

Lab#2: Guide to Characterizing the Spectrometer

Introduction

The USB 2000 spectrometer is a simple optical instrument based on a diffraction grating and a one-dimensional CCD detector array. The CCD array has 1×2048 pixels so the spectrum reads out as a list of 2048 data numbers. The spectrometer box is shown in Figure 1 and depicted schematically in Figure 2. Light enters via a slit located at the bottom of a threaded receptacle, which can be used to connect an optical fiber that is terminated with a SMA plug. This instrument achieves a spectral resolution of about 0.6 nm between wavelengths of 370 to 700 nm. The spectrograph is based on a Czerny-Turner optical design, which has no moving parts.



Figure 1: The Ocean Optics USB 2000 spectrometer. The spectrometer entrance slit is located at the rear of the SMA 905 type threaded connector. Commands to expose the CCD are sent via a USB connection and the data are returned via the same route.

Connecting to a PC or laptop loaded with Ocean Optics' SpectraSuite operates the spectrometer via a USB serial interface. Windows, Linux, and Mac versions of this software are available.

Do not plug the spectrometer into a PC that does not have the SpectraSuite software installed.

Spectrometer check out procedure

We only have one USB 2000 spectrometer. If it gets lost or damaged it cannot be replaced, and it will be impossible to complete the associated lab exercise. For that reason the spectrometer will only be run from AB105. The spectrometer must be treated with care—it is a delicate optical instrument that is sensitive to shock and contamination.

Inside the “back box”

Figure 2 shows a schematic of the USB 2000 spectrometer from the Ocean Optics web page¹. Light from a fiber enters the optical bench through the SMA connector (1). Light from the fiber passes through a slit (2), which acts as the entrance aperture. An optical filter (3) is installed between the slit and the aperture in the SMA connector. This filter blocks light that would be diffracted in the second- and third-orders by the grating. A collimating mirror (4) matches to the 0.22 numerical aperture ($F/2.3$) of the optical fiber. Light reflects from this mirror, as a collimated beam, toward the grating. The grating (5) is installed on a rotating platform that selects wavelength range. After assembly, the grating platform is fixed to eliminate mechanical shifts or drift. A mirror (6) focuses the first-order spectra on the detector plane. A cylindrical lens (7) is fixed to the detector to focus the light from the tall slit onto the shorter detector element ($14\ \mu\text{m} \times 200\ \mu\text{m}$ pixels), increasing light-collection efficiency. A 2048-element Sony ILX511 linear CCD array detector (8) pixel responds to the wavelength of light that strikes it.

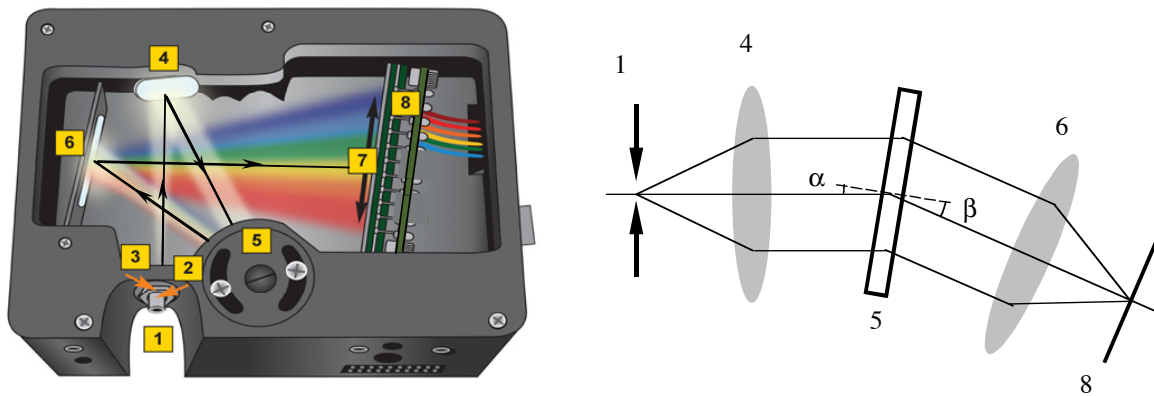


Figure 2: *Left:* The interior of the USB 2000 spectrometer, showing the optical layout. The key optical components are the entrance aperture (1), the collimating mirror (4) the grating (5), the camera mirror (6) and the detector array (8). *Right:* equivalent optical diagram using lenses. The angle of incidence and diffraction at the grating (α and β) are shown such that $m\lambda/\sigma = \sin\alpha + \sin\beta$, where m is the order (1, 2, 3...), λ is the wavelength, and σ is the grating groove spacing (for a transmission grating replace the plus sign with minus.)

