Lab #2 "Introduction to Spectroscopy"

Lab report is due at 4pm on Nov 1 (Monday). Submission on Quercus.

Of all objects, the planets are those which appear to us under the least varied aspect. We see how we may determine their forms, their distances, their bulk, and their motions, but we can never know anything of their chemical or mineralogical structure; and, much less, that of organized beings living on their surface...
Auguste Comte, The Positive Philosophy, Book II, Chapter 1 (1842)

1. Overview and Goals

Spectroscopy is a fundamental tool used by all physical sciences. For astrophysicists, spectroscopy is essential for characterizing the physical nature of celestial objects and the universe. Astronomical spectroscopy has been used to measure the chemical composition and physical conditions (temperature, pressure, and magnetic field strength) in planets, stars, and galaxies, as well as their velocities. One of the key aspects of spectroscopy is wavelength calibration. In this lab, you will conduct two types of wavelength calibrations, one with Neon lamp for 1-dimensional spectra and the other with OH telluric sky lines for 2-dimensional spectra, to determine the temperature of a blackbody spectrum and velocity of ionized iron gas from a supernova explosion.

Schedule: This is a four-week lab between October 4 and November 1. There will be no class on October 11 for Thanksgiving. Group-led discussions will happen on October 18 and 25. (More information on Group-led discussion will be given separately.)

2. Key Steps

1. Understand how spectroscopy is done, especially wavelength calibration.
2. Obtain a wavelength solution (= mapping solution between the detector pixels and wavelengths) of Neon spectrum taken with a spectrograph equipped with a 1-dimensional detector (= linear detector) using the known wavelengths of Neon lines.
3. Apply the wavelength solution to determine the temperature of a perfect blackbody spectrum taken with the same spectrograph.
4. Obtain a wavelength solution of OH sky lines for a 2-dimenaional dispersed image in the near infrared.
5. Apply the wavelength solution to obtain the velocity of ionized iron gas by comparing the intrinsic wavelength of [Fe II] 1.644 micron and the measured wavelength.
6. Write a report on your work. (See the document on lab report writing.)

2.1 Wavelength solution of 1-dimisional Neon spectrum and blackbody temperature

Figure 1 shows a simple laboratory setup for spectroscopy. Photons from the light source (e.g., Neon lamp, blackbody source) are transferred to the entrance of the USB4000 spectrograph by optical fiber. Inside the spectrograph, the entered photons are dispersed by grating (component ⑤) before they are recorded in 1-dimensional detector (component ⑨). The detector has **1024 pixels**. (Note that there are other optical components inside the spectrograph that reflect, collimate, and focus the photons.) The spectrograph is configured to be sensitive to photons roughly in the range of 500–800 nm.

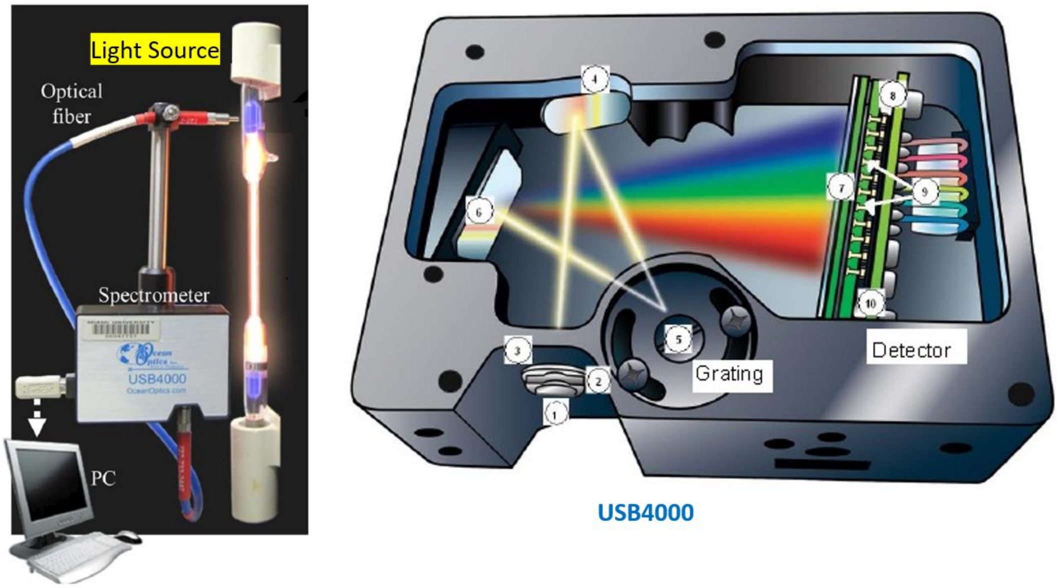

Figure 1. (Left) Experimental setup for laboratory spectroscopy using USB4000 spectrograph. (Right) Internal configuration of the USB4000 spectrograph.

