Understanding Spectrometer Signal to Noise

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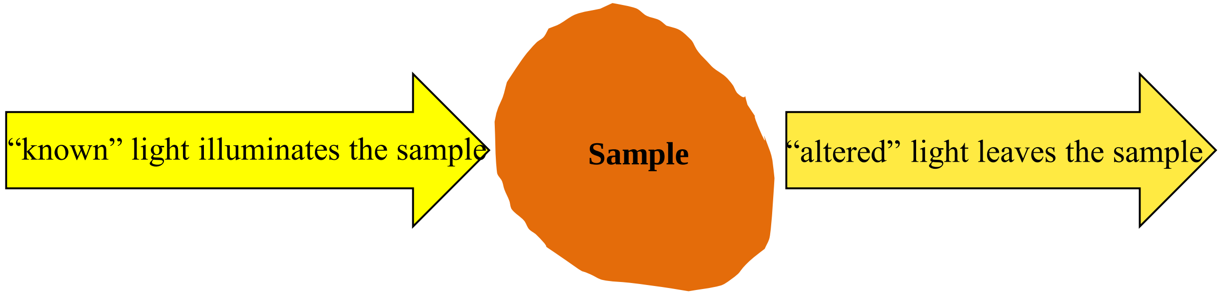
- Application Examples
- Spectrometer Fundamentals
- Spectrometer Signal generation
- Digital Data Considerations
- Practical examples

Application Examples

Spectroscopy Techniques

- Divided into two broad classes: **absorption spectroscopy** and **emission spectroscopy.**
- In absorption spectroscopy, "known" light illuminates the sample. The light may pass through (transmit) the sample or reflect from it. The transmitted or reflected light differs from the "known" light. The change, among other factors, is a function of the sample's chemical composition.

Basic Idea of Absorption Spectroscopy



Absorption Spectroscopy

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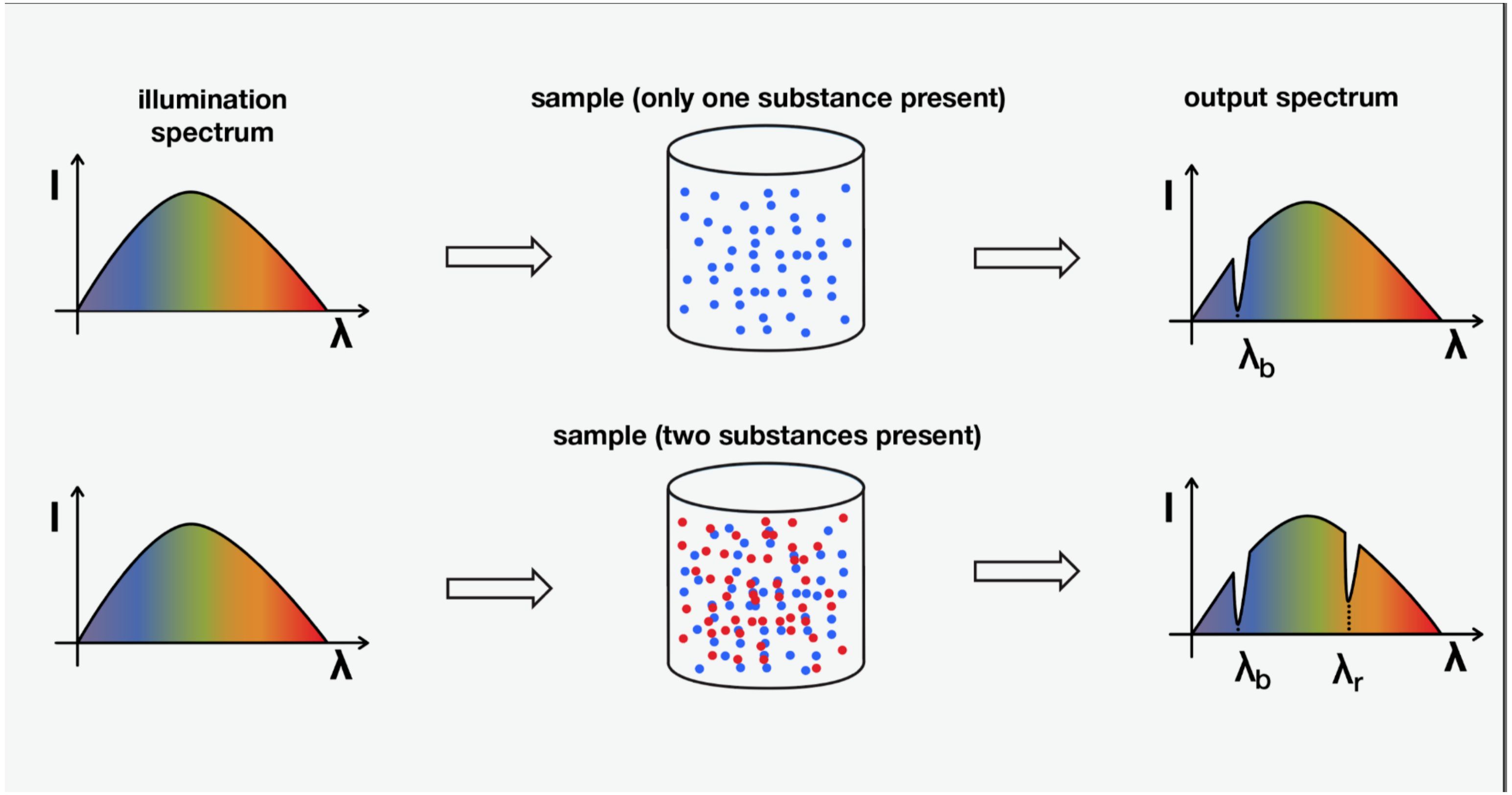
- Each substance has a unique spectral signature. The output spectrum will show the absorption features only if the incoming illumination contains the wavelengths at for which absorption occurs.

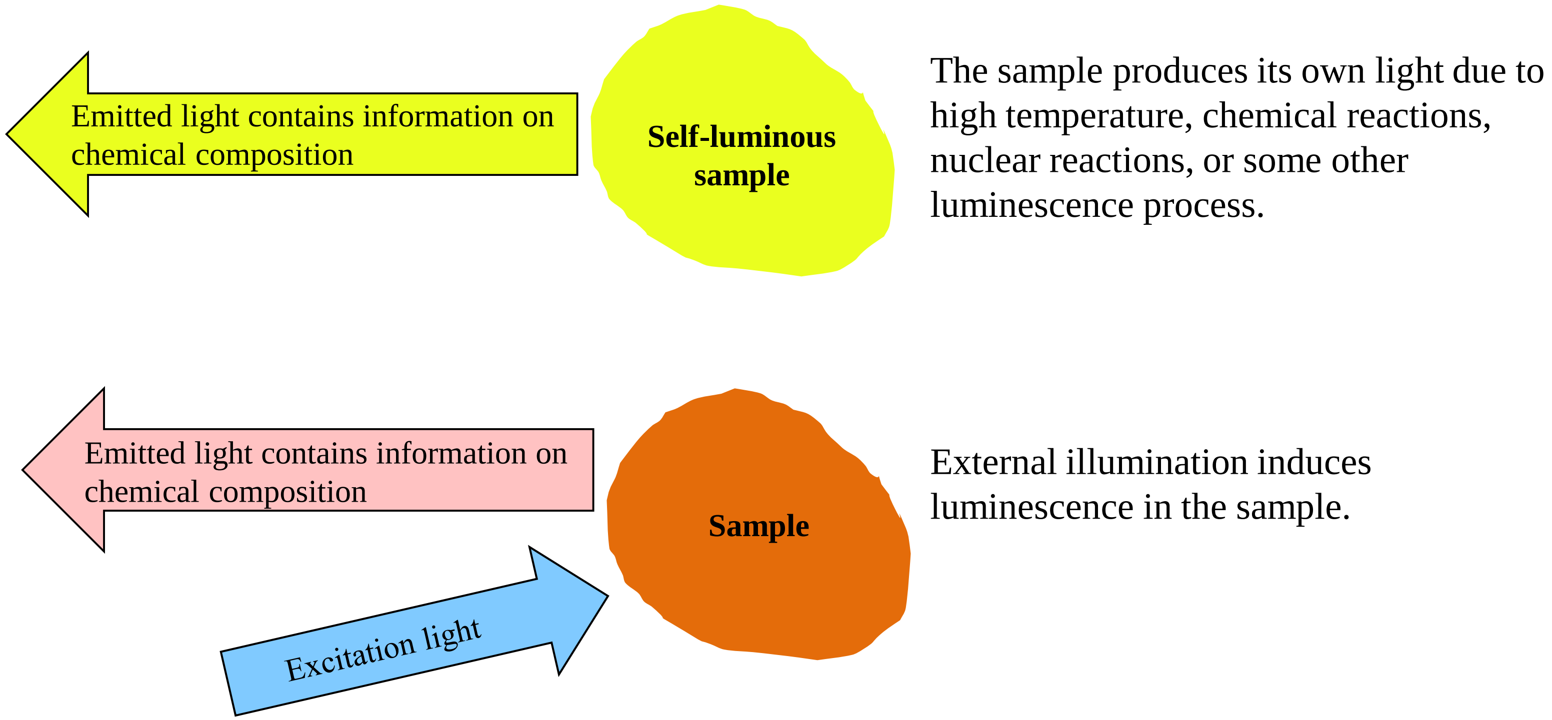


$$AU = \log\left(\frac{Illumination\ Spectrum}{Output\ Spectrum}\right)$$

Emission Spectroscopy

- The sample either produces its own luminescence or the external illumination (e.g., laser light) induces luminescence in the sample. The emitted light contains information a the sample's chemical composition.

Basic Idea of Emission Spectroscopy



Spectrometer Selection

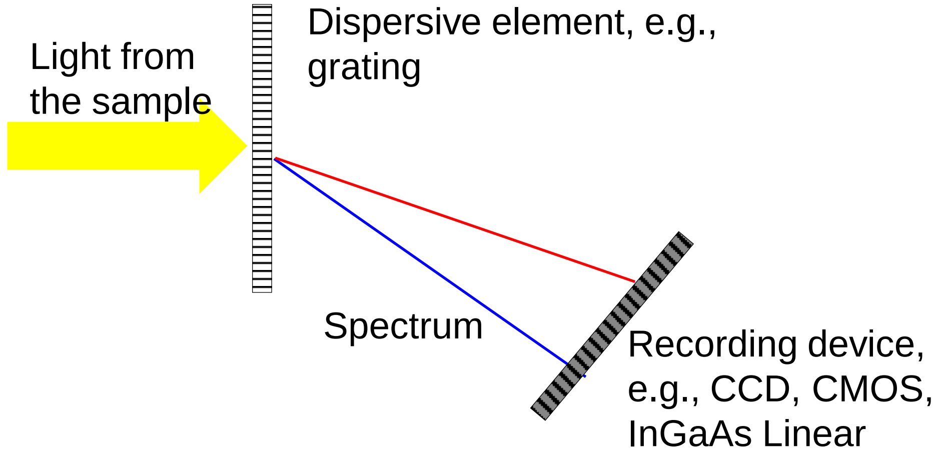
Key Spectrometer Parameter	Absorption Spectroscopy	Emission Spectroscopy
Wavelength & Optical Resolution	Spectrometer meeting the application wavelength range and optical resolution	
Timing	Lower scan rates, mSec order and above	Timing considerations, excitation event (LIBS)
SNR and Dynamic Range	Detecting small changes on a large signal.	Often times associated with low light conditions.
Light Intensity	Spectrometer with large signal to noise ratio	Select spectrometer with low noise (readout noise)

Spectrometer Fundamentals

Spectroscopy -Creating Optical Spectrum

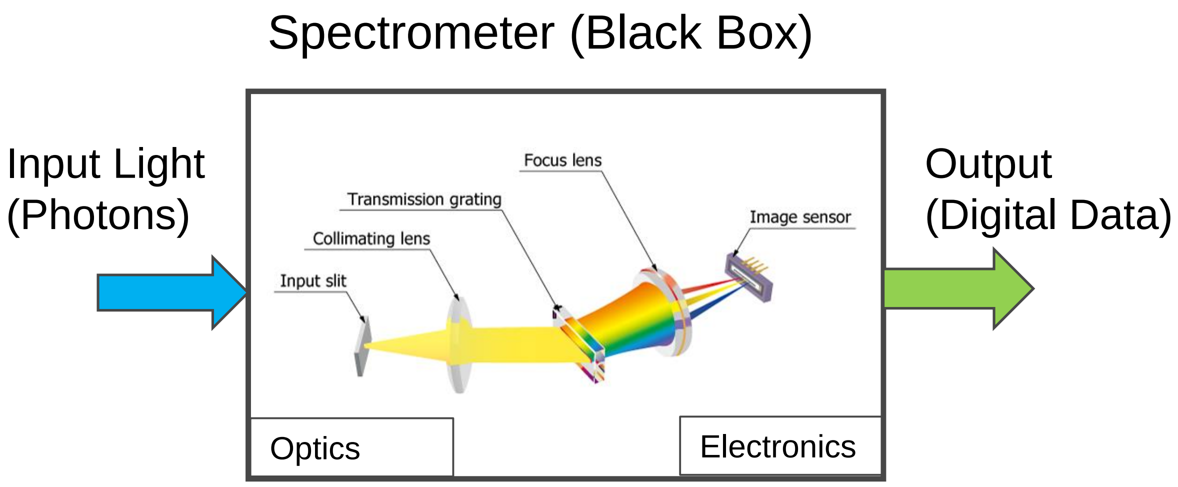
- In a dispersive spectroscopy, a dispersive element (e.g. prism or grating) takes in a beam of light from the sample and separates the constituent wavelengths in angle. In other words, it produces a spectrum.
- Convolution of optical efficiency, photodetector quantum efficiency and amplifier gain determine the signal.

Basic Setup of Dispersive Spectroscopy



Spectrometer Operating Principles

- Perform spectral separation.
  - Gratings
  - Fabry-Pérot Interferometer (FPI)
  - Michelson interferometer (FTIR)
- Vast majority of grating based spectrometers use charge storage.
  - $Q=CV=I*\Delta T$
- FPI and FTIR generally use some form of averaging
- Ultimately supply digital data to micro-control or computer.



