Supplementary Information: Calibration of the Spectrometer

Calibration Needs

Each spectrometer is manually assembled using 3D printed parts to hold the collimator, LVF and photodiode array together. The manual assembly, and the variation in the parts used, leads to some variability from spectrometer to spectrometer. Before meaningful data can be extracted, calibration measurements need to be taken with each spectrometer. Calibration measurements include: 1. measurement of a wavelength standard, 2. measurement of the resolution 3. dark current measurement, 4. bright field measurement

Alongside bright field measurements, dark current measurements are necessary because dark current and responsivity vary from pixel to pixel due to variations in the InGaAs and the electronics used. These variations are accounted for through dark current subtraction and bright field (or flat field) correction. The dark current measurements were taken illumination source off. Traditional bright field correction is performed by illuminating all pixels with equal light and measuring the varied responses. However, this cannot easily be done once the linear variable filter (LVF) is in place. Thus, modified bright field measurements were performed by illuminating the spectrometer with a source of known broad spectrum that illuminates every wavelength region of the spectrometer.

The spectrometer studied in this work outputs the intensity data in an analog video signal where the intensity measured at each pixel is represented by a voltage with each pixel corresponding to a particular wavelength. Thus, wavelength calibration is required to determine the wavelength of light measured by each pixel. For this calibration, a krypton calibration lamp with a known spectrum and clearly defined sharp peaks is used. Dark current measurements are taken in a lab and in a temperature controlled chamber to get noise characteristics. Finally a bright field spectrum from a broad tungsten halogen bulb is used to calibrate the spectrometer for measurements.

Calibration Methods

The data collection was done using the development board provided by Hamamatsu corporation and the Teensy microcontroller-based data collection system described earlier[31]. Wavelength calibration was done using a Krypton arc lamp. The spectrometer was placed 25 mm away from the lamp and a spectrum was taken with an integration time of 8.5 ms. The peaks of the measured spectrum correspond to known wavelengths[32], allowing certain pixels to be matched to the known wavelengths. A linear calibration vector was then built and used for a pixel-to-wavelength conversion.

The dark current was measured by taking several spectrums while the spectrometer was not illuminated. The cycle time was 10 ms, with an integration period of 8.5 ms and a data collection period of 1.5 ms. The spectra were averaged together to yield a dark current offset.

Spectrometer noise performance and temperature dependance were characterized in a temperature-controlled chamber at 25 °C. To characterize noise, dark current was measured in a temperature-controlled chamber for 20+ hours. The charge from each pixel was converted to an analog video signal and all 128 pixels were recorded every 10 ms by the microcontroller.

The temperature dependence of the spectrometer dark signal was measured. In this test the chamber temperature was varied in a controlled manner in the range of 0-40°C while collecting data with the non-illuminated spectrometer. As with the noise measurements, data was recorded every 10 ms.

Bright field calibrations are done by illuminating the spectrometer with a broad tungsten halogen (Ocean Optics LS-1) source. To mimic the expected applications and eliminate shadowing by the collimator, the light was scattered using a diffuse reflector (Thorlabs DG10-120-P01) prior to detection (Figure S1). The spectrum was collected using the Hamamatsu development board with an integration time of 8.5 ms. The resulting spectrum is then used to make a brightfield calibration vector to correct for the pixel-to-pixel variation. First, the dark current is subtracted from the spectrum, then because the source should have a smooth continuous spectrum a 5-boxcar average is used to smooth each pixel giving us a bright field value for each pixel. The value is divided by the non-averaged pixel value to get a vector that can be multiplied by a spectrum to correct for the bright field.

