

PHYS-4007/5007: Computational Physics
Course Lecture Notes
Section VI

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Abstract

These class notes are designed for use of the instructor and students of the course **PHYS-4007/5007: Computational Physics** taught by Dr. Donald Luttermoser at East Tennessee State University.

VI. Methods of Data Fitting

A. Methods of Fitting “Local” Data.

1. There are two main types of data fitting:
 - a) **Local data fitting** means that you are just fitting a few points in the complete population of data points presented. We will look at three types of local data fitting in the class: *Interpolation*, *Lagrangian Interpolation*, and *Cubic Splines*.
 - b) The second type of data fitting is **global data fitting**. Here we fit the entire population of data points to an assumed analytic function. We will investigate two types of global data fitting: Fitting data to *Gaussian profiles* (or distributions) and to linear equations using the method of *linear least squares*.

2. Linear Interpolation.

- a) There are times when we may wish to know the value of an unmeasured datum that lies between two measured data in a population. The easiest way to do this is to draw a straight line between the two known data points and fit the unmeasured point on that straight line.
- b) Let’s say that we have two measured data, $P_1(x_1, y_1)$ and $P_2(x_2, y_2)$, and we wish to determine the y -value of the data that lies on x , such that, $x_1 < x < x_2$.
- c) To determine this, we just set up the following ratio:

$$\frac{y - y_1}{x - x_1} = \frac{y_2 - y_1}{x_2 - x_1} = m . \quad (\text{VI-1})$$

- d) Then solving for y , we get

$$y = y_1 + \frac{y_2 - y_1}{x_2 - x_1} (x - x_1) = y_1 + m(x - x_1) . \quad (\text{VI-2})$$

- e) There may be times when you need a regularly spaced grid of data points (*i.e.*, $x_j - x_i = \text{constant}$, where $j - i = 1$) to pass to another function (such as an integration routine, see §VII of the notes). You would then need to interpolate your data to determine your data's y values at the regularly spaced x values from your original (uneven) data. Such is the time when you would need a linear interpolation procedure. The IDL function `INTERPOL` will carry out such an operation for you.

3. Lagrange Interpolation.

- a) Suppose that the data on either side of the unknown point we are interested in is not following a linear distribution, but instead, is following a curved path. Then a straight line is not the best representation of your data.
- b) In such cases, it is better to fit to a polynomial instead of a straight line. This leads us to an interpolation scheme developed by Lagrange.
- c) One can fit an $(n - 1)$ -order polynomial,

$$f_i(x) \simeq a_0 + a_1x + a_2x^2 + \cdots + a_{n-1}x^{n-1}, \quad (x \simeq x_i), \quad (\text{VI-3})$$

to n values of the function $f(x)$ evaluated at points x_i .

- d) The formula is written as the sum of polynomials

$$f(x) \simeq f_1\lambda_1(x) + f_2\lambda_2(x) + \cdots + f_n\lambda_n(x) , \quad (\text{VI-4})$$

where

$$\lambda_i(x) = \prod_{j(\neq i)=1}^n \frac{x - x_j}{x_i - x_j} = \frac{x - x_1}{x_i - x_1} \frac{x - x_2}{x_i - x_2} \cdots \frac{x - x_n}{x_i - x_n}, \quad (\text{VI-5})$$

and note that

$$\sum_{i=1}^{\infty} \lambda_i = 1. \quad (\text{VI-6})$$

- e) For 3 points, Eq. (VI-4) provides a second-degree polynomial, while for eight points, it gives a seventh-order polynomial. It is easy to see that for 2 points, Lagrange interpolation just reduces to the linear interpolation described above.
- f) The Lagrange interpolation has no constraints that the data be evenly spaced.
- g) The difference between the value of the polynomial evaluated at some x and that of the actual function is equal to the *remainder*:

$$R \approx \frac{(x - x_1)(x - x_2) \cdots (x - x_n)}{n!} f^{(n)}(\zeta), \quad (\text{VI-7})$$

where ζ lies somewhere in the interval of interpolation, but is otherwise undetermined.

- h) Lagrangian interpolation is typically used to fit only *local* data, though it can be use to fit the data *globally*. However, there are better ways to fit nonlinear global data \implies polynomial least square fitting (which we are not going to have time to cover in this class).

4. Interpolation with Cubic Splines.

- a) A sophisticated variation of the $n = 4$ Lagrange interpolation, known as **cubic splines** sometimes offers superior fits to nonlinear data.