The final goal of this experiment is to determine the temperature of a blackbody source by analyzing its spectrum obtained with the spectrograph. In the folder linked to the following address

https://drive.google.com/drive/folders/1jbY0PQxzgxmCrSX19NPH5nHL_NBzOvVs?usp=sharing

you can find a file named "**Group_?_BB.dat**" which is the spectrum of the blackbody source for your group. If you plot the spectrum, it looks like the following

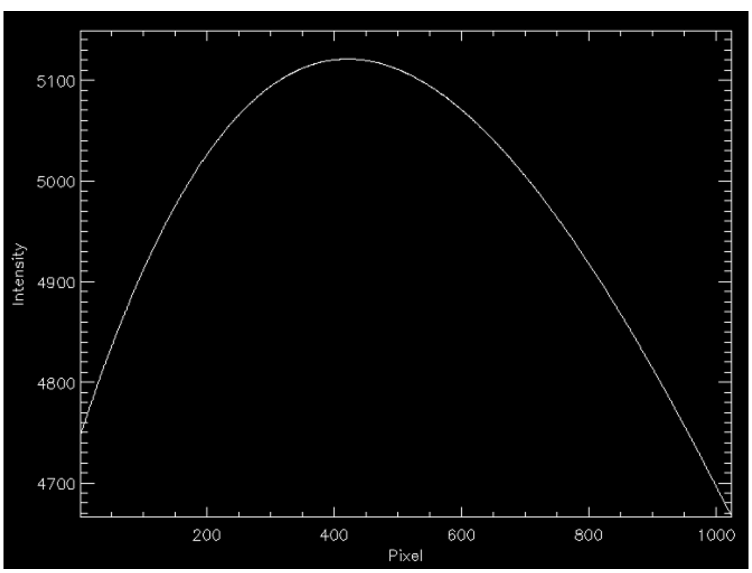

Figure 2. Example spectrum of the blackbody source obtained with the spectrograph.

In order to estimate the temperature of your blackbody source, you need to obtain the wavelength solution since temperature determines the wavelength depednece of a blackbody spectrum. In the same web page above, you can find a file named "**Ne_calib.dat**," and it is a spectrum of a Neon lamp obtained with the same specrtrograph. Its spectrum looks like the following

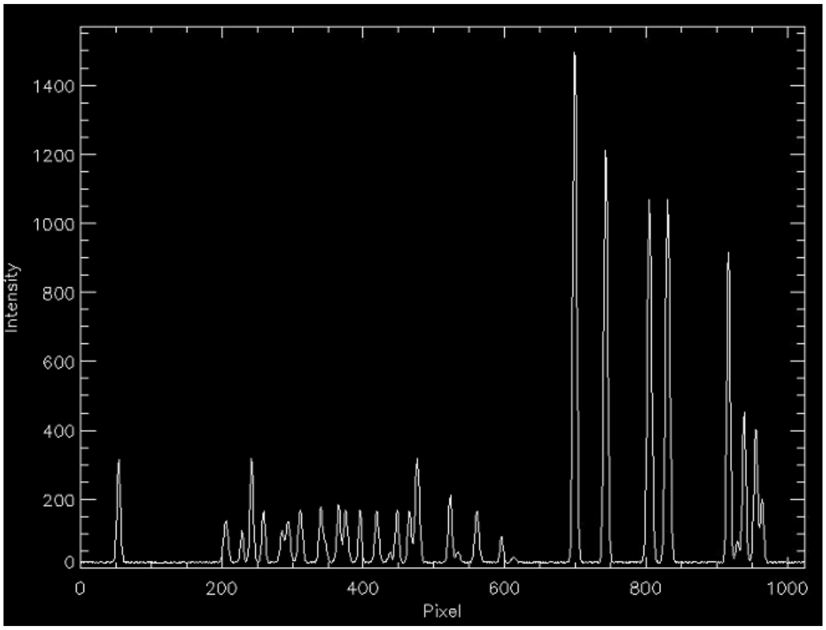

Figure 3. Spectrum of a Neon lamp in "Ne_calib.dat."

