued)

- good choice of a, b
- number of students as N(t) = a + bt where t is the year $\Rightarrow a$ gives number of students for year 0
- sums involving x_i -values are very large \Rightarrow subtracting them from one another (as in computing Δ) easily leads to roundoff errors
- errors in a and b will be highly correlated: small change in b changes a dramatically in one direction
- prevent both problems by centering time interval around point of fitting, i.e. N = a + b(t 1994)
- avoids round-off errors and correlation of variations are minimized
- good practice in astronomy to define time with respect to some fiducial point near middle of measurements

Linear Models with Errors in Both Coordinates

x_i may also have errors ⇒ minimize

$$\chi^{2}(a,b) = \sum_{i=1}^{N} \frac{(y_{i} - a - bx_{i})^{2}}{\sigma_{y_{i}}^{2} + b^{2}\sigma_{x_{i}}^{2}}$$

- weighted sum of variances in denominator from error propagation
- a determined from setting partial derivative to zero

$$a = \left[\sum_{i=1}^{N} \frac{(y_i - bx_i)^2}{\sigma_{y_i}^2 + b^2 \sigma_{x_i}^2}\right] / \sum_{i=1}^{N} \frac{1}{\sigma_{y_i}^2 + b^2 \sigma_{x_i}^2}$$

- b determination more complicated because equation becomes non-linear ⇒ numerical solution to minimize with respect to b
- at each iteration ensure that minimum with respect to b is also minimized with respect to a
- complicated errors in parameter estimates ⇒ use apprach to be discussed for general case

General Linear Least Squares Problem

Linear Models

- model y_i^m is linear combination of M given functions of x
- example: polynomial of degree M-1: $y(x) = a_1 + a_2x + a_3x^2 + ... + a_Mx^M$
- general form

$$y(x) = \sum_{k=1}^{N} A_k X_k$$

- $X_1(x), \dots, X_M(x)$ arbitrary (non-linear!) fixed functions of x
- minimize

$$\chi^{2} = \sum_{i=1}^{N} \frac{y_{i} - \sum_{k=1}^{N} a_{k} X_{k}(x_{i})}{\sigma_{i}^{2}}$$

design matrix

$$A_{ij} = \frac{X_j(x_i)}{\sigma_i}$$

Linear Models (continued)

- in general, A has more rows than columns (N > M)
- vector \vec{b} of length N:

$$b_i = \frac{y_i}{\sigma_i}$$

 minimum of chi-squared where derivatives with respect to all M parameters vanishes leads to

$$(A^TA)\vec{a} = A^T\vec{b}$$

• inverse matrix of positive definite matrix $A^T A$

$$C = (A^T A)^{-1}$$

• errors in parameters then given by

$$\sigma^2(a_i) = C_{ii}$$

• off-diagonal elements C_{jk} are covariances between a_i and a_k

Linearizing Models

- apparently nonlinear problems can be linearized
- example: $y(x) = ae^{bx}$ becomes $\log y(x) = c + bx$
- warning: transformations does not make Gaussian errors into Gaussian errors
- warning: watch out for degenerate parameters, e.g. $v(x) = ae^{bx+d}$