- b)** In this method, cubic polynomials are fit to the data points representing some polynomial function in each interval, with the constraint that the first and second derivatives of the polynomials be continuous from one interval to the next.
- c)** This continuity of slope and curvature makes the spline fit particularly eye-pleasing.
- d)** The basic approximation of splines is the representation of the function $f(x)$ in the subinterval $[x_i, x_{i+1}]$ with a cubic polynomial:

$$f(x) \simeq f_i(x), \quad \text{for } x_i \leq x \leq x_{i+1}, \quad (\text{VI-8})$$

$$f_i(x) = f_i + f^{(1)}(x - x_i) + \frac{1}{2}f^{(2)}(x - x_i)^2 + \frac{1}{6}f^{(3)}(x - x_i)^3, \quad (\text{VI-9})$$

where $f^{(1)}$, $f^{(2)}$, and $f^{(3)}$ are the first-, second-, and third-derivatives of the function $f(x)$ evaluated at x_i .

- e)** The computational chore is to determine these derivatives in terms of the N tabulated values of f_i .
- f)** The matching of f_i from one interval to the next (at the *nodes*) provides the equations:

$$f_i(x_{i+1}) = f_{i+1}(x_{i+1}), \quad i = 1, \dots, N - 1. \quad (\text{VI-10})$$

- g)** Also, the first and second derivatives must be continuous at the nodes:

$$f_{i-1}^{(1)}(x_i) = f_i^{(1)}(x_i), \quad f_{i-1}^{(2)}(x_i) = f_i^{(2)}(x_i). \quad (\text{VI-11})$$

- h)** Finally, an additional equation is needed to determine all of the constants. For this, the third derivatives are found

by approximating them from the second derivatives:

$$f_i^{(3)} \simeq \frac{f_{i+1}^{(2)} - f_i^{(2)}}{x_{i+1} - x_i} . \quad (\text{VI-12})$$

- i) In practice, it is better to use a cubic spline routine supplied by the programming language (*e.g.*, **SPLINE** in IDL) or math library.

B. Data Fitting: Gaussian Distributions.

1. The most important probability distribution for use in statistical analysis of data is the **Gaussian** or **normal error distribution**.
 - a) Mathematically, it is an approximation to the binomial distribution for the special limiting case where the number of possible different observations, n , become infinitely large and the probability of success, p , for each is finitely large so that $np \gg 1$.
 - b) Physically, it is useful because it seems to describe the distribution of random observations for most experiments.
 - c) In spectra, it describes the shape of many spectral lines.
2. This type of data fitting can be considered both a “global” and a “local” data fitting technique, depending on what is being fitted. In the case of spectra, one often finds either absorption lines and or emission lines superimposed on a gradually varying continuum. Often, it is useful just to isolate the individual lines from the continuum and fit these lines to the proper profile distribution. More times than not, such lines follow a *Gaussian distribution*.
3. Figure VI-1 shows the Gaussian profile and labels the various components to this distribution. The Gaussian distribution func-

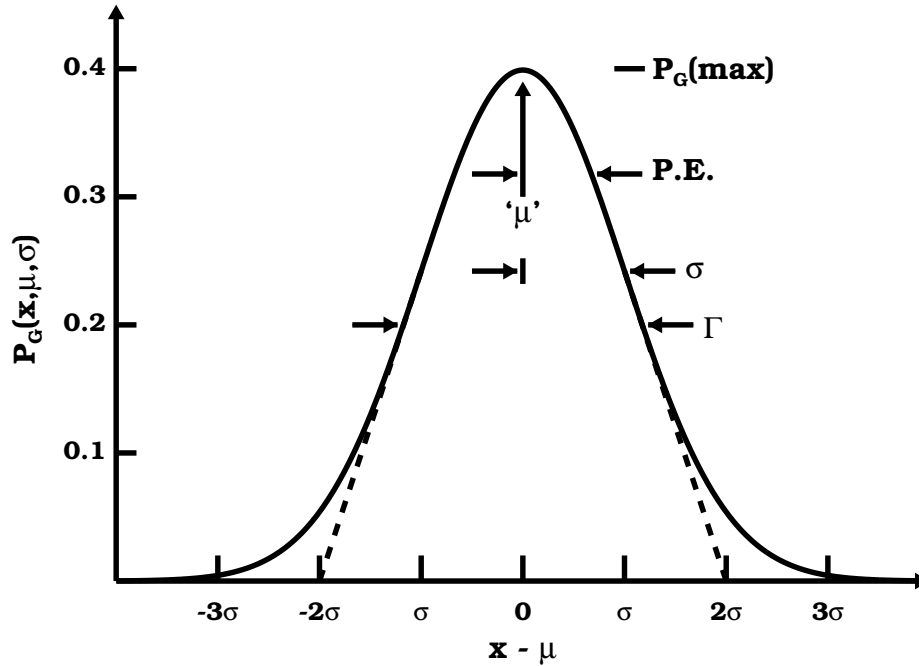


Figure VI-1: The Gaussian distribution function.