Neon has many line transitions in the wavelength range of 500–800 nm as listed in Figure 4,

511.367	**640.225**
511.650	**650.653**
540.056	**653.288**
576.441	**659.895**
582.015	**667.828**
585.249	**671.704**
588.189	**692.947**
594.483	**703.241**
597.553	**717.394**
602.000	**724.512**
607.433	**743.890**
609.616	**747.244**
612.884	**748.887**
614.306	**753.577**
616.359	**754.404**
621.728	837.761
626.649	849.536
630.479	878.375
633.442	1117.752
638.299	1152.275

Figure 4. Wavelengths (in nm) of bright Neon lines. (The source is https://www.oceaninsight.com/globalassets/catalog-blocks-and-images/manuals--instruction-old-logo/wavelength-calibration-products-v1.0_updated.pdf)

and the relative strengths of these lines are shown in Figure 5.

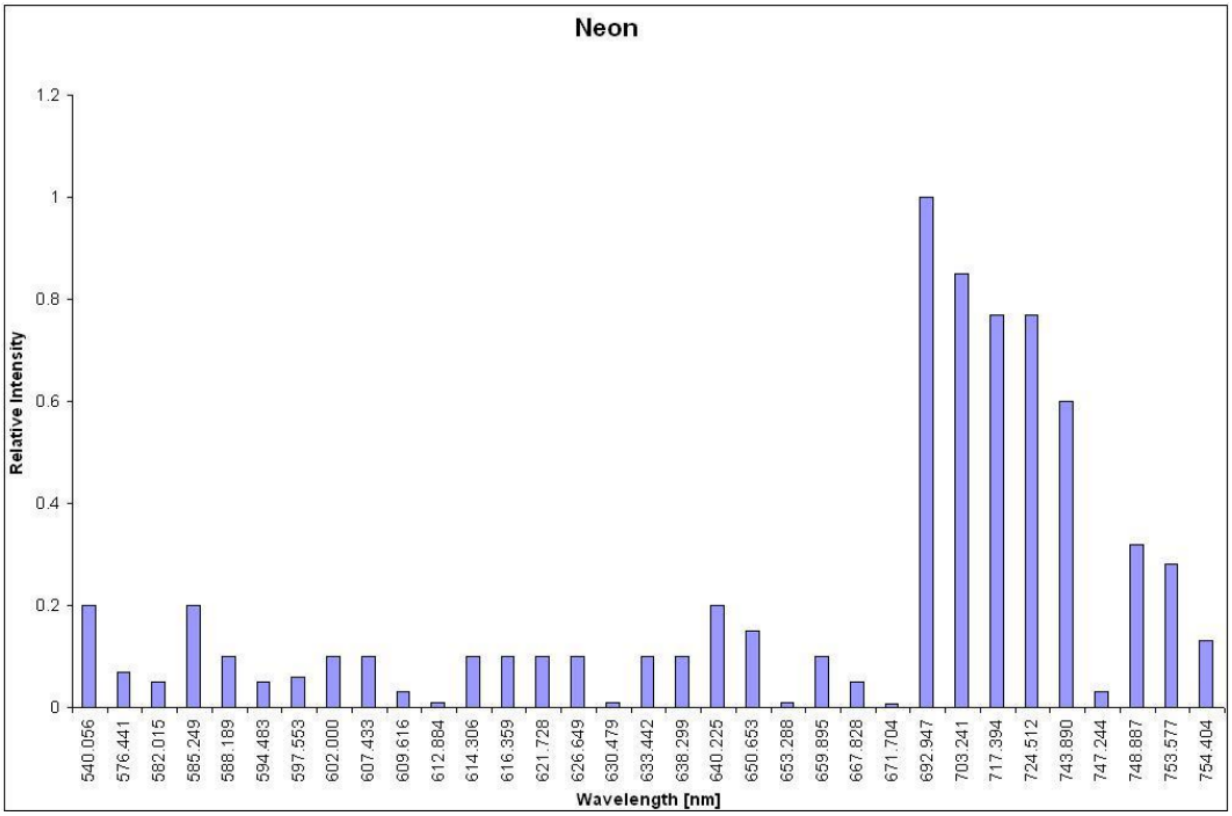

Figure 5. Relative intensities of the Neon lines above. This plot is from the same source as Figure 4.

Now you can obtain the wavelength solution of the spectrum in Figure 3 and determine the temperature of your blackbody. You need to follow the following steps for this.

1. Identify the wavelengths of the Neon lines in Figure 3 as many as possible using the information in Figure 4 and 5. Some nearby lines may overlap if their wavelengths are close.
2. Determine the *centroids* (i.e., pixel positions) of the lines. (There could be many different ways to do it.)
3. Obtain a linear least square fitting (= straight line fit; see below in Appendix) between the pixel positions of the Neon lines that you identified and their wavelengths. How good is the fitting? The linear fitting is the wavelength solution.
4. Apply the wavelength solution that you obtained in step 3 above to your blackbody spectrum. Now you know the wavelengths of the blackbody spectrum. What is the temperature of your blackbody?

