

Flexible Trade-offs in Maximizing SNR and Resolution in TI DLP® Technology-Based Spectrometer Systems

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ABSTRACT

Signal-to-noise ratio (SNR) and resolution are two key performance metrics for any spectrometer. While SNR is typically quoted as a single ratio in a typical condition, the SNR for a particular condition may differ from the quoted value based on the following factors:

- The scan time and other settings or operational modes used for a scan;
- · The wavelength inspected;
- How much signal enters the instrument, which is affected by the illumination, sampling method, and the particular sample under test.

Understanding how the settings and operational modes of an instrument affect SNR helps users utilize their instrument in the most effective way for their application. It also helps instrument designers optimize the system design so that users of their systems can achieve the desired tradeoff between SNR, resolution, and scan time. Design choices which affect SNR equally in all instrument setup conditions are covered in the DLP Spectrometer Design Considerations application note, and are not the subject of this document. Examples of those factors are: light source stability, light source intensity, optical engine efficiency, and detector and analog front end noise, the last of which is covered in more detail in the Optimizing the DLP Spectrometer Signal Chain application note. Instead, this document focuses on SNR and resolution evaluation methods and the functionality offered by DLP technology in spectroscopy. DLP technology can dynamically optimize the classic spectrometer performance tradeoffs of SNR versus resolution and SNR versus scan time. This allows spectrometers based on DLP technology to achieve maximum performance for each application they encounter.

Measurement methods and specific steps are provided for the DLP NIRscan™ and DLP NIRscan Nano evaluation modules (EVMs). For more information on the stated specifications of these EVMs, please refer to the respective EVM User's Guide. With this information, the reader should be able to easily evaluate the performance of instruments based on DLP technology and benchmark them against other spectrometer instruments.

Finally, a model is presented which simulates the tradeoff between the instrument settings and their effect on SNR for a particular sampling setup. This model is verified with test data from the DLP NIRscan Nano. Spectrometers using DLP technology offer features such as multiplexed patterns, variable pattern width, and variable integration time which are not present in more traditional portable spectrometer technologies. This flexibility due to the programmability of spectrometers using DLP technology brings many advantages, including a digital slew scan functionality where particular regions of wavelengths can have different scan definitions to perform different tradeoffs between these factors. Understanding how these features operate and how they affect SNR and resolution is vital to maximizing application performance of spectrometers based on DLP technology. Understanding this flexibility and the trade-offs at the time of system design and usage is beneficial for both the system designer and the advanced user of the instrument.



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www.ti.com SNR Measurement

1 SNR Measurement

In order to consistently measure SNR, a metric is defined. Details on the measurement technique for the DLP NIRscan and DLP NIRscan Nano EVMs are then provided.

1.1 SNR Metric

We define the SNR of a spectrometer system as the ratio of the measured signal amplitude at a particular wavelength of a stable input source to the stability or short-term consistency of repeated measurements at that wavelength of that stable input source as shown in Equation 1:

$$SNR\left[\lambda_{n}\right] = \frac{mean\left(Int\left[\lambda_{n}\right]\right)}{\frac{\sigma\left(Int\left[\lambda_{n},s_{m}\right]-Int\left[lambda_{n},s_{m-1}\right]\right)}{\sqrt{2}}} = \frac{\frac{\sum_{m=1}^{k}\left(Int\left[\lambda_{n},s_{m}\right]\right)}{k}}{\sqrt{\frac{\sum_{m=2}^{k}\left(Int\left[\lambda_{n},s_{m-1}\right]\right)^{2}}{\sqrt{2}}}}$$

$$\frac{\sqrt{\sum_{m=2}^{k}\left(Int\left[\lambda_{n},s_{m-1}\right]\right)^{2}}}{\sqrt{2}}$$
(1)

where the scan period between successive scans approaches the scan time being tested and,

 $SNR\left[\lambda_{n}
ight]$ — SNR at wavelength n for this configuration and scan time

 $Int\left[\lambda_{n},s_{m}\right]$ — The intensity of wavelength n during scan m

k — The number of scans taken during the SNR test

The stability of the signal is taken as the standard deviation of the difference vector between successive scans divided by the square root of two. This is done in order to focus on instrument variability rather than long-term effects. These longer term drift effects may impact system performance, but they are not included in this definition because they are highly dependent on signal drift sources that are outside of the control of the spectrometer optical engine. Examples are lamp brightness, large environmental changes, variation in sampling technique, and others. This noise term is divided by the square root of 2 because each element in the difference vector is an RMS combination of two noise measurements.

