Peering through the OH Forest: public release of sky-residual subtracted spectra for SDSS DR7

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Abstract

The Sloan Digital Sky Survey (SDSS) automated spectroscopic reduction pipeline provides >1.5 million intermediate resolution, $R \simeq 2000$, moderate signal-to-noise ratio (SNR), SNR ~ 15 , astronomical spectra of unprecedented homogeneity that cover the wavelength range 3800-9200 Å. However, there remain significant systematic residuals in many spectra due to the sub-optimal subtraction of the strong OH sky emission lines longward of 6700 Å. The OH sky lines extend over almost half the wavelength range of the SDSS spectra, and the SNR over substantial wavelength regions in many spectra is reduced by more than a factor two over that expected from photon counting statistics. Following the OH line subtraction procedure presented in Wild & Hewett (2005, WH05), we make available to the community sky-residual subtracted spectra for the Sloan Digital Sky Survey Data Relase 7. Here we summarise briefly the method, including minor changes in the implementation of the procedure with respect to WH05. The spectra are suitable for many science applications but we highlight some limitations for certain investigations. Details of the data model for the sky-residual subtracted spectra and instructions on how to access the spectra are provided.

1 Introduction

The Sloan Digital Sky Survey (SDSS; York et al. 2000) represents the most impressive application yet of wide-field multi-object spectrographs to provide spectroscopic samples of quasars, galaxies and stars of unprecedented size. The final data release (DR7; Abazajian et al. 2009) provides >1.5 million science-target spectra, nearly 1.3 million of which form part of the SDSS Legacy Survey.

Despite the high quality of the SDSS spectra, visual inspection reveals significant systematic sky-subtraction residuals longward of 6700 Å in many spectra. For fainter objects in particular, the sky-subtraction residuals, which exhibit strong non-Gaussian properties, are the dominant source of uncertainty over a wavelength interval of some 2000 Å. The wavelength range affected includes features of significant astrophysical interest; examples include the Calcium triplet (8500, 8544, 8665 Å), a powerful diagnostic of stellar populations in low-redshift galaxies, and the H β + [OIII] 4960, 5008 Å emission region in active galactic nuclei (AGN) in the redshift interval 0.4 < z < 0.8.

The fundamental problem is the difficulty associated with the removal of OH emission features from spectra in which the line profiles are barely resolved. Combined with sub-pixel changes in the pixel-to-wavelength calibration between spectra, sharp (positive/negative) residuals often remain following sky subtraction. The sky-subtraction residuals arise from the subtraction of two essentially identical tooth-comb signatures that have been very slightly misaligned, leading to well-defined residual patterns. In WH05 we presented a method to remove the dominant OH sky-subtraction residuals in the SDSS spectra based on Principal Component Analysis (PCA). PCA takes advantage of the correlations present as a function of wavelength, offering significant advantages over simply masking the affected pixels.

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In this document we describe the release to the astronomical community of FITS-files containing the sky-residual subtracted fluxes. We briefly summarise the main steps of the procedure in Section 2, including details of the object-feature masks used and minor alterations to the original method. In Section 3 we describe the data model and how to access the data. The core code, written in the IDL language, is also released for reference.

2 Method

Here we outline the main points of the procedure, and refer the reader to WH05 for full details. For each observation of a SDSS spectroscopic plate, 32 fibres, 16 for each of the 2 spectrographs, are normally assigned to blank sky regions, selected from areas containing no detected objects in the SDSS imaging survey. During the SDSS pipeline processing, the sky spectra are combined to create a "master-sky" spectrum for each spectroscopic plate, which is then scaled and subtracted from each of the 640 spectra, producing 608 sky-subtracted object spectra and 32 sky-subtracted sky spectra, all of which are part of the standard SDSS data releases. Throughout the remainder of the paper we will refer to the sky-subtracted sky spectra as "sky spectra", and the sky-subtracted object spectra as "object spectra". The purpose of our technique is to remove the tooth-comb residuals which remain after the SDSS pipeline master sky subtraction.