2.2 Wavelength solution of 2-dimisional dispersed image using OH sky lines and the velocity of ionized iron gas

As we learned in the class, one convenient way to obtain a wavelength solution in the near-infrared waveband is to use the OH sky telluric emission lines. So, let's apply this method to real data. In the same web page above, you can download a file named "**Near-Infrared.fits**" which is a real data file of a 2-dimensional dispersed image of ionized iron gas (= Fe II) from a supernova explosion saved in the FITS (= Flexible Image Transport System) file format. (The FITS format is the standard data format in astronomy.) The file looks like the following if you use a FITS viewer program like DS9 available at https://sites.google.com/cfa.harvard.edu/saoimageds9. (*Note that adjusting scale and changing contrast is important to see images in DS9. You can try ZScale and move mouse on the image with the right button pressed to adjust contrast.*)

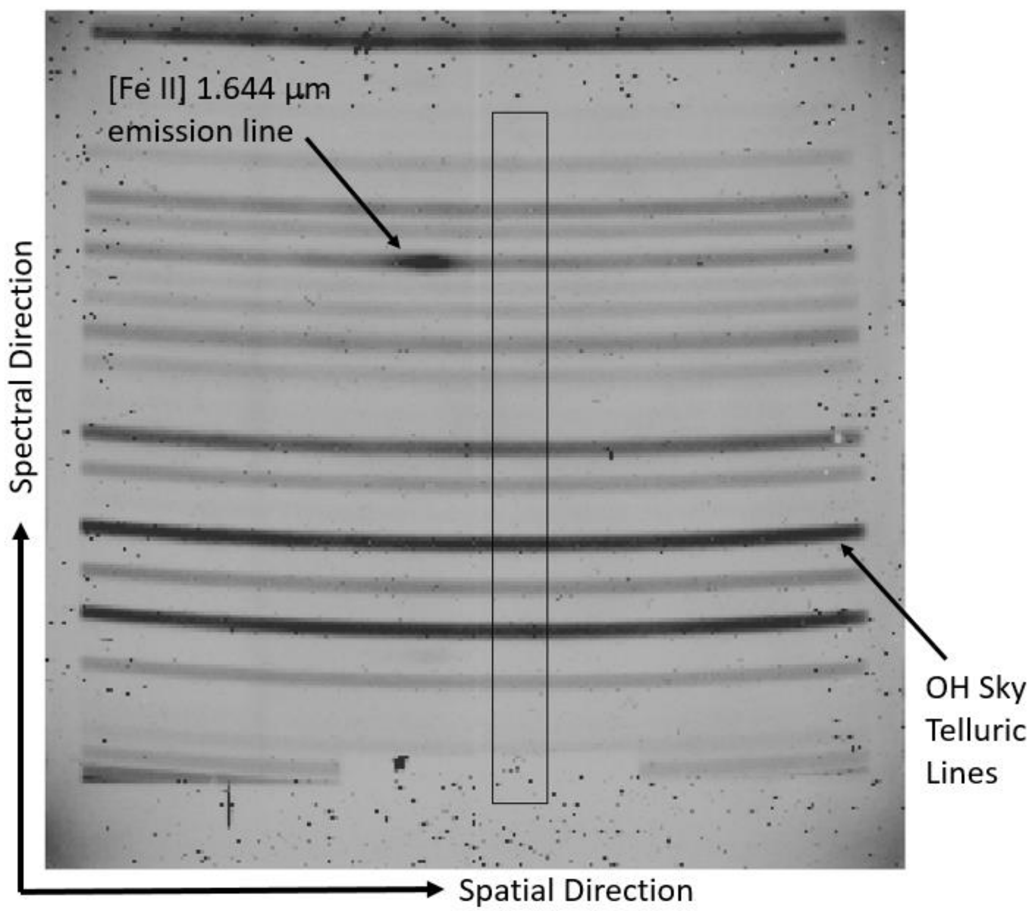

Figure 6. Dispersed image of ionized iron gas from a supernova explosion.

You can see that it is dominated by the OH sky lines, but there exists clear [Fe II] 1.644 micron emission almost overlapping with one of the OH lines. Figure 7 is a spectrum of the OH lines in Figure 6 created by using the area in the rectangle Figure 6 by taking the median value of each row in the rectangle.