tion is defined by

$$P_G(x, \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right]. \quad (\text{VI-13})$$

- a) It is a continuous function describing the probability that from a parent distribution with a mean μ and a standard deviation σ , the value of the random observation would be x .
- b) The probability function is properly defined such that the probability $dP_G(x, \mu, \sigma)$ that the value of a random observation will fall within the interval dx around x is given by

$$dP_G(x, \mu, \sigma) = P_G(x, \mu, \sigma) dx. \quad (\text{VI-14})$$

- c) Gaussian distributions are bell shaped and characterized by the *full-width-at-half-maximum* (FWHM), which is generally called the *half-width* $\Gamma \implies$ the range of x between

the values which P_G is half the maximum value:

$$P_G\left(\mu \pm \frac{1}{2}\Gamma, \mu, \sigma\right) = \frac{1}{2} P_G(\mu, \mu, \sigma) , \quad (\text{VI-15})$$

$$\Gamma = 2.354 \sigma . \quad (\text{VI-16})$$

- d) A tangent drawn along the portion of steepest decent of the curve intersects the curve at the $e^{-1/2}$ points $x = \mu \pm \sigma$ and intersects the x axis at points $x = \mu \pm 2\sigma$ (see dashed lines in Figure VI-1):

$$P_G(\mu \pm \sigma, \mu, \sigma) = e^{-1/2} P_G(\mu, \mu, \sigma) . \quad (\text{VI-17})$$

4. The mean and standard deviation of the Gaussian distribution of Eq. (VI-13) are given by the μ and σ parameters respectively.
5. The **probable error** (P.E.) is defined to be the location on the Gaussian distribution where half of the observations will fall between $\mu \pm$ P.E. Mathematically, it can be shown that

$$\text{P.E.} = 0.6745 \sigma = 0.2865 \Gamma . \quad (\text{VI-18})$$

6. The **integral probability**, $A_G(x, \mu, \sigma)$, is defined as the probability that the value of any random measurement x_i will have a deviation from μ less than $z\sigma$, where z is the dimensionless range $z = |x - \mu|/\sigma$. It is found with

$$A_G(x, \mu, \sigma) = \int_{\mu-z\sigma}^{\mu+z\sigma} P_G(x, \mu, \sigma) dx = \frac{1}{\sqrt{2\pi}} \int_{-z}^z e^{-\frac{1}{2}x^2} dx , \quad (\text{VI-19})$$

and normalized such that

$$A_G(z = \infty) = 1 . \quad (\text{VI-20})$$

7. Note that the smaller σ is, the more “precise” our observations and/or calculations will be. The standard deviation σ is often referred to as the *best estimate* of x_i representing the actual value.

8. Gaussian Distributions in Nature: Absorption and Emission Lines.

- a) In many cases in nature and in the laboratory (*e.g.*, stellar spectra and emission discharge tubes), dark and/or bright “lines” are seen in the spectra objects emit.
- b) Often, the shapes of these lines, in either wavelength, frequency, or energy space, follow a Gaussian shape.
- c) If a spectral line has a *rest* (also called “lab”) wavelength λ_o , we can describe a **line profile**, $\phi(\Delta\lambda)$, such that it is normalized over the entire profile:

$$\int_{-\infty}^{+\infty} \phi(\Delta\lambda) d\Delta\lambda = 1 , \quad (\text{VI-21})$$

where

$$\Delta\lambda = \lambda - \lambda_o \quad (\text{VI-22})$$

and λ represents the wavelength at a specific point along the profile.

- i) In practice (*i.e.*, computer programming), one does not carry the integration from $-\infty$ to $+\infty$, but instead, just carries the integration across the line profile (*i.e.*, $\pm(\Delta\lambda)_{\max} \approx 3\sigma$ to 5σ).

- ii) Also note that

$$\phi(\Delta\lambda) d\Delta\lambda = -\phi(\nu) d\nu , \quad (\text{VI-23})$$

where $\nu (= c/\lambda)$ is the frequency of the line profile.