Spectrometer Optical Resolution

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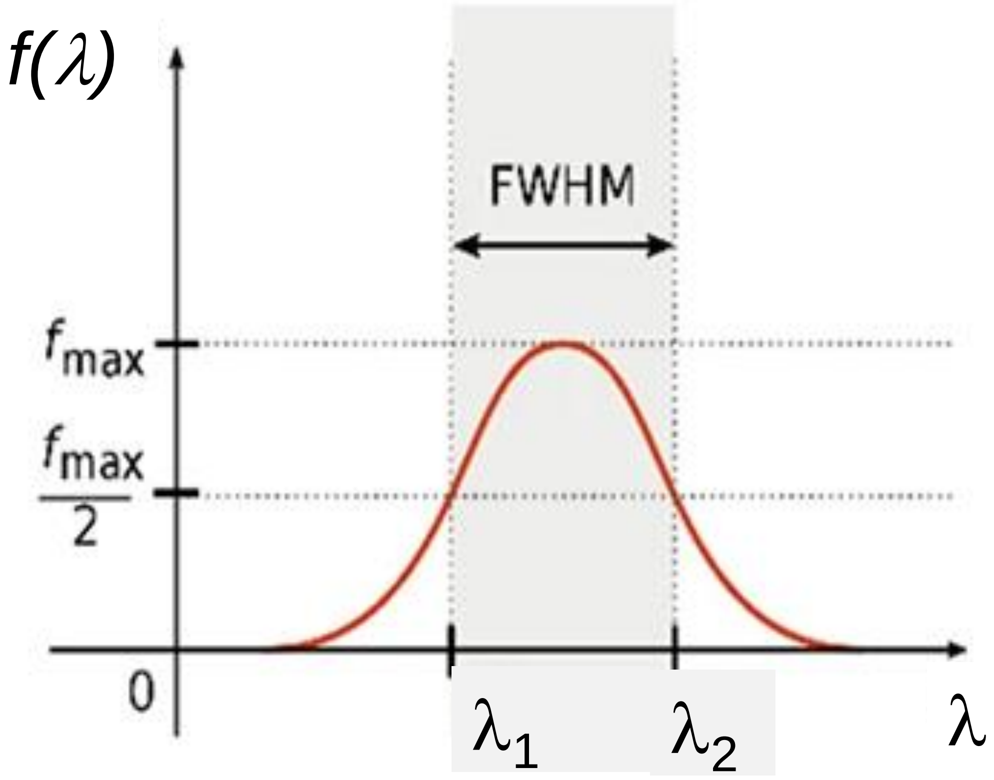
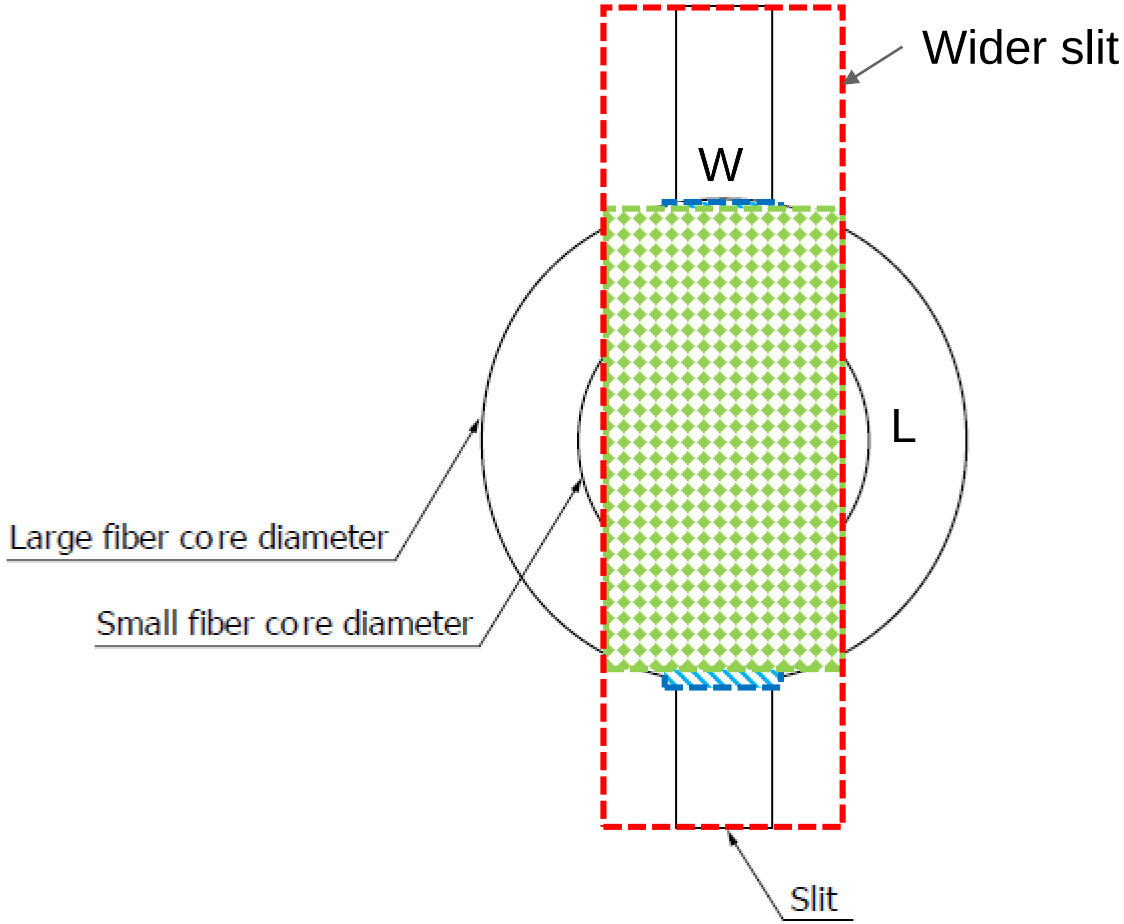
- Ability to determine the natural widths of individual emission lines and to distinguish neighboring peaks.
- Spectral features smaller than the resolution cannot be directly distinguished.
- Result of the spectrometers optical design and image sensor pixel size.
- Resolution factors;
  - Slit Width
  - Grove density
  - Focusing optics
  - Quality of components (aberrations)

Often definite as Full Width Half Maximum (FWHM)



Spectrometer Signal Considerations

- Tradeoffs between light throughput, often perceived as “sensitivity” and optical resolution.
- Larger slit wide, with sufficient fiber core, increase light collection.
- Optical power density, at spectrometer entrance slit, W/cm^2
- Simple approximation as area of rectangle, L x W.



Spectrometer Resolution & Slit Width Tradeoffs

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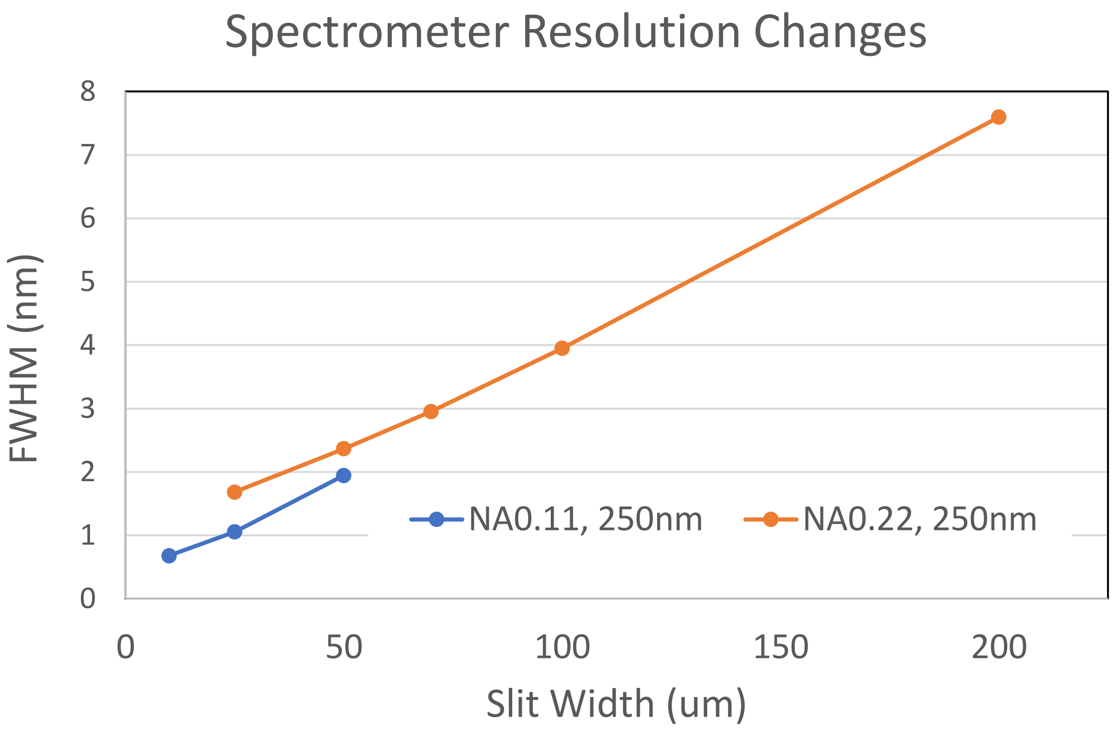
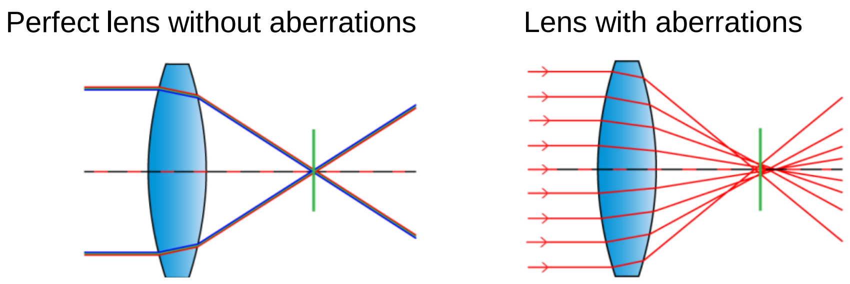
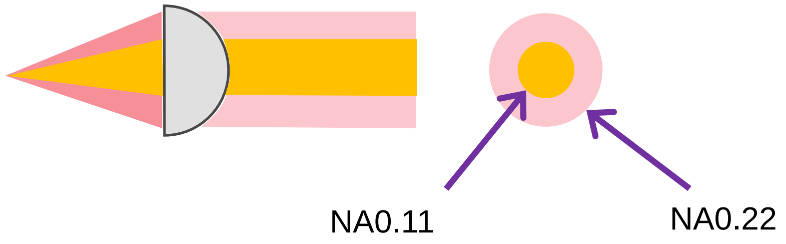
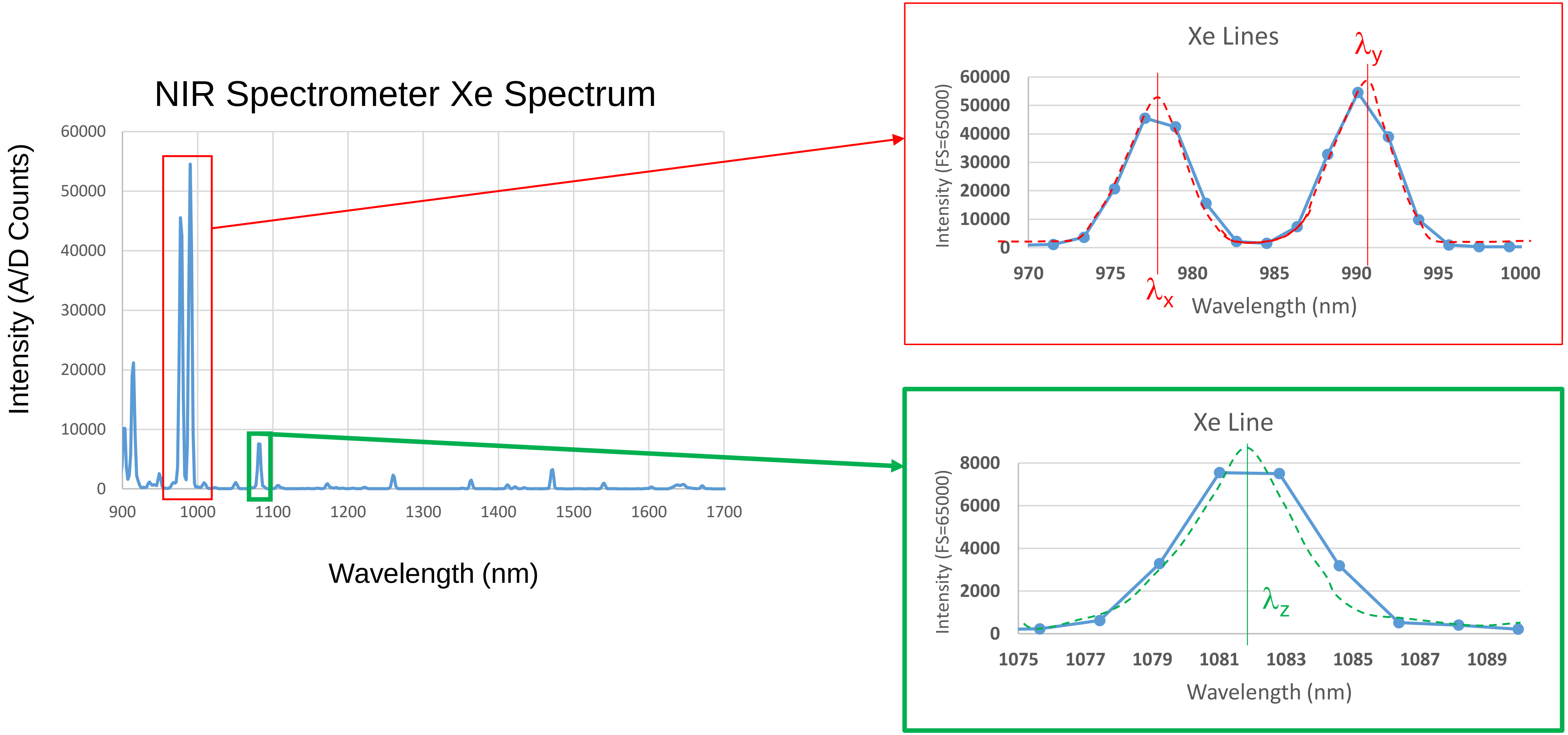
- Higher resolution, meaning lower FWHM, enables the instrument to better resolve narrow spectral lines (peaks).
- The non-linear slit width, FWHM is caused by optical aberrations.