Getting started

The USB2000 spectrometer should be plugged into the linux laptop USB port, then fire up the SpectraSuite control software. You should immediately see the control window, which is shown in Figure 3. Connect the spectrometer only to a PC or laptop that you know has the Ocean Optics control software installed. If no device shows up in the data sources window (top left) select Spectrometer/Rescan Devices from the menu. If you started the software before plugging in the spectrometer, quit the software and then plug in the spectrometer and try again.

¹ http://www.oceanoptics.com/products/benchoptions_usb4.asp

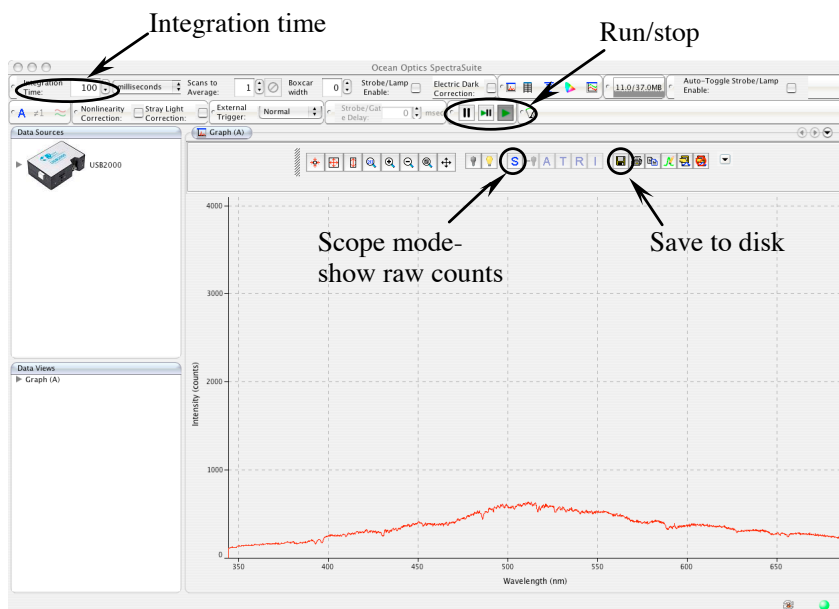


Figure 3: The default form of the SpectraSuite control software when it starts up. The red line is a graphical display of the spectrum. The x-axis is displayed in nm, computed using the nominal wavelength scale measured by the manufacturer. Pressing the scope mode button displays unprocessed data. Make sure that the following are turned off: Nonlinearity correction; Stray light correction; Electric Dark Correction. Set the following: Scans to average (1); Boxcar width (1).

Taking a spectrum

In the default operating mode the spectrometer runs in continuous acquisition mode, which as the name suggests, is like an oscilloscope: the spectrum is continuously scanned at a cadence equal to the integration time. If its spectrum is shown select File/New/Spectrum Graph. To take an spectra of your desired object using the fiber cable to point to your source. But remember that the fiber optical cable is VERY FRAGILE so do not excessively bend the cable!

Click the blue **S** button to make sure that the plotted spectrum shows raw counts from the CCD (see Figure 3). (Pressing the other buttons to the right of **S** activates various processing options such as dark subtraction, which we do not want.)

The spectrum display is “live,” and updates with each new exposure. Wave your hand in front of the entrance aperture and note the change in brightness. The default exposure time is 100 ms, so you should see an immediate response on the plot.

Try changing the integration time in the upper left window from the default 100 ms to a longer time and view the results. Use the set of icons just above the graph to adjust the x- and y-scaling of the graph. If you have a scroll wheel on your mouse, you can use this to zoom in and out.

The easiest way to use the spectrometer is to inspect the live graphical display. This is a very handy option because, for example, it lets you see immediately if the light source is bright enough to yield useful data. The plot has some handy tools. For example you can right-click on a feature within the plot window, and a vertical green line will appear. This cursor can be used to read off the wavelength of a feature—when you click this updates the text box at the bottom

of the plot with the wavelength in nm and the intensity in counts. **By default the plot appears with the x-axis labeled in nm. Choose Processing/X-axis Units... to select pixels (or press cntrl-3).**

What you really want is to save data so that you can read them into Python. No self-respecting AST-325/6 astronomer would trust a black box program like SpectraSuite! When you are happy with the exposure time and other details of the measurement, click the floppy disk icon above the spectrum. Click the “browse” button to select the path and then type a file name in the dialog box. From the “Desired Spectrum” menu, select “Processed Spectrum”—to make sure that you save is raw counts make sure that you have clicked the blue **S** button. You have several options for file type to save. The handiest choice is to generate columns of tab-delimited ASCII text.