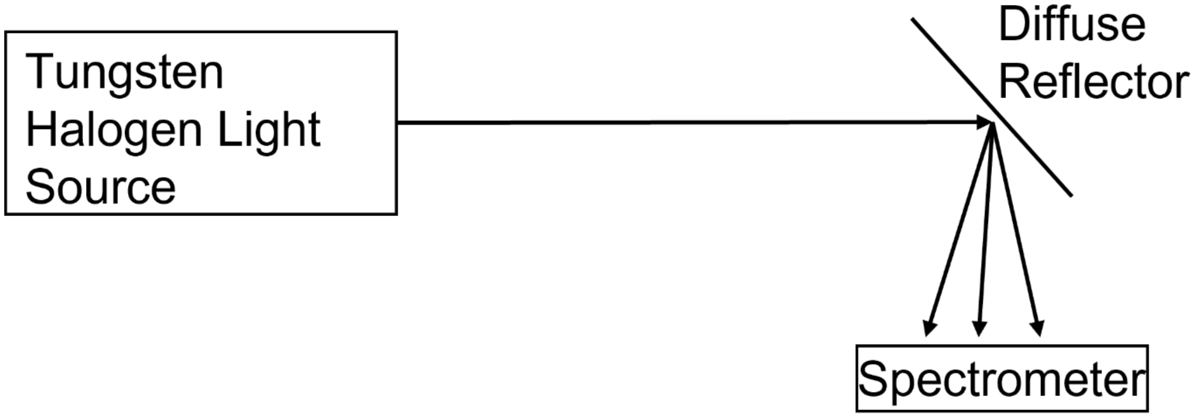


Figure S1) Setup for bright field testing. Using a tungsten halogen bulb and a diffuse reflector, a scattered broad spectrum illuminates the spectrometer. The resulting data can be used to calculate the bright field correction for the spectrometer.

The resolution of the spectrometer was calculated using a spectrally narrow source at various wavelengths. In the main text this was done with a monochromator; here it was also done using the krypton arc lamp. The resolution of the spectrometer is determined by the full width half max (FWHM) of the sharpest peak (1363 nm).

Using the diffuse reflector to scatter light from five LEDs (Marktech 1050 nm, 1300 nm, 1550 nm, 2x 1650 nm), the effect of dark current and bright field corrections are shown. The raw spectrum from the LEDs is collected using the Hamamatsu development board. The dark current is then subtracted from the spectrum and the bright field correction applied.

Calibration Results

A Krypton arc lamp gives off a known spectrum with narrow peaks at known wavelengths (such as 975 nm, 1363 nm, 1442 nm, 1523 nm). A spectrum collected from our spectrometer when illuminated by a Krypton arc lamp is shown in figure S2. The collected spectrum is overlaid with the peaks using a peak-finder application and their relative sizes. This gives multiple calibration points from which the rest of the wavelengths are extrapolated assuming a linear fit in between data points. The pixel-to-pixel spacing is approximately 6 nm.

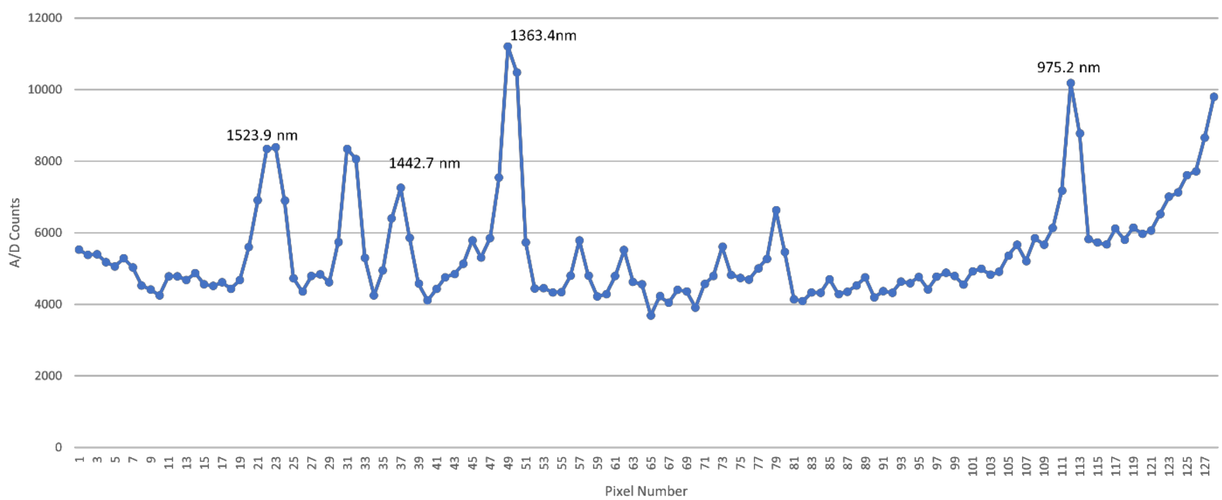


Figure S2) The spectrum of light collected from a kypton arc lamp. Light is collected from a krypton arc lamp and a spectrum measured. The peaks in the spectrum match with known peaks from the krypton source.