To test SNR at a particular scan setting, the following procedure can be used, as illustrated in Figure 1 and Table 1:

- 1. Execute scan k times with scan time t and no time between scans.
- 2. Compute difference vector of the intensities at wavelength n.
- 3. Compute the average of the intensity measurements at wavelength n.
- 4. Compute the SNR as shown in Equation 1.

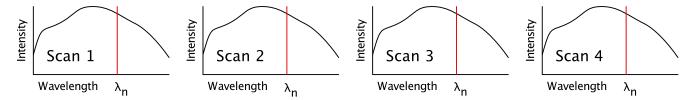


Figure 1. SNR Scan Process



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Table 1. SNR Scan Process Example

	$Int\left[\lambda_n,s_m\right]$	$\int Int \left[\lambda_n, s_m\right] - Int \left[\lambda_n, s_{m-1}\right]$				
Scan 1	210					
Scan 2	215	215 - 210 = 5				
Scan 3	212	212 - 215 = -3				
Scan 4	213	213 - 212 = -1				
Mean	212.5					
Standard Deviation		4.2				
SNR = Mean / Standard Deviation = 212.5 / 4.2 = 50.6						

This allows the computation of the SNR at any wavelength, at the tested resolution, for a particular scan time. SNR at other wavelengths, resolutions, and scan times, can be measured by altering those parameters and repeating the test.

1.2 Measurement Constraints

For instruments which include a light source like the DLP NIRscan and DLP NIRscan Nano, 'stable input source' refers to a mechanically stable sample that yields maximum signal as illuminated by the included lamp. For transmittance sampling, data is taken with no sample in the sampling path. For reflectance sampling, data is taken with a known diffuse reflectance standard which is near 100% reflective in the waveband being tested. An example of a material commonly used in visible and near-infrared (NIR) regions is Spectralon™. Instruments which do not include a light source should be evaluated with the external source and sampling instrument used during measurements.

Since the signal average and standard deviation vary as a function of wavelength, the SNR will also vary as a function of wavelength. For simplicity, instrument companies usually quote SNR only at the peak response of the instrument. The requirements of a particular application may require a minimum SNR at wavelengths other than the peak wavelength. In this case, modeling and testing at the wavelengths of interest may be necessary.

Various other SNR metrics are used for different applications and by different instrument suppliers. Many instruments do not have an integral illumination head, and instead include a fiber input. Because of this, some of these instruments only quote dynamic range, which is typically defined as the ratio of the digital full scale input if the instrument were saturated to the dark noise of the instrument with the slit blocked. This is typically much higher than if the SNR of the same instrument were measured as defined earlier.

Other applications define SNR utilizing communications theory, where the power of a narrow wavelength signal is compared to the power of the signal measured outside of the expected bandwidth of the narrow wavelength signal. This is useful in some applications, but it has a tendency to measure both SNR and stray light performance in a single measurement. When stray light is high, the SNR by this definition would be lower than by the definition proposed in this application note. To have an accurate view of a system's performance, it is helpful to separate SNR and stray light into two different metrics.

1.3 Measurement Procedure

To properly measure the SNR of a system, multiple scans must be taken immediately after each other. Manual collection of this data is tedious. It also introduces human variability in the time between successive scans, and limits the speed at which scans can be taken. This section shows the methods we use to characterize the SNR of our DLP NIRscan and DLP NIRscan Nano EVMs in an automated manner for consistent data collection with short and measurable integration times. For comparison with other instruments, SNR measurements should be done in a similar manner by capturing back-to-back scans.



www.ti.com SNR Measurement

1.3.1 DLP NIRscan

In the DLP NIRscan EVM, the included HTML control interface does not directly allow for automated repeated scan measurements and export of the raw data. However, the DLP NIRscan EVM runs a Linux operating system, and there is a command line application (dlp_nirscan) included which does allow this lower level control. To access this, it is necessary to gain shell access to the unit.