Note, that you can choose the ASCII version to come with a header that includes the following information:

```
SpectraSuite Data File
+++++
Date: Fri Sep 23 15:34:36 EDT 2011
User: jrg
Dark Spectrum Present: No
Reference Spectrum Present: No
Number of Sampled Component Spectra: 1
Spectrometers: USB2+H05261
Integration Time (usec): 100000 (USB2+H05261)
Spectra Averaged: 1 (USB2+H05261)
Boxcar Smoothing: 0 (USB2+H05261)
Correct for Electrical Dark: No (USB2+H05261)
Strobe/Lamp Enabled: No (USB2+H05261)
Correct for Detector Non-linearity: No (USB2+H05261)
Correct for Stray Light: No (USB2+H05261)
Number of Pixels in Processed Spectrum: 2048
>>>>Begin Processed Spectral Data<<<<
0.0  940.90
1.0  940.90
2.0  940.90
3.0  912.81
4.0  905.79
5.0  891.79
...
...
2046.0 4011.68
2047.0 3983.59
>>>>End Processed Spectral Data<<<<
```

This example is for a 0.1 s, unprocessed spectrum (no dark; no reference; no boxcar smoothing; no electrical dark subtraction; no stray light correction). By inspecting the header you can check if you really have raw data. The first number of each pair is the pixel number; the second is the measured signal in data numbers. The default units for the first column is the wavelength computed from the pixel number using the manufacturer’s wavelength calibration. In this

example the file is truncated after the first three pairs of data. You can read the SpectraSuite ASCII format with the following call to the numpy function `loadtxt`:

```
data = np.loadtxt(filename, skiprows=17, usecols=(0,1) )
```

where `filename` is a python variable containing the file name.

When the integration time is longer than a few seconds the “scope” mode can be inconvenient. The method for taking single exposures is accessed from View/Toolbars/Acquisition Controls. The buttons are shown in Figure 4. For a single shot press the center button.

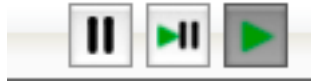


Figure 4: To change from continuous acquisition mode to single shot mode push the center button. Each time you push the center button a new exposure is recorded in memory. To return to continuous acquisition mode push the right hand button. To pause, push the left button. Save your spectrum by clicking the floppy disk icon on the menu bar above the spectrum.

A convenient option can be found in Tools/Options/SpectraSuite Settings/Current Working Directory, which allows you to set the default directory where data are written. If you don’t set this you’ll find that a lot of clicking through menus is needed every time you save a file.

A third choice for saving spectra is found using the File/Save/Save Spectrum option. This menu allows lots of flexibility, perhaps the most useful of which is the ability to take multiple spectra (see Figure 8).

Processing options

The default is that SpectraSuite software saves the data as raw “data numbers,” i.e., a number that is proportional to the number of photoelectrons detected. However, the SpectraSuite software also supports some processing options. Even though these should be disabled, it is a good idea to understand what these are and **make sure that the processing options are turned OFF before you collect any data for detailed analysis**. These options are selected by pushing the button to the right of the blue **S** button.

The most basic corrections are “dark” and “reference”. In general a “dark” is a spectrum that is subtracted from the raw data and the “reference” is a spectrum that is used to divide the spectrum, i.e., the i -th pixel in a processed spectrum, P , is of the form

$$P_i = \frac{R_i - D_i}{S_i - D_i}, \quad (1)$$

where R is the raw spectrum, S is a reference, and D is a dark. Thus, if you turn off processing, then $P = R$, and you get raw data, which is what you want. As you can perform all processing operations in Python, it is recommended that you do not select dark subtraction or reference. You can also average multiple scans or boxcar-smooth the spectra; make sure that these are not

enabled either. Other, more advanced corrections include non-linearity correction, “electrical dark” subtraction, and stray light correction. The non-linearity correction applies a polynomial correction to the raw data values. The stray light correction is not documented, and should be turned off.

The electrical dark appears to be a bias correction. The first 24 pixels are used to estimate the mean dark level (these pixel are not illuminated), and this mean level is subtracted from the rest of the spectrum. As the dark current varies from pixel to pixel this only provides a first order correction.

My first spectrum & wavelength calibration

The fluorescent strip lights in AB 105 are gas-discharge lamps. A potential difference of 110 V is sufficient to partially ionize low-pressure mercury (Hg) vapor that is contained in the tube, and the resultant flow of electric current excites Hg atoms to radiate, predominantly in the UV at 184.9 and 253.6 nm. A phosphorescent material that is painted on the inside of the tube absorbs these UV lines and glows at visible wavelengths producing useful illumination. The chemical composition of phosphors is often complex and is typically includes rare earths, such as terbium (Tb), cerium (Ce) and europium (Eu). Not surprisingly the resultant spectrum is quite complex (see Figure 5). In addition to the UV Hg I lines the spectrum also includes some narrow, visible wavelength atomic Hg lines, which are useful to us for wavelength calibration (Table 1.)