- d) If an object that is emitting a spectrum is moving with respect to the observer, the “rest” wavelength (*i.e.*, line center) gets shifted via the **Doppler effect**:

$$\frac{\Delta\lambda}{\lambda_o} = \frac{\lambda - \lambda_o}{\lambda_o} = \frac{v_r}{c} = z , \quad (\text{VI-24})$$

where here λ is the observed line center, λ_o is the line center as measured in the lab, v_r is the radial velocity of the moving object, c is the speed of light in the vacuum, and z is a parameter called the **redshift**.

i) If a line is *redshifted*, $\lambda > \lambda_o$ and $v_r > 0 \implies$ the object is moving away from us.

ii) If a line is *blueshifted*, $\lambda < \lambda_o$ and $v_r < 0 \implies$ the object is moving toward us.

iii) Note that Eq. (VI-24) is valid only when $v_r \ll c$ (*i.e.*, the motion is nonrelativistic).

e) We also can write a more general expression for the redshift,

$$z = \frac{\Delta\lambda}{\lambda_o} = \frac{\sqrt{1 + v_r/c}}{\sqrt{1 - v_r/c}} - 1 . \quad (\text{VI-25})$$

where, here, we have included the *relativistic* (*i.e.*, $v_r \lesssim c$) correction for the Doppler Effect.

i) Rewriting this relativistic formula, we can express velocity as a function of redshift:

$$\frac{v_r}{c} = \frac{(z + 1)^2 - 1}{(z + 1)^2 + 1} . \quad (\text{VI-26})$$

ii) You will note that there is no way a velocity calculated from the relativistic form of the Doppler effect can exceed the of light \implies the special theory of relativity is not violated!

f) If an absorption/emission line has a Gaussian distribution, its profile function follows the form

$$\phi(\Delta\lambda) = \frac{1}{\sqrt{\pi} \Delta\lambda_G} \exp\left(-\frac{\Delta\lambda^2}{\Delta\lambda_G^2}\right) \quad (\text{VI-27})$$

- i) The parameter $\Delta\lambda_G$ is referred to as the Gaussian (or Doppler, see below) width. From a comparison of Eqs. (VI-27) and (VI-13), we see immediately that

$$\Delta\lambda_G = \sqrt{2}\sigma . \quad (\text{VI-28})$$

- ii) With this bit of information, we can show that the line profile half-width is

$$\Delta\lambda_{1/2} = 1.665 \Delta\lambda_G . \quad (\text{VI-29})$$

- iii) The Gaussian profile has a peak value of $1/(\sqrt{\pi} \Delta\lambda_G)$.

9. Sometimes, line profiles are a conglomerate of other line profiles just as the total error can be the sum of different individual random errors.

- a) In such cases, we must **convolve** the individual profiles together with the convolution integral:

$$\phi(\Delta\lambda) = \int_{-\infty}^{+\infty} \phi_1(\Delta\lambda - x) \phi_2(x) dx . \quad (\text{VI-30})$$

- b) The convolution of two Gaussian profiles with $\Delta\lambda_{G1}$ and $\Delta\lambda_{G2}$ (at the same λ_0) yields another Gaussian profile with $\Delta\lambda_G^2 = \Delta\lambda_{G1}^2 + \Delta\lambda_{G2}^2$.

10. Spectrographs are a “hardcopy” version of the **Fourier transform** function \implies it breaks white light up into its component colors.

- a) From this analogy, the spectrograph acts as a convolution integral, convolving the instrument profile with the profile from the emission source.

- b) Since “good” spectrographs are designed to have Gaussian instrument profiles, the Gaussian from the source is

convolved with the Gaussian of the spectrograph.

- c) Spectrographs with $\Delta\lambda_{1/2} < 1 \text{ \AA}$ ($1 \text{ \AA} = 10^{-10} \text{ m}$) are said to be *high-resolution* or high-dispersion spectrographs.
 - d) Spectrographs with $\Delta\lambda_{1/2} > 1 \text{ \AA}$ are said to be *low-resolution* or low-dispersion spectrographs.
 - e) $\Delta\lambda_{1/2}$ effectively determines whether two spectral lines separated by $\Delta\lambda$ can be split into individual lines.
 - i) If $\Delta\lambda < \Delta\lambda_{1/2}$, the two spectral lines will appear as one in a spectrum.
 - ii) If $\Delta\lambda > \Delta\lambda_{1/2}$, the two spectral lines will appear as two individual lines.
11. Line profiles emitted from a gas tend to have Gaussian shapes due to the fact that the atoms and molecules that make up the gas are randomly moving in the gas \implies they are said to be following a Maxwellian or a Maxwellian-Boltzmann distribution.
- a) As individual particles absorb and emit photons, the photons are shifted via the Doppler effect based on their relative thermal motion with respect to the observer.
 - b) As such, Gaussian profiles are often referred to as **Doppler broadening** of a spectral line.
 - c) Since the particles are following a Maxwellian distribution in velocity space, they have a Gaussian distribution in wavelength or frequency space, where the Gaussian (or Doppler) width is equal to the thermal Doppler width

$$\Delta\lambda_G = \Delta\lambda_D = \Delta\lambda_{\text{th}} = \lambda_o \frac{\sqrt{2kT/m_\beta}}{c} \quad (\text{VI-31})$$

where $k = 1.38062 \times 10^{-23}$ J/K is Boltzmann's constant, T is the temperature of the gas, c is the speed of light, and m_β is the mass of the radiating particle.