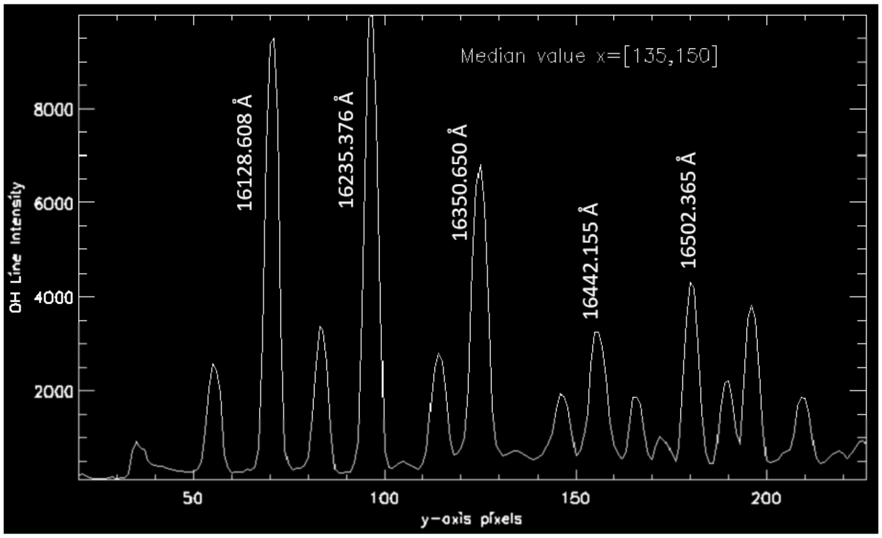

Figure 7. Spectrum of the OH telluric sky lines in Figure 6. Five bright lines are identified with their wavelengths.

Five bright OH sky lines are easily identifiable using the relative intensities of the known OH lines in Figure 8.

