Resolution- and throughput-enhanced spectroscopy using high-throughput computational slit

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Abstract

There exists a fundamental tradeoff between spectral resolution and the efficiency or throughput for all optical spectrometers. The primary factors affecting the spectral resolution and throughput of an optical spectrometer are the size of the entrance aperture and the optical power of the focusing element. Thus far collective optimization of the above mentioned has proven difficult. Here, we introduce the concept of high-throughput computational slits (HTCS) for improving both the effective spectral resolution and efficiency of a spectrometer. The proposed HTCS approach was experimentally validated using an optical spectrometer configured with a 200 $\mu$m entrance aperture, test, and a 50 $\mu$m entrance aperture, control, demonstrating improvements in spectral resolution of the spectrum by $\sim$20% over the control spectral resolution and improvements in efficiency of $>2$ times the efficiency of the largest entrance aperture used in the study while producing highly accurate spectra.

The spectral resolution and efficiency of an optical spectrometer, which affects the ability to distinguish closely spaced spectral features such as transmission lines, absorption lines, and emission lines, are controlled by a number of different factors such as the size and shape of the entrance aperture, the optical characteristics of the dispersive element, the optical characteristics of the collimating optics the focusing optics, and the size and shape of the detector’s pixels. In particular, the size of the entrance aperture (e.g., width of slit used as entrance aperture) and the optical power of the focusing element are the primary factors affecting the tradeoff between spectral resolution and efficiency or throughput of a spectrometer. A focusing element that can create a very sharp focused spot can be useful in increasing the spectral resolution of a spectrograph but, there exists fundamental limitations in manufacturing and designing of focusing elements with high optical powers (small focal ratio, f-number or large numerical aperture) therefore more efforts have been put forth in decreasing the effective size of the entrance aperture in order to increase the spectral resolution.

The spectral resolution of the spectrometer can be increased by decreasing the size of the entrance aperture. The decrease in size, width, is only necessary along the spectral dispersion axis. By decreasing the width of the entrance aperture of the spectrometer the width of the resulting focused spectral spots are also decreased therefore subtending a smaller portion of the detector array to allow closely spaced spectral features to be distinguished. However, this decrease in size of the entrance aperture also decreases the amount of light that enters the spectrometer -as less light is able to enter the spectrometer- therefore resulting in a decrease in light throughput of the resulting spectrum. The depletion of light can be detrimental to application that are photon-starved -where the amount of light available to the spectrometer is low- yet demand extremely high spectral resolution such as Raman spectroscopy [1-3], biomedical spectroscopy [4,5], and astronomy [6,7] among many other applications. Thus, spectroscopic methods that allow for an increase in spectral resolution while maintaining and allowing for high light throughput are sought after.

Previous methods of improving both the spectral resolution and efficiency of spectrometers have focused primarily on the design of analog optical slicers situated before the dispersive element of the spectrometer. Some optical slicers use specialized prisms to slice a light beam [8], where the performance depends on the optical properties of the prism which is wavelength dependent and can limit its use in broadband light conditions. Some optical slicers-often referred to as integral field slicers- make use of slicer mirror arrays, lenslet arrays, or fiber optical bundles, in the image space, to redirect portions of the light to their respective spectrometer, thus slicing the light beam into portions with at least one of the spatial dimensions smaller than the received light beam. However, such optical slicers can be large in size and limited in getting high spectral information from all the different beam portions [9,13].