- d) As a result of this, one can determine the temperature of a gas by measuring the half-width of a line arising from a gas (after, of course, one has subtracted off the instrument profile).
- e) In practice, life isn't quite this easy since other line broadening mechanisms may also be involved, some following the **Lorentz** (dispersion, damping) **profile** given by

$$\phi(\Delta\lambda) = \frac{\Delta\lambda_L}{2\pi} \frac{1}{\Delta\lambda^2 + \Delta\lambda_L^2/4}, \quad (\text{VI-32})$$

with

$$\Delta\lambda_L = \frac{\lambda_o}{\omega_o} \gamma = \left(\frac{\lambda_o^2}{2\pi c} \right) \gamma, \quad (\text{VI-33})$$

where γ is the damping constant.

- i) The Lorentz profile has a *peak value* of $2/(\pi\Delta\lambda_L)$ and a FWHM of $\Delta\lambda_L$.
- ii) The convolution of 2 Lorentz profiles with γ_1 and γ_2 (and same λ_o) yields another Lorentz profile with $\gamma = \gamma_1 + \gamma_2$.
- iii) Convolution of a Gaussian and Lorentzian (with same λ_o) yields a **Voigt profile**. See any book on radiative transfer for details on the Voigt function.
- f) **Radiation** (natural) **broadening** of a line results from an excited state having a finite width or probability distribution due to the Heisenberg Uncertainty Principle. It approximately yields a Lorentz profile with a damping

constant

$$\gamma_{\text{rad}} = \gamma_i + \gamma_j , \quad (\text{VI-34})$$

where γ_i and γ_j are the damping constants for the i -th and j -th levels. These damping constants are determined either quantum mechanically or by experiment.

- g) Collisional broadening** caused by the interaction of radiating particles with surrounding matter. The E -fields of the perturbing particles affect the *level thicknesses* of the radiating particle, hence broadening the line. These collisional broadening events give rise to *Lorentzian* profiles. There are 4 types of collisional broadening events:
- i)** Linear Stark effect in a hydrogen-like particle due to a charged perturber.
 - ii)** Resonance interaction between two identical particles.
 - iii)** Quadratic Stark effect due to a charged perturber.
 - iv)** Van der Waals interaction between two particles of different species.
- h) Rotational broadening**, is a broadening of a spectral line due to the rotation of the emitting object. It must be taken into account if $v_{\text{rot}} \gtrsim v_{\text{th}}$, where v_{th} is the thermal velocity. Rotational broadening follows a Gaussian distribution similar to thermal Doppler broadening, except the rotation velocity replaces $\sqrt{2kT/m_\beta}$ in Eq. VI-31.
- i) Instrument broadening** due to attributes of the optical system (*i.e.*, diffraction, filter characteristic, pixel size, etc.). One determines an *instrument profile* by tak-

ing a comparison spectrum of an emission lamp with “infinitely” sharp lines (that is, the natural broadening dominates atomic broadening mechanisms and the natural broadening is much less than the instrument profile). Generally an instrument profile is Gaussian in shape, but doesn’t necessarily have to be. This determines the dispersion of the spectrum (see §VI.B.10).

- j) Beside the above mentioned broadening mechanisms, there are other processes that can affect a line profile. Magnetic fields (*e.g.*, *Zeeman effect*) and e^- interactions with nucleus (*i.e.*, *hyperfine structure*) are two such examples.

12. Most of the math-oriented programming languages have functions that will fit data to a Gaussian profile. In IDL, there are 2 intrinsic functions dealing with fitting Gaussians:

- a) The GAUSSFIT function computes a non-linear least-squares fit to a function $f(x)$ with from 3 to 6 unknown parameters. $f(x)$ is a linear combination of a Gaussian and a quadratic; the number of terms is controlled by the keyword parameter NTERMS. The syntax for this function is

```
Result = GAUSSFIT(X, Y [, A] [, CHISQ=variable]
                [, ESTIMATES=array] [, YERROR=variable]
                [, MEASURE_ERRORS=vector] [, SIGMA=variable]
                [, NTERMS=integer(3 to 6)])
```

(Note that the square brackets ‘[]’ here means optional parameters.)