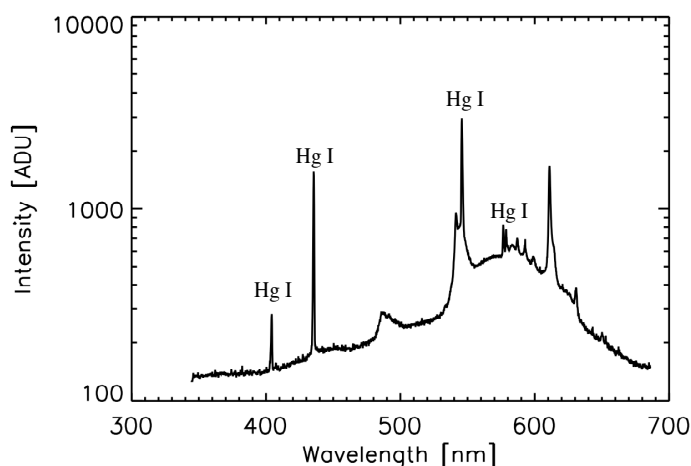


Figure 5: A 200 ms exposure spectrum of the fluorescent lamps obtained with the USB2000 spectrometer. Prominent, narrow lines of atomic mercury (Hg I) are visible together with a broad emission from the lamp phosphor. Not all the narrow lines are from Hg I, but are associated with the rare earths in the (Tb, Ce, and Eu). The wavelength scale here is the nominal factory calibration. Note the y-axis is plotted on a logarithmic scale.

There are no prominent Hg lines the red part of the spectrum; therefore, it is impossible to calibrate the wavelength scale across the entire range of the spectrometer using only the room lights. However, a commonly available Ne lamp has a rich spectrum of lines (Figure 6) in the red (hence the orange glow) and the combination of the blue Hg lines and the red lines from a neon lamp provides complete coverage.

A wavelength solution for the USB 2000 spectrograph can be constructed by combining the atomic data in Table 1 and Table 2 with measurements of line positions (see **Error! Reference source not found.** and Figure 7). The details of the wavelength solution are discussed in the Appendix.

Table 1: Bright atomic mercury lines². The pixel position is the measured line position.

Relative Intensity	Air wavelength (nm)	Pixel	ID	Relative Intensity	Air wavelength (nm)	Pixel	ID
600	365.0153	101.7	Hg I	100	434.7494		Hg I
70	365.4836		Hg I	1000	435.8328	479.1	Hg I
50	366.3279		Hg I	500	546.0735	1115.2	Hg I
400	404.6563	310.2	Hg I	50	576.9598	1306.4	Hg I
60	433.9223		Hg I	60	579.0663	1319.8	Hg I

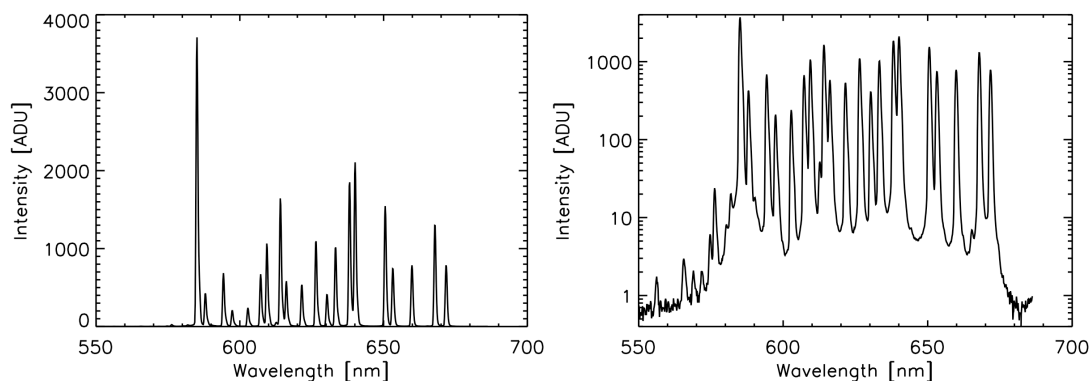


Figure 6: Spectrum of a Ne lamp showing bright emission lines. This is an average of 1000, 60-ms exposures. The data have been dark subtracted. The left hand spectrum is on a linear scale. The right hand plot uses a log scale on the y-axis to show weak features.

Table 2: Bright Ne I lines and measured pixel positions on the USB 2000 spectrometer. Lines without measurements are either too faint or blended with adjacent lines.