With a means of calibrating each spectrometer, we can look at the spectrometer-to-spectrometer variations between builds. With the pixel pitch of the photodiode array being 50 µm, a slight shift during assembly will result in a shift in wavelength. A few devices were calibrated and compared to each other by plotting them on the same scale as shown in figure S3. The location of the peaks varies by up to two pixels. The height and width of the peaks also vary. Note that the LVF was oriented in the opposite direction as figure S2. All the devices were measured under the same conditions, but the spectrum of each device is unique and need to be normalized for use.

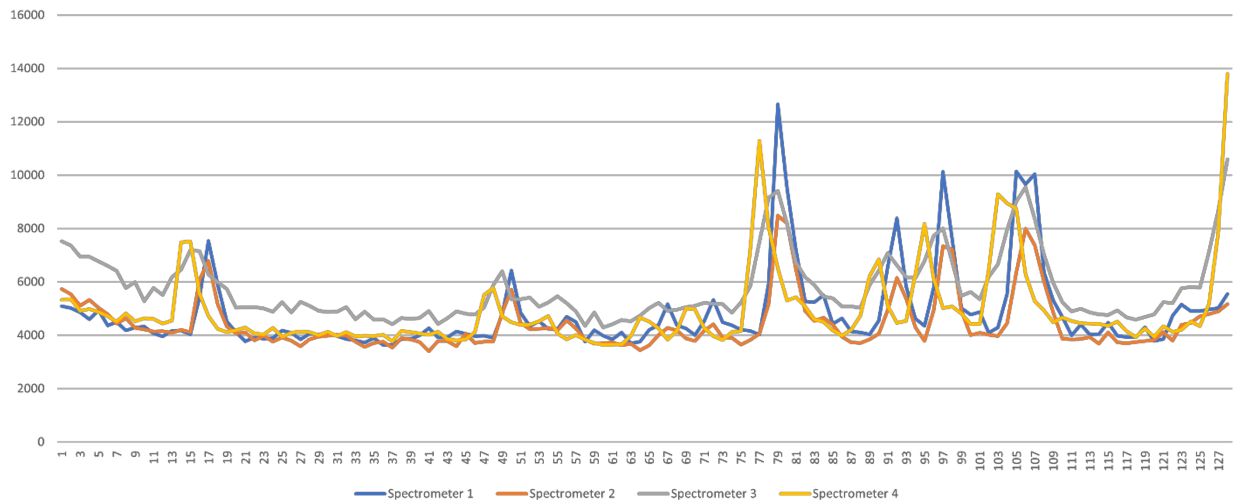


Figure S3) Four different spectrometers measure the same spectrum from a krypton arc lamp. The krypton spectrum can be used as a way to see the differences in the spectrometers from build to build.

Dark current measurements allowed for the development of a dark current correction vector. The dark spectrum was collected every 10 ms for three second total. These spectra were then averaged together to produce figure S4. Figure S4 shows the different dark current from pixel to pixel. This spectrum is subtracted from an illuminated spectrum to perform the dark current correction.

For a time period of 20+ hours the spectrometer collected data at constant temperature in 10 ms intervals. The spectrometer was blocked from light to study the noise in the dark current. The mean (over multiple

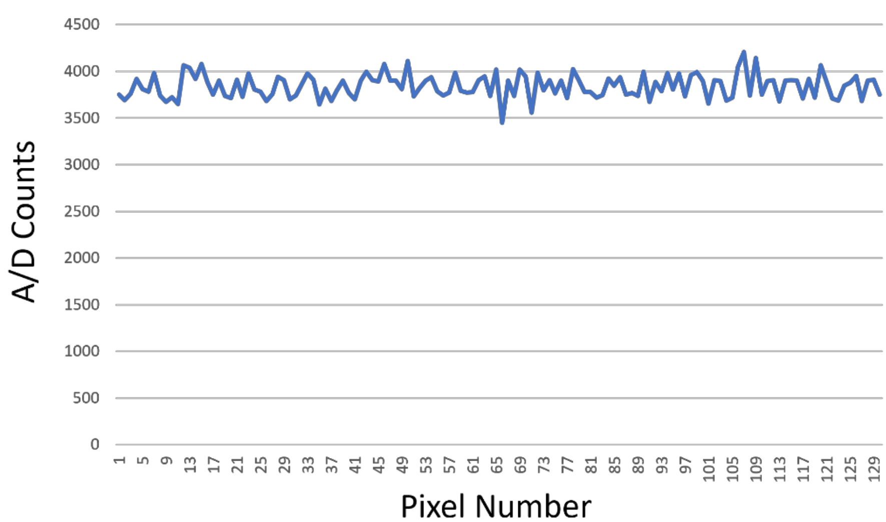


Figure S4). A dark current measurement. By taking measurements with the spectrometer with the light source turned off a signal that is due to the dark current in the electronics. This spectrum can be subtracted from any spectra collected by the spectrometer to improve the signal