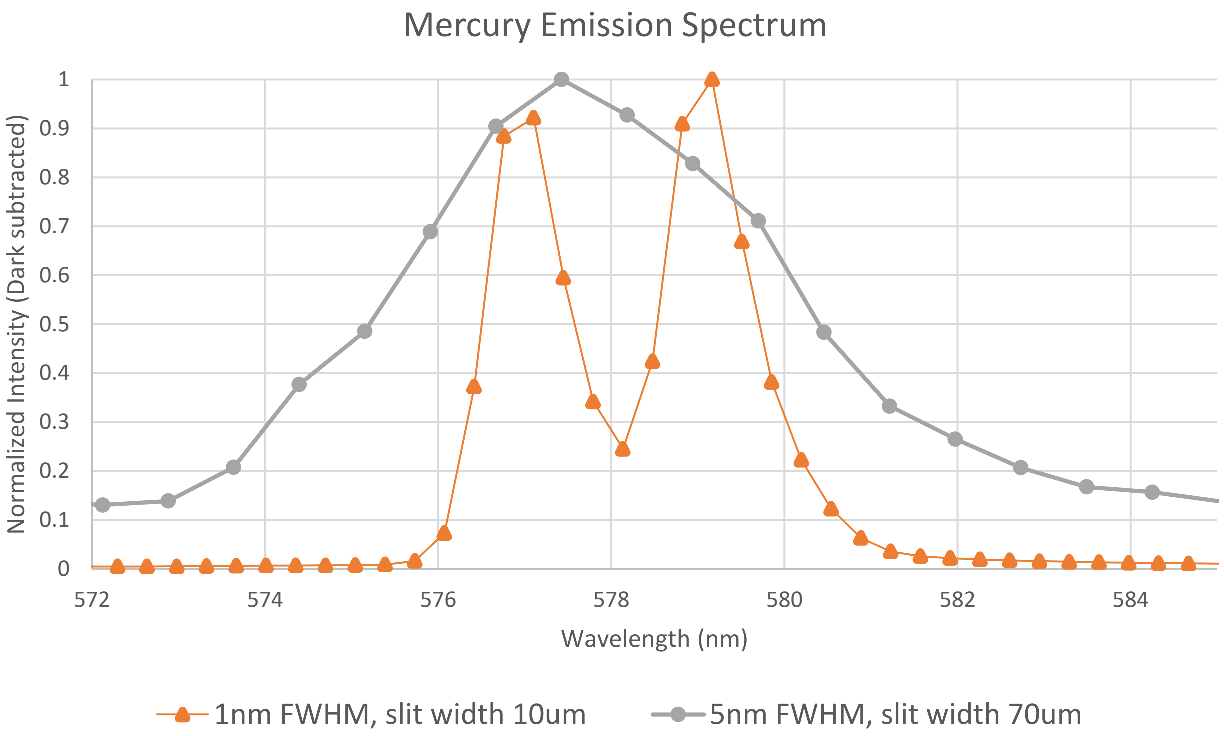


Gaussian Fitting



Optical Resolution, Distinguishing Spectral Features

- Mercury emission lines, known doublet 576.9nm and 579.0nm
- Intensity scale is normalized.
- Red is a spectrometer with 1nm resolution.
- Gray is a spectrometer with 5nm resolution.
- Necessary to apply spectral fitting techniques.
- Calculate Signal to Noise at each pixel (wavelength).



Introduction of Opto-Electronic Terminology

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Parameter	Brief Definition
Readout Noise	In image sensors, the readout noise is introduced when the charge packet is converted to a voltage by means of electronic amplifier. Unlike dark shot noise, readout noise is the fundamental noise source that cannot be eliminated.
Full Well Capacity (FW)	Also commonly referred to as saturation, full well capacity is the amount of charge (electrons) the image sensor (CCD) can handle.
Dark Current	Finite thermal carrier generated, by an image sensor, in the absence of light (photons).
Dynamic Range (DR)	Figure of merit as it is essentially an unachievable value. Calculated by dividing the Full Well Capacity by the Readout noise.
Signal to Noise Ratio (SNR)	Differs from DR in that one determines the total noise at a given signal level. The SNR is the signal divided by the noise at the signal level.
Conversion Gain	An image sensors ability to convert stored electrons to a voltage, by infernal (monolithic) or external amplification. Expressed in micro-volts per electron.
Numerical Aperture (NA)	In an optical system (lens), NA refers to the light acceptance cone.

Explanation of Image Sensors Offset

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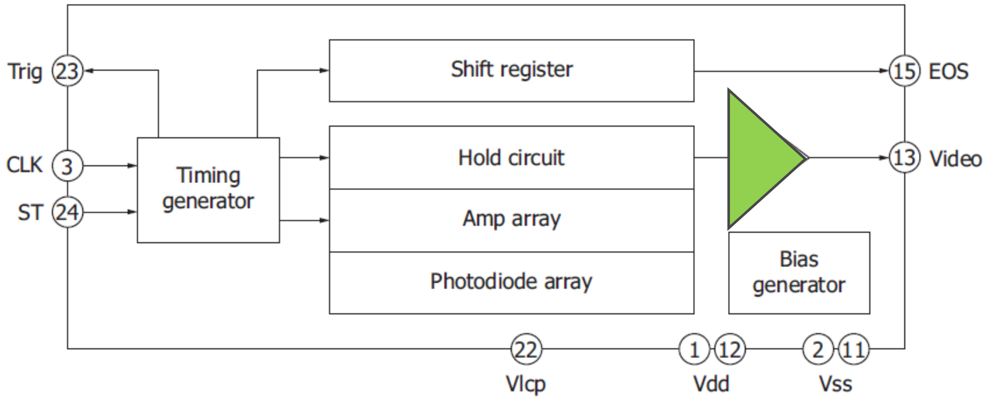
- Image sensor –Internal and external electronics create an offset.
- Assure incoming analog signal is greater than zero.



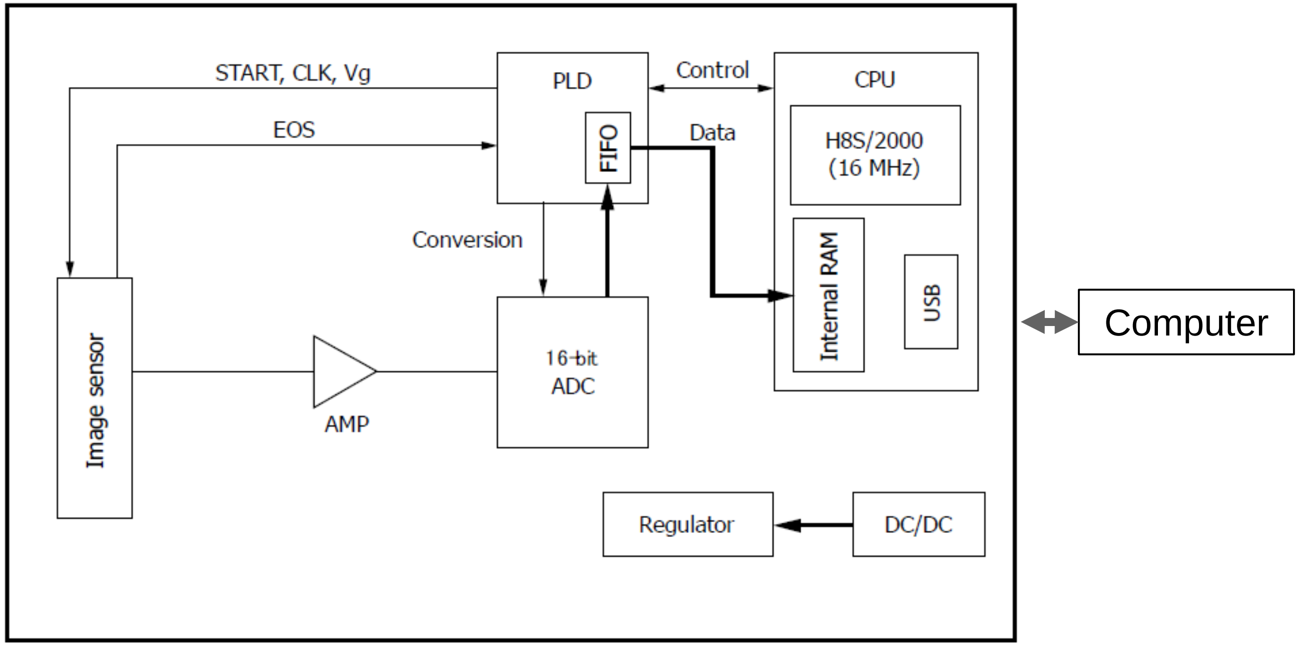
Block diagram of a CMOS- Active Pixel image sensor

Electrical and optical characteristics [Ta=25 °C, Vdd=5 V, V(CLK)=V(ST)=5 V, f(CLK)=10 MHz]

Parameter	Symbol	Min.	Typ.	Max.	Unit
Spectral response range	λ		200 to 1000		nm
Peak sensitivity wavelength	λp	-	700	-	nm
Photosensitivity*4	S	-	1300	-	V/(lx·s)
Conversion efficiency*5	CE	-	25	-	μV/e-
Dark output voltage*6	Vd	0	0.2	2.0	mV
Saturation output voltage*7	Vsat	1.7	2.0	2.5	V
Readout noise	Nread	0.1	0.4	1.2	mV rms
Dynamic range 1*8	Drange1	-	5000	-	times
Dynamic range 2*9	Drange2	-	10000	-	times
Output offset voltage	Voffset	0.3	0.6	0.9	V
Photoresponse nonuniformity*4 *10	PRNU	-	±2	±10	%
Image lag*11	Lag	-	-	0.1	%

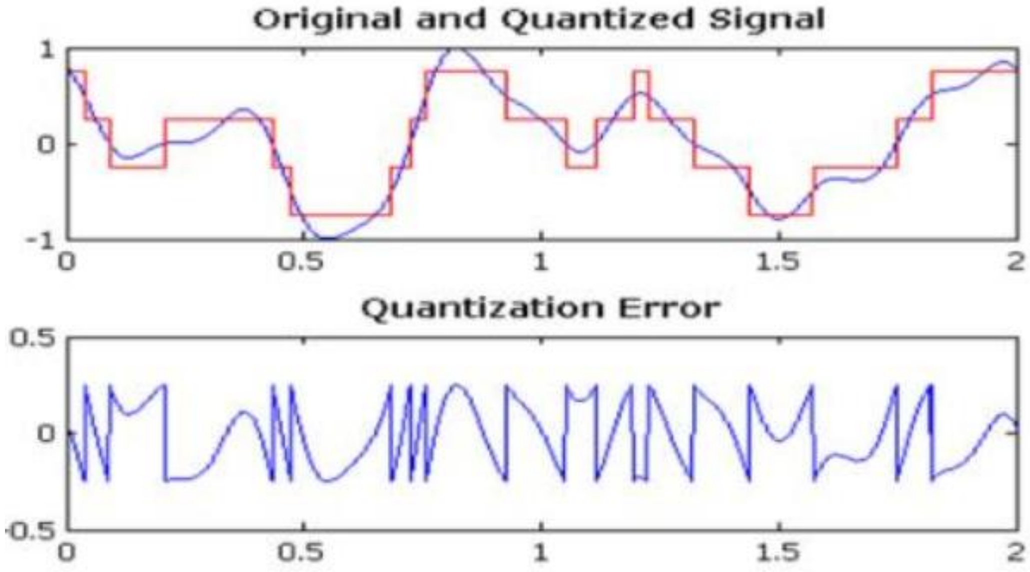
Spectrometer Electronics Block Diagram (CCD)

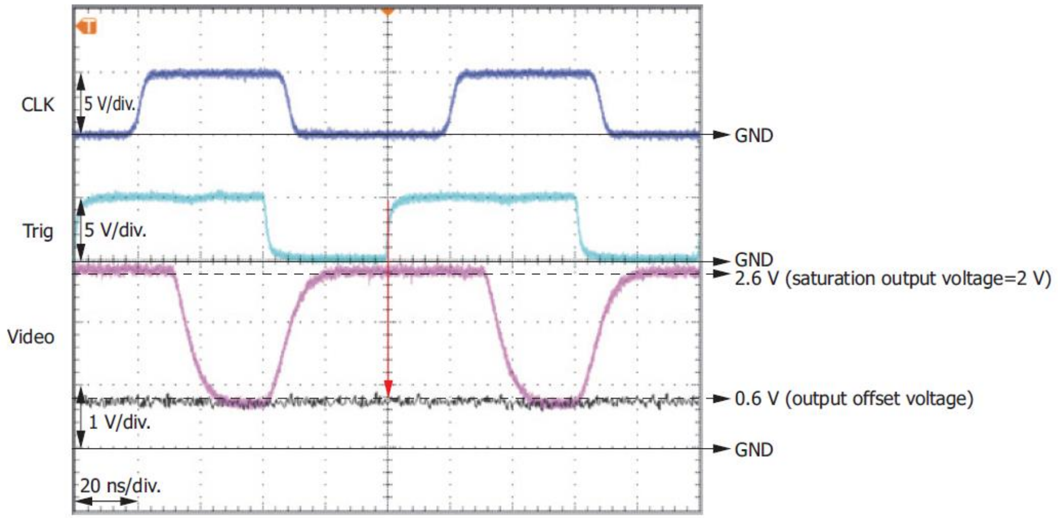
- Analog Signal Processing Chain
- Need to know;
  - Input voltage range of A/D
  - Resolution of A/D (12 bit, 16 bit)
  - Amplifier gain
  - Image sensor conversion factor
  - Convert A/D Counts into Reflect the A/D counts
- Reflect the A/D counts back to image sensor output
- Determine system gain (e-/DN)



Analog to Digital Converter Considerations

- Sampling frequency – how often do we read the analog signal.
- Quantization noise is the difference between the converted value and the actual.
- ADC sampling rate must be at least twice the signal frequency. (Nyquist Criteria)
- Image sensors and spectrometers- synchronize the ADC reading with the pixel ready timing.