Relative Intensity	Air wavelength (nm)	Pixel	ID	Relative Intensity	Air wavelength (nm)	Pixel	ID
200	540.05618	1078.5	Ne I	100	614.30626	1547.1	Ne I
200	585.24879	1358.6	Ne I	100	616.35939	1560.6	Ne I
50	587.28275		Ne I	100	621.72812	1596.4	Ne I
100	588.18952		Ne I	100	626.6495	1629.5	Ne I
50	594.48342	1417.8	Ne I	100	633.44278	1675.4	Ne I
50	596.5471		Ne I	100	638.29917	1708.6	Ne I
50	597.46273		Ne I	200	640.2248	1721.7	Ne I
60	597.5534		Ne I	150	650.65281	1794.0	Ne I
100	602.99969		Ne I	100	659.89529	1858.8	Ne I
100	607.43377		Ne I	50	667.82762	1915.1	Ne I

² Data from the National Institute of Standards (NIST)

<http://physics.nist.gov/PhysRefData/Handbook/Tables/mercurytable2.htm>

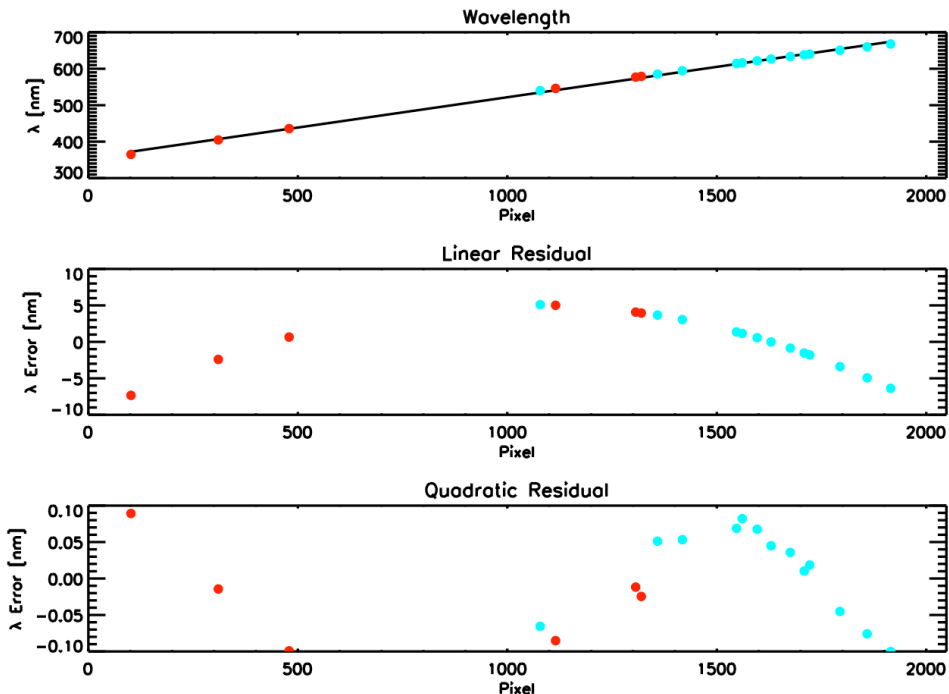


Figure 7: Combined line positions from Hg I lines (red) and Ne I lines (cyan). The central panel shows the deviation between the data and a straight line fit. The bottom panel shows the residual from a quadratic fit. Evidently, a higher order polynomial fit is called for.

Taking multiple spectra

You can take multiple spectra by clicking on the disk icon and selecting the save information each time. This quickly gets tiresome, so you should use the “File/Save/Save Spectrum” option to collect multiple files (Figure 8). Figure 8 shows the setup for saving a sequence of 100 scans. Each scan is automatically given a file name that includes a number that is incremented by one after every new scan. To collect an additional set of data press control-S—the file numbers will automatically increment so that your original data are not overwritten.

Note if you have pressed that pause button data acquisition will not start until you push the green “go” button (Figure 4). However, continuous acquisition mode will continue, even after all your files have been written to disk. Once you have used this option use “File/ Save/ Configure Export” to change base file name or the number of files that you want saved.

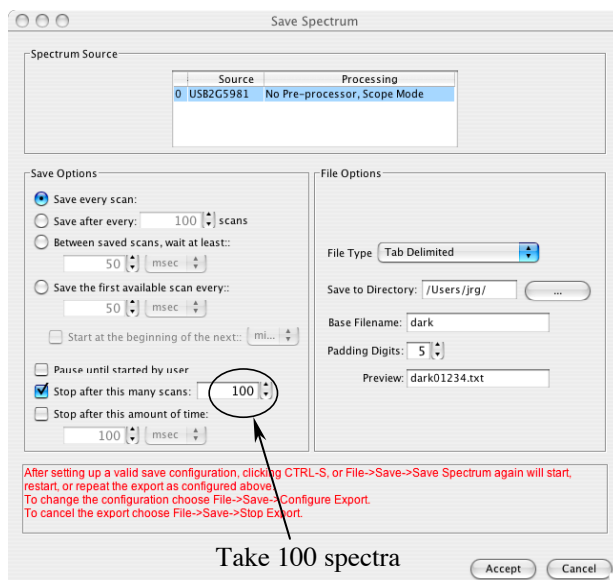


Figure 8: The Save Spectrum window lets you save multiple scans automatically. The example shown here will save 100 frames starting with file name /Users/jrg/dark00000.txt. The files are saved as plain ASCII text.