measurements) dark current (~1200 ADC counts) was subtracted from each data point (figure S5 top). Grouping the results into 1000 equal size bins the standard deviation was calculated and plotted in S5 bottom. The standard deviation was calculated to be 6 ADC counts, which coverts to a noise level of -28 dB.

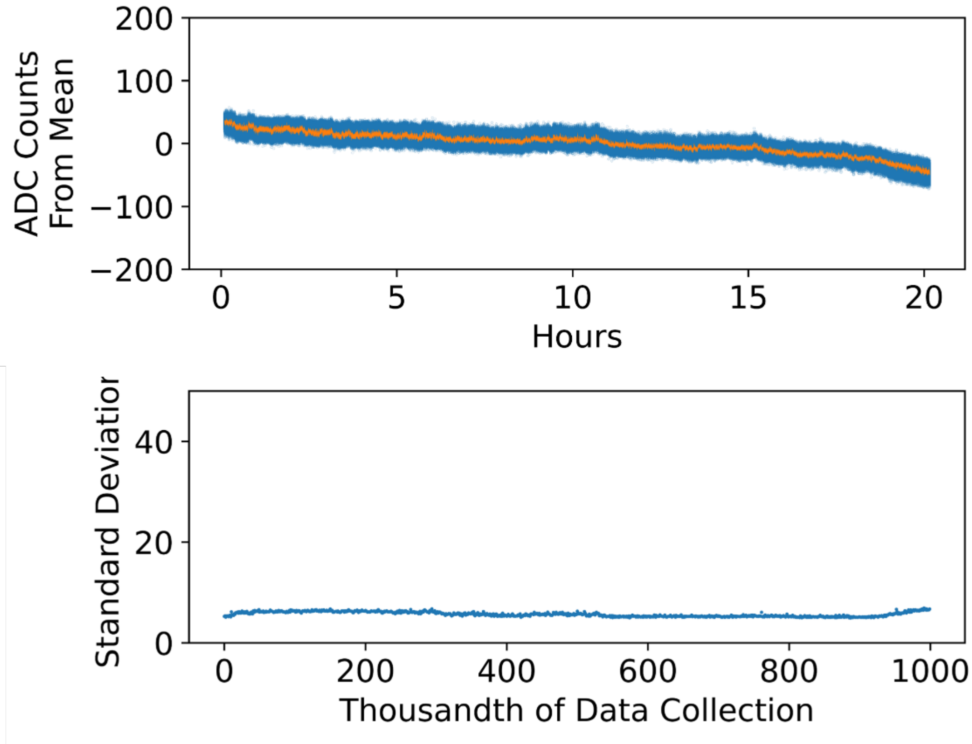
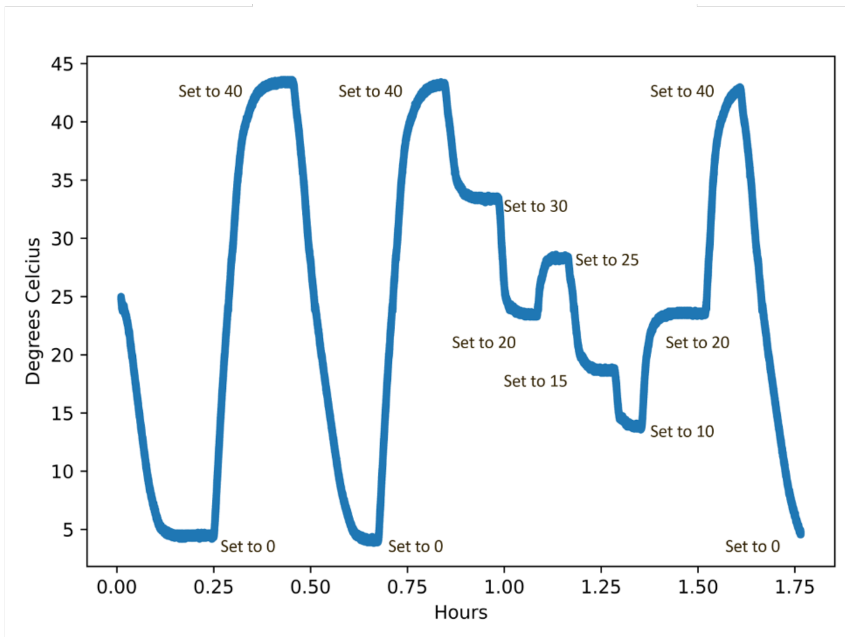