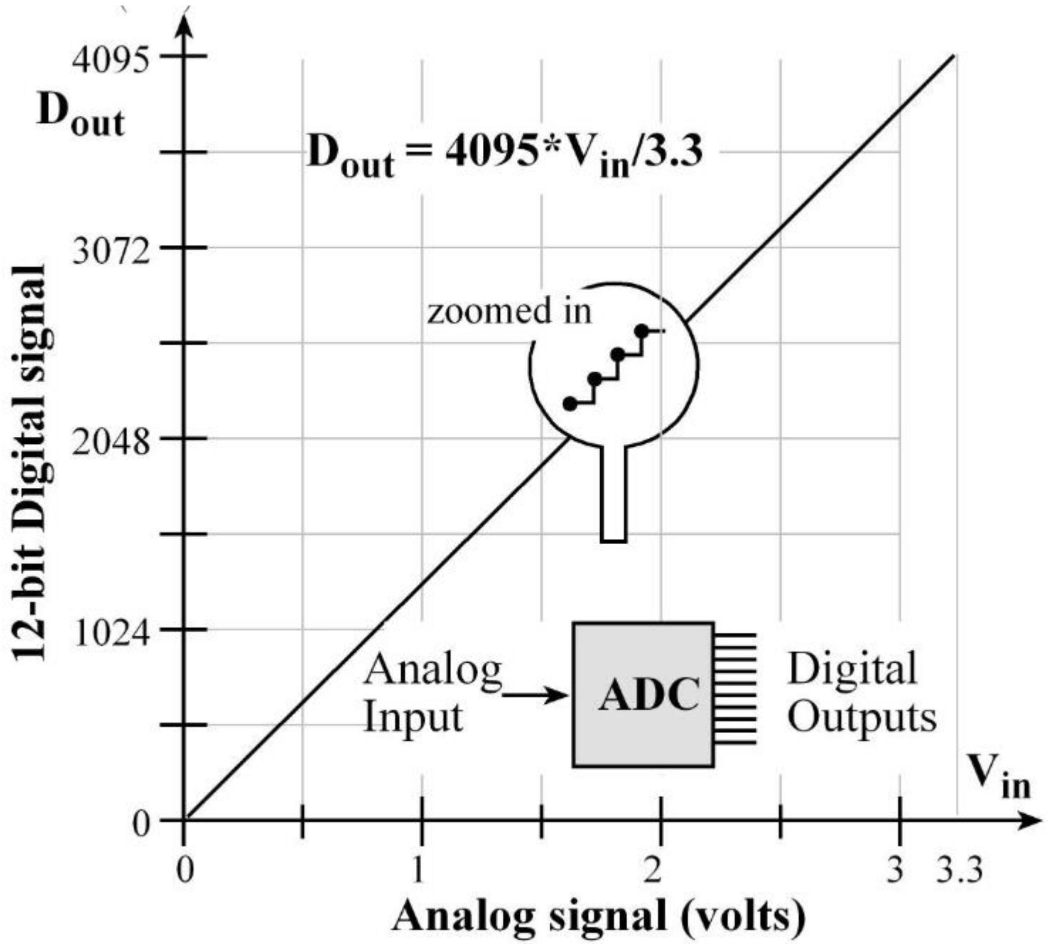




Analog to Digital Converter Considerations

- ADC resolution, the number of steps used to digitally represent the analog signal.
- Calculated as (2^N – 1), where N is the bit depth.

Bit Depth	Digital Signal	ADC Conversion (FS=3.3V)
8	255	12,941uV/DN
12	4095	805.9uV/DN
16	65,535	50.3uV/DN
24	16,777,215	19.7uV/DN



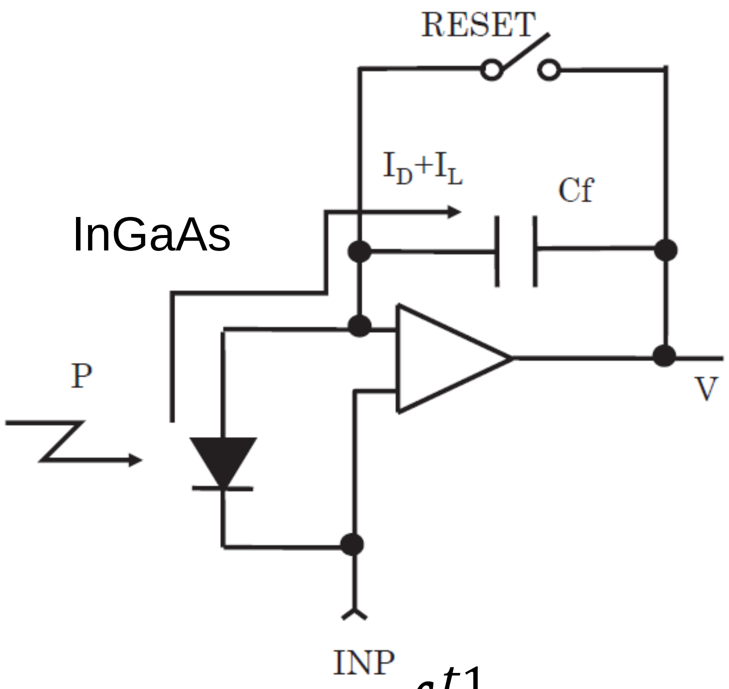
Selecting Appropriate Bit-Depth ADC

Part Number	Full Well	Readout Noise	Dynamic Range	Maximum Signal to Noise	Sufficient ADC	Comment
S10121 (CMOS-PDA)	165pC ~1030Me-	~ 10,000e- RMS (depends on circuit designer)	103K	32,000	2^{18} = 262,144 (18 bit ADC)	An 18 bit converter is twice the sensors dynamic range.
S10420 (BT-CCD)	Horizontal 300Ke-	6e- rms	50K	550	2^{16} = 65536	16 bit ADC is greater than sensor dynamic range.
S11639-01 (CMOS-APS)	2V/(25uV/e-) ~80Ke-	0.4mV/(25uV/e-) ~16e-rms	5K	280	2^{12} = 4096	A 12-bit converter almost coverts the sensors dynamic range, but for marketing reasons, almost no one uses a 12-bit ADC.

Spectrometer Signal Generation

Spectrometer Operating Principles – Signal Generation

- Charge is stored in the feedback capacitance of charge amplifier.
- Charge is integrated over a period of time, this is known as the integration time or exposure time.
- Readout noise represents the noise floor.
- Within any given spectrometer there is an offset.
- $I(t) = I_L + I_D$
- Increase input slit width to allow more light to enter.



$$Q = CV = \int_{t0}^{t1} I(t)dt$$

$$Q = CV = I * \Delta t$$

Spectrometer Digital Signal Calculations

$$Signal = P_i * S_s * \Delta T$$

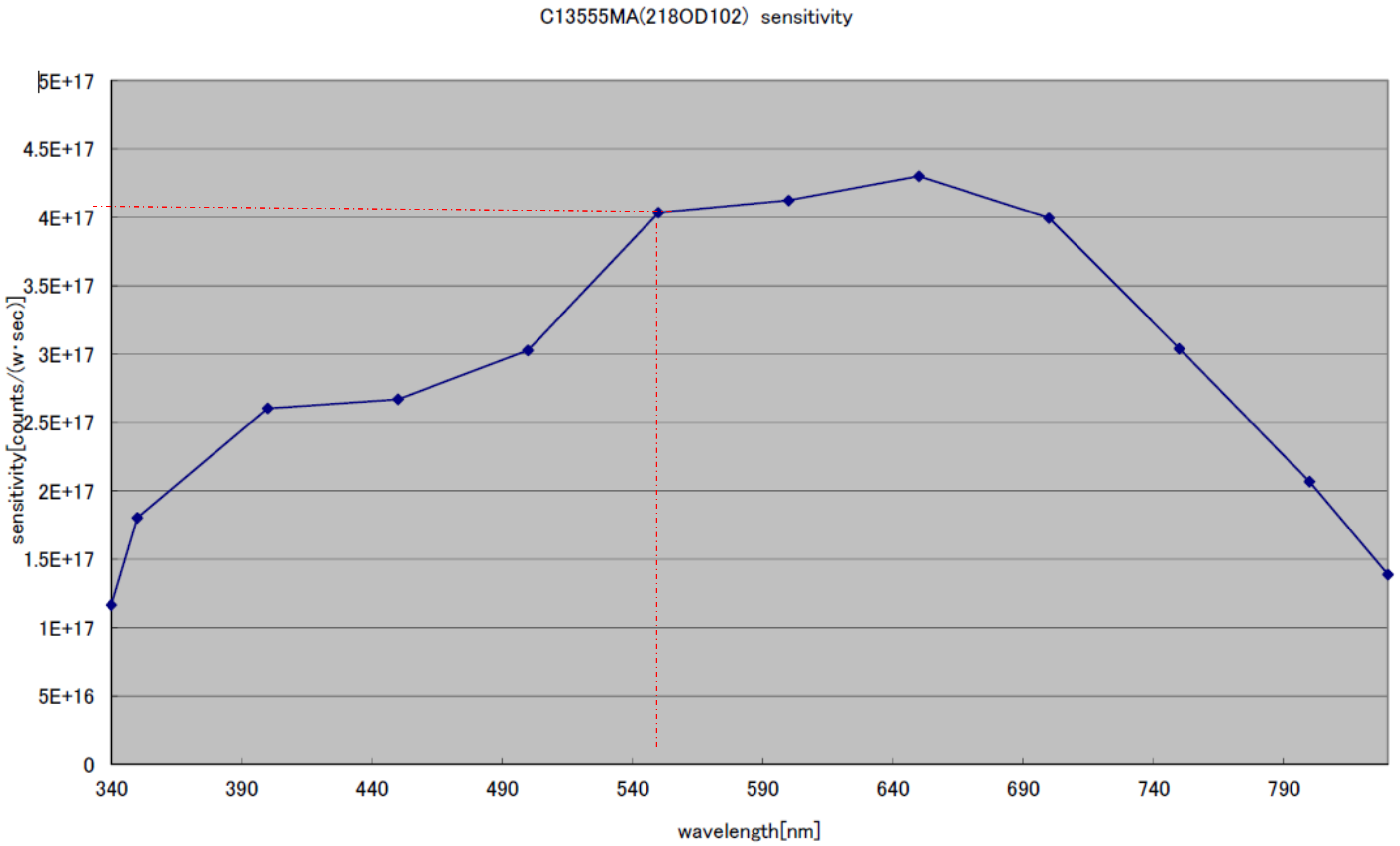
- ΔT: Integration time
- S_s: Spectrometer Sensitivity
- P_i: Optical power

$$Signal = \{\frac{Counts}{(\cancel{Watts} * \cancel{Sec})}\} * \cancel{Watts} * \cancel{Sec}$$

Watts and Sec cancel, left with Counts

Spectrometer Signal

- Spectrometer sensitivity (S_s) expressed in units of; **{Counts/(Watt*Sec)}**



$$Signal = P_i \ * \ S_s \ * \ \Delta T$$

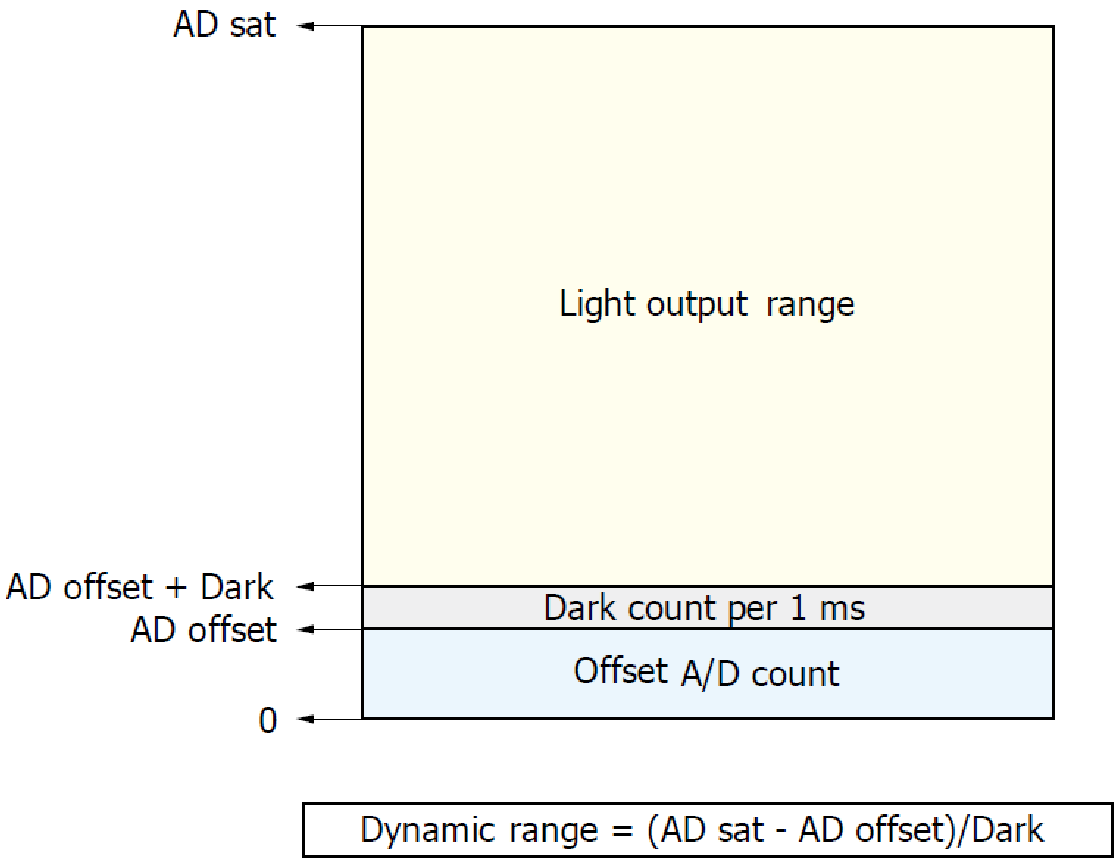
$$Signal = \ 4x10^{17}(Counts/Watts * Sec) \ * 1pW \ \ * 100mSec$$

$Signal =$ 40,000 AD Counts

Spectrometer Digital Data Considerations

Spectrometer Useable Dynamic Range

- Offset is a fixed value to assure spectrometer output is always greater than zero.
- Because it's a constant, offset does not contribute to shot noise.
- Dark signal (dark current) is above the offset.
  - Practical tip- use minimum integration setting to approximate the offset.



AD sat: saturation A/D count
AD offset: offset A/D count
Dark: dark count

Spectrometer Useable Dynamic Range

- Image sensor output and A/D considerations
- Understand does the image sensor reach saturation before the A/D?
- Reverse scenario, A/D saturate before the image sensor?