Read noise & Gain

Figure 9 shows the spectrum of a desk lamp equipped with a quartz halogen lamp. The spectrum should be continuous without any sharp features, so the wiggles seen in the spectrum represent the spectral response of the spectrograph due to the optical filter transmission, the grating efficiency, and transmission of the anti-reflection coating on the CCD, all of which vary with wavelength. This plot is formed from the average of 1024 individual spectra, which have been dark subtracted. Note that even the fine wiggles are common to both spectra: these are likely due to pixel-to-pixel variations (flat field).

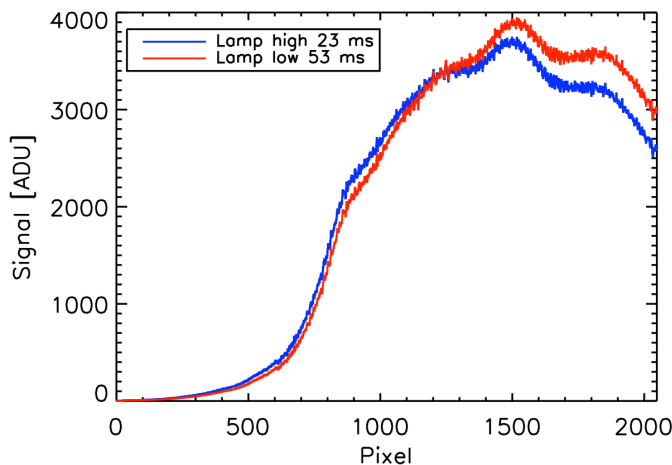


Figure 9: Two spectra of a quartz halogen desk lamp. The lamp has two brightness settings, denoted here high and low. These spectra are the average of 1024 individual spectra. The spectra have been dark subtracted. Note that the spectrum of the lamp in the low setting is “redder.” The small-scale fluctuations reproduce from spectrum to spectrum suggesting that these represent pixel-to-pixel gain variation across the array (flat field variations). Note that in the low setting the spectrum is redder than in the high setting.

The noise properties of the spectrograph can be investigated by computing the mean and variance for each pixel from the time sequence. Figure 10 gives an example for pixel number 1000 of the time sequence of samples from which these statistics are computed. It is important to examine such sequences to make sure that the variance is not dominated by external factors, such as varying illumination.

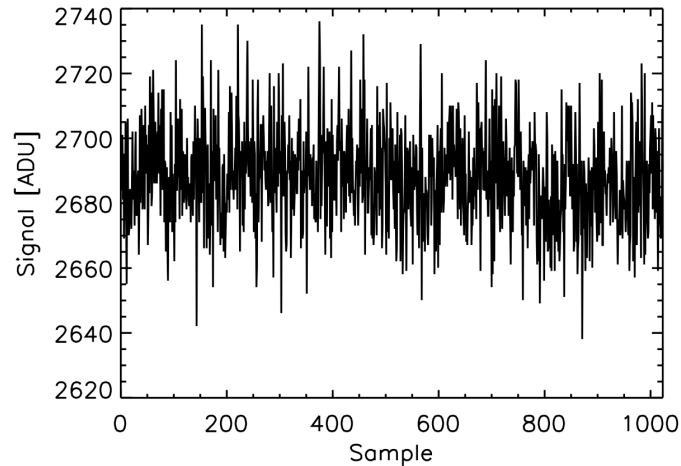


Figure 10: The time series of pixel values (dark subtracted) for pixel 1000 in the array. The mean and variance for all 2048 pixels is show in Error! Reference source not found..

Figure 11 shows the associated average Fourier power spectrum. The spectrum is flat showing that the noise is largely uncorrelated (white noise). There is a strong harmonic peak, which may correspond to aliased 60 Hz power line variation.