Figure S5). Dark current measurements at a constant temperature. Top) Showing one pixel measured in time, the dark current fluctuations are plotted with the mean dark current removed. Bottom) The data from the top graph is grouped into 1000 bins of equal size and the standard deviation calculated and plotted. The mean standard deviation was found to be 6 ADC counts, which equates a noise of -28 dB.

A shorter run of 1.75 hours with varying temperatures measured the change in the dark current with temperature (Figure S6 bottom). The temperature-controlled chamber was programmed with the temperature profile in figure S6 top. While ranging the temperatures from 0-40 °C, the dark current of a single pixel varied from 600 ADC to 1600 ADC counts. As temperature increases the ADC counts also increase. While the base ADC counts do not directly correlate with a given temperature, large changes in temperature yield more drastic changes in ADC counts.



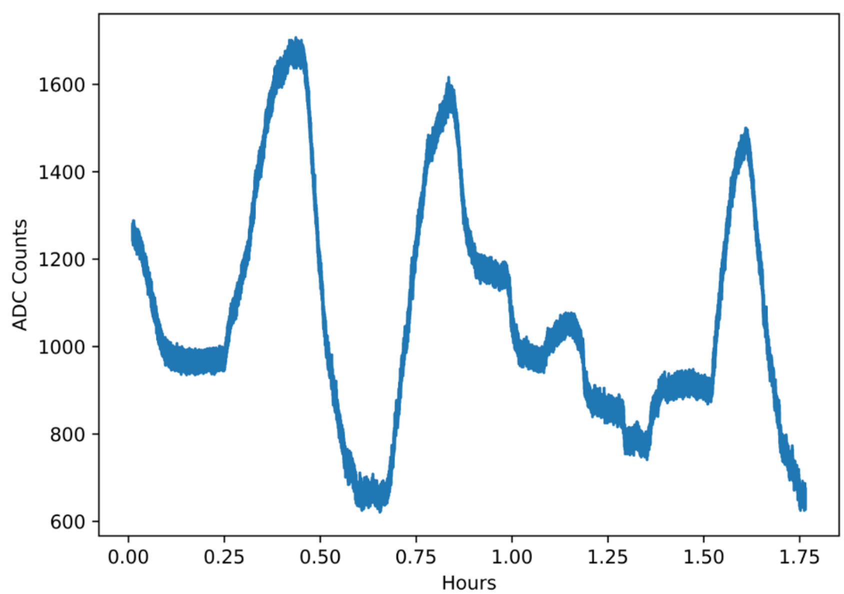


Figure S6) Dark current measurements with changing temperature. Top) The temperature profile input into the temperature controlled chamber. Bottom) The dark current measurements for 1 pixel with changing temperature.

Bright field calibration is developed from a measurement made by illuminating the spectrometer with a tungsten halogen light source (Figure S7). In the raw spectrum, there are some noticeable pixel-to-pixel fluctuations.

After dark current subtraction, a pixel-by-pixel vector is developed to normalize the spectrum to match the light source. This is then applied to future measurements.