The analysis that follows is applied only to the red part of the SDSS spectra (6700-9180 Å), as the strong emission features blueward of 6700 Å are small in number and easily masked. Additionally, only pixels which may have been contaminated by night sky lines, termed "sky-pixels", are cleaned. Those pixels which lie between sky lines, termed "non-sky pixels", are not altered by the procedure and are used simply as reference points during the reconstruction of the OH features in the sky-pixels.

2.1 The eigensystem

The SDSS sky spectra are used to calculate the eigensystem. The first stage is to form an estimate of the Poisson noise spectrum for each plate from the median of the error arrays of the 32 sky spectra on that plate. The reason for such an approach, rather than using the individual noise arrays of each sky spectrum, is the difficulty of separating the sky noise component from the object noise component in the object error arrays. Thus, a single Poisson noise spectrum is used for all objects on the same plate. This Poisson noise spectrum is corrected for the rescaling applied by the SDSS reduction pipeline at the position of the OH lines (see WH05). With a robust estimate of the Poisson noise spectrum available for each plate, each sky spectrum is then normalised by the expected Poisson noise. Failure to do so would result in over-subtraction of flux in sky pixels, with "corrected" pixels apparently exhibiting fluctuations below the Poisson limit (see WH05).

The sky-subtraction method then proceeds by performing a PCA of the Poisson error normalised sky spectra to produce a set of orthogonal components that provides a compact representation of the systematic residuals caused by the OH emission lines. In our updated method, a robust and iterative PCA procedure is used, which is presented in Budavári et al. (2009). The algorithm essentially replaces the least-squares minimisation solved by traditional PCA with the minimisation of a new robust function of the data, which employs a robust Cauchy-type function to limit the impact of outliers. The iterative nature of the algorithm allows us to greatly reduce the computational time for the eigensystem; only ~ 3000 sky spectra are required for the eigensystem to converge.

A single set of eigenspectra are created for the entire SDSS DR7. During development of this release, attempts were made to create sets of eigenspectra for different plates, and for groups of fibres which exhibit similar fluctuations. However, no substantial improvement in the final result was found and therefore the simplest (and original) method was adopted.

2.2 Cleaning of object spectra

Once the eigensystem has been created from the sky spectra, the second step of the procedure involves adding the components in linear combinations to remove the systematic sky residuals from the spectra of target objects, such as galaxies, quasars and stars.

The number of components to use in the reconstruction is not well defined. The use of too many components results in the artificial suppression of noise below the Poisson limit, with the PCA acting as an (undesirable for most science applications) high-frequency filter. The use of too few components means that the removal of sky residuals is sub-optimal and, in some cases, the overall quality of the spectra can decrease. The reduction of the noise in the sky pixels below the noise in the non-sky pixels is clearly unphysical, and we therefore estimate the number of components to employ in the reconstruction of each spectrum by adopting the non-sky pixels of that spectrum as a reference. The number of components is determined using the root-mean-square (RMS) of the (flux-continuum)/error array for both the sky, and non-sky pixels. All RMS-values are calculated after subtraction of the object continuum, using a 71-pixel running median filter, masking of potential line features as described below, and removal of bad (error=0) pixels. Despite these precautions, a robust estimator of the RMS is still required, therefore the 90th percentile of the absolute (flux-continuum)/error array is used as our "RMS" estimator. This simplifies slightly the procedure of WH05. The error array used in this section has been rescaled to empirically remove the rescaling applied during the SDSS pipeline reduction at the position of the OH lines (see WH05 for more details). All three RMS values are included in the FITS-headers described in Section 3.

The reconstruction of a spectrum proceeds one component at a time, with the RMS-ratio calculated between the sky-residual subtracted spectrum and the non-sky pixels as reference. The reconstruction is stopped when the RMS-ratio reaches unity, i.e. when the noise weighted flux RMS is the same for the sky and non-sky pixels. The scheme is largely self-calibrating. For example, in spectra with high SNR the systematic sky residuals typically contribute only marginally to the sky-pixel noise, the RMS-ratio thus starts close to unity and only a small number of components are necessary to achieve equality in the RMS-ratio.