- i) **X**: An n -element vector of independent variables (data).
- ii) **Y**: A vector of dependent variables (same vector length as **X**).

- iii) **A**: A named optional variable that will contain the coefficients A of the fit (see below).
- iv) **CHISQ**: Set this keyword to a named variable that will contain the value of the reduced chi-square goodness-of-fit statistic.
- v) **ESTIMATES**: Set this keyword equal to an array of starting estimates for the parameters of the equation. If **NTERMS** keyword is specified, the **ESTIMATES** array should have **NTERMS** elements. If **NTERMS** is not specified, the **ESTIMATES** array should have 6 elements. If the **ESTIMATES** array is not specified, estimates are calculated by the **GAUSSFIT** routine. *Note*: If **ESTIMATES**[2] (the Gaussian width) is zero, then **GAUSSFIT** will automatically compute a best guess for the starting value for this term.
- vi) **YERROR**: Set this keyword to a named variable that will contain the standard error between **YFIT** and **Y**.
- vii) **MEASURE_ERRORS**: Set this keyword to a vector containing standard measurement errors for each point $Y[i]$. This vector must be the same length as **X** and **Y**. *Note*: For Gaussian errors (*e.g.*, instrumental uncertainties), **MEASURE_ERRORS** should be set to the standard deviations of each point in **Y**. For Poisson or statistical weighting, **MEASURE_ERRORS** should be set to **SQRT(Y)**.

viii) **SIGMA**: Set this keyword to a named variable that will contain the 1-sigma error estimates of the returned parameters. *Note*: If **MEASURE_ERRORS** is omitted, then you are assuming that a polynomial is the correct model for your data, and therefore, no independent goodness-of-fit test is possible. In this case, the values returned in **SIGMA** are multiplied by $\text{SQRT}(\text{CHISQ}/(\text{N}*\text{M}))$, where **N** is the number of points in **X**, and **M** is the number of coefficients. See Section 15.2 of *Numerical Recipes in C* (Second Edition) for details.

ix) **NTERMS**: Set this keyword to an integer value between 3 and 6 to specify the function to be used for the fit. The values correspond to the functions shown below. In all cases:

$$z = \frac{x - A_1}{A_2} .$$

- **NTERMS=6**:

$$f(x) = A_0 e^{-z^2/2} + A_3 + A_4 x + A_5 x^2 .$$

NTERMS=6 is the default setting. Here, A_0 is the height of the Gaussian, A_1 is the center of the Gaussian, A_2 is the width of the Gaussian, A_3 is the constant term, A_4 is the linear term, and A_5 is the quadratic term.

- **NTERMS=5**:

$$f(x) = A_0 e^{-z^2/2} + A_3 + A_4 x .$$

- **NTERMS=4**:

$$f(x) = A_0 e^{-z^2/2} + A_3 .$$

- NTERMS=3:

$$f(x) = A_0 e^{-z^2/2} .$$

Note that this last value just fits the data to a Gaussian profile.

Tip: The full-width-at-half-maximum (FWHM) of the Gaussian may be computed as $2*\text{SQRT}(2*\text{ALOG}(2))*A2$.

- b) `Result = GAUSSINT(X)` evaluates the integral of the Gaussian probability function and returns the result. The Gaussian integral is defined as:

$$\text{GAUSSINT}(X) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt .$$

If X is double precision, the result is double precision, otherwise the argument is converted to floating-point and the result is floating point. The result has the same structure as the input argument, X .

C. Data Fitting: The Method of Least Squares.

1. **Introduction.** Here we will discuss fitting data to a straight line. See your textbook for a more general discussion of Least Squares for higher-order equation fits.

- a) If the data measurements are a linear function of some other variable, we can use the method of **linear least-squares fit**.
- b) The data will contain errors in their measurement, as such, we will need to calculate a *goodness of fit*.
- c) Let's say that $y = f(x)$ in a linear sense, then

$$y = a_1 + a_2 x , \quad (\text{VI-35})$$

then, our task is the figure out a_1 (*i.e.*, the y -intercept), a_2 (*i.e.*, the slope), and their uncertainties from the data. Note that some authors use the $y = A + Bx$ notation and others use $y = b + mx$ notation. These, of course, are all the same equation with $a_1 = A = b$ (*i.e.*, y -intercepts) in the three equations and $a_2 = B = m$ (*i.e.*, the slopes).

- d) The method of least-squares also is called **linear regression**.