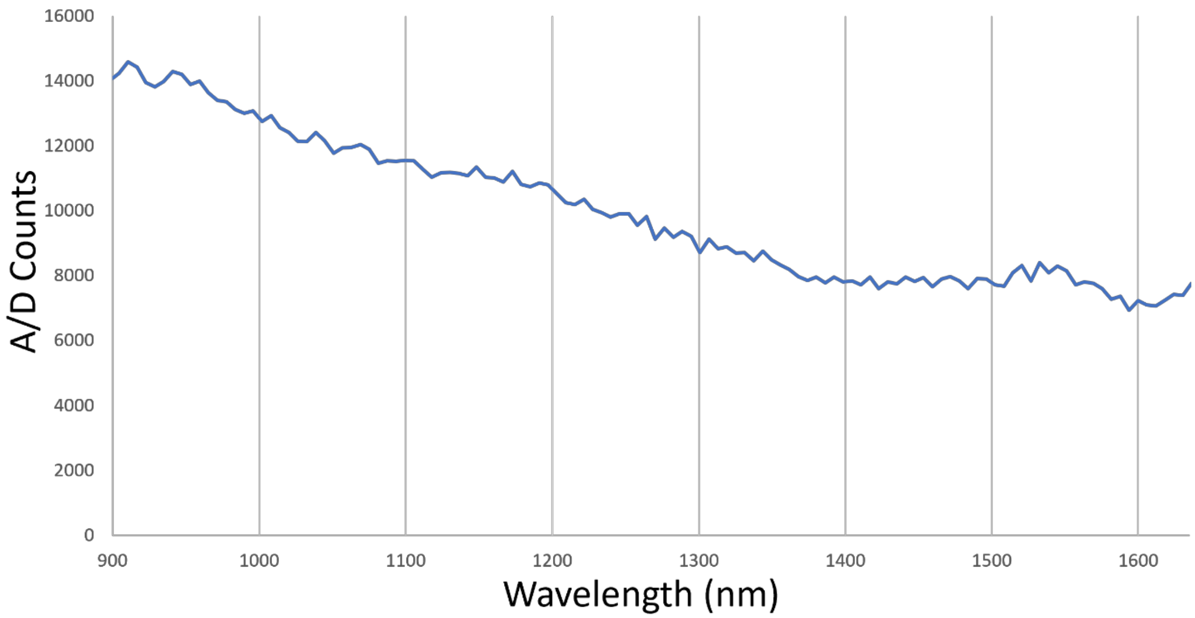


Figure S7) The spectrum collected from a tungsten halogen source. The bright field vector is calculated using the spectrum and averaging the nearest pixels in a 5-boxcar average.

Using five LEDs the spectrometer is illuminated off a diffuse reflector to collect a spectrum (Figure S8 top). The spectrum in figure S8 has artifacts of both the dark current and the variations in pixel responsivity. Most notable is the dip in the spectrum just before 1500 nm. Applying the dark field subtraction and bright field calibration to the original spectrum, we get a corrected spectrum (Fig S8 bottom). This corrected spectrum is smoother than the raw spectrum collected. Looking just before 1500 nm, the raw waveform has a dip in intensity, after calibration that dip is no longer there. The “roughness” of the signal around 1200 nm is also reduced after calibration.