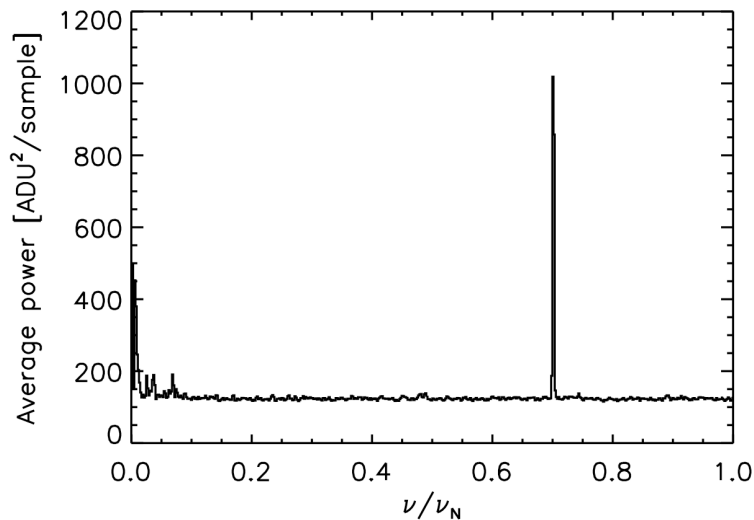


Figure 11: Average Fourier power spectrum of all 2048 pixel time series—Figure 10 shows an example of one such time series. The x -axis is in units of the Nyquist frequency. Assuming no lag between exposures this corresponds to $0.5/23\text{ms} = 21.7\text{ Hz}$, and the strong peak at 0.70 lies at 15.2 Hz . This may represent aliased power from 60 Hz line frequency as $21.7(0.70 + 2) = 59\text{ Hz}$.

You will be using the relation between the variance and the mean of your data values to determine the readnoise and gain of the spectrometer’s detector.

At low signal levels the noise is independent of signal. Above about 100 ADU the noise starts to increase and continues through about 40,000 ADU. In this interval the relation between variance and mean is approximately linear, indicating that Poisson noise dominates. The data from these 2048 pixels is well described by a linear relation between the measured variance, s^2 , and the mean pixel value, x .

$$s_{ADU}^2 = s_0^2 + kx_{ADU}$$

Here the intercept s_0 represents a constant additive measurement noise (the read noise) and k , which depends on the “gain”, i.e. the conversion from photoelectrons to ADU. At the highest flux levels, it is evident that the noise falls below the Poisson value, which strongly suggest that the signal is no longer proportional to the incident flux. The maximum signal value is $2^{16}-1 = 65535$, i.e., the analog to digital converter is 16-bit, but between 40,000 ADU and this hard cut-off the turn over in noise suggest that the CCD, the amplification stage, or the analog to digital converter itself exhibits non-linear behavior.

Appendix A: Manufacturer’s Specifications

The data sheet provided by Ocean Optics with the USB 2000 spectrometer lists the nominal properties given in Table 3.

Table 3: Nominal spectrometer properties

Property	Value
Model	USB 2000
Serial No.	USB2+H05261
Grating	1200 line holographic VIS
Bandwidth	350-660 nm
Options	L2 lens, 25 μm slit, WG305 filter
CCD	Sony ILX511 1 \times 2048 pixel
Pixel size	14 μm \times 200 μm
Pixel well depth	62,500 electrons
A/D resolution	16-bit
Dark noise	2.5 counts RMS
Focal length	42 mm input, 68 mm output
Integration time	1 ms—65 s

The image sensor is a 2048-pixel linear CCD manufactured by Sony, part number ILX511. The ILX511 is a rectangular reduction-type CCD designed for bar code hand scanners and optical measuring equipment use. The pixel size is 14 μm \times 200 μm . The chip has a built-in timing generator and clock drivers and packaged in a 22 -pin DIP.

Appendix B: Manufacturer's wavelength calibration

The spectrometer has a built in processor that uses pre-measured third-order polynomial to convert pixel number to wavelength, so you actually get two columns in the data file, where the first number is an estimate of the wavelength in nm based on a polynomial expression of the form

$$\lambda_i = \sum_{j=0}^3 a_j i^j = a_0 + a_1 i + a_2 i^2 + a_3 i^3 \dots, \quad (2)$$

where i is the pixel value. The manufacturer's values are given in Table 1.

Table 4: Manufacturer's wavelength calibration

Coefficient	Value
a_0	365.7268923
a_1	0.197792654
a_2	-1.44488×10^{-5}
a_3	-5.63994×10^{-10}

To check whether or not the nominal values are loaded go to Spectrometer/Spectrometer Features and inspect the table that appears when you click the Wavelength tab (Figure 12). Check that the wavelength table contains the nominal values. Also inspect the stray light and nonlinearity values under their respective tabs to make sure that these are all set to zero, otherwise the data that you retrieve from the spectrometer will be confusing!

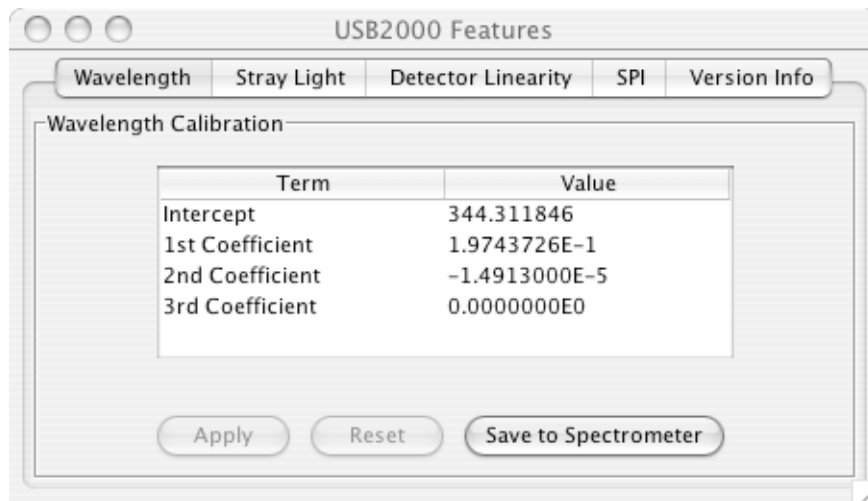


Figure 12: The wavelength calibration coefficients in use can be view via the menu item Spectrometer/Spectrometer Features.