2. The Goodness of Fit: χ^2 .

- a) The **chi-squared** test also is called the *Method of Maximum Likelihood*. It is the assumption that the observed set of measurements is more likely to have come from the parent distribution than some other distribution or random event.
- b) The χ^2 is determined with

$$\begin{aligned}\chi^2 &\equiv \sum_{i=1}^N \left(\frac{\Delta y_i}{\sigma_i} \right)^2 = \sum_{i=1}^N \left(\frac{y_i - f(x_i)}{\sigma_i} \right)^2 \\ &= \sum_{i=1}^N \left[\frac{1}{\sigma_i^2} (y_i - a_1 - a_2 x_i)^2 \right],\end{aligned}\quad (\text{VI-36})$$

where N represents the total number of data measurements.

- c) The best fit to the assumed functional dependence will occur when χ^2 is at a minimum:

$$\frac{\partial \chi^2}{\partial a_m} = 0, \quad (m = 1, M), \quad (\text{VI-37})$$

where M is the maximum number of terms in our polynomial fit.

- d) Since we are only interested in straight lines here, $M = 2$, so

$$\begin{aligned}\frac{\partial}{\partial a_1} \chi^2 &= \frac{\partial}{\partial a_1} \sum_{i=1}^N \left[\frac{1}{\sigma_i^2} (y_i - a_1 - a_2 x_i)^2 \right] \\ &= - \left[\sum_{i=1}^N \frac{2}{\sigma_i^2} (y_i - a_1 - a_2 x_i) \right] = 0 \quad (\text{VI-38})\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial a_2} \chi^2 &= \frac{\partial}{\partial a_2} \sum_{i=1}^N \left[\frac{1}{\sigma_i^2} (y_i - a_1 - a_2 x_i)^2 \right] \\ &= - \left[\sum_{i=1}^N \frac{2x_i}{\sigma_i^2} (y_i - a_1 - a_2 x_i) \right] = 0 . \quad (\text{VI-39})\end{aligned}$$

Note that if the uncertainties of each measurement are the same, we could just label $\sigma_i = \sigma$ and take it outside the summation sign. At this point, we will not make that assumption and leave the uncertainty in the summation.

- e) These equations can be rearranged to yield a pair of simultaneous equations:

$$\begin{aligned}\sum_{i=1}^N \frac{y_i}{\sigma_i^2} &= \sum_{i=1}^N \frac{a_1}{\sigma_i^2} + \sum_{i=1}^N a_2 \frac{x_i}{\sigma_i^2} \\ &= a_1 \sum_{i=1}^N \frac{1}{\sigma_i^2} + a_2 \sum_{i=1}^N \frac{x_i}{\sigma_i^2} \quad (\text{VI-40})\end{aligned}$$

$$\begin{aligned}\sum_{i=1}^N \frac{x_i y_i}{\sigma_i^2} &= \sum_{i=1}^N a_1 \frac{x_i}{\sigma_i^2} + \sum_{i=1}^N a_2 \frac{x_i^2}{\sigma_i^2} \\ &= a_1 \sum_{i=1}^N \frac{x_i}{\sigma_i^2} + a_2 \sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} . \quad (\text{VI-41})\end{aligned}$$

- f) Solving Eqs. (VI-40) and (VI-41) for a_1 and a_2 will give the coefficients for which χ^2 , the sum of the square of the deviations of the data points from the calculated fit, is a minimum. One way to solve these equations is to use the method of determinants:

$$a_1 = \frac{1}{\Delta} \begin{vmatrix} \Sigma(y_i/\sigma_i^2) & \Sigma(x_i/\sigma_i^2) \\ \Sigma(x_i y_i/\sigma_i^2) & \Sigma(x_i^2/\sigma_i^2) \end{vmatrix}$$

$$\begin{aligned}
&= \frac{1}{\Delta} \left(\sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} \sum_{i=1}^N \frac{y_i}{\sigma_i^2} - \sum_{i=1}^N \frac{x_i}{\sigma_i^2} \sum_{i=1}^N \frac{x_i y_i}{\sigma_i^2} \right) \\
&= \frac{S_{xx} S_y - S_x S_{xy}}{\Delta} \tag{VI-42}
\end{aligned}$$

$$\begin{aligned}
a_2 &= \frac{1}{\Delta} \left| \begin{array}{cc} \Sigma(1/\sigma_i^2) & \Sigma(y_i/\sigma_i^2) \\ \Sigma(x_i/\sigma_i^2) & \Sigma(x_i y_i/\sigma_i^2) \end{array} \right| \\
&= \frac{1}{\Delta} \left(\sum_{i=1}^N \frac{1}{\sigma_i^2} \sum_{i=1}^N \frac{x_i y_i}{\sigma_i^2} - \sum_{i=1}^N \frac{x_i}{\sigma_i^2} \sum_{i=1}^N \frac{y_i}{\sigma_i^2} \right) \\
&= \frac{S S_{xy} - S_x S_y}{\Delta} \tag{VI-43}
\end{aligned}$$