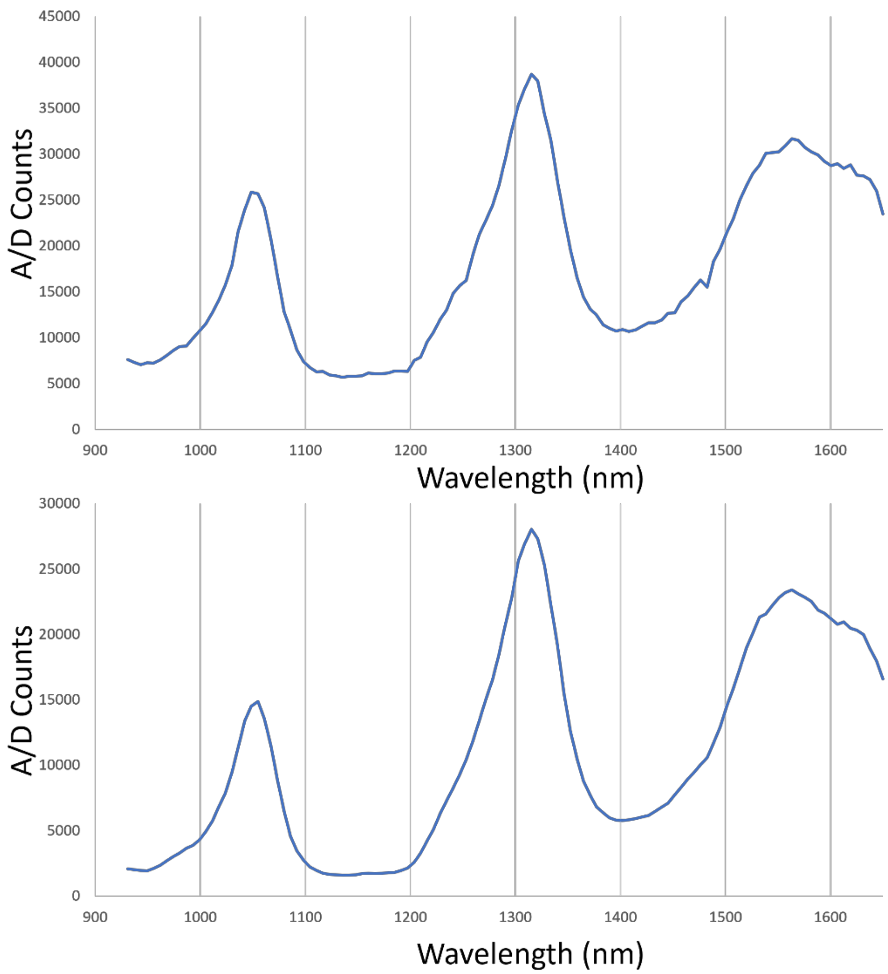


Figure S8) Bright field calibrations. Top) The raw spectrum collected from the LEDs off a diffuse reflector. Bottom) The spectrum from the LEDs off a diffuse reflector after dark current subtraction and bright field correction.

Discussion

A krypton arc lamp provides a reliable metric to test each spectrometer build, to both calibrate each device by wavelength and determine the spectrometer-to-spectrometer variations in wavelength and resolution. The spectra from figure S2 to S3 are flipped, due to the orientation of the LVF in reference to the photodiode array. The orientation of the LVF to the photodiode array is arbitrary during assembly. If careful care is not taken, the spectrometers can output spectral features at very different pixel numbers. In figure S3 there appears to be a 2-pixel shift from spectrometer 1 to 4; this would result in about a 12 nm shift between spectrometers. The linear calibration vector assumes that the change in wavelength is linear between two known points. While this assumption is accurate when the points are close, the further their distance the more error in the assumption. We use as many if the features that are resolved in the krypton spectrum to minimize this error.

After wavelength calibration, the resolution of the spectrometer can be calculated by looking at a sharp peak like the one at 1363 nm. By taking the full width half max of the peak, we determine the resolution of the spectrometer at that wavelength. A typical spectrometer has a resolution of 13-14 nm at the 1363nm peak. Spectrometer 3 is unique, as the majority of the spectrum is higher than the other 3 spectrometers and its peaks are broader. This indicates that the collimator used to build this spectrometer was shorter than the rest, allowing more light through while broadening each peak. This is also represented in the much lower resolution of this device (~20 nm). This method of testing spectrometers allows for an analysis of the unit as a whole, which could help with quality control of the devices.

The dark current measurements are straightforward; due to laboratory light outputting little to no light in the 900-1700 nm range, a dark current measurement could be made in an open indoor room while the spectrometer illumination sources are off. The InGaAs photodiode is nonresponsive to light outside the 900-1700 nm range. Several dark scans were collected and averaged to minimize noise in the dark measurement.

The integration time for the noise performance was chosen to be 8.5 ms as this is the expected application-based integration time. All the measurements thus far were collected using the development board provided by Hamamatsu. Hamamatsu also provided the collection software, but that software was designed to take single spectra or continuous spectra for a minute or two. This was not suitable for a long multi-hour run. We solved this by building a collection system using a Teensy 3.5 microcontroller. The collection system was designed to have lower noise than the expected noise from the Hamamatsu detector.

The standard deviation of the collection system noise was -28dB. Calculations based on datasheets of the Hamamatsu detector found the primary source of the noise to be the write noise of the device. While it would be preferential to be shot noise limited, the write noise was related to the read out integrated circuit (ROIC) on the Hamamatsu diode and was not alterable for this work. Further optimizations could be possible but were not the focus of this work as the noise is small compared to the full scale.

InGaAs detectors have sensitivity to changes in ambient temperature. It was important to verify the dependance for future temperature-based calibrations. Using the temperature-controlled chamber, temperatures could be reliably varied. Figure S6 gives a clear temperature dependance with the base A/D counts rising with increased temperature. The counts had a range of about 1000 A/D counts from 0-40°C. Even small changes in temperature had large changes in the dark current offset when compared to the noise. The spectrometer seemed to become less sensitive to high temperature swings as the experiment continued. This can be seen as the peaks get lower with each 40 °C measurement. This may be due to shorter time at each point, which may have been too short for the temperature to stabilize.