- 1. Connect and gain shell access by one of the following options:
 - (a) RNDIS (Remote Network Driver Interface Specification) over USB
 - (i) Connect USB cable between the DLP NIRscan and a computer as if you were going to access the HTML interface.
 - (ii) Power on the DLP NIRscan.
 - (iii) Initiate an SSH terminal session with the following credentials and no password:

```
server IP address— 192.168.0.10
username— root
password— N/A
```

- (b) Ethernet
 - (i) Connect Ethernet cable between the DLP NIRscan and your network.
 - (ii) Connect USB cable between the DLP NIRscan and a computer to access the HTML interface.
 - (iii) Power on the DLP NIRscan.
 - (iv) In the information screen, note the IP address which the DLP NIRscan has obtained from the network's DHCP server.
 - (v) In a computer connected to the same local network which the DLP NIRscan is connected to, initiate an SSH terminal session with the following credentials and no password:

```
server IP address— (obtained in previous step)
username— root
password— N/A
```

2. Navigate to a directory and create a directory where we will store the images:

```
cd /usr/share
mkdir -p SNR-test/patterns
```

3. Generate and load patterns for scan (this generates patterns for a 100-pattern scan, where each pattern is exposed for 10ms):

```
dlp_nirscan -A32 -Z1800 -N100 -E10000
cd patterns
dlp_nirscan -P scan.sdf
dlp_nirscan -15
cd ..
```

- 4. Ensure nothing is in the sample holder (empty)
- 5. Set the PGA gain of the ADC to the highest value where samples do not exceed digital full scale:

```
dlp_nirscan -g16
```

6. Execute scan command for 100 scans:

```
dlp_nirscan -S100 -freadings.txt -L100 -E10000
```

7. Copy files to host PC. With the same credentials used in step 1, you may connect to the DLP NIRscan EVM with an FTP program over SFTP. This will allow you to navigate to the directory where the scans were executed from and copy the output text files to a local machine.

Once this data resides on a host PC, the output text files include the intensity readings for each pattern. These can be imported and processed with the tool of your choice in order to compute SNR based on the earlier explanation.



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1.3.2 DLP NIRscan Nano

The DLP NIRscan Nano EVM GUI available for download at ti.com allows the user to execute scans and modify the settings for those scans, which we call scan configurations. The user's guide lists a USB command which launches a special SNR measurement scan sequence implemented in the firmware of the DLP NIRscan Nano EVM. This is done so that successive scans can be executed without the standard lamp warm-up and turn-off time between scans. This function both executes the scans necessary to compute the SNR and computes the SNR within the DLP NIRscan Nano. After the scans are performed, the computed SNRs are transferred to the PC. This involves executing a sequence of the following commands:

- 1. Set the desired scan configuration to test. Pattern width may be adjusted, but the measured integration times are set within the Tiva application processor firmware to test integration times of 17 ms, 133 ms, and 600 ms. The total number of patterns must be set to SNR_PATTERNS, and the number of scans or number of repeats must be 720.
- 2. Start the scan.
- 3. Wait for scans to complete.
- 4. Read the data.

This process is handled in the GUI source for both column and Hadamard scans by the MainWindow::DoSNRComputation() function.



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1.4 Scan Types

The two basic scan types implemented for both DLP NIRscan and DLP NIRscan Nano are column and Hadamard. Hadamard scans direct energy toward the detector from multiple wavelengths simultaneously in a way that the spectrum can be mathematically determined from these measurements. Since the individual regions of pixels measuring a particular wavelength is the same size and shape in both Hadamard and Column scans, the measured resolution does not differ between the two methods, while the measured SNR is different. For more information on the implementation of Hadamard scans, see the DLP Spectrometer Design Considerations application note.

The wavelength-multiplexing nature of Hadamard scans does direct much more light to the detector during each measurement. This typically yields higher SNR than column scans, but in Hadamard scans the noise is not directly proportional to the wavelength as it is during column scans since the intensity received by the detector for each pattern no longer has a one to one relationship with a single wavelength. The SNR gain is also related to the number of independent patterns being measured and other scan factors, so the degree of improvement may vary based on these scan configuration parameters. Figure 2 shows measured column and Hadamard SNRs in the DLP NIRscan EVM.