$$\begin{aligned}
\Delta &= \left| \begin{array}{cc} \Sigma(1/\sigma_i^2) & \Sigma(x_i/\sigma_i^2) \\ \Sigma(x_i/\sigma_i^2) & \Sigma(x_i^2/\sigma_i^2) \end{array} \right| \\
&= \sum_{i=1}^N \frac{1}{\sigma_i^2} \sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^N \frac{x_i}{\sigma_i^2} \right)^2 \\
&= S S_{xx} - S_x^2 \tag{VI-44}
\end{aligned}$$

3. Combining Statistical and Experimental Errors.

- a) In the equations above, y_i corresponds to individual measurements each with their own **statistical errors** \implies statistical fluctuations in the collection of finite numbers over a finitely long interval of time $\implies \sigma_i(y_i)$.
- b) Note that there also can be uncertainties in our independent variable x_i .
 - i) For example, y_i might be displacement measurements and x_i the times the measurements are made.
 - ii) Since the time measurement also has an uncertainty, $\sigma_i(x_i)$, we have 2 uncertainties to worry about.
 - iii) $\sigma_i(x_i)$ is referred to as the **experimental error**.

- c) As such, the σ_i 's in Eqs. (VI-42) through (VI-44) are the combination of these 2 uncertainties which is found with

$$\sigma_i^2 = \sigma_i^2(x_i) + \sigma_i^2(y_i) . \quad (\text{VI-45})$$

4. If we known the statistical and experimental errors, or have determined an approximate σ from the sample variance from your fitted function, the theory of least squares then gives an expression for the *variance* or uncertainty in the deduced parameters:

$$\sigma_{a_1}^2 = \frac{S_{xx}}{\Delta} , \quad \sigma_{a_2}^2 = \frac{S}{\Delta} . \quad (\text{VI-46})$$

5. A measure of the dependence of the parameters on each other is given by the **correlation coefficient**:

$$\rho(a_1, a_2) = \frac{\text{cov}(a_1, a_2)}{\sigma_{a_1} \sigma_{a_2}} , \quad (\text{VI-47})$$

$$\text{cov}(a_1, a_2) = \frac{-S_x}{\Delta} . \quad (\text{VI-48})$$

- a) Here $\text{cov}(a_1, a_2)$ is the *covariance* of a_1 and a_2 and vanishes if a_1 and a_2 are independent.
- b) The correlation coefficient $\rho(a_1, a_2)$ lies in the range $-1 \leq \rho \leq 1$.
- i) Positive ρ indicates that the errors in a_1 and a_2 are likely to have the same sign.
- ii) Negative ρ indicate opposite signs.
6. The preceding analytic solutions for the parameters are of the form found in statistics books, but are not optimal for numerical calculations because subtractive cancellation can make the answers unstable. We can improve the stability of the calculations

by rearranging some terms and introducing the averages of the measurements (\bar{x}, \bar{y}) to the solution:

$$a_1 = \bar{y} - a_2 \bar{x}, \quad a_2 = \frac{S_{xy}}{S_{xx}}, \quad (\text{VI-49})$$

$$S_{xy} = \sum_{i=1}^N \frac{(x_i - \bar{x})(y_i - \bar{y})}{\sigma_i^2}, \quad S_{xx} = \sum_{i=1}^N \frac{(x_i - \bar{x})^2}{\sigma_i^2}, \quad (\text{VI-50})$$

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i, \quad \bar{y} = \frac{1}{N} \sum_{i=1}^N y_i. \quad (\text{VI-51})$$

7. Math oriented programming languages always have least-square functions or subroutines available, either as a *built-in* command or in a math library.
 - a) The books titled *Numerical Recipes* show how to code your own subroutine for least squares should you need to do it: See FIT and LFIT in any of the *Numerical Recipes* books.
 - b) IDL has built-in functions: LINFIT() and REGRESS(). See the IDL ‘Help’ utility to see the details of these two functions.

8. Though we won’t do it here, there are least-square methods to fit non-linear functions. In IDL, see the internal functions:
 - CURVEFIT() — Non-linear least-squares fit to a function.
 - GAUSSFIT() — Fits sum of a Gaussian and quadratic.
 - POLY_FIT() — Polynomial least-squares fit.
 - SFIT() — Determine a polynomial fit to a surface.