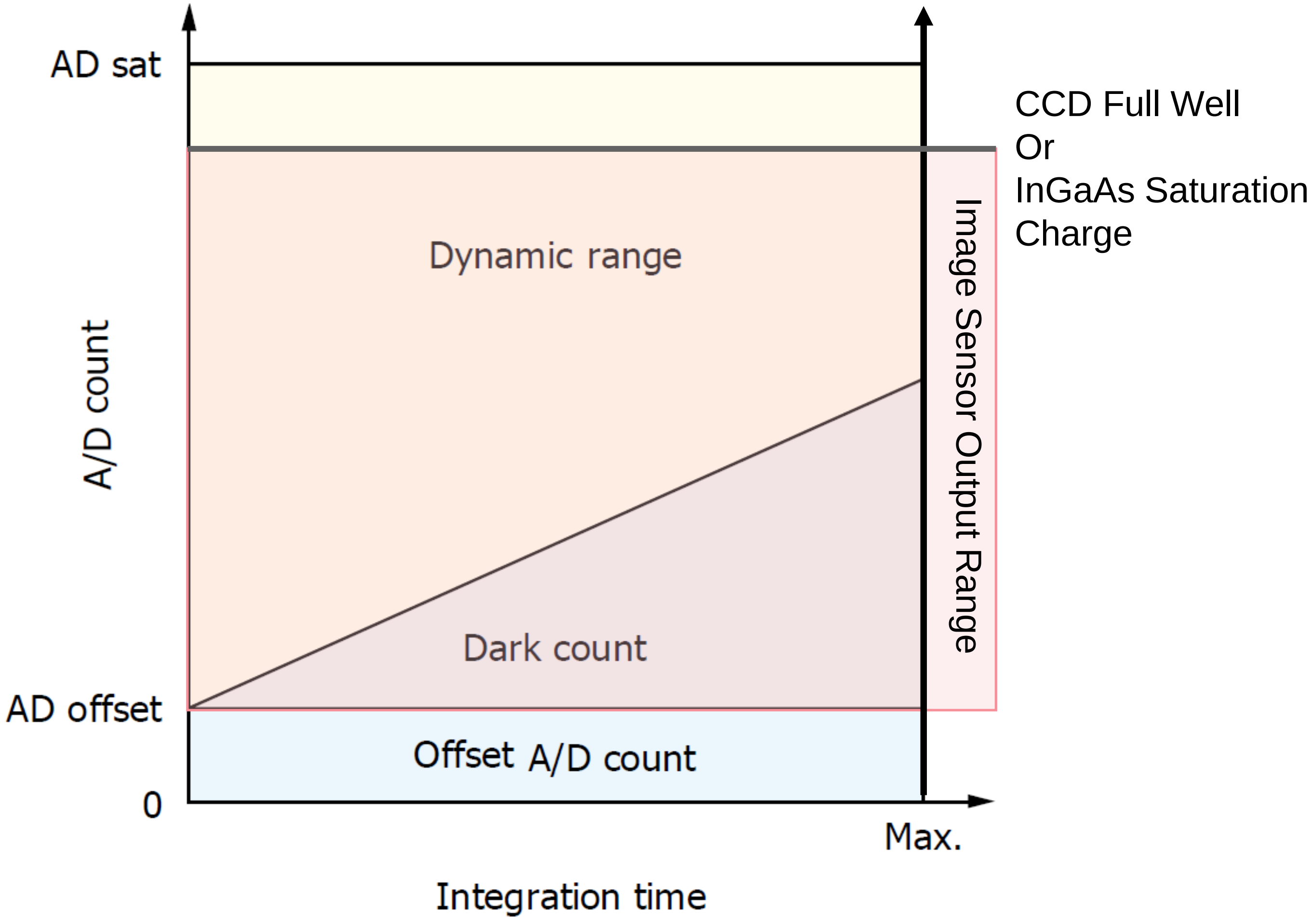
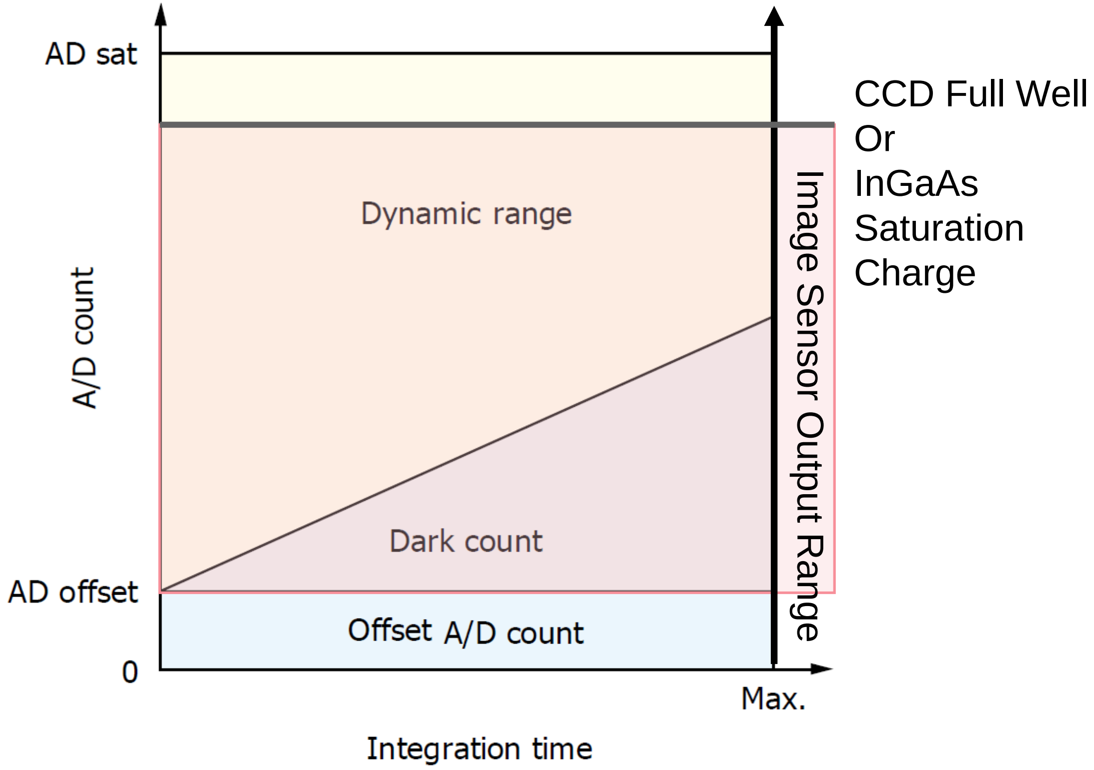
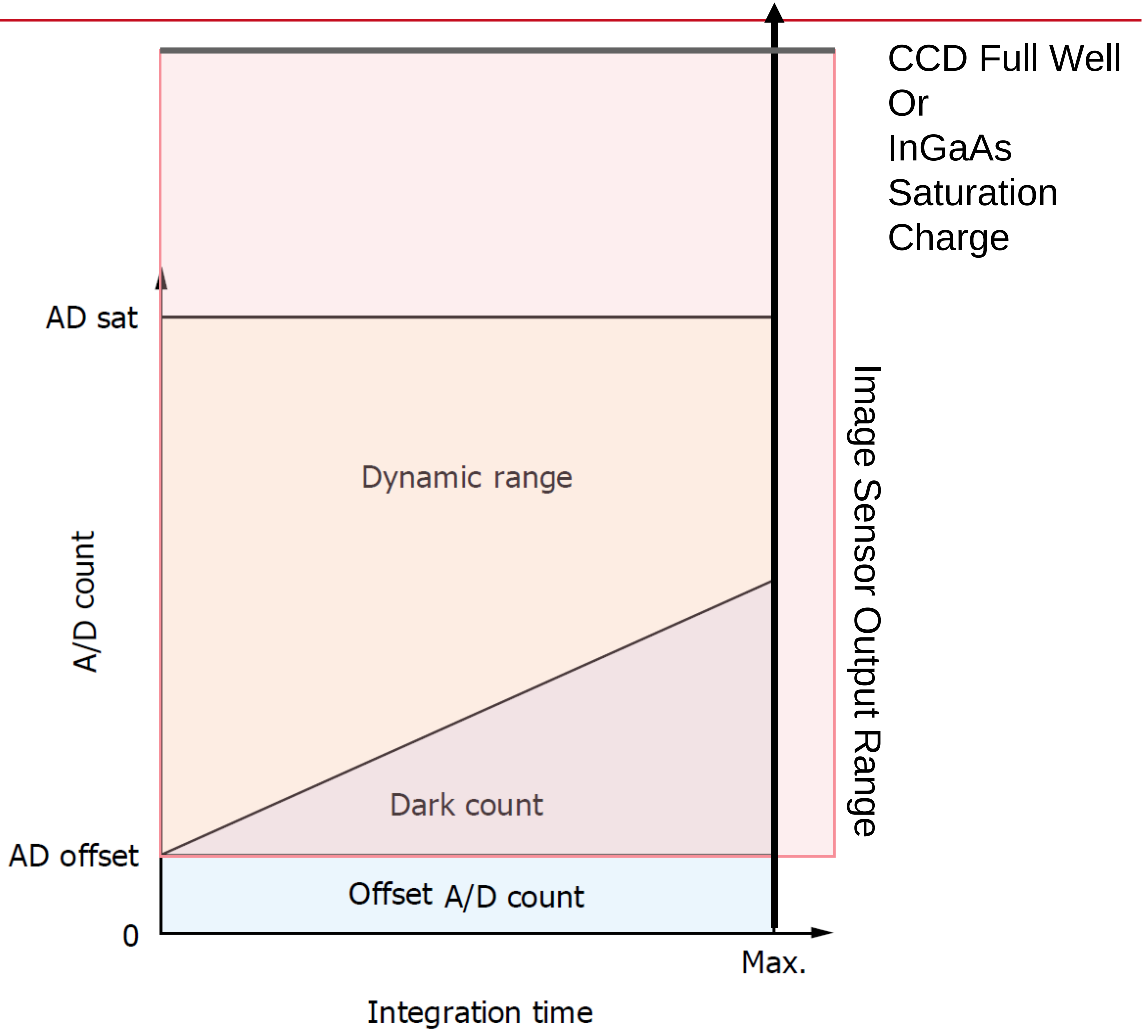


Image Sensor and ADC Saturation Contrasts



Left – Image sensor dynamic range matched within the limits of A/D full scale.



Right – Image sensor dynamic range exceeds the limits of A/D full scale.

Spectrometer Noise Analysis

Total Noise

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- Shot noise follows Poisson distribution.
- Discrete nature of electrons and photons.
- Noise analysis based on ideal optics as first order.
  - Stray Light can also introduce noise.
- ADC quantization noise.
  - Not an issue with proper electrical design.

$$N_t = \sqrt{N_r{}^2 + N_d{}^2 + \underbrace{\cancel{Np}^2}_{0} + \underbrace{\cancel{Nsys}^2}_{0}}$$

Nr – Readout Noise
Nd – Dark shot noise
Np – photon shot noise
Nsys – System noise

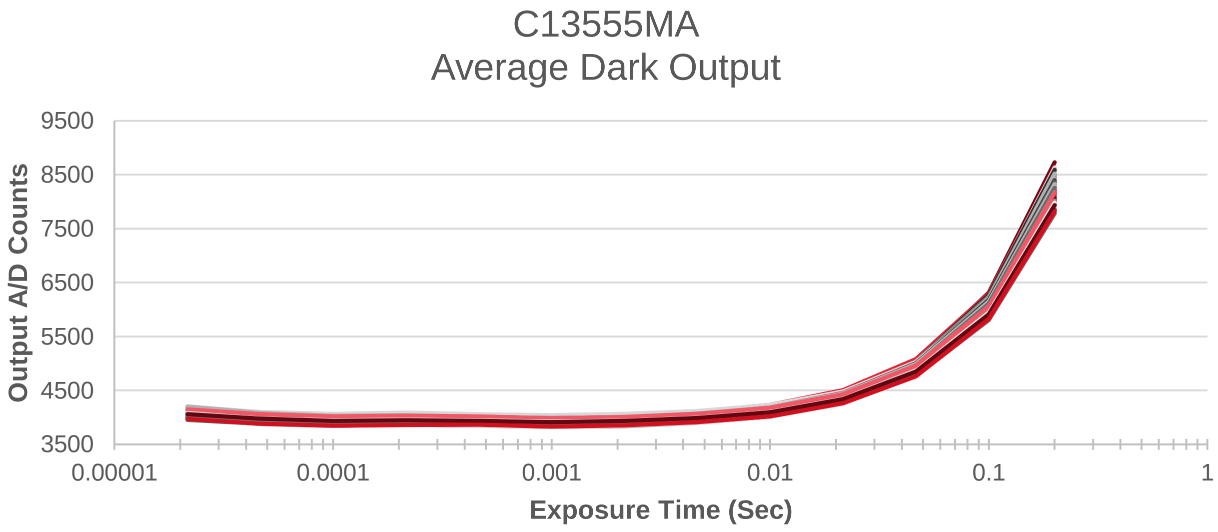
$$N_{td} = \sqrt{N_r{}^2 + N_d{}^2}$$

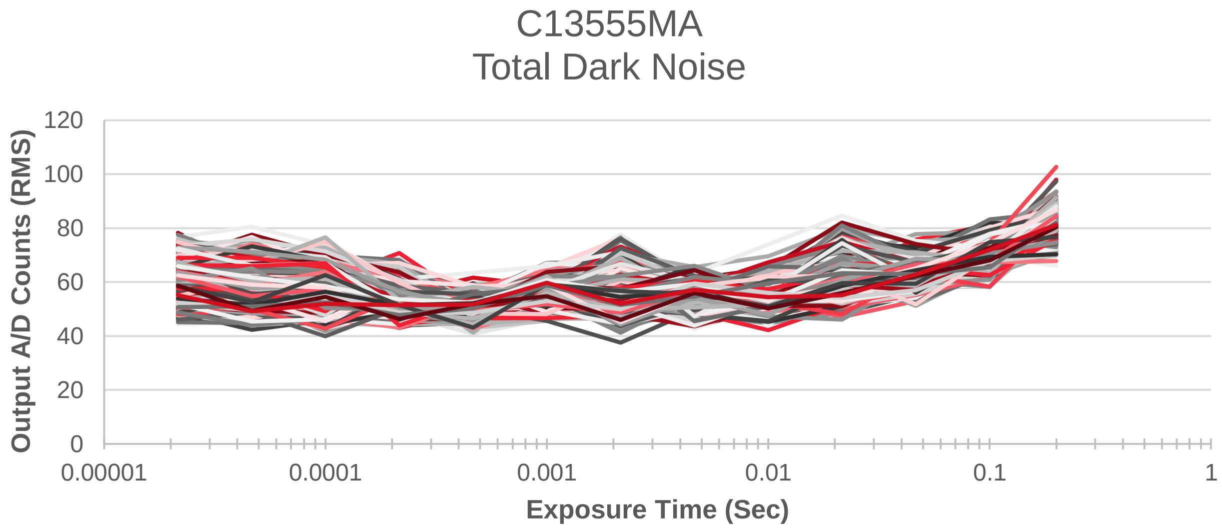
N_{td} – Total Dark Noise

Shot noise can be calculated by taking the square root of the number of electronics, following Poisson distribution. Only when converted to electronics. One cannot take the square root of AD counts correctly compute noise.