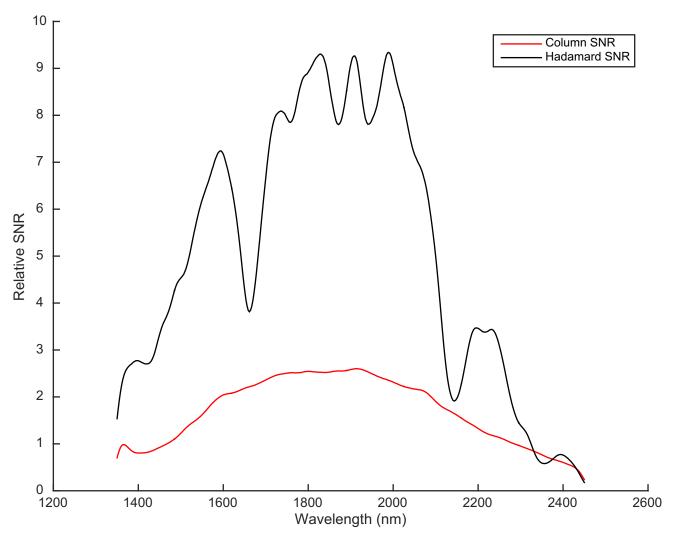


Figure 2. Hadamard SNR vs. Column SNR in DLP NIRscan EVM



Resolution Measurement www.ti.com

2 Resolution Measurement

The resolution of a spectrometer impacts the minimum distance between two peaks so that they are measured as two separate peaks. The minimum required resolution depends on the material being inspected, since different materials contain combinations of absorbance peaks of different widths.

2.1 Method

The resolution of a spectrometer is typically specified in full-width half-max (FWHM) of the measured width of a zero-width input source. This is a convenient measure because as shown in Figure 3 when two independent peaks are closer to each other than the system resolution of the instrument, they are resolved as a single peak instead of two independent peaks. Broadly, this means that the target system resolution in FWHM should be smaller in nanometers than the distance between two peaks that need to be resolved.

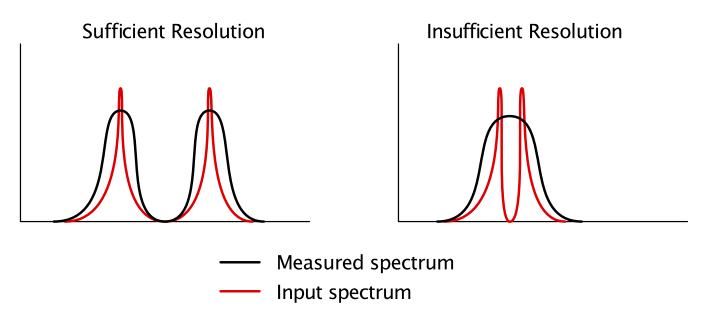


Figure 3. Required FWHM Determination

A narrow-band excitation source is required for accurate resolution measurements. The narrowest available sources are wavelength calibration sources which excite various rare gases and metal vapors, or high quality narrow-bandwidth lasers. If the width of the source is known, it can be deconvolved with the measured peak or removed by assuming that the FWHM of the measured spectrum is the root mean square (RMS) addition of the spectrometer's FWHM and the source's FWHM. However, it is always better to start with a narrow excitation source to reduce the potential magnitude of this error.



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The FWHM of the DLP NIRscan Nano EVM is tested at the factory by scanning an Argon source which provides narrow lines at several wavelengths within the measurement bandwidth of 900-1700 nm. Specifically, the widths of the following excitation wavelengths are measured:

- 965.7 nm
- 1371.9 nm

These are measured with a scan configuration with the following settings:

Start wavelength- 900 nm

End wavelength— 1700 nm

Pixel width of patterns— 5 px

Number of wavelength points— 427

Number of scans to average— 50

Scan type— column

For the data presented here, no deconvolution for removal of the excitation width has been performed.

2.2 Results

Table 2 shows the measured FWHM in nanometers of several DLP NIRscan Nano units.

