Lab #2 "Introduction to Spectroscopy"

Lab report due: Wednesday, 2019 November 6th 11:59pm
(e-submission to astrolab@astro.utoronto.ca)

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 known 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

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. Characterizing a spectrograph's instrumental parameters is a key for deriving the intrinsic spectra from a source. In this lab you will use a spectrograph to collect data from common light sources (room lights and gas discharge lamps), establish a wavelength scale, investigate the noise properties of the detector, and (hopefully) measure astronomical spectra of stars and planets. In class we will explore the fundamentals of diffraction, dispersion elements, 2D detectors (e.g, CCDs), telescopes, and review the celestial coordinate systems.

2 Schedule

This is a four-week lab between October 7 (Monday) and November 6 (Wednesday). There will be no class on October 14 and November 4 because of Thanksgiving and Reading Week, respectively. Group-led discussions will happen on October 21 and 28. Starting the week of October 21, we will attempt to obtain astronomical spectra using the campus telescope. The details of the Campus Telescope Sessions will be announced later in the class and on its web page.

3 Goals

Use a simple, visible light (350−700 nm) spectrometer to explore the spectra of laboratory and astrophysical sources. We will conduct wavelength calibration of the Ocean Optics spectrometer, which will introduce the concept of spectroscopy and linear least square fitting. We will then learn how to acquire data from a telescope and acquire spectra of astronomical sources. In the process, we will learn the basic steps of astronomical data reduction (e.g., dark subtraction, flat fielding, wavelength solution) using the SBIG spectrograph on the MP telescope.

3.1 Reading assignments

- USB 2000 spectrometer handout (class web page)
- Lecture/notes on statistics and error analysis and least square fitting (class web page)
- Notes on CCDs and their noise properties (class web page)

- *Reference*: Chapters 1−4 “Handbook of CCD Astronomy,” S. B. Howell, Cambridge University Press. There are two copies in Gerstein and more copies may be available in AB 105. Pay special attention to §§3.4−3.8 and §§4.2−4.3, & 4.5.
- *Reference*: “To Measure the Sky,” F. R. Chromey, Cambridge University Press. In particular, Chapters 6 on Astronomical Telescopes, Chapter 8 on Detectors, and Chapter 11 on Spectrometers.

4 Key Steps

1. Learn to operate the USB 2000 spectrometer using the Spectral Suite software in one of the lab tutorials during the first week of the lab.
2. Save spectra and read them into Python for plotting and analysis.
3. Observe and compare spectra of common sources—incandescent lamp, fluorescent strip light, gas discharge lamps, and sunlight.
4. Determine the wavelength calibration of the spectrometer, i.e., the mapping between pixel number and wavelength. Do this by measuring the *centroids* (i.e., pixel positions) of bright Neon (and Hydrogen, if available) lines with respect to their known wavelength. Then use the method of linear least squares to determine a polynomial fit to these data to derive the wavelength solution.
5. Attend one of the telescope sessions and use the SBIG spectrometer at the campus observatory to collect spectra of the moon, Arcturus, Vega, and/or Jupiter and other bright stars.
6. Reduce the SBIC spectra of the astronomical sources and compare and contrast these spectra.
7. Write up your report.

5 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.

5.1 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

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

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

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

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.

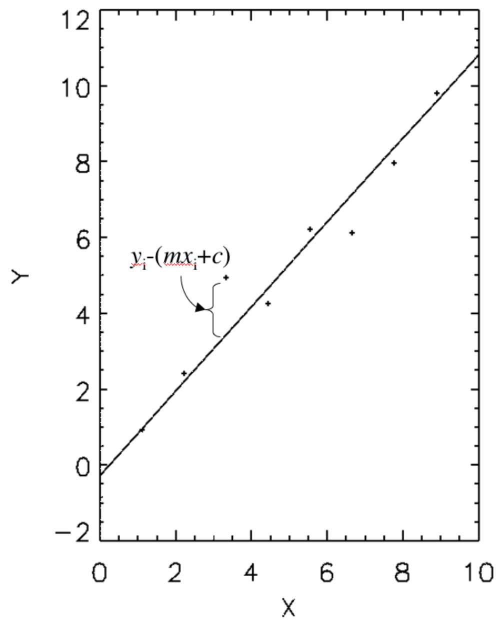

Figure 1: Example data with a least squares fit to a straight line. A typical deviation from the straight line is illustrated.