Spectrometer Dark Noise Practical Example

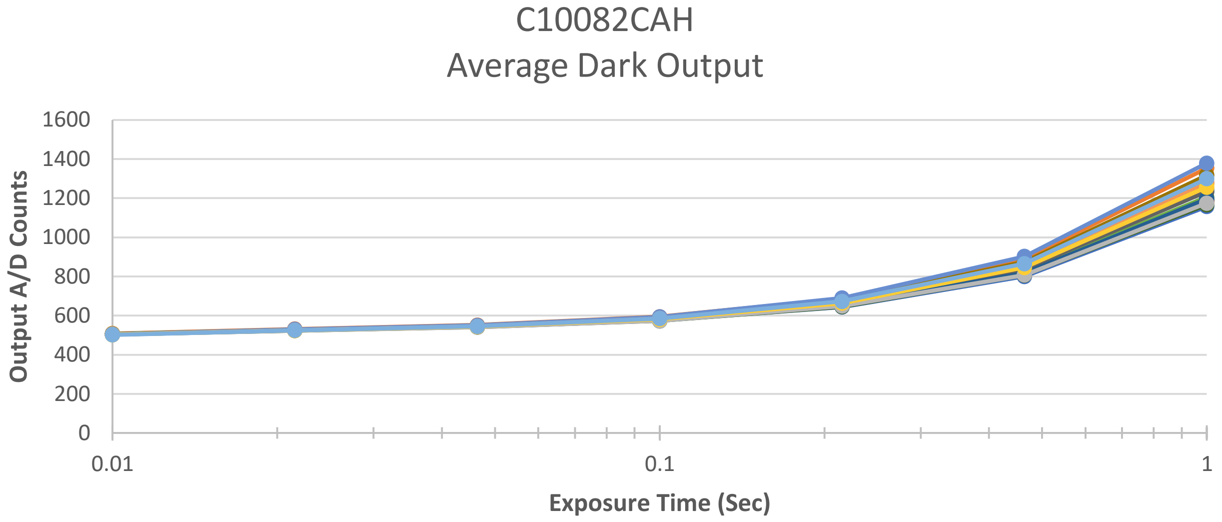
- UV-Visible spectrometer using CMOS-APS technology.
- Black box – 16 bit ADC with USB interface.
- Acquire 100 readings at each exposure time, calculate the average value and the standard deviation (noise).
- Benefit of performing dark noise analysis as a bench mark.

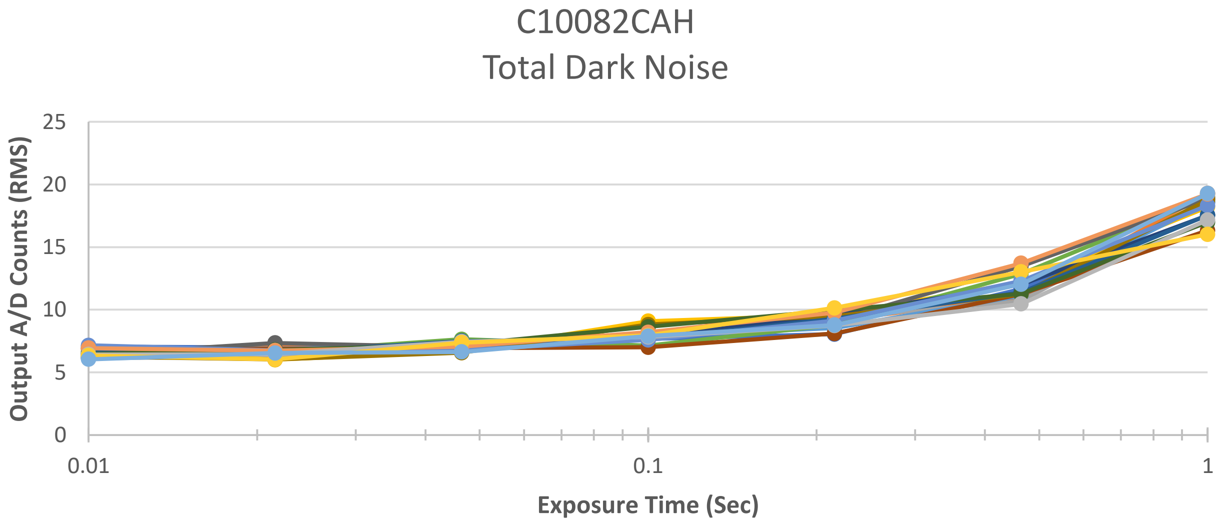




Spectrometer Dark Noise Practical Example

- UV-Visible spectrometer using BT-CCD technology.
- Black box – 16 bit ADC with USB interface.
- Acquire 100 readings at each exposure time, calculate the average value and the standard deviation (noise).
- Dark output non-linear due to spectrometer offset.





Why is Signal to Noise Important

- Represents the instrument or systems accuracy.
- Signal to Noise must be greater than unity.
- No dimensions –Ratio
- The larger the SNR, the more precisely measurements.
- Provides a uniform comparison amongst spectrometers / manufacturers.

Final Signal to Noise

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$$\boldsymbol{SNR = \frac{S_m}{Nt}}$$

$$S_m = P_i \; * \; S_s \; * \; \Delta T$$

S_m - Measured Signal = $S_s \; - (Dark + Offset)$

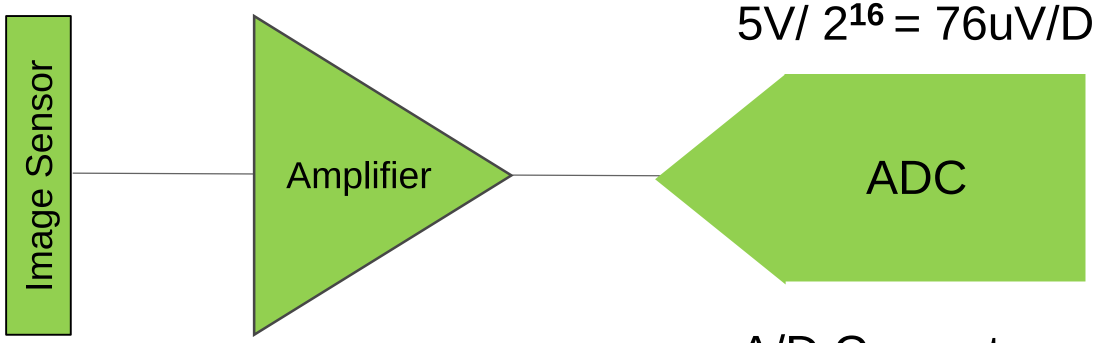
$$Nt = \sqrt{2Nr^2 + Nd^2 + Np^2 + Nsys^2}$$

Nr – Each readout sequence contains readout noise. To calculate the absolute signal measured value, the different between two readings are taken (Signal+Dark+offset) and (Dark+Offset). This introduces a factor of 2 read noise.
Nd – Dark shot noise
Np – (Photo-electrons + Dark electrons + Offset) ; Shot noise is included in the dark electronics and must be included to accurately calculate the total noise.
Nsys – System noise, light source drift, temperature changes, etc.

System Gain – Calculation Example

5V/ 2^{16} = 76uV/DN

S10420-xxxx (BT-CCD)
Conversion Gain =
6.5uV/e-



Amplifier Gain = 3.5

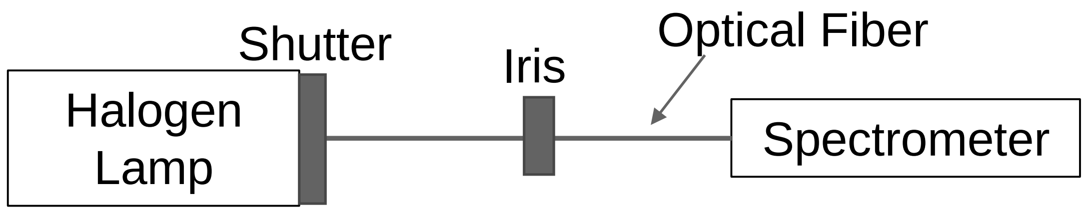
A/D Converter;
16 bits → 2^{16} = 65636
Input range 0 → 5V

$$System\ Gain = \frac{ADC\ Conversion\left(\frac{uV}{DN}\right)/Amp\ Gain}{Conversion\ Gain\ (uV/e^{-})}$$

$$= \frac{76\left(\frac{uV}{DN}\right)/3.5)}{6.5\ (uV/e^{-})} = 3.35\ \ (e^{-}/DN)$$

Experimental Results

Signal to Noise Experimental Set-up

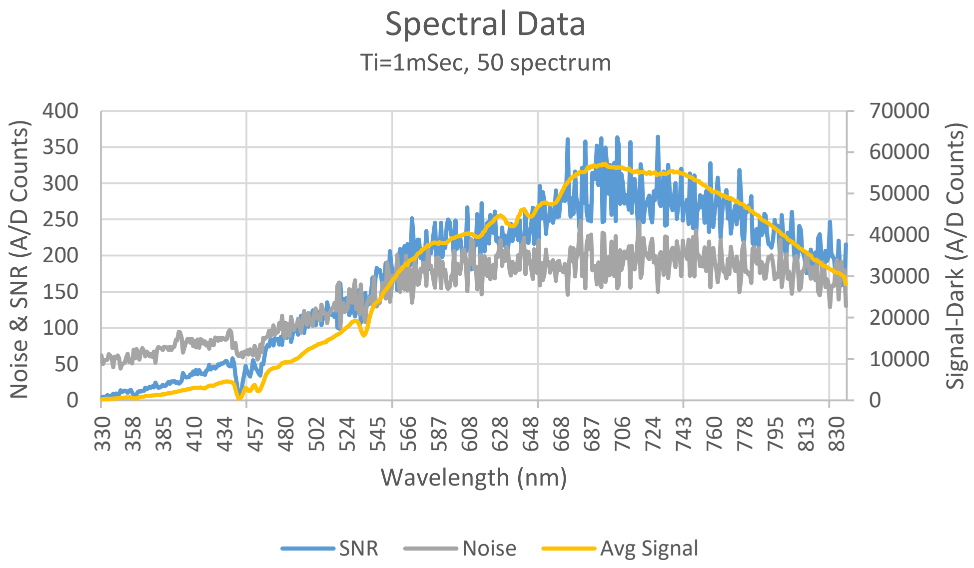


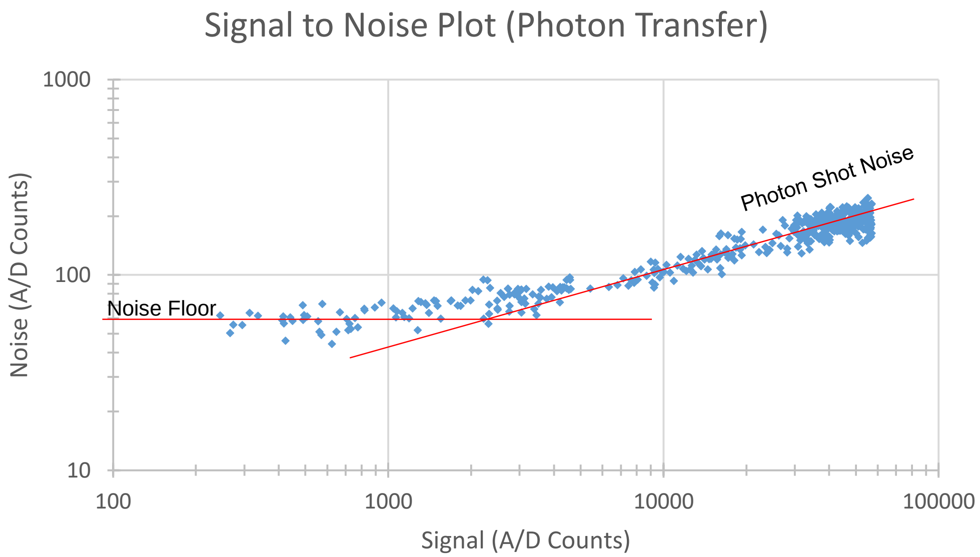
- Procedure
  - Verify lamp stability
  - Set exposure time to minimum value.
  - Adjust light intensity, vary iris (maintain color temperature).
  - Semi-automated data collection routine, minimum 100 spectra.
  - Calculate average signal at each pixel (wavelength).
  - Compute the standard deviation (noise) at each pixel.

- Equipment
  - Halogen lamp
  - Optical fiber
  - Optical attenuator (iris)
  - Spectrometer
  - Computer

Experimental Results

- Average signal over spectrometers wavelength range (all pixels)
- Each wavelength (pixel) corresponds to varying signal levels.
- Maximum SNR occurs in the region of highest signal level, ~700nm.
- Low signal levels, as signal increases, the total noise remains fairly constant. An indication total noise dominated by readout noise.
- As signal increases, we see the total noise becomes dominated by photon shot noise.





