Improving the observing efficiency of SINFONI and KMOS at the VLT by factors of 2 to 4: sophisticated sky subtraction algorithms

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ABSTRACT

Accurate subtraction of the bright night sky emission lines in the near-infrared is crucial, given that the object being observed is often several magnitudes fainter than the sky background. Most integral field spectrographs (IFS) have a modest field of view (FoV), and it is often not possible to achieve good sky subtraction by nodding the object within the FoV, as is common practice for long slit spectrographs. In principle, it should be possible to use sky background information from one part of the FoV (typically the periphery) to subtract the sky from all other parts of the IFS FoV. However, this has never been achieved in practice.

We show that the reason on-IFU sky subtraction does not work is that the spectrograph spectral response function (line spread function, or LSF) varies strongly with wavelength, position within the field of view, and telescope pointing (flexure). By micro-stepping the grating of the SINFONI IFS at the ESO-VLT, we have been able to hyper-sample the spectral PSF and reconstruct detailed LSF profiles for all wavelengths and all field points for SINFONI H band data. Using this information, we can conclusively demonstrate improvements in observing efficiency by over a factor of two. Our technique not only removes the need for separate sky exposures, but can also improve the noise of the sky background measurement itself, providing further potential gain over pairwise frame subtraction. We explain our algorithms, including non-parametric descriptions of the LSF, and present the results from applying our method to archival SINFONI data.

Keywords: near-infrared, observing efficiency, sky subtraction, B splines, line spread function, integral field, spectroscopy, hyper-sampling.

1. MOTIVATION

The SINFONI and KMOS spectrographs operate in the near-infrared (~1.0–2.4 μm). Over most of this wavelength range, the night sky background is very bright, often many magnitudes brighter than the object signal that is being sought. The night sky emission is almost entirely in narrow, unresolved, emission lines of OH and other atmospheric species. Whilst the sensitivity of all ground based observing is limited by the added shot noise from these emission lines, even achieving this level of excess noise is extremely difficult, as it requires correctly subtracting the sky background flux for all field points at all wavelengths. Classically, sky subtraction is done by beam switching, also termed nodding, where observations of “source+sky” are alternated with those of “blank sky”. If the source size is small enough compared to the field of view (FoV), the source can be nodded within the FoV, thus maximizing the exposure time on the target. In either case, this yields accurate background subtraction independent of detailed knowledge of the instrumental spectral response function (line spread function - LSF), as “blank sky” flux is subtracted from “source+sky” flux for the same detector pixel. However, the night sky emission is temporally variable on relatively short time scales (~1 minute), requiring the use of super-sky or line group flux scaling methods to correctly account for the temporal flux changes. The length of time between the “source+sky” and “blank sky” exposure is also limited by instrument flexure, as the latter can lead to “P-Cygni” type residuals when the wavelength mis-alignment between the two frames exceeds a few percent of the line width.

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Integral field spectrographs (IFS) like SINFONI and KMOS often have a modest field of view, as only the linear extent of the detector is available for both dimensions of spatial information (at least in the more popular type using image slicers). Consequently, the amount of “blank sky” within the field of view is limited, and it is often not possible to nod the object within this limited field of view. As a result, most observations with SINFONI and KMOS need to spend half the time observing “blank sky” to measure the sky background spectrum with sufficient accuracy for scaling (to account for the temporal variation) and subtraction.

Of course, as there is only a single sky spectrum relevant to observations with all spatial elements (the entire FoV of the SINFONI IFU, or all 24 IFUs of KMOS), it should, at least in theory, be possible to use information from a fraction of spatial elements (spaxels) that point to blank sky to correctly subtract the sky spectrum for all spatial elements (spaxels), thus eliminating the need for sky observations entirely. Although this has been tried several times (e.g. with SINFONI at the VLT), it has never been successfully achieved for an IFS.

If we could successfully use information from a part of the IFS FoV that points to blank sky to accurately estimate the sky spectrum, and subtract it from all spaxels of the IFU, we would eliminate the need for blank sky exposures, thus improving observing efficiency by a factor of two. Furthermore, if we could combine the information from all blank sky spaxels to produce a very high signal-to-noise ratio sky spectrum, we could almost eliminate the excess noise associated with the sky subtraction process, thus improving the observing efficiency by another factor of two.