5.2 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.

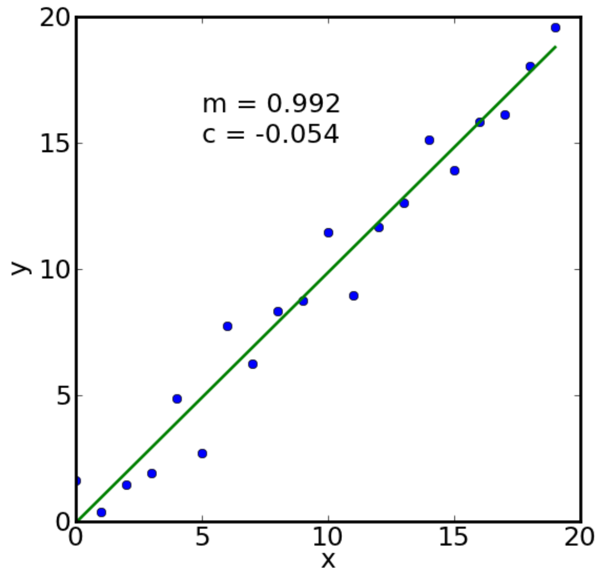

Figure 2—Least squares straight line fit. The true values are *m* = 1 and *c* = 0.

5.3 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

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

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.,

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

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.

6 Night time observing

For nighttime astronomy, we will use a spectrograph that is located on the 16-inch telescope on the 16th floor of the McLennan Physics tower. Michael Williams (williams@astro.utoronto.ca), who is in charge of the lab equipment and telescope operation, will be there to set up the telescope and help you collect your data. Separate documents describing this spectrograph and the observing procedure are available on the class web page.

Example spectra taken with the SBIG spectrograph attached to the 16-inch telescope are shown in Figure 3. The top spectrum is for a quartz halogen lamp, and shows the response of the spectrometer to an approximately 3200 K black body. (*In this example, the short wavelength flux* *from the lamp may be suppressed by a built-in UV filter, so the blackbody assumption may not be valid in the blue part of the spectrum*.) Note the overall variation of responsivity and fine scale pixel-to-pixel fluctuations. The subsequent astronomical spectra are corrected for the spectrometer response assuming that the lamp radiates like a black body with temperature equal to the color temperature. Thus we compute for each pixel, P_i, the quantity

$$P_i = \frac{R_i - D_i}{L_i - D_i} B(\nu_i, T)$$

where R_i is the raw signal, D_i is the dark count, and L_i is the lamp, and $B_\nu(T)$ is the Planck function

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}$$

where $\nu_i = c/\lambda_i$ is the frequency of the *i-th* pixel. (Note that in this case the lamp spectrum is used for flat fielding – see lecture slides).