During projection of the eigenspectra onto the object spectra, bad pixels (error=0) and pixels which may have been affected by a narrow emission or absorption feature, not removed by the 71-pixel median filter, are masked (Section 2.4). However, OH emission line residuals are still removed from these pixels via subtraction of the contiguous PCA components, the amplitudes of which are determined using the rest of the wavelength range. The effective correction of pixels which include astrophysical features is a major benefit of the PCA subtraction scheme compared to the application of a high-pass filter or masking out pixels affected by OH residuals completely.

As in WH05 we have imposed an upper limit on the number of components used of 300. Any spectrum which reaches this upper limit (see header keyword NRECON in the FITS files, see Table 3) should be treated with suspicion, as it is possible that the stopping criteria has failed due to some real unmasked feature in the spectrum, such as strong intervening absorption lines in quasars. In a very small number of spectra, the final reconstruction after 300 components has a sky pixel RMS that is worse than prior to subtraction. No correction is applied to such spectra, which may be identified by inspection of the FITS header keywords SKYVAR1 and SKYVAR2 (i.e. SKYVAR1=SKYVAR2, see Table 3). The reliability of the PCA reconstructions deteriorates significantly when a substantial fraction of all the pixels are unavailable, therefore no correction is applied to spectra where the combined fraction of bad and masked pixels in the range $6700-9180\,\text{Å}$ exceeds 20 per cent.

2.3 Samples

In the inital public release (Version 1.0) we have made available spectra for two science samples: galaxies and quasars. Galaxies have been selected as all objects in DR7 possessing spSpec FITS-files, with header keyword SPEC_CLN= 2. Quasars are selected from the FITS header keyword SPEC_CLN= 3 or 4. Additionally, spectra of additional objects not selected by the latter criterion, but included in the DR7 quasar catalogue (Schneider et al. 2010) have also been treated as quasars. Sky spectra (SPEC_CLN= 5) and spectra without classification (SPEC_CLN= 0) have also been processed and are included in the release.

2.4 Masks

Narrow features, intrinsic to object spectra, that are not subtracted by the median-filter derived "continua" (Section 2.2) can effect the determination of the sky- and non-sky-pixel RMS values and bias the reconstruction of the sky-residuals. To mitigate both effects, narrow features, notably emission and absorption lines, are masked during the projection of the eigenspectra and calculation of the RMS values. The masked pixels are still subject to the sky-residual correction

but their presence is not allowed to influence the projection of the eigenspectra. Details of the mask applied for each spectrum are included in the third row of the FITS data files (see Table 4).

Individually tailored masks can be generated for each object spectrum, depending on the specific science application. However, for the majority of science applications, the use of a liberally-defined mask results in only a minor degredation in the quality of the sky-residual subtraction while minimising the probability of undesirable bias, due to the influence of unmasked features on the projections.

Thus, for galaxies, a single mask has been used which includes all the common emission and absorption features found in galaxy spectra that are detectable at the resolution and SNR of the SDSS spectra. Details of the features, their vacuum wavelengths and the rest-frame extent of the masked region are given in Table 1. Redshifts, necessary to calculate the observed-frame wavelengths of the masked regions, are taken from the SDSS FITS file primary headers. The same philosophy has been applied for the quasar sample although redshifts are taken from the DR7 quasar catalogue of Schneider et al. (2010) where available. Vacuum wavelengths and the rest-frame extent of the masked regions for quasars are given in Table 2¹. The advantage of using the sky-residual subtracted spectra can be appreciated by inspection of Figs. 2, 3 and 4.

It is important to recognise that the spectra resulting from the use of the generic masking procedure described above are not suitable for science investigations where additional narrow features are present at a different redshift to the science object. Examples include quasar absorption line catalog generation and the identification of spectra consisting of multiple object components, such as galaxies with gravitationally lensed background sources. The potential problems are demonstrated via inspection strong MgII absorption systems at z_{abs} =2.191 and z_{abs} =1.485 in the original and sky-residual-subtracted spectra of spSpec-52282-0518-495 and spSpec-52282-0328-472 respectively. In the former case, the absorption system is virtually eliminated, while in the latter case, the absorber doublet ratio alters dramatically.