Measured Examples of Signal vs Noise (Photon Transfer)

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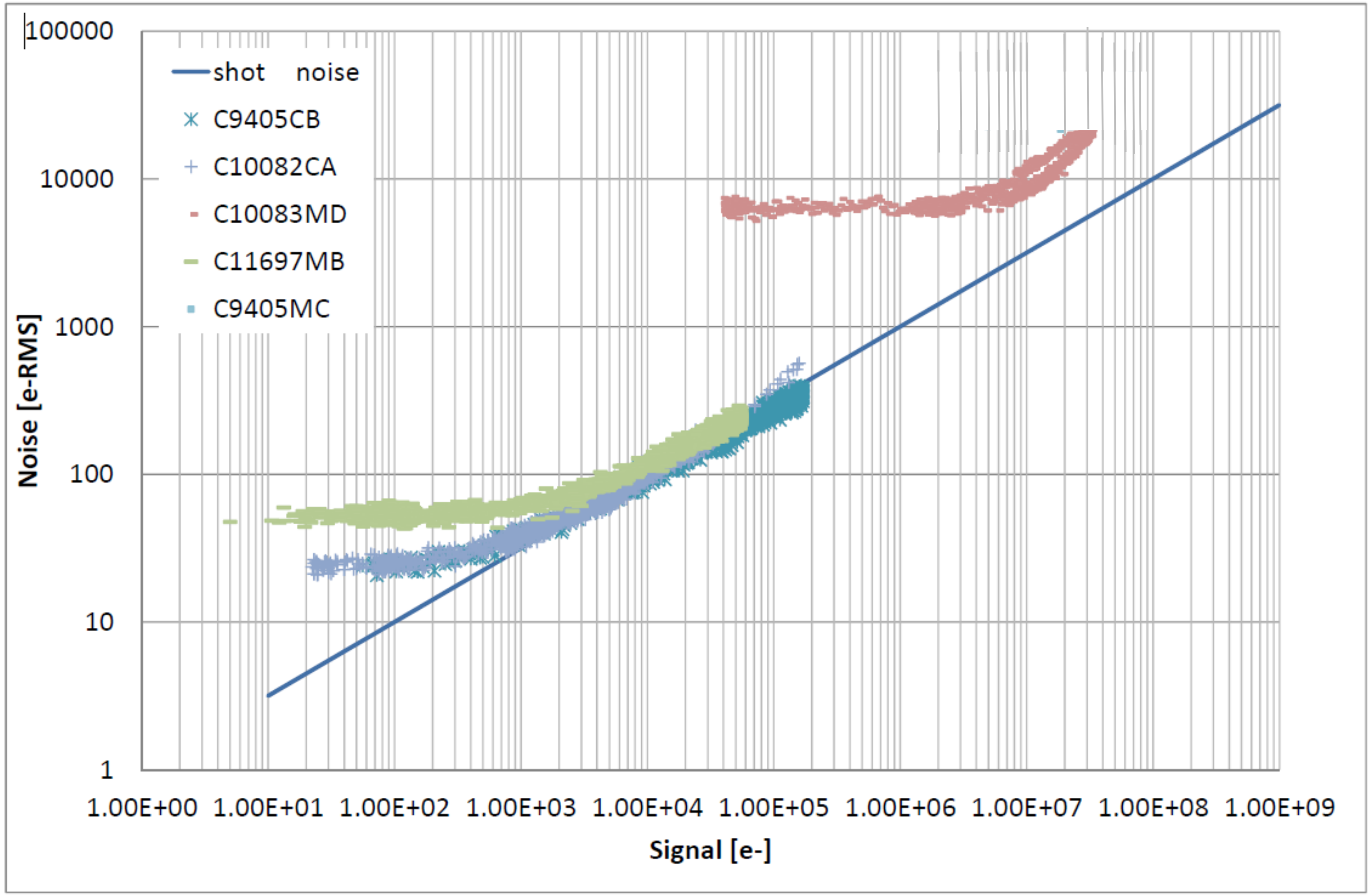
- The plateau (flat) region, dominate noise is circuit noise, readout noise.
- As the signal increase we see the impact of photon shot noise, giving rise to total noise.
- Blue – BT-CCD, noise floor on the order of 20-30e-



Techniques to Improve Signal to Noise

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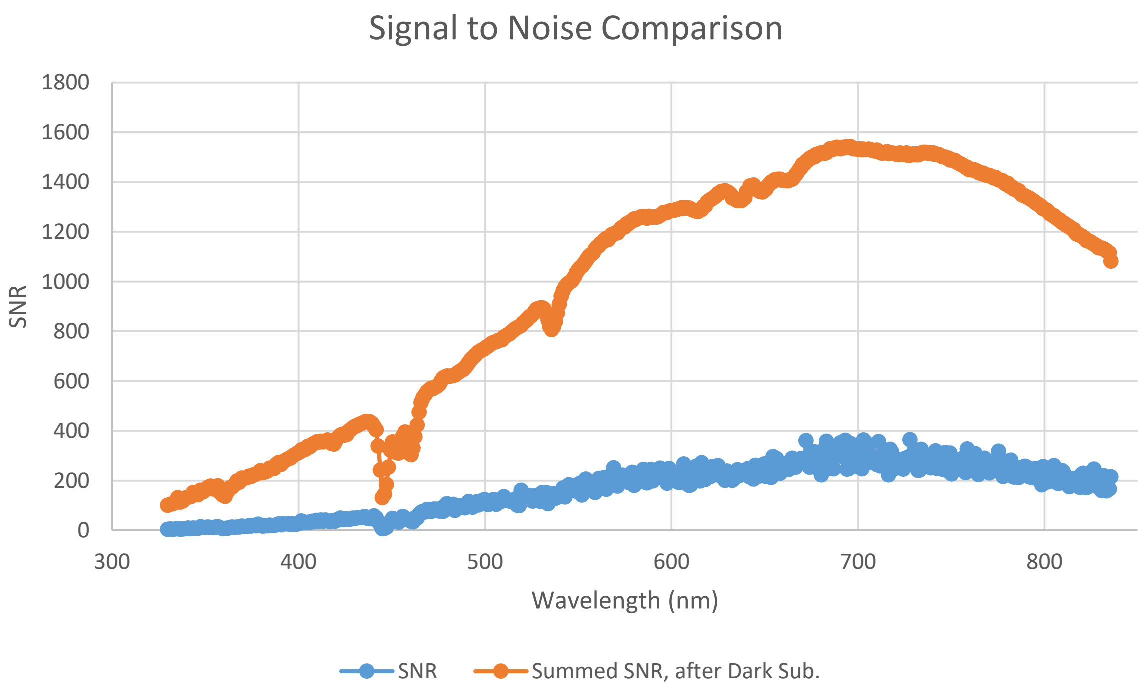
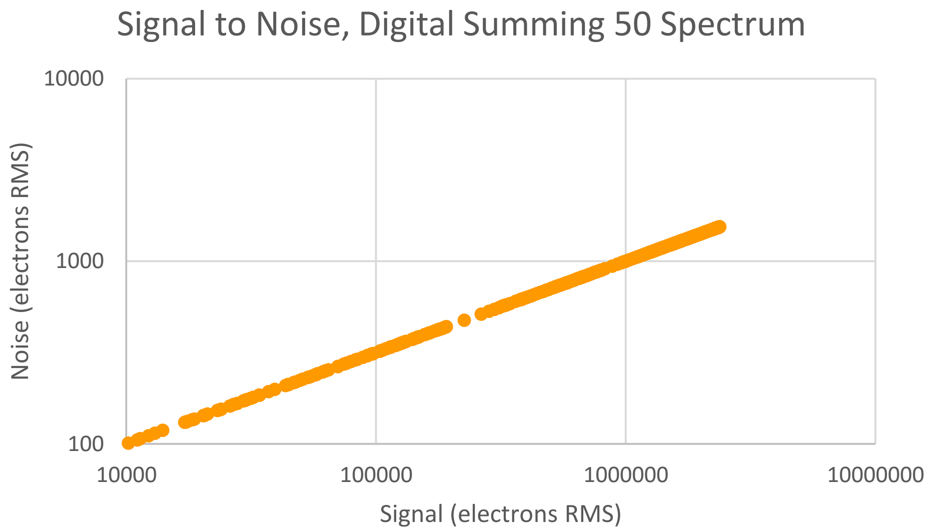
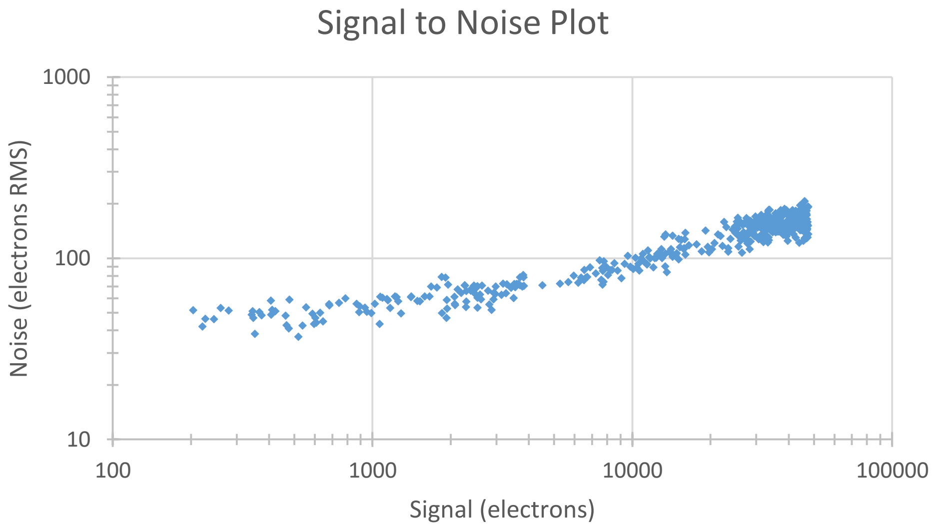
- Summing multiple spectrum.
- Signal is additive.
- Readout noise will also increase.