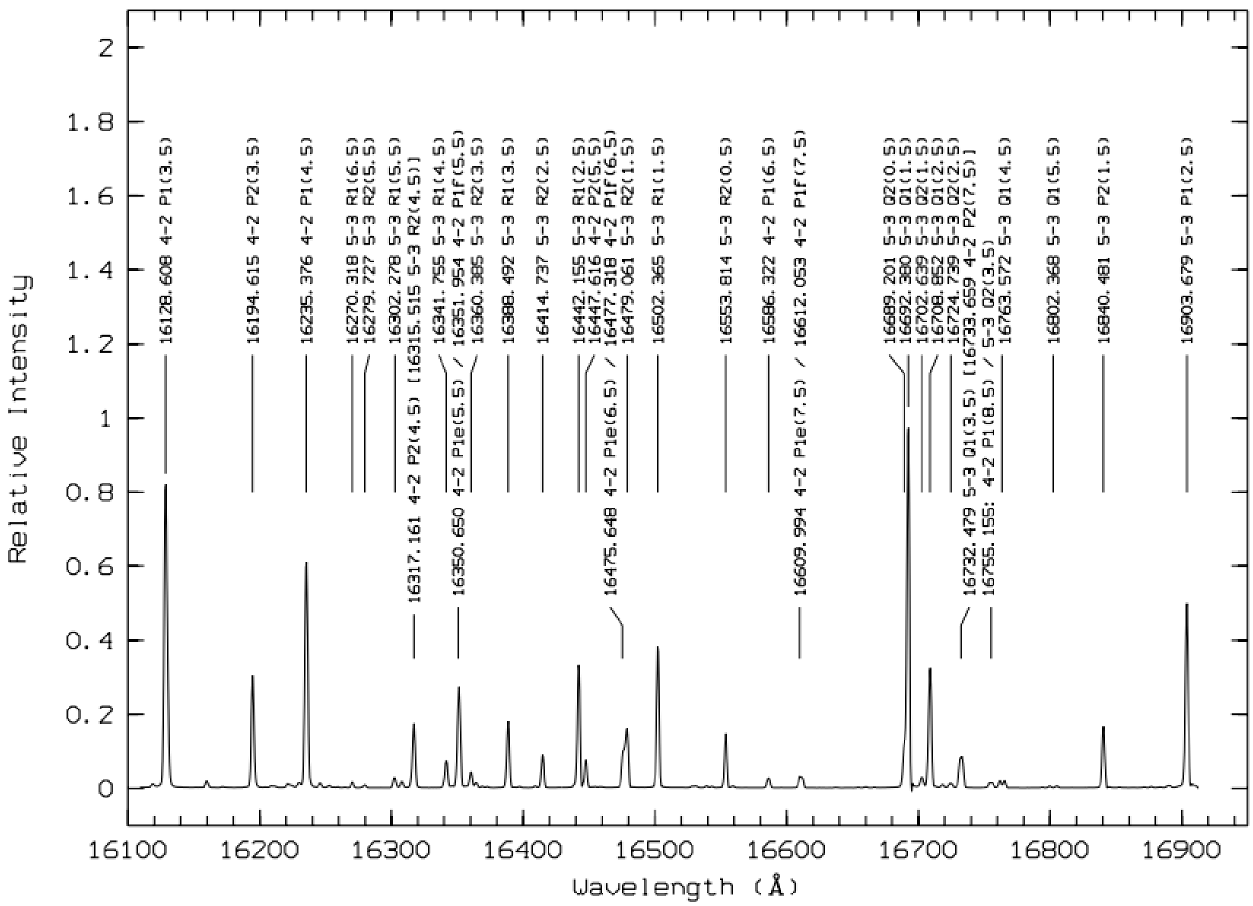

Figure 8. Relative intensities of known the OH telluric sky lines in the wavelength range of 1.610-1.690 micron from the paper of Rousselot et al. 2000. (Note that this paper is linked in the class web page.)

Now you can calculate the velocity of the iron gas in Figure 6 using the observed wavelength of the [Fe II] 1.644 micron line. You need to follow the following steps for this:

1. In addition to the five already identified OH lines, identify as many more OH lines as possible from a region near the [Fe II] emission (e.g., the rectangular box) in Figure 6.
2. Determine the central positions (in terms of y-axis pixel numbers) of the identified lines, and then conduct polynomial fitting of the central positions to the wavelengths. This gives a wavelength solution, which is mapping between the pixel positions and wavelengths. You can choose the degree of the polynomial fit between 1 (= linear least fit) and 3.
3. How good is your wavelength solution, or what is the uncertainty of your wavelength solution?
4. Determine the central position of the [Fe II] emission in Figure 6 in y-axis, and then apply the wavelength solution that you already obtained above using OH sky lines to estimate the wavelength of [Fe II] emission in Figure 6. The intrinsic wavelength of the [Fe II] 1.644 μm line emission is 1.6439981 μm. What's the velocity of the gas emitting the [Fe II] emission in Figure 6?

Appendix: Linear Least Squares Fitting

One of the primary skills we will learn in this lab is the use of linear least squares fitting. Often observations and experimental measurements are undetermined, which means that they are limited by the number of observations or sampling to calculate an undetermined parameter space. To correct for this, we use an equation to model a set of data, and compare the difference between the observed values to the fitted values from the model. This difference is referred to as residuals. The term "least-squares" refers to minimizing the *square of the residuals* to determine the best-fit model to the observed data set.

In this lab, we will first focus on linear-least squares where the model is a straight line, but we will generalize the least squares method to other non-linear functions. It is important that in this lab you do not use a canned least-squares routine and you write your own least-square routine.

1. A Straight Line Fit

Suppose that we have a set of N observations (x_i, y_i) where we believe that the measured value, y, depends linearly on x, i.e.,

$$y = mx + c.$$

For example, suppose a body is moving with constant velocity, what is the speed (m) and initial (c) position of the object?

Given our data, what is the best estimate of m and c? Assume that the independent variable, x_i, is known exactly, and the dependent variable, y_i, is drawn from a Gaussian probability distribution function with constant standard deviation σ_i = const. Under these circumstances the most likely values of m and c are those corresponding to the straight line with the total minimum square deviation, i.e., the quantity

$$\chi^2 = \sum_i \left[y_i - (mx_i + c)\right]^2$$

is minimized when m and c have their most likely values. Figure 1 shows a typical deviation.

The best values of m and c are found by solving the simultaneous equations,

$$\frac{\partial}{\partial m}\chi^2 = 0, \quad \frac{\partial}{\partial c}\chi^2 = 0$$

Evaluating the derivatives yields

$$\frac{\partial}{\partial m}\chi^2 = \frac{\partial}{\partial m}\sum_i \left[y_i - (mx_i + c)\right]^2 = 2m\sum_i x_i^2 + 2c\sum_i x_i - 2\sum_i x_i y_i = 0$$

$$\frac{\partial}{\partial c}\chi^2 = \frac{\partial}{\partial c}\sum_i \left[y_i - (mx_i + c)\right]^2 = 2m\sum_i x_i + 2cN - 2\sum_i y_i = 0.$$

This set of equations can conveniently be expressed compactly in matrix form,

$$\begin{pmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & N \end{pmatrix} \begin{pmatrix} m \\ c \end{pmatrix} = \begin{pmatrix} \sum x_i y_i \\ \sum y_i \end{pmatrix}$$

and then solved by multiplying both sides by the inverse,

$$\begin{pmatrix} m \\ c \end{pmatrix} = \begin{pmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & N \end{pmatrix}^{-1} \begin{pmatrix} \sum x_i y_i \\ \sum y_i \end{pmatrix}$$

The inverse can be computed analytically, or in Python it is trivial to compute the inverse numerically, as follows.