This paper seeks to demonstrate that we can certainly achieve the first factor-of-two gain, virtually eliminating the need for separate sky exposures. We have also made significant progress towards achieving an almost noise-less sky spectrum measurement, thus recovering most of the second factor-of-two gain. Section 2 provides an overview, section 3 describes the method employed, section 4 presents the results achieved so far, and section 5 provides conclusions and a plan for future work.

1.1 Knowing the LSF

The primary reason that on-IFU sky subtraction does not work is because the spectrograph’s LSF (spectral PSF) varies strongly with wavelength and position within the field of view. To demonstrate this, we need to measure the spectrograph LSF with sufficient sampling along the spectral axis. Typically, integral field spectrographs just satisfy the Nyquist sampling criterion in the spectral direction, with two samples per resolution element. We have used spectrally hyper-sampled data from SINFONI to accurately reconstruct LSFs for all sky emission lines at all field points (similar hyper-sampling has been achieved with DEIMOS, NIRSPEC, and LRIS on Keck\textsuperscript{3}). The shapes are strongly non-Gaussian (figure 1), and vary substantially with wavelength and field position (figure 2). It is self-evident that this strong variation in LSF leads to large residuals when spectra observed at one location on the detector are subtracted from other locations, even if the correct wavelength shift and flux scaling can be determined in an accurate manner.

![Typical SINFONI line spread function](image1)

![Variation in SINFONI line spread function](image2)

Figure 1: Hyper-sampled line spread function for the SINFONI spectrograph in the H band. The red line is a smooth curve through the hyper-sampled data points (black), while the blue line represents the best fit Gaussian. There are substantial departures from a Gaussian profile.

Figure 2: Hyper-sampled line profiles for a single H band night sky emission line at three different spatial positions within the SINFONI FoV. The variation in width and LSF shape is self-evident.
2. OVERVIEW

2.1 Overview
We have developed a new technique to improve the sky subtraction of IFU data while simultaneously increasing the observing efficiency by eliminating the need to take separate/simultaneous night sky observations. We first constructed a hypersampled data frame by combining a series of wavelength-shifted night sky exposures. From this hypersampled frame we separately modelled the line profiles of each of the ~100 brightest lines in each slitlet, constructing a database of line profiles. We performed the sky subtraction on science data by identifying regions on the science frame dominated by sky flux, scaling and shifting our hypersampled line profiles to match the observed data in these regions and then subtracting the scaled and shifted hypersampled frame from the science frame. We tested our technique on H-band SINFONI observations and found that it results in a sky subtraction with accuracies better than 1 per cent, comparable to those achievable with separate sky exposures.

2.2 Observations and initial reduction
To construct the hypersampled data frame we obtained a series of IFU observations with the SINFONI IFU at the European Southern Observatory Very Large Telescope in Paranal, Chile. Over two nights (4 July 2010 and 02 Aug 2010) we obtained 26 H-band exposures of blank sky at zenith, each with 300 s exposure time. In each subsequent exposure the central wavelength of the grating was shifted by ~0.1 spectral pixels, corresponding to ~0.1Å. The final dataset spans a range in central spectral pixel of ~1.5 pixels, with ~0.05 spectral pixel sampling (see Figure 3).

![Figure 3: Measurement of the line centroid for an isolated line for the 26 data frames. The X axis gives the peak location in detector pixel units, while the Y axis shows the value read back from the grating encoder.](http://proceedings.spiedigitallibrary.org/)

We constructed a bad pixel map and high S/N flat field frame from the standard SINFONI calibration data taken on the nights of our observations. The bad pixel map includes static bad pixels (taken from the SINFONI reference bad pixel map from the ESO QC archive), hot pixels and non-linear pixels (identified by comparing the flux in a series of lamp flat frames of increasing exposure time). The high S/N flat field frame was produced by combining 10 lamp frames, while masking bad pixels and rejecting cosmic rays by median-filtering each frame before median-combining. Using a bootstrapping analysis we determined that the noise in the final flat-field frame was ~0.1 per cent. Each of the 26 science exposures was then dark subtracted and flat-fielded by dividing through by the high S/N flat frame.

3. METHOD

3.1 Constructing a hypersampled frame
We combined the 26 separate sky exposures into a single hypersampled SINFONI frame, by placing each frame on a common spectral axis. In order to achieve our target accuracy of 1 per cent in the final sky subtraction it was necessary to align the frames to ≤0.1 spectral pixels. Initial attempts to achieve this by placing each frame on a common wavelength scale did not meet this target. Instead we opted to carry out the hypersampling in pixel space without making...
the transformation to wavelength space. This eliminates the additional source of errors incurred by comparing line positions to a line list and fitting a smoothly varying wavelength solution.