In [14], Meade et al. introduced a pupil-based optical slicer, comprising of a beam reformatter, a beam compressor and a beam expander to improve spectral resolution while allowing for high throughput via a large entrance aperture by negating the use of a light limiting slit. The beam reformatter receives a full aperture of collimated light beam and splits it into two or more beam portions in the dimension of dispersion. These beam portions, each containing similar spectral information, are then reformed into a vertical stack which has a narrower width in the direction of dispersion. An asymmetric beam expander then changes the width of the stack to match the original width of the original full aperture. While such optical slicing methods do improve both spectral resolution and throughput, they come at the expense of the introduction of additional analog optical elements that increase not only the complexity of the spectrometer, but also increases the cost of the spectrometer as well [15]. These optical components (e.g., lenses, reflective surfaces, etc.) along with the associated mounting apparatus will introduce aberrations and other performance issues (i.e. alignment) to the device. Therefore, a method that allows for an increase in both spectral resolution and throughput without the introduction of additional analog optical components and associated mounting apparatus, such as that in an optical slicer, to the spectrometer is highly desired.
In this study, we introduce the concept of high-throughput computational slit (HTCS) for improving both the effective spectral resolution and efficiency of the resulting spectrum. An overview of the proposed concept of HTCS is shown in Fig. 1. In HTCS light enters an entrance aperture (pinhole), similar to any other spectrometer, however the size of the aperture need not to be limited by the desired spectral resolution, thus, increasing the amount of light that enters the system. The light diverging out of the entrance aperture encounters a collimating element to produce a collimated light beam. The collimated light beam then continues on and is then projected onto a dispersive element, which splits the input light beam into its spectral components in the form of multiple collimated light beams traveling...
Figure 2: The improved spectral characteristics resulting from the HTCS implementation. (a) The spectra of the light source at one second exposure time using a 200 µm and a 50 µm entrance aperture and the HTCS implementation on the 200 µm entrance aperture. At wavelength of interest, 613 nm, the peak signal of the spectrum produced by the HTCS method is > 2 times and > 30 times larger than the spectrum of 200 µm and a 50 µm entrance aperture, respectively. (b) The spectra of the 200 µm and a 50 µm entrance aperture and the HTCS implementation on the 200 µm entrance aperture, normalized at 546 nm, which is a doublet. It can be observed that the spectral features from the HTCS implementation closely resembles the features observable in the 50 µm spectrum.

at different angles depending on the wavelength of light. The spectral beams then arrive at a camera which focuses the light using a focusing element and records the information on a detector. The detector recordings are then used to form digital representations of the beams that entered the detector, and the digital beams are then reformed numerically such that they appear as to have passed through a slit with the desired morphology, imposed by the spectral resolution requirement, in the first place. By passing the digital beams numerically through a high-throughput computational slit that is narrower than the physical entrance aperture of the spectrometer, improved spectral resolution can be achieved while reaping the light throughput benefits of a much larger entrance aperture.

Figure 1a shows the image of the dispersed light that is formed on the detector, from which the spectrum is extracted, note that since the size of the input aperture is not limited in the dispersion direction there is an overlap of the spectral features which tends to decrease the spectral resolution. In other words the uniqueness of wavelengths is not discernible. But given the HTCS method, a higher-resolution spectrum can be produced, resulting in highly separable spectral features, Figure 1b.

In this study a Mercury vapor fluorescent lamp was used as the source, the high-resolution spectrum of which is shown in Figure 1c. The proposed HTCS operates analogous to changing the morphology the entrance aperture of the system from a circular aperture, Figure 1d, to an elliptical aperture, Figure 1e, in this case. The spectrum of the lamp was measured using a spectrometer with a 200 µm and a 50 µm entrance aperture and the resulting exposure time independent spectra are shown in Figure 1f. It is clear that with larger entrance aperture more light is allowed to enter the spectrometer hence producing a spectrum with much higher signal. Conversely, a small entrance aperture would result in a spectrum of improved spectral resolution. Figure 1g (normalized spectra), as more spectral features can be observed. Quantitatively, using the spectral feature at ∼ 613 nm in Figure 1f, it is observed that the signal of the spectrum from the larger aperture is > 14 times higher than the signal from the smaller aperture. Additionally, according to the spectral feature at ∼ 438 nm in Figure 1g, the spectral resolution is > 4 times higher for the spectrum of the smaller aperture, 7 nm for 200 µm and 1.7 nm for 50 µm entrance apertures. This is the tradeoff that has plagued the field since its inception.