Table 2. DLP NIRscan Nano Measured Resolution

Unit Under Test	FWHM at Stated Wavelength				
Onit Onder Test	965.7 nm	1371.9 nm			
DLP NIRscan Nano #1	9.76 nm	10.81 nm			
DLP NIRscan Nano #2	9.81 nm	10.37 nm			
DLP NIRscan Nano #3	9.72 nm	10.23 nm			



3 Trading Off SNR and Slit Width

In dispersive spectroscopy, there is an inherent tradeoff between resolution and SNR. This is because the resolution of an instrument is the convolution of three factors: slit width, optical resolution as defined by the point spread function, and the width of the wavelength selector element, which is the pattern on the digital micromirror device (DMD) which directs the energy toward the detector. This is shown in Figure 4:

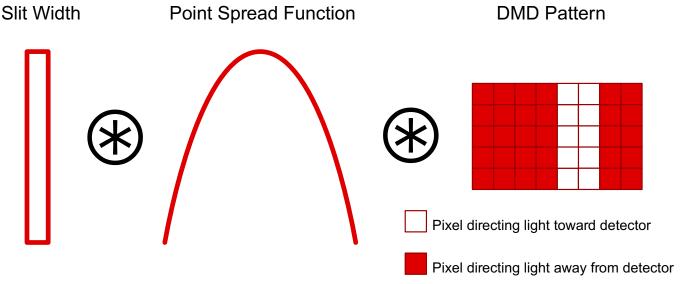


Figure 4. System Resolution By Convolution

In the case of an array detector spectrometer, the width of the wavelength selector is the pixel width of a single detector element. In the case of a spectrometer based on DLP technology, it is the width of a single DMD mirror column which directs a wavelength of light to the single pixel detector.

Improving system resolution by improving the optical resolution typically incurs some combination of the following changes to the optics and mechanics of the optomechanical module:

- Increased size
- Increased complexity
- Increased cost
- Reduction in throughput which decreases SNR

3.1 Classic Approach: Slit Width

The optical design of an instrument is fixed once a unit is produced. For array-based instruments, the width of the array detector pixels is also fixed. Therefore, the only way to trade off SNR versus resolution in these instruments is to replace the input slit. Replacing the input slit is troublesome, because for smaller instruments the placement of the slit has a very tight tolerance. Misaligning the slit by only 20-30 microns when changing slits could cause a wavelength shift of 15nm or more, depending on the size of the dispersed image plane and the optical magnification between the slit and image plane. For this reason, recalibrating the system for wavelength accuracy is often necessary after replacing a slit.

Large scanning monochromator-based systems were sometimes physically robust enough and at a large enough scale that manual replacement of the input and exit slits was possible without too much degradation in wavelength accuracy. In a monochromator, the width of the exit slit is the wavelength selector width.

As a result, array detector instruments must choose an input slit narrow enough to generate the minimum required FWHM with a fixed size detection pixel width in the most stringent resolution requirement that instrument will be used.



3.2 DLP Approach: Slit Width + Pattern Width

The optical design of the DLP NIRscan Nano, shown in Figure 5, disperses the spectrum on the DMD, and then light from selected wavelengths is directed toward the detector and measured. This compact form factor retains the capability of high system optical resolution because of the high spatial resolution DMD. The high resolution two dimensional DMD array allows fine control of the width of the wavelength selector by turning on different numbers of adjacent DMD columns per measured spectrum point. The DLP2010NIR DMD has mirrors that measure only 5.4 µm across. The dispersion from the grating is slightly nonlinear, such that the relationship between the horizontal position at the image plane on the DMD and the wavelength imaged there is slightly nonlinear. In the case of the DLP NIRscan Nano optical design for 900-1700 nm bandwidth, this translates to each pixel spaning between 0.96nm and 1.31nm at the extents of the designed bandwidth. This allows the system designer to pick the largest slit which will yield the required minimum resolution using only a few DMD columns, while higher SNR can be achieved for scans which do not require a high resolution by using more columns per wavelength. This tradeoff can be better visualized through a convolution-based model for SNR, slit width, DMD pattern width, and resolution.