We first identified the centroids of all lines in a single column on a single frame by resampling each sky frame on to a finer grid (by a factor of 100) and convolving the data with an antisymmetric function similar to the one used in IRAF task center1d. We refer to the resampled pixels, where 100 resampled spectral pixels corresponds to a single SINFONI spectral pixel, as hypersampled pixels. The width of the convolution function was matched to that of the observed sky lines. Line centroids are identified by the zero-crossing of the convolved spectrum, with emission lines corresponding to negative-to-positive transitions (and absorption features positive-to-negative). We select all lines above a threshold of 200 counts, to avoid incorrectly identifying noise features or bad pixels as sky emission features. This process was repeated for each column in the frame, then for each of the 26 sky frames, to form a list of line centroids. By comparing the variation in the measured line centroids between frames we estimate this technique is accurate to 0.03 spectral pixels.

Because the sky brightness varies on short timescales (< 300s) it is not sufficient to combine the sky frames by placing them on a common spectral scale - they must also be placed on a common flux scale. An example of a line profile formed by combining the 26 sky frames without correcting for sky brightness variations is shown in the left panel of figure 4. Here each colour corresponds to data from a single sky frame and the two symbols used distinguish data taken on the two different nights. Significant differences in the line flux are clearly visible, both between the two nights (~15 per cent) and during a single night (~7 per cent).

To correct for variations in the line flux between observations we normalised the data from each sky frame to a common level on a line-by-line basis. For each line centroid identified in the previous step we extracted a 20 pixel (2000 hypersampled pixel) region around the centroid position. We fit a single Gaussian function to each line profile to determine the Gaussian flux within the line. We then normalised the 26 line profiles, one from each of the separate sky frames, to a common flux level. Using a Gaussian fit to parameterise the line fluxes was found to produce smoother profiles than using the total or peak line fluxes. The 26 normalised line profiles were then placed on a common spectral axis by aligning the line centroids determined above. We show an example of a flux-scaled, hypersampled line profile in the right panel of figure 4. The scaled, hypersampled profile is much smoother than the unscaled profile, though individual bad datapoints can still be distinguished. The detailed structure of the line profile emerges here, with clear deviations from a Gaussian profile evident. This process was repeated for all lines identified above. Finally each line profile is placed into a hypersampled frame (with 2048 spatial pixels, corresponding to 32 slitlets of width 64 pixels and 204,800 hypersampled spectral pixels). The process was unsuccessful for a limited number of cases, particularly for lines close to the edge of a slitlet where contamination by light from the adjacent slitlet becomes an issue and also for lines strongly affected by bad pixels or cosmic rays.
3.2 Fitting line profiles

We observe that the SINFONI H band LSFs are often asymmetric, with shoulders and other features that deviate substantially from a Gaussian profile. Consequently, we were interested in characterizing the line spread function in a non-parametric manner, as it was essential to accurately represent the line shape to avoid residuals from the sky subtraction. Doing this in the presence of measurement noise (and the occasional bad data point) requires “fitting” the data points with a “smooth” function, but without a restrictive functional form. B splines have been used to super-sample data when employing sky subtraction in multi-object spectrographs\(^2\), and we employed a similar technique. We used an iterative method, first fitting the flux scaled hyper-sampled line profile (right panel of figure 4) with a set of B splines. Deviations from the smooth curve were used to weed out bad points. We noticed that the line spread function varied smoothly with wavelength and spatial position on the detector, differences within one slitlet were negligible. Consequently, we combined all the valid data points (output from the steps above) within one slitlet, after appropriately shifting and scaling data for each spaxel. This produced an LSF with even better sampling, and B splines could be fit to this data set, again weeding out bad points that were outliers. The result was a smooth line spread function for each isolated spectral line, and for each slitlet. As the variation in LSF with wavelength is smooth, we could use LSFs computed using isolated lines for very nearby crowded regions, without any noticeable degradation in performance.