Appendix C: Polynomial wavelength calibration

The manufacturer uses a polynomial wavelength solution. Why is this approximation an appropriate choice? The grating equation determines the position of a given wavelength on the detector array given an angle of incidence, α , wavelength, λ , and groove spacing, σ ,

$$m\lambda/\sigma = \sin \alpha + \sin \beta, \quad (3)$$

assuming that the incident light is perpendicular to the grooves on the ruling. The pixel location corresponding to some angle of diffraction, β , is determined by the focal length, f , of the camera

$$p = p_0 + f \tan(\beta - \beta_0), \quad (4)$$

where p_0 is some reference pixel where the wavelength is λ_0 . Thus,

$$p = p_0 + f \tan[\arcsin(m\lambda/\sigma - \sin \alpha) - \beta_0]. \quad (5)$$

The residuals to a non-linear least squares fit to Eq. (5) using the data listed in Table 1 and Table 2 is shown in Figure 13. The residuals to a polynomial fit are also shown. Figure 13 shows that Eq. (5) is not a complete description of our spectrometer: perhaps there are errors in the photolithographic mask used to make the CCD or more likely the camera optics exhibit distortion such that the focal length is a function of field angle.

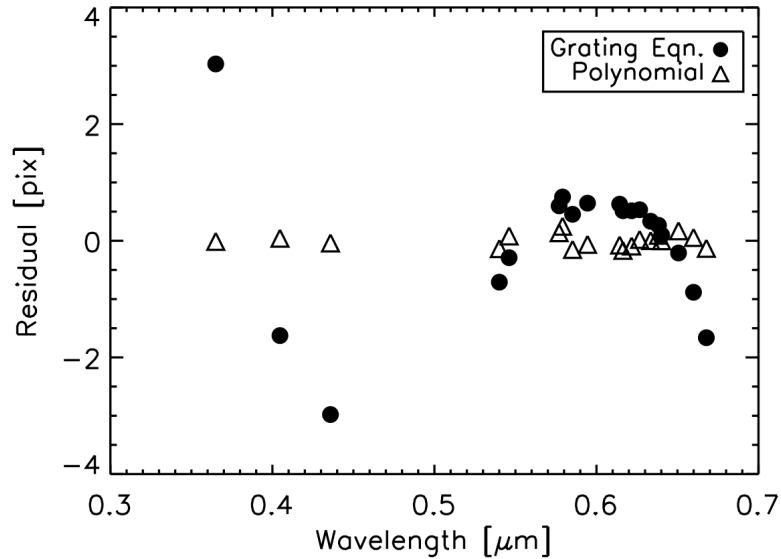


Figure 13: Wavelength residuals to a fit to the Ne I and Hg I data listed in Table 1 and Table 2 using Eq. (5). The fit assumes $m = 1$, 1200 grooves per mm, $14 \mu\text{m}$ pixels, and a semi-opening angle of $\phi = 15^\circ$. The best fit parameters are the camera focal length, $f = 61.6 \pm 0.2$ mm and $\theta = 9.9 \pm 0.1^\circ$, where $\alpha = \theta + \phi$ and $\beta = \theta - \phi$. The residuals are 1.2 pixels rms. A strong cubic residual is evident. A fifth order polynomial fit is much superior, with residuals of 0.1 pixels rms.

A polynomial solution is justified, by making a Taylor expansion about λ_0 , which yields

$$\begin{aligned}
 p = p_0 &+ f \frac{m}{\sigma \cos \beta_0} (\lambda - \lambda_0) \\
 &+ \frac{f}{2} \frac{m^2 \tan \beta_0}{\sigma^2 \cos^2 \beta_0} (\lambda - \lambda_0)^2 \\
 &+ \frac{f}{2} \frac{m^3}{\sigma^3 \cos^5 \beta_0} (\lambda - \lambda_0)^3 \\
 &+ O((\lambda - \lambda_0)^4).
 \end{aligned}$$

Evidently the wavelength solution can be approximated by polynomial. Note that both odd and even powers are present in the expansion. The coefficients are not independent, but this information is discarded when a polynomial solution is adopted.