3 Data model

Conscious of the significant data volume of the SDSS Legacy Survey spectra we have deliberately opted for a data model that minimises the duplication of information contained in the original Legacy Survey FITS spSpec files. Our new files include a direct copy of the primary FITS header from the SDSS spSpec file, with the addition of the FITS header keywords listed in Table 3. Three NAXIS1-pixel floating-point data arrays, of the same length as the original SDSS spectra, are included: the sky-residual subtracted spectrum flux array as the first row; the re-scaled error array as the second row; the mask information as the third row (see Table 4). Only those pixels where the sky-residual correction has been applied have had their flux and error values altered, all other pixels remain unchanged from the original SDSS spSpec file.

The sky-residual subtracted spectra have the same naming convention as the SDSS spSpec files, i.e. one file per spectrum, labeled by the mjd, plate and fiberid of the spectrum. The file names include the tag "_skysub" to prevent any confusion with the original SDSS spSpec files. Individual files are stored in directories according to their plate number.

The reduction of the number of data arrays per spectrum from five to three, combined with the elimination of the extensive FITS-header units (containing information about emission and absorption features detected in the spectrum) results in a file size just under half that of the original SDSS Legacy Survey spSpec files.

3.1 Data Access

The data files may be accessed through the Johns Hopkins University SDSS server at the address

http://www.sdss.jhu.edu/skypca/spSpec

Subsequent versions will be stored in the subdirectories v1/, v2/ etc. with the main directory given above pointing to the latest version at all times.

 $^{^1}$ A region centred on 4984 Å is masked to exclude artificial "absorption" resulting from the continuum-subtracted spectra of objects possessing strong [O III] $\lambda\lambda$ 4960,5008 emission.

Table 1: Galaxy Mask

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Central Wavelength	Size	Species
(Å)	(Å)	0
3728.30	20.0	O II
3798.4	15.0	$H\theta$
3836.2	15.0	${ m H}\eta$
3869.9	15.0	[Ne III]
3889.00	15.0	$H\zeta$
3934.8	33.0	Ca K
3969.6	33.0	ca H
3971.19	15.0	$H\epsilon$
4102.9	20.0	$H\delta$
4305.6	30.0	G-band
4341.7	20.0	${ m H}\gamma$
4364.44	15.0	[O III]
4472.5	15.0	Не і
4862.68	30.0	$^{\mathrm{H}eta}$
4960.30	15.0	[O III]
5008.24	20.0	[O III]
5176.7	30.0	Mg B
5200.0	10.0	[N I]
5272.0	20.0	
5877.4	15.0	Не і
5891.58	20.0	Na 1
5897.56	20.0	Na 1
6302.3	15.0	[N II]
6498.0	20.0	
6549.86	15.0	[N II]
6564.6	30.0	$H\alpha$
6585.27	15.0	[N II]
6680.4	15.0	
6718.3	20.0	[S II]
6732.7	20.0	[S II]
7066.4	15.0	Не і
7138.4	15.0	[Ar III]
7321.5	15.0	[O II]
7331.6	15.0	[Ar sc iv]
7753.5	10.0	[Ar III]
8500.36	20.0	Ca II
8544.38	25.0	Ca II
8664.52	25.0	Ca II
9018.0	15.0	
9072.0	15.0	[S III]

Table 2: Quasar Mask

Central Wavelength	Size	Species
(Å)	(Å)	
1216.0	40.0	$Ly\alpha$
1241.0	40.0	NV
1305.0	40.0	O I
1400.0	40.0	Si IV+O IV
1549.0	40.0	C IV
1909.0	40.0	C III]
2798.0	40.0	Mg II
3427.0	20.0	[Ne V]
3729.0	20.0	O II
3870.0	20.0	[Ne III]
4103.0	40.0	${ m H}\gamma$
4342.0	40.0	${ m H}\delta$
4863.0	40.0	$H\beta$
4960.0	40.0	[O III]
4984.0	40.0	_
5008.0	40.0	[O III]
5878.0	20.0	Не і
6302.0	20.0	[O I]
6550.0	20.0	[N II]
6565.0	40.0	$H\alpha$
6585.0	20.0	[N II]
6725.0	40.0	[S II]
7139.0	20.0	[Ar III]