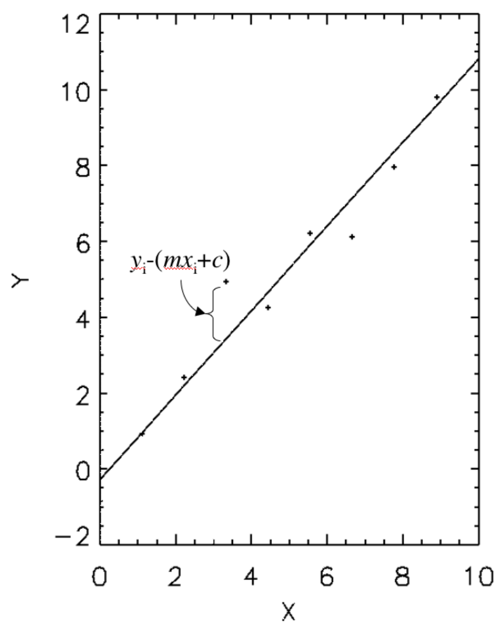

Figure 1: Example data with a least squares fit to a straight line. A typical deviation from the straight line is illustrated.

2. Example Python Script

```
# Test least squares fitting by simulating some data.
import numpy as np
import matplotlib.pyplot as plt

nx = 20          # Number of data points
m = 1.0          # Gradient
c = 0.0          # Intercept
```

```
x = np.arange(nx,dtype=float)         # Independent variable
y = m * x + c                         # dependent variable

# Generate Gaussian errors
sigma = 1.0                           # Measurement error

np.random.seed(1)                     # init random no. generator
errors = sigma*np.random.randn(nx)    # Gaussian distributed errors
ye = y + errors                       # Add the noise

plt.plot(x,ye,'o',label='data')
plt.xlabel('x')
plt.ylabel('y')

# Construct the matrices
ma = np.array([ [np.sum(x**2), np.sum(x)],[np.sum(x), nx ] ]  )
mc = np.array([ [np.sum(x*ye)],[np.sum(ye)]])

# Compute the gradient and intercept
mai = np.linalg.inv(ma)
print 'Test matrix inversion gives identity',np.dot(mai,ma)
md = np.dot(mai,mc)     # matrix multiply is dot

# Overplot the best fit
mfit = md[0,0]
cfit = md[1,0]
plt.plot(x, mfit*x + cfit)
plt.axis('scaled')
plt.text(5,15,'m = {:.3f}\nc = {:.3f}'.format(mfit,cfit))
plt.savefig('lsq1.png')
```

See Figure 2 for the output of this program.

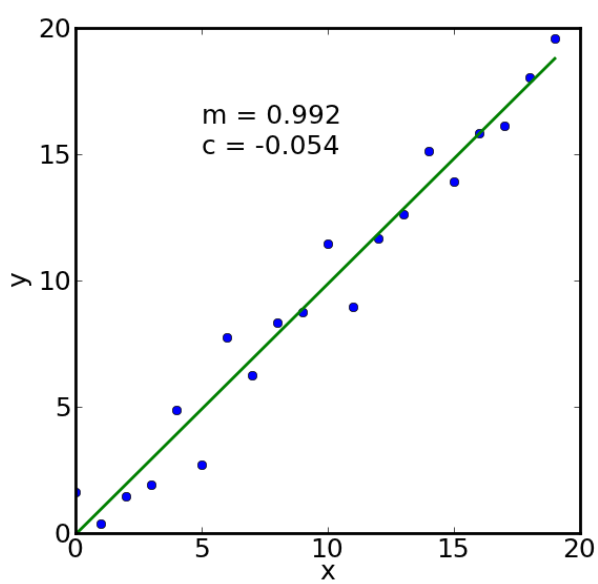

Figure 2—Least squares straight line fit. The true values are *m* = 1 and *c* = 0.

3. Error Propagation

What are the uncertainties in the slope and the intercept? To begin the process of error propagation we need the inverse matrix

$$\begin{pmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & N \end{pmatrix}^{-1} = \begin{pmatrix} N\Big/\left[N\sum x_i^2 - \left(\sum x_i\right)^2\right] & \sum x_i\Big/\left[N\sum x_i^2 - \left(\sum x_i\right)^2\right] \\ \sum x_i\Big/\left[\left(\sum x_i\right)^2 - N\sum x_i^2\right] & \sum x_i\Big/\left[N\sum x_i^2 - \left(\sum x_i\right)^2\right] \end{pmatrix},$$

so that we can compute analytic expressions for *m* and *c*,

$$\begin{pmatrix} m \\ c \end{pmatrix} = \begin{pmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & N \end{pmatrix}^{-1} \begin{pmatrix} \sum x_i y_i \\ \sum y_i \end{pmatrix} = \begin{pmatrix} \dfrac{\sum x_i \sum y_i - N\sum x_i y_i}{\left(\sum x_i\right)^2 - N\sum x_i^2} \\ \dfrac{\sum x_i \sum x_i y_i - \sum x_i^2 \sum y_i}{\left(\sum x_i\right)^2 - N\sum x_i^2} \end{pmatrix}.$$