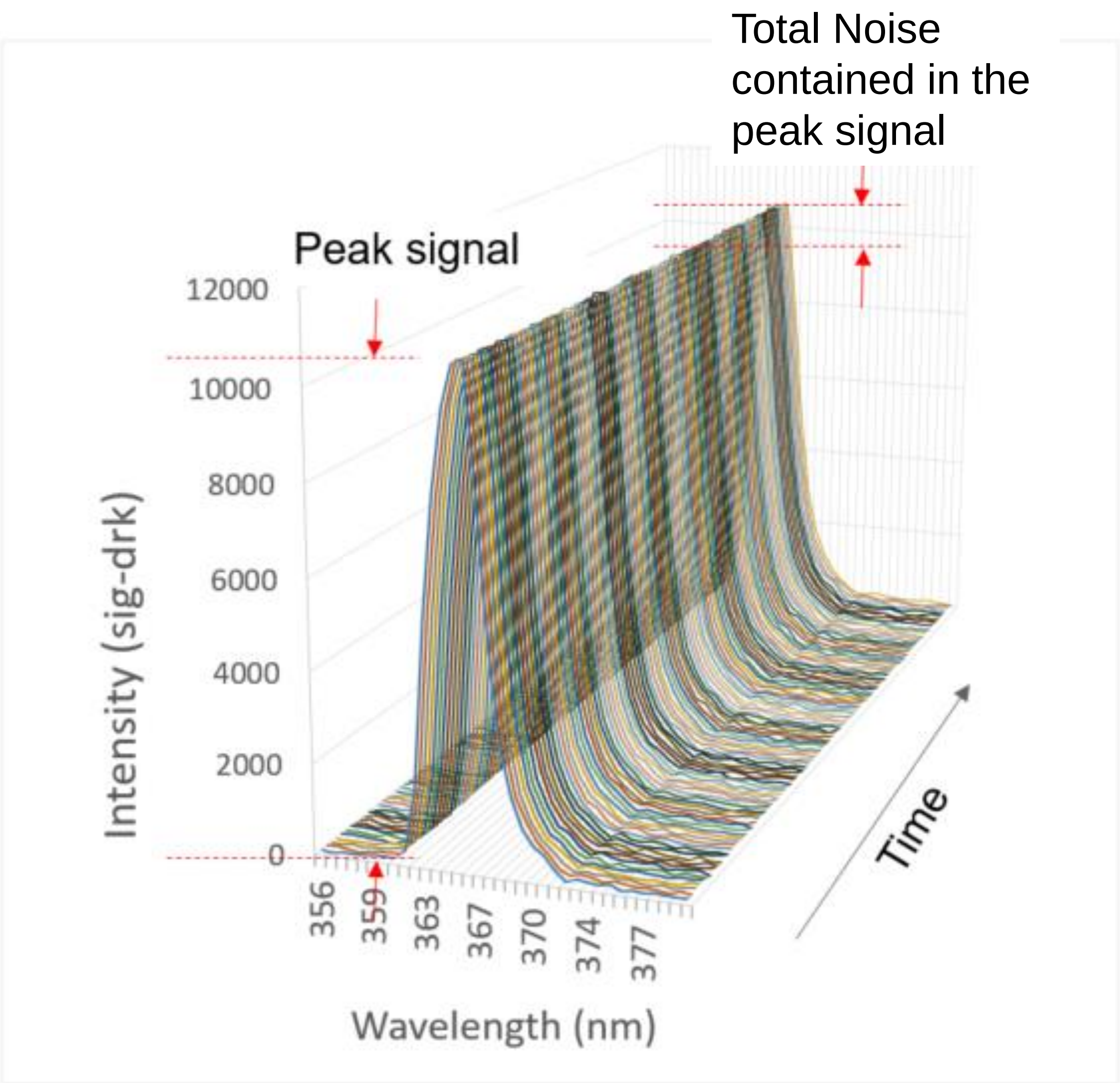




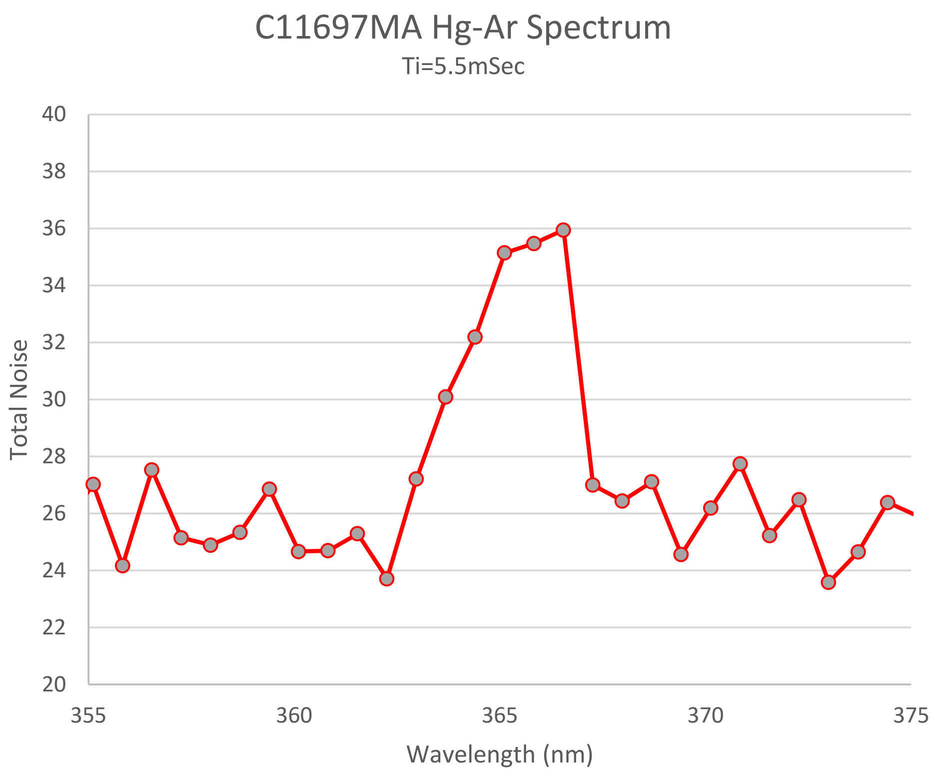


Signal to Noise Example, Emission Spectroscopy

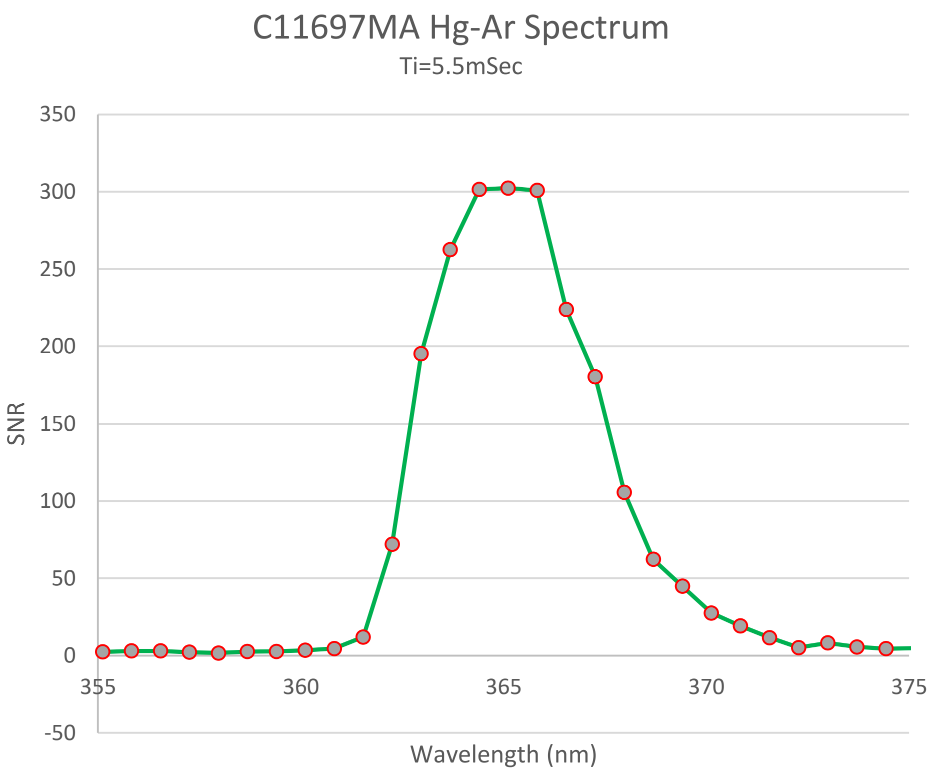
- 3D surface plot showing peak intensity fluctuations (noise) over time.
- Peak signal, an average of 100 scans.
- Calculate the total noise contained in each pixel (wavelength), this includes dark current.



Signal to Noise Example, Emission Spectroscopy



Total measured noise



Signal to Noise Ratio `~ 300

Where would Signal to Noise be the greatest?

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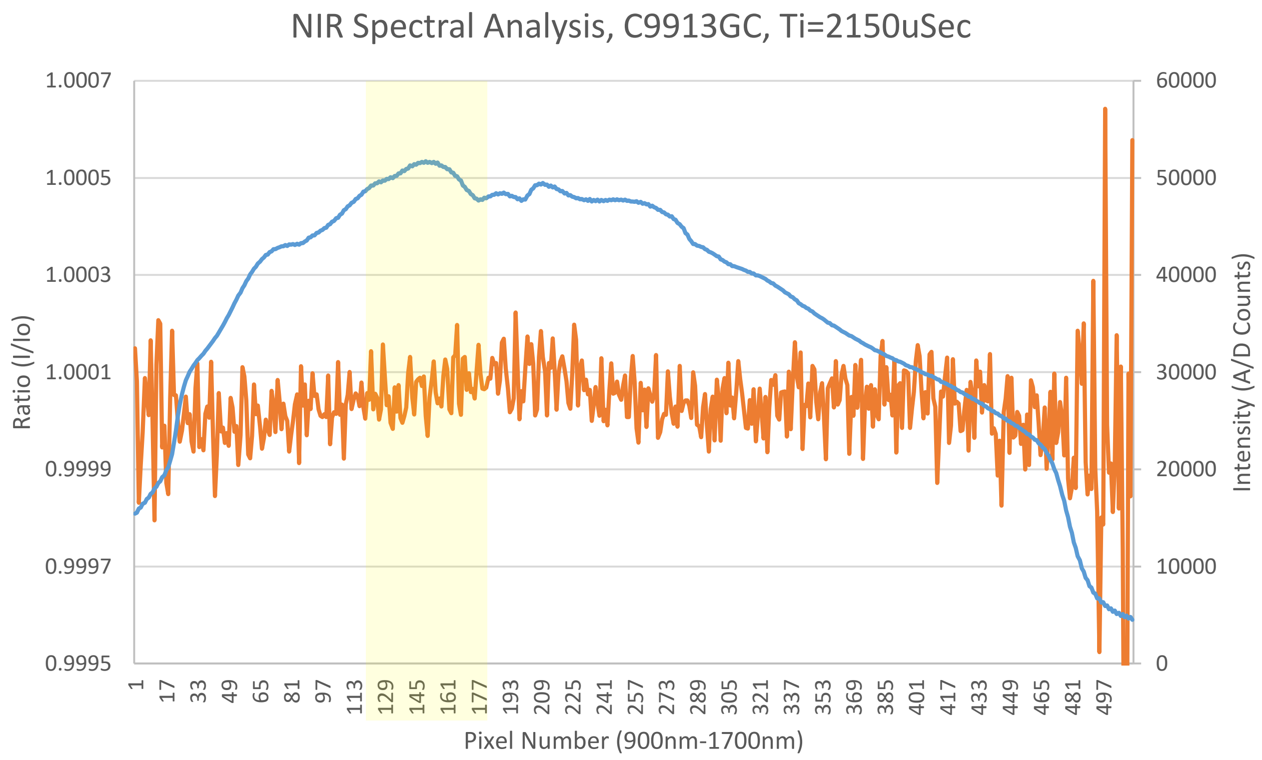
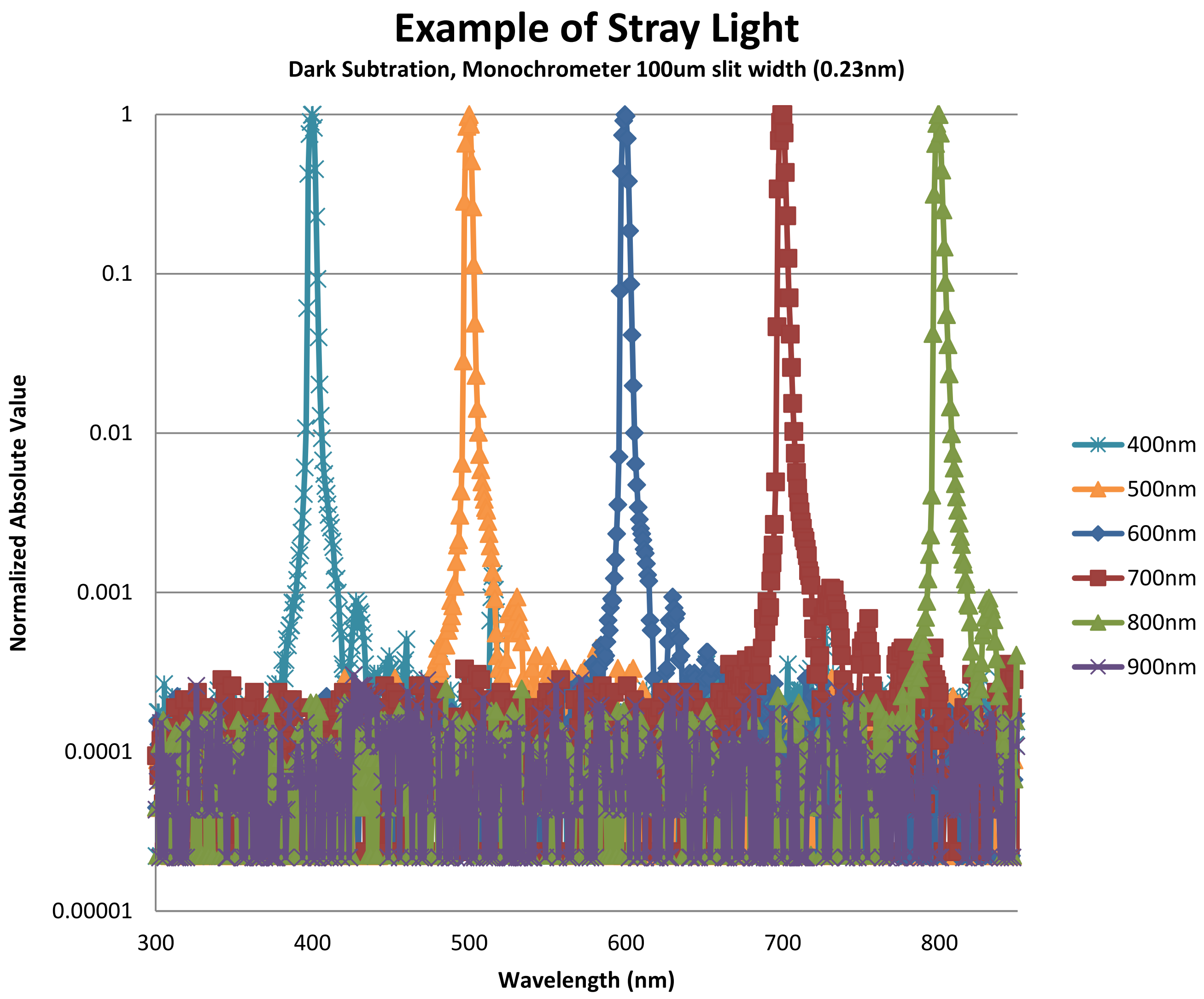
- Constant illumination source, acquire consecutive 100 spectrum.
- Maximum signal to noise occurs at highest signal level.
- Ideally we are operating within a Photon Shot noise limit.
- Highlighted region of interest represents the expected highest SNR
- Where is the noise the largest?
- What is the noise on the edges?



Troubleshooting – When Measurement doesn’t match Theory

- Narrow down noise source.
  - Check dark noise performance?
  - Plot temporal distribution (signal vs time).
- Assess spectrometer stray light contributions.
  - Light wonders to unexpected region.
- What impact does temperature have on your measurements?
  - Keep measurement interval as short as possible to minimize the impact of temperature drift.



Troubleshooting – When Measurement doesn’t match Theory

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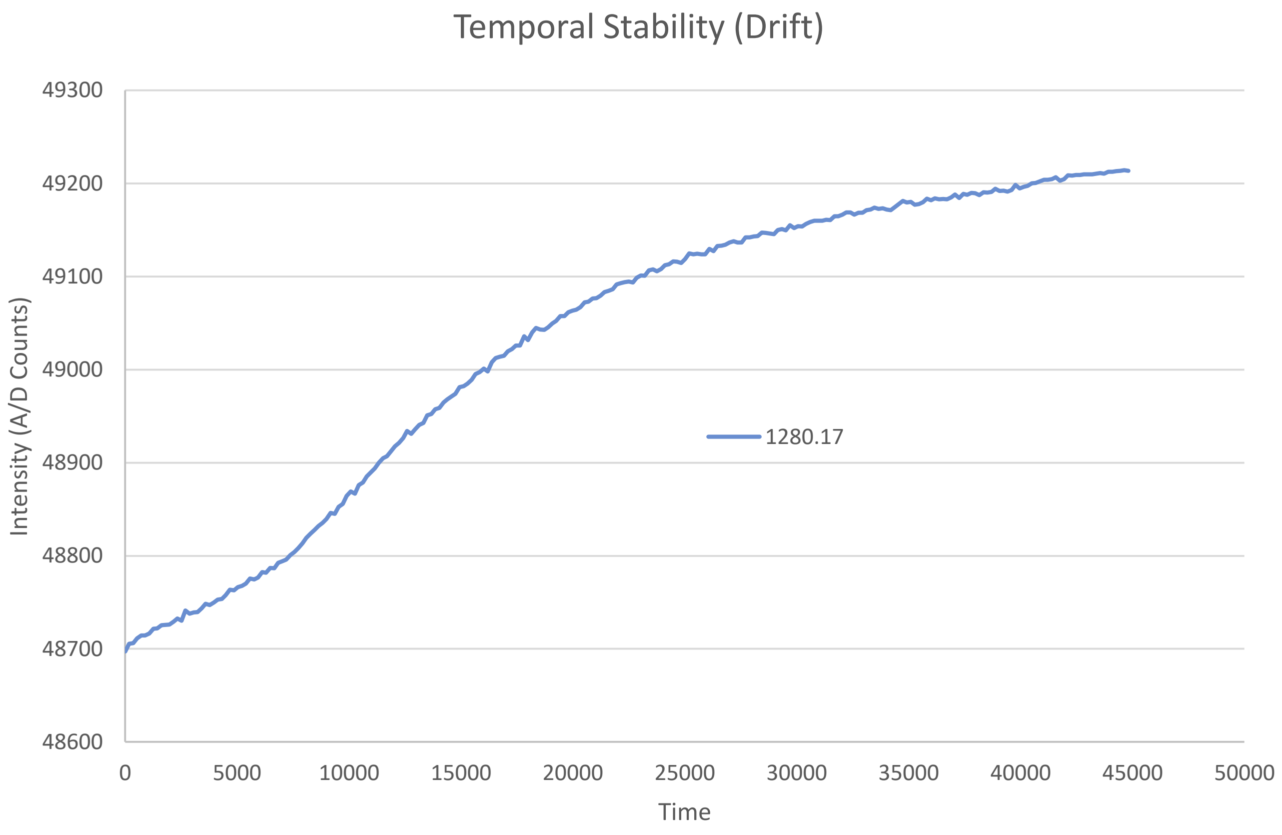

Closing Remarks

- Signal to Noise is one of the most important parameters to consider when performing spectroscopic analysis.
- Many factors involved with SNR analysis.
- Measured data and analysis need to be carefully considered for accurate results.
- For single scan applications, the maximum SNR is the square root of the number of electronics.

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1 Weeks Break				
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5	Introduction to Image Sensors	2	30-Jun-20	02-Jul-20
1 Weeks Break				
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