Table 3: FITS file primary header keywords

Keyword	Description
SKYVAR0	Non-sky pixel variance
SKYVAR1	Sky pixel variance before correction error
SKYVAR2	Sky pixel variance after correction
NRECON	Number of components in reconstruction

Table 4: FITS file data content

Data row	Content	Equivalent SDSS data row
1	Object flux array	1
2	Object error array	3
3	Sky-correction mask	_

Table 5: FITS sky-correction mask values and their meanings

Mask value	Meaning
0	outside wavelength range $6700-9180\text{Å}$ for sky-correction
1	non-sky pixels: inside wavelength range but not subject to sky-correction
2	sky pixels: inside wavelength range and subject to sky-correction
3	masked non-sky pixels: pixel masked due to object feature or SDSS bad pixel
4	masked sky pixels: pixel masked due to object feature or SDSS bad pixel

The files are easily accessible via the "wget" command. Several file lists have been prepared for the convenience of the user and can be found in the main directory given above:

wget_all.lis To download all reduced spectra.

wget_dr7qsocat.lis To download the spectra of the DR7 quasar catalog.

wget_specobj_specclass2.lis All spectra spectroscopically classified as galaxies (SPECCLASS=2) in the CAS SPECOBJ view, except for 20 objects classified as galaxies in the CAS catalog, but not in their FITS file headers.

wget_specobjall_specclass2.lis All spectra spectroscopically classified as galaxies (SPECCLASS=2) in the CAS SPECOB-JALL table (i.e. includes duplicates), except for objects on plate 1631 for which the spectra of the same mjd as in the catalog do not exist, and the 20 objects noted above.

After downloading the individual file list to your computer or creating your own, a command such as:

```
wget -x -nH --cut-dir=2 -a logfile.txt -i wget_all.lis
```

will download all the files in that file list to your machine, creating the file logfile.txt to keep track of the progress.

The DR7 QSOs may additionally be accessed from the DR7 Value Added Catalogue web page.

4 Conclusion

We have released to the community a set of SDSS DR7 spectra with significantly improved subtraction of OH sky lines. The PCA-based technique employed takes advantage of the correlation of OH lines as a function of wavelength and sky subtraction close to the Poisson noise limit is achieved for many spectra. Our procedure is generally more effective than simply employing a high-pass filter or simple feature-exclusion mask. Release Version 1.0 includes galaxies, quasars, sky and "unknown" spectra. Future releases will incorporate improved redshifts for the quasars and the masking of intervening absorption features in quasar spectra.

5 Acknowledgements

We would like to thank Alex Szalay and Tamas Budavari at Johns Hopkins University for kindly organising the hosting of the data files for public access, and Jan Vandenberg and Rich Ercolani for their time setting up the web access. Gordon Richards enabled the spectra for the SDSS DR7 quasar catalogue to be made available as part of the SDSS DR7 Legacy Release website 'Added Value' data page.

References

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York D. G., Adelman J., Anderson J., et al 2000, AJ, 120, 1579

A Figures

Here we include a repeat of some of the figures presented in WH05, for easy reference, and to allow direct comparison between the results before and after the re-reduction of the entire data set by the SDSS team.

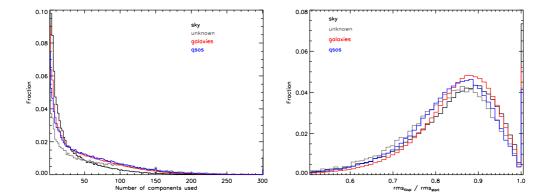


Figure 1: *Left:* Histogram of the number of components used to reconstruct the sky signal in the sky, unknown, galaxy and quasar samples. The y-axis is truncated in order to show the majority of the objects. Twenty-three per cent of the unknown spectra require zero components, demonstrating the importance of employing appropriate object-specific masks (Section 2.4). *Right:* Histogram of the ratio between the root mean square noise of the pixels affected by OH lines before and after application of the sky-residual subtraction procedure.