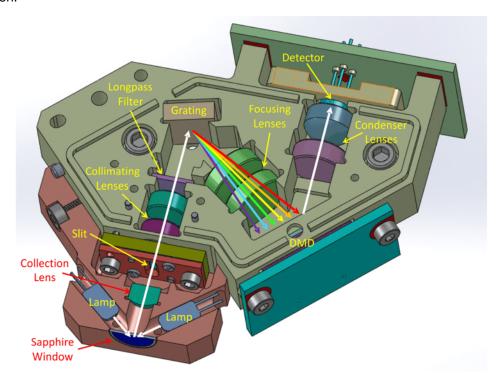


Figure 5. DLP NIRscan Nano Optical Layout



3.2.1 Model Design

In order to accurately model the optical system, a Zemax OpticStudio™ simulation was run with several different slit widths. This simulation took a field source of monochromatic light and imaged it through to the DMD. The output of the model is the energy distribution of that monochromatic slit imaged at the DMD as a function of the wavelength inspected.

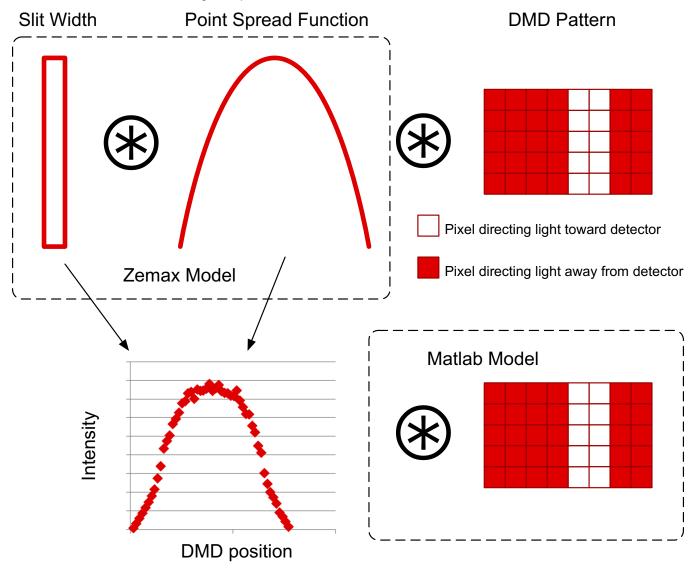


Figure 6. Resolution Model

The output of this Zemax model was then convolved with the square wave shape of different DMD pattern widths as shown in Figure 6. The photon noise in a shot-limited detection system increases proportionally with the square root of the signal. Therefore, SNR increases as shown in Equation 2:

$$RelativeSNR = \frac{signal}{\sqrt{signal}} = \sqrt{signal}$$
 (2)



For each point plotted in Figure 7, the relative SNR is then computed and normalized to the mean SNR shown in the plot. This view allows one to visualize what line within this surface is achievable for a system, given a fixed input slit width. For reference, a horizontal plane showing the intersection of a fixed 10.5 nm and 8 nm resolution with the solution space is provided. For instance, 10.5 nm resolution can be achieved at a physical slit width of 25 μ m and a pattern width of 4 pixels, or a slit width of 15 μ m and a DMD pattern width of 10 pixels. When a broader resolution of 12 nm is targeted, using a 25 μ m slit and 10 pixel wide patterns yields a higher SNR than a 15 μ m slit and a 12 pixel wide DMD pattern.

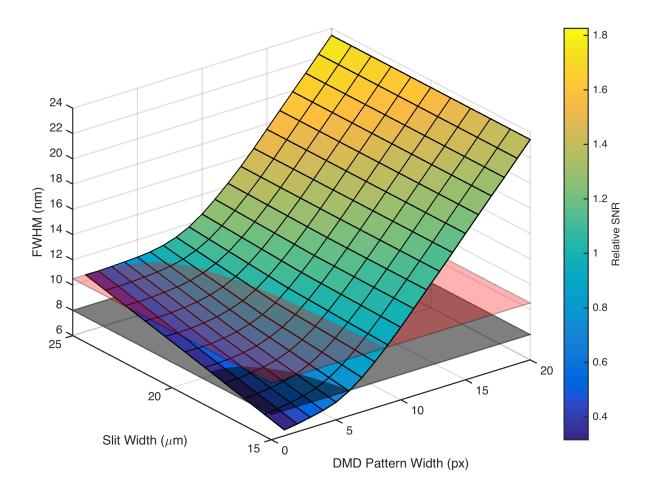


Figure 7. SNR and Resolution Model



3.2.2 Model Verification

Three slit widths were then tested with column scan patterns at various DMD pattern widths in a DLP NIRscan Nano EVM as shown in Figure 8. The marker's vertical deviation from the surface signifies the tested FWHM deviation in nanometers from the model. The marker color is the measured relative SNR, in the same scale as the model surface, and the area of each marker is scaled to the percentage deviation of the measured SNR versus the model SNR.