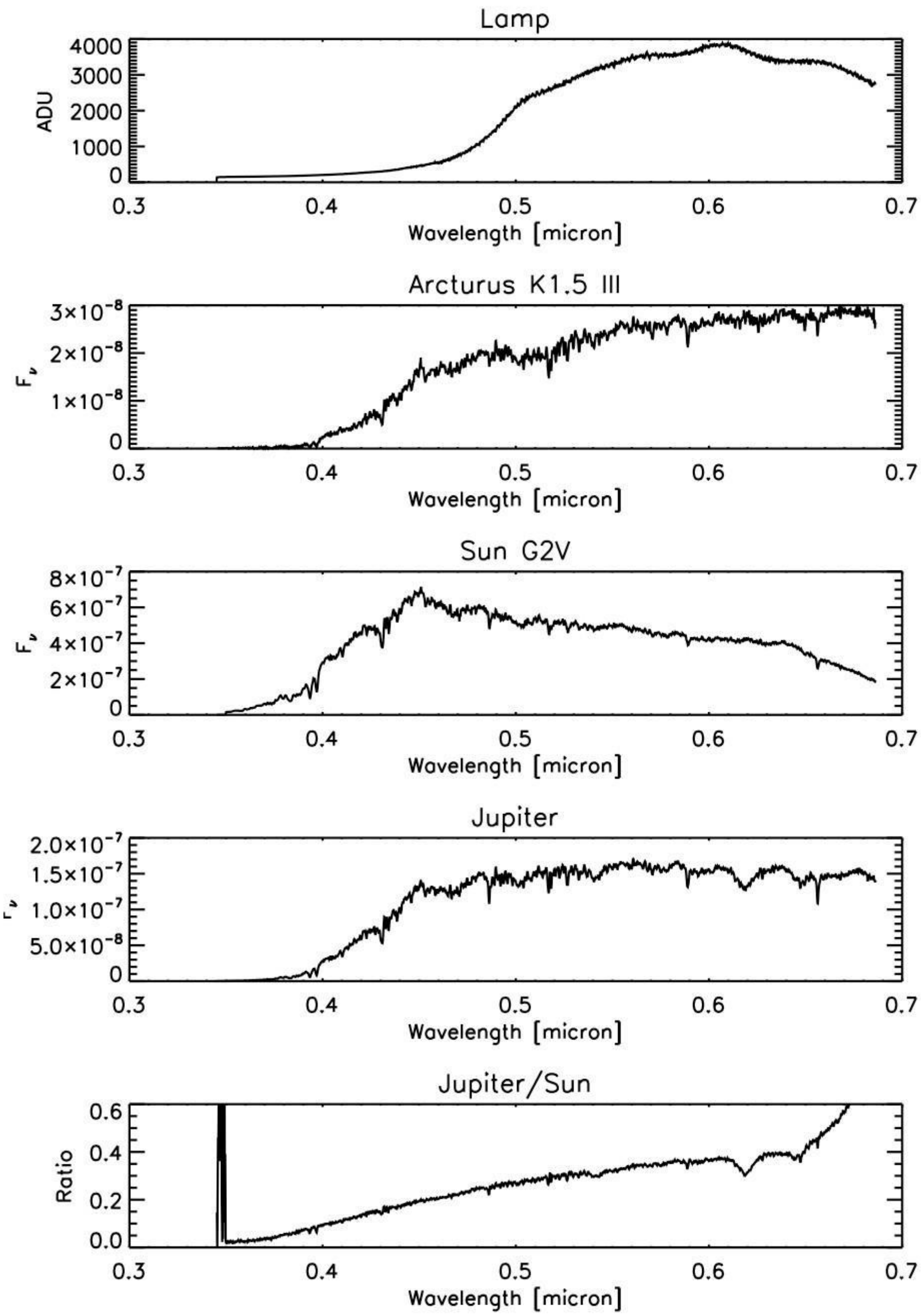

Figure 3. Spectra of a lamp and some astronomical sources. Comparison of Arcturus (4300 K) and the Sun (5800 K) shows the effect of Wien's law. The stellar spectra show both the underlying continuum emission and many microscale absorption lines. In the solar spectrum Ca II H&K 393.37, 396.85 nm, the G band 430.8 nm, Hβ 486.1 nm, the b and E bands (Mg + Fe) 517, 527 nm, Na D 588.995, 589.592 nm, and Hα 656.2 nm are all visible. The spectrum of Jupiter is red, with strong methane absorption at 619 nm. The exposure times are: lamp 23 ms, 1000 frames; Arcturus & Jupiter 500 ms, 100 frames; sun 3 ms, 100 frames. The astronomical spectra are dark subtracted, divided by the lamp spectrum, and multiplied by a 3200 K black body.