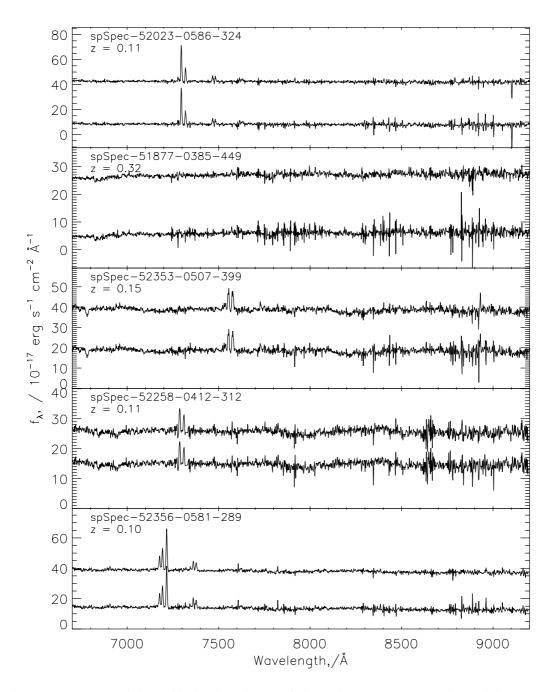


Figure 2: Examples of sky residual subtraction applied to galaxy spectra. In each panel the lower spectrum is the raw SDSS data and the upper spectrum is after application of the sky-residual subtraction procedure. The upper sky-residual subtracted spectrum is offset for clarity.

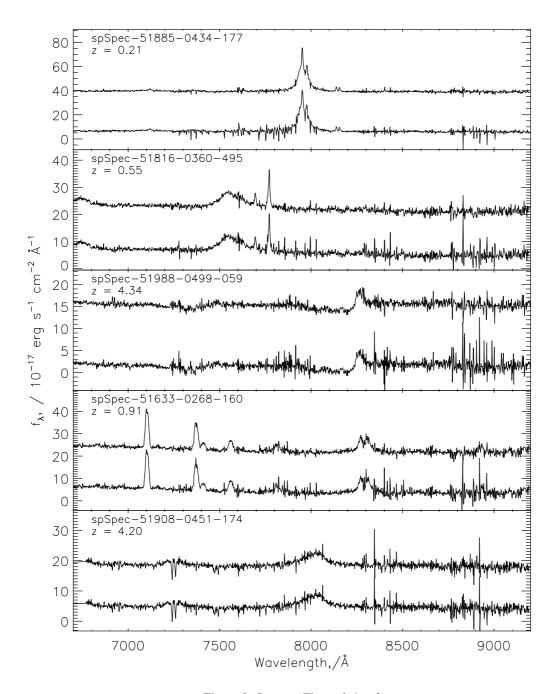


Figure 3: Same as Figure 2, but for quasars

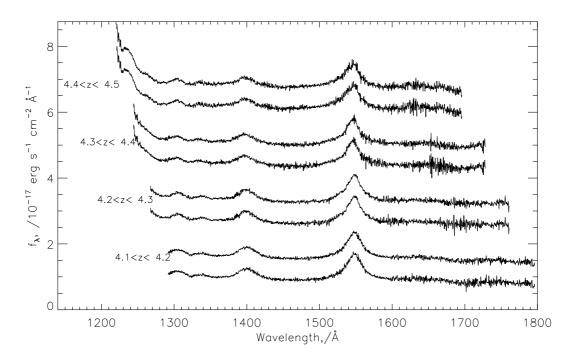


Figure 4: Composite spectra of $z\sim 4$ quasars. The observed frame spectra fall at wavelengths $>6700 \mbox{Å}$. For each pair of spectra, the lower composite is created directly from the SDSS spectra, and the upper composite from the same spectra after subtracting the sky residuals.