Bright field measurements were collected using a tungsten halogen source as it was a smooth broad source. The assumption was made that the illumination intensity for a nearby pixel was expected to be the same, justifying the use of the boxcar average. While not an ideal bright field, it is close and can still improve data quality. In a production setting, a bright field would be collected before spectrometer assembly; this would enable a flat field measurement to be taken and averaged. This was not practical as several spectrometers have been built and there is not a straightforward way to identify the individual photodiodes when not a part of a spectrometer. This would not be an issue in a production environment. A possible source of error in this calibration depends on how normal the spectrometer is to the brightfield. If the spectrometer is at an angle there will be a skew in the bright field. We minimized this effect by only accounting for nearby pixels.

Using the dark current and bright field calibrations, the quality of the measured spectrum can be improved. The spectrum collected from LEDs can be smoothed out. LEDs were chosen as a baseline for the spectrum going into the body for human subjects testing. The calibration also gives more meaning to the individual intensity values as the gain from pixel to pixel is accounted for. All of the calibrations shown here are important to have done for each spectrometer to ensure quality control and quality data.

Conclusions

A method of calibrating each spectrometer built, while establishing a means to look at the quality control of a group of spectrometers is shown. While none of the techniques used here were novel in their approaches, they were important steps in calibrating and validating the spectrometer shown in this work.

We have shown that wavelength calibration is important as a quality control for each spectrometer because of the variation in the alignment of the linear variable filter with the photodiode array and height of the collimator. A small shift in the filter location can offset a wavelength peak by 1 to 2 pixels, which corresponds to 6-12 nm. The quality control can also act as a check for validating that the collimator heights between units are within a given tolerance, as shorter collimators will have larger base ADC counts and broader peaks.

We have shown the importance of dark current and bright field calibrations as well as quantifying the dark current noise. The dark current noise was small at -28dB but does limit the signal to noise if used in a highly sensitive measurement. Temperature fluctuations will need further study to quantify the expected change with temperature in a wearable application. Using the spectrometer in a well understood test we were able to develop calibration vectors to improve the quality of measured signals. We are able to reduce the "jaggedy" nature of the raw waveform to more accurately represent the collected spectrum. The calibration gives more meaning to the data by translating pixels to wavelengths and by decreasing inaccuracies related to variation in intensity. It is important moving forward for these calibrations to be performed for each spectrometer.

CAD models for Spectrometer holders

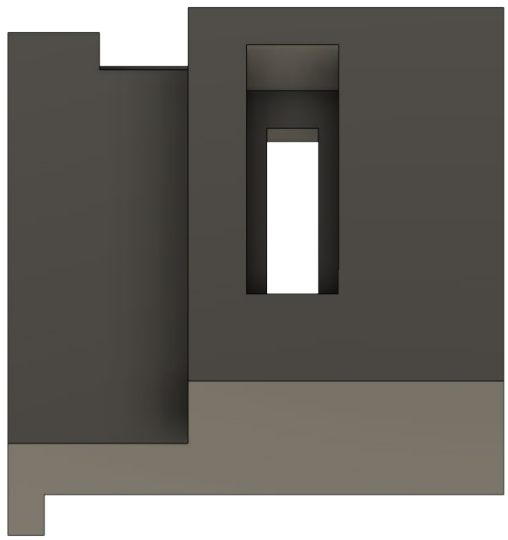


Figure S9). *CAD model of spectrometer holder for LEDs. A holder for the spectrometer with a flat to be able to place an LED board on.*

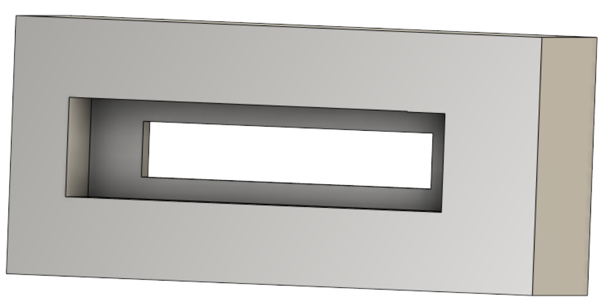


Figure S10). *CAD model of spectrometer holder. A spectrometer holder for experiments that do not require LEDs*