The analysis of error propagation shows that if $z = z(x_1, x_2, .. x_N)$ and the individual measurements x_i are uncorrelated (they have zero covariance) then the standard deviation of the quantity z is

$$\sigma_z^2 = \sum_i \left(\partial z/\partial x_i\right)^2 \sigma_i^2 .$$

If the data points were correlated then we would have a covariance matrix. The diagonal elements of this matrix are the standard deviations σ_{ii}^2 and of the off diagonal elements $\sigma_{ij}^2 = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$.

Thus, ignoring any possible covariance

$$\sigma_m^2 = \sum_j \left(\partial m/\partial y_j\right)^2 \sigma_j^2 \quad \text{and} \quad \sigma_c^2 = \sum_j \left(\partial c/\partial y_j\right)^2 \sigma_j^2.$$

The expression for the derivative of the gradient, *m*, is

$$\frac{\partial m}{\partial y_j} = \frac{\partial}{\partial y_j}\left(\frac{\sum x_i \sum y_i - N\sum x_i y_i}{\left(\sum x_i\right)^2 - N\sum x_i^2}\right) = \frac{\sum x_i - N x_j}{\left(\sum x_i\right)^2 - N\sum x_i^2}$$

because $\left(\partial y_i/\partial y_j\right) = \delta_{ij}$., where δ is the Kroneker If we assume that the measurement error is the same for each measurement then

$$
\begin{aligned}
\sigma_m^2 &= \sigma^2 \sum_j \left(\frac{\sum x_i - N x_j}{\left(\sum x_i\right)^2 - N \sum x_i^2} \right)^2 \\
&= \frac{\sigma^2}{\left[\left(\sum x_i\right)^2 - N \sum x_i^2\right]^2} \sum_j \left[\left(\sum x_i\right)^2 - 2N x_j \sum x_i + N^2 x_j^2 \right] \\
&= \frac{\sigma^2}{\left[\left(\sum x_i\right)^2 - N \sum x_i^2\right]^2} \left[N\left(\sum x_i\right)^2 - 2N\left(\sum x_i\right)^2 + N^2 \sum x_i^2 \right] \\
&= \frac{N\sigma^2}{N\sum x_i^2 - \left(\sum x_i\right)^2}
\end{aligned}
$$

Similarly, for the intercept, c,

$$
\frac{\partial c}{\partial y_j} = \frac{\partial}{\partial y_j} \left(\frac{\sum x_i \sum x_i y_i - \sum x_i^2 \sum y_i}{\left(\sum x_i\right)^2 - N \sum x_i^2} \right) = \frac{x_j \sum x_i - \sum x_i^2}{\left(\sum x_i\right)^2 - N \sum x_i^2}
$$

and hence

$$
\begin{aligned}
\sigma_c^2 &= \sigma^2 \sum_j \left(\frac{x_j \sum x_i - \sum x_i^2}{\left(\sum x_i\right)^2 - N \sum x_i^2} \right)^2 \\
&= \frac{\sigma^2}{\left[\left(\sum x_i\right)^2 - N \sum x_i^2\right]^2} \sum_j \left[x_j^2 \left(\sum x_i\right)^2 - 2x_j \sum x_i \sum x_i^2 + \left(\sum x_i^2\right)^2 \right] \\
&= \frac{\sigma^2}{\left[\left(\sum x_i\right)^2 - N \sum x_i^2\right]^2} \left[\sum x_i^2 \left(\sum x_i\right)^2 - 2\left(\sum x_i\right)^2 \sum x_i^2 + N\left(\sum x_i^2\right)^2 \right] \\
&== \frac{\sigma^2 \sum x_i^2}{N\sum x_i^2 - \left(\sum x_i\right)^2}.
\end{aligned}
$$

If we do not know standard deviation, σ *a priori*, the best estimate is derived from the deviations from the fit, i.e.,

$$
\sigma^2 = \frac{1}{N-2} \sum_i \left[y_i - (m x_i + c) \right]^2 .
$$

Previously, when we compute the standard deviation the mean is unknown and we have to estimate it from the data themselves; hence, the Bessel correction factor of $1/(N-1)$, because there are N-1 degrees of freedom. In the case of the straight line fit there are two unknowns and there are N-2 degrees of freedom.