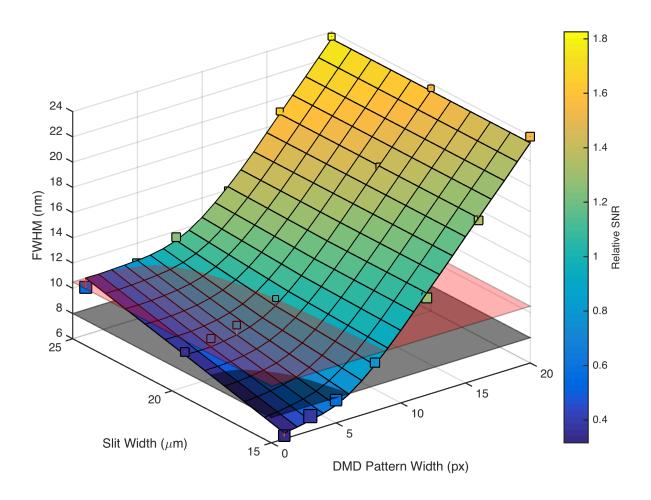


Figure 8. SNR and Resolution Tested Results: Column Scan

Table 3. SNR and Resolution Tested Results: Column Scan

Slit Width	Deviation	DMD Pattern Width (px)						
(nm)		1	3	5	8	12	16	20
15	FWHM (nm)	-0.22	+0.34	+0.41	+0.18	-0.39	-0.18	+0.50
15	Relative SNR	-0.07	-0.19	-0.15	-0.10	+0.18	+0.10	+0.11
20	FWHM (nm)	+0.25	+0.68	+0.78	+0.58	-0.52	-0.03	+0.22
20	Relative SNR	-0.03	+0.04	+0.04	+0.02	+.10	+0.04	-0.04
25	FWHM (nm)	-0.74	-0.54	-0.26	+0.25	-0.30	+0.20	+0.18
23	Relative SNR	+0.16	+0.07	+0.14	+0.09	+0.06	+0.06	+0.06



Hadamard scans were then tested and shown in Figure 9, showing good conformance to the model.

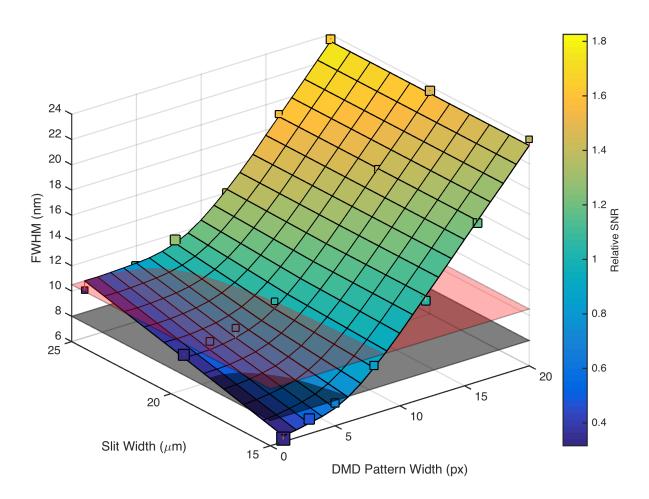


Figure 9. SNR and Resolution Tested Results: Hadamard Scan

Table 4. SNR and Resolution Tested Results: Hadamard Scan

Slit Width	Deviation	DMD Pattern Width (px)						
(nm)		1	3	5	8	12	16	20
15	FWHM (nm)	-0.22	+0.34	+0.41	+0.18	-0.39	-0.18	+0.50
13	Relative SNR	-0.11	-0.08	-0.05	-0.06	-0.08	-0.09	-0.04
20	FWHM (nm)	+0.25	+0.68	+0.78	+0.58	-0.52	-0.03	+0.22
20	Relative SNR	-0.07	+0.04	-0.03	+0.02	+0.03	+0.06	-0.16
25	FWHM (nm)	-0.74	-0.54	-0.26	+0.25	-0.30	+0.20	+0.18
25	Relative SNR	-0.01	+0.14	+0.12	+0.15	+0.11	-0.06	-0.16