In the HTCS method, let $I^\alpha$ denote the predicted beam that would have been projected on the detector if it had passed through the desired computational slit, and let $I^\beta$ denote the beam projected on the detector having passed through the physical slit. We treat the problem of numerical beam reforming as a probabilistic state prediction problem, where the goal being to predict the most probable $I^\alpha$ given $I^\beta$, computational slit function $S$ that models the shape
Figure 3: The improved spectral resolution resulting from the HTCS implementation. The spectra of the 200 µm and a 50 µm entrance aperture and the HTCS implementation on the 200 µm entrance aperture, normalized at 546 nm, which is a doublet. It can be observed that the HTCS implementation is able to clearly resolve the doublet, resulting in a 5 times and 1.23 times spectral resolution improvement over the spectra measured using the 200 µm and a 50 µm entrance apertures, respectively. 

of the beam exiting a computational slit with the desired morphology, and optical transfer function O. Modeling \( I^\alpha \) and \( I^\beta \) as stochastic processes, the probabilistic state prediction problem can be formulated as

\[
\hat{I}^\alpha = \arg\max_{I^\alpha} \ p \left( I^\alpha | I^\beta, S, O \right),
\]

where \( p \left( I^\alpha | I^\beta, S, O \right) \) is the conditional probability of \( I^\alpha \) given \( I^\beta, S, \) and \( O. \)

Accounting for quantum photon emission statistics, the morphology of the computational slit, and nonstationary of \( I^\alpha \) and \( I^\beta \), we introduce the following \( p \left( I^\alpha | I^\beta, S, O \right): \)

\[
p \left( I^\alpha | I^\beta, S, O \right) = \prod_{x \in X} \left( \frac{1}{I^\beta_x!} \left( \frac{1}{\sqrt{2\pi(\sigma^\beta_x)^2}} \right)^{I^\alpha_x} I^\alpha_x! \right) \exp \left[ -\frac{1}{2(\sigma^\beta_x)^2} \left( I^\alpha_x - \frac{1}{\sqrt{\sigma^\beta_x}} \right)^2 \right]
\]

where \( X \) denotes a set of sensor locations in the detector, \( x \in X \) denotes a specific sensor location in the detector, and \( \bar{\sigma} \) denotes nonstationary expectation. In this study, an iterative EM solver is used to solve Eq. 1 and is performed until convergence.

For this study, a computational slit function \( S \) corresponding to a 5µm slit was used. By utilizing a computational slit with a width narrower than the physical entrance aperture, the idea is that the spectral resolution of the resulting spectrum would be enhanced while maintaining the high light-throughput enabled by the large entrance aperture.

The proposed HTCS system, implemented as described above, was examined on the spectrum of the fluorescent lamp using the 200 µm entrance aperture the results of which are shown in Figure 2 which demonstrates that not only the spectrum resulting from the HTCS system has a higher power than the original 200 µm spectrum but it has higher spectral resolution than the 50 µm spectrum. The exposure time independent spectra are shown in Figure 2 which demonstrates that the power of the HTCS spectrum is > 2 times and > 30 times higher than the 200 µm and 50 µm spectra, respectively. The spectral resolution of the HTCS spectrum, which is 1.38 nm, is 5 times and 1.23 times higher than the spectral resolution of the 200 µm (7 nm) and 50 µm (1.7 nm) spectra, respectively. This resolution enhancement can be observed in the intensity-normalized spectra, at 546 nm, shown in Figure 3 where a doublet feature at ∼ 550 nm is examined closely. This feature is not resolved in the 200 µm spectrum and is barely resolved in the 50 µm but it is clearly resolved using the HTCS system. Lastly, in order to demonstrate that the HTCS system has no adverse effects on the fidelity of the measured spectrum the correlation coefficient between all of the measured spectra and the ground truth spectrum presented in Figure 1c was evaluated. The correlation coefficient which determines the statistical relationship, likeness, between two entities is evaluated to be 94.13%, 87.69%, and 97.83% for the spectra
measured using the 50 µm entrance aperture, 200 µm entrance aperture, and HTCS compared to the ground truth spectrum presented in Figure [1]. This demonstrates that not only the HTCS improves the throughput and spectral resolution of a spectrometer, it preserves the underlying features of a spectrum and is capable of creating highly accurate spectra.

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Author Contribution

A.W. and F.K. have equally contributed to this work.

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