After producing B-spline fits to each hypersampled line in each slitlet we revisited the production of the hypersampled frame, using the B-spline line profiles to improve the accuracy of the line centroiding and flux normalisation. On the individual sky frames we fit the hypersampled data for a single line within a single column with the corresponding B-spline line profile, allowing a linear shift along the spectral axis and a multiplicative scaling of the flux. We repeated this on the data for each of the 26 separate sky frames, resulting in a set of relative spectral shifts and flux scalings more accurate than those determined from the line centroiding and Gaussian fitting. Using the new line centroids and flux scalings, we produced a new hypersampled line profile as above. Using a fixed line profile we were able to determine hypersampled line profiles for lines that the initial technique had failed on. The process of producing a hypersampled frame and constructing B-spline fits of the line profiles was iterated until hypersampled profiles were available for all bright lines in all slitlets and the determined line centroids and flux scalings no longer varied.

Information from all 26 sky frames was combined to produce a database of line spread functions, for each sky emission line and for each slitlet. The line spread functions have very fine sampling and are high signal to noise. In addition, we have accurate relative positions and fluxes as a function of spaxel number (running from 1 to 2040 across the detector) for each spectral line. The creation of this database is depicted in the grey flowchart on the left hand side of figure 5.

![Figure 5: block diagram showing the steps in the new sky subtraction algorithm. The parts designated in grey (on the left) create the LSF database, and need only be performed infrequently. The parts on the right (with blue-green background) apply the technique to each science exposure.](http://proceedings.spiedigitallibrary.org/ on 01/13/2013 Terms of Use: http://spiedl.org/terms)
3.3 Subtracting sky emission lines

To use the hypersampled LSF database to subtract the sky emission lines from real science data, it is first necessary to identify regions of the science frame dominated by sky flux. This limits the technique to science frames where the science object does not completely fill the field-of-view. We process the science frame one night sky emission line at a time, the procedure for each spectral line is depicted in the blue-green boxes on the right half of figure 5. We mask out all spaxels of the science frame that might contain object flux. For the remaining spaxels (corresponding to blank sky), we determine a single shift and scale of the science frame so that it best fits the hypersampled database for that line. Note that the science frame is sparsely sampled, both spectrally and spatially, with respect to the corresponding section of the hypersampled frame. Once the required shift and scale can be ascertained, it can be applied to all spaxels. The relative positions of the line centroids for all spaxels are already accurately known, this information being stored separately for all sky emission lines. The shifted and scaled hyper sampled frame can then be sampled at the wavelength points appropriate for each spaxel, using the information on the relative offsets of the line centroids. This results in a robust estimate of the night sky emission for that particular line, which can be subtracted from the science frame.

If ~10% of the spaxels correspond to blank sky, and can be used to estimate the flux scaling, we can gain a factor of ~14 in estimating the sky flux level in each line. Furthermore, if many sky lines are known to vary together\(^1\), then we can further improve the sky flux estimate. In the following section we apply this technique to real science data comparing it to other common sky subtraction techniques, as well as examining the overall sky subtraction accuracy we achieve with this technique.

4. RESULTS

4.1 Detailed look at subtracting individual lines

Figure 6 shows the results of applying our technique to a 600 sec science exposure obtained from the ESO VLT archive. The science target for these observations was a distant emission line galaxy, and the continuum is not detected in a single exposure. We chose a night sky emission line well separated in wavelength from the region containing object flux. Thus, for our purposes, the archival data represent a set of blank sky exposures. The results from applying our technique are shown in the top panel of figure 6. The brick-wall pattern of the SINFONI slicer is clearly visible, including the different wavelength offsets of the central two spaxels. In this test, only every other slitlet has had the night sky emission line subtracted from it. The middle panel represents the original data, and the bottom panel represents the result from subtracting the subsequent science exposure for the same target, taken immediately after the first science exposure. It is obvious that the night sky has varied between the two exposures, resulting in a large negative residual from the pair-wise subtraction of the subsequent frame. This can be corrected by scaling the flux from the second frame prior to subtraction. We compare the residuals from our technique with such a scaled pair-wise subtraction in the next section.

Figure 6: comparison of our proposed sky subtraction algorithm with a "nodding" scheme. The three panels are separated by white bars. The red ovals highlight one of the regions where sky subtraction has been performed.
4.2 Comparison of our technique with nodding-on-IFU for real science data

Figure 7: Residuals resulting from subtraction of a single night sky emission line. Data from all spaxels has been overlaid in this plot, using the line centroid of the hypersampled line as a reference. The red lines indicate the expected 2-sigma limits for pair-wise subtracted frames. The blue line is a histogram of the fraction of points that fall within the red curves, with the dashed pink lines representing 100% and 90% respectively. The left hand panel shows the result from subtracting a scaled version of a subsequent science exposure, while the right panel shows the residuals from using the proposed technique.