The coefficient of determination for FWHM and SNR was:

FWHM R²— 0.9988

Column SNR R2— 0.9550

Hadamard SNR R²— 0.9553

These types of models for a particular optical design allow a system to be designed to enable a range of different pairs of minimum SNR and resolution specifications. The high resolution of the DMD allows a system which might require infrequent scans at a high resolution to use a wider physical input slit and reduce the DMD pattern width. This achieves a minimum FWHM value while preserving higher SNR performance for more common scans because the size of the physical input slit is maximized, maximizing the amount of light on the detector.



4 Trading Off SNR and Scan Time

As the integration time is increased and there is sufficient signal to be read noise limited, SNR is proportional to the square root of the integration time, as shown in Equation 3:

$$\frac{SNR(t_1)}{SNR(t_2)} = \frac{\sqrt{t_1}}{\sqrt{t_2}} \tag{3}$$

Instrument implementation may change this integration time by several methods:

- Increase the time spent integrating charge from the photodetector before measuring the signal;
- Increase the time spent sampling the current from the photodetector, averaging together multiple ADC samples;
- · Perform multiple scans, and average the results for each wavelength into a single spectrum.

The second and third methods are supported in the DLP NIRscan and DLP NIRscan Nano evaluation modules.

When analyzing a sample, the SNR of each spectral point is relative to its intensity at that wavelength. Since most spectrums of interest have absorbance bands where much less light is transmitted or reflected from the sample, this causes a condition where the observed SNR of a sample scan in a real application is higher in areas of lower absorbance, and lower in areas of high absorbance. If the noise in the high absorbance areas is not sufficiently low for the application, it must be reduced with one of the following approaches.

4.1 Classic Approach: All Time Increases/Decreases Together

In linear array spectrometers, the classic way to reduce noise once an instrument has been produced is to increase the sampling time or average multiple scans together. This can be effective, as SNR is inversely proportional to the square root of the exposure time. However, in situations where fast scans are required, system requirements may limit the minimum scan time possible. to increase the scan time by the square of the required SNR increase. For instance, increasing SNR by a factor of 4, the exposure time would need to be increased by a factor of 16.

4.2 DLP Approach: Increase Time Only Where You Need It

The DLP NIRscan and DLP NIRscan Nano EVMs also have a digital slew scan method, where these pattern widths and integration times can be set differently for different regions of the spectrum, allowing SNR and resolution to be optimized for different constraints over the entire spectrum. This brings functionality previously only available in large laboratory scanning grating systems into a robust, compact, and portable form factor.

Digital slew scan functionality provided in both the DLP NIRscan and DLP NIRscan Nano EVMs allows a user to choose independent exposure times for particular patterns or regions of the spectrum. This can then be used to reallocate scan time from an area of the spectrum with lower SNR requirements to an area with higher SNR requirements. The sampling time can be increased only in wavelengths where the sample is highly absorbent which might represent only 10% of the waveband. When using the slew scan function to increase SNR only in that area of interest comprising 10% of the waveband, the SNR could be raised by a factor of 4 by only increasing the total scan time by a factor of 2.5. Achieving a similar performance gain through increasing the global integration time would require increasing the scan time by a factor of 16.

5 Applications of Programmability

The programmability of spectrometers based on DLP technology allow the system designer and user to tailor the exposure time and width of different patterns in unique combinations in order to optimize the scan for a substance. Since these scans are programmable, the possibility exists for systems to define new optimized scans in a real-time, iterative nature, based on the approximate spectrum they capture. For instance, if a quick scan reveals an area requiring very high SNR or narrow resolution, additional data can be captured by adapting the scan settings so that the necessary data is captured in the shortest amount of time possible.

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