Figure 7 shows the accuracy of the sky subtraction achieved by using the proposed technique (right panel), by comparing the residuals with a scaled pair-wise subtraction of two science exposures. For each spaxel, we plot the residuals over a range of +/- 9 spectral pixels relative to the line peak. Data for each spaxel are re-centered, so that the line peak lies at the same location (hypersampled pixel 5500) for all spaxels. The proposed technique achieves higher sky subtraction accuracy than scaled pair-wise subtraction of science frames, without the need for a separate sky exposure! One can notice a slight excess of residuals top left and bottom right of the peak, for the pairwise subtracted data. This indicates the presence of measurable instrument flexure, even within the short time span of 10 minutes. We note that pairwise subtraction (scaled or not) only works in the absence of instrument flexure, as the latter can cause systematic shifts in the spectra, that cannot be accounted for in the subtraction procedure.

5. CONCLUSIONS

We have demonstrated a new technique to perform sky subtraction for near-infrared integral field spectrographs that removes the need for dedicated blank sky exposures, thus making near-infrared observing similar in observing methodology and efficiency to observations at visible wavelengths. The technique relies on detailed measurements of the spectrograph line spread function for all spaxels and at all wavelengths corresponding to night-sky emission lines. Once a database can be populated with the required information for all night sky emission lines, science data can be sky subtracted in a quick and robust manner. An improvement in observing efficiency of a factor of two has already been demonstrated, and more may be possible if the sky flux estimate and flat field accuracy can be further improved.

5.1 Summary of the technique

Integral field spectrographs have a high density of information on the near-infrared detector, with spectra recorded for all spaxels covering a two-dimensional field of view. However, variations in the spectrograph point spread function across the detector result in substantial variations in the line spread function, as a function of both spatial position and wavelength. This effect, combined with the poor spectral sampling inherent to integral field spectrographs, makes it impossible to use information in one part of the field to accurately subtract night sky emission lines in other parts of the field.

We have used the fine movement afforded by the SINFONI grating drive, coupled with the slow variation of line spread function across the detector, to produce hypersampled line spread functions for all H band night sky emission lines, for all spaxels. The hypersampling was achieved by placing 26 distinct night sky exposures, each with a slight (~0.1 pixel) wavelength offset, on a single hypersampled grid with 0.01 pixel steps, after correctly accounting for flux scaling for
each exposure. The resulting database provides all the information required to accurately subtract the sky from science data.

Armed with the database giving the line spread function shape for each slitlet in each spectral line, we can sky subtract science data by determining the required shift and scale that best fits the science data to the database, once for each spectral line. The shift and scale is determined using observed line positions and strengths derived from spaxels that point to “blank sky”. By obviating the need for sky exposures, the proposed technique can improve observing efficiency by at least a factor of two. Further gains can be realized if the noise in the sky estimate can be further reduced, by grouping night sky lines known to vary together.

5.2 Implications for IFU observing

The next step will be to demonstrate an improvement in the observed spectrum of a science target, combining multiple science exposures. Once this has been achieved, it should pave the way to making the proposed technique a standard tool for the analysis of SINFONI data. Creating the database of line spread functions requires night time observations for each grating. We fully expect the line spread function shapes, relative intensities and relative positions to be stable over long periods of time, requiring re-calibration only every few months, or if an intervention has been made to the instrument. The small amount of time required to carry out these calibrations will be well worth the increased observing efficiency of all observations made with the SINFONI IFS.

5.3 Extension to KMOS and other IFUs

Our proposed technique can be extended to other medium resolution near-infrared integral field spectrographs. In particular, it can be applied to KMOS\(^1\), the multi-object integral field spectrograph about to be commissioned at the ESO VLT. The key measurement required to hypersample the line spread function relies on being able to shift the spectra on the detector by fractions of a pixel. While this can be easily done for SINFONI, given the extremely high angular resolution of the grating drive mechanism, it is much more difficult for KMOS, where no such mechanism exists. Luckily, we can use instrument flexure to advantage, and if measurements are made at many different instrument rotator settings, the resulting flexure is just enough to compute a well-sampled LSF. Similar techniques may be applied to other IFUs.

REFERENCES