LSDCat: Detection and cataloguing of emission-line sources in integral-field spectroscopy datacubes

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ABSTRACT

We present a robust, efficient, and user-friendly algorithm for detecting faint emission-line sources in large integral-field spectroscopic datacubes together with the public release of the software package Line Source Detection and Cataloguing (LSDCat). LSDCat uses a three-dimensional matched filter approach, combined with thresholding in signal-to-noise, to build a catalogue of individual line detections. In a second pass, the detected lines are grouped into distinct objects, and positions, spatial extents, and fluxes of the detected lines are determined. LSDCat requires only a small number of input parameters, and we provide guidelines for choosing appropriate values. The software is coded in Python and capable of processing very large datacubes in a short time. We verify the implementation with a source insertion and recovery experiment utilising a real datacube taken with the MUSE instrument at the ESO Very Large Telescope.

Key words. methods: data analysis – techniques: imaging spectroscopy

1. Introduction

One motivating driver for the construction of the current generation of optical wide-area integral-field spectrographs such as the Multi Unit Spectroscopic Explorer at the ESO VLT (MUSE, in operation since 2014; Bacon et al. 2014; Kelz et al. 2016) or the Keck Cosmic Web Imager (KCWI, under construction; Martin et al. 2010) is the detection of faint emission lines from high-redshift galaxies. The high-level data products from those instruments are three-dimensional (3D) arrays containing intensity-related values with two spatial axes and one wavelength axis (usually referred to as datacubes). So far, efficient and robust methods and detection cataloguing software for faint-line-emitting sources in such datacubes is not publicly available. To remedy this situation we now present the Line Source Detection and Cataloguing (LSDCat) tool, developed in the course of our work within the MUSE consortium.

Automatic source detection in two-dimensional (2D) imaging data is a well-studied problem. Various methods to tackle it have been implemented in software packages that are widely adopted in the astronomical community (see reviews by Bertin & Arnouts 1996; Masias et al. 2012, or the comparison of two frequently used tools by Annunziatella et al. 2013). A conceptually simple approach consists of two steps: first, the observed imaging data is transformed in order to highlight objects while simultaneously reducing the background noise. A particular transformation that satisfies both requirements is the matched filter (MF) transform. Here the image is cross-correlated with a 2D template that matches the expected light distribution of the sources to be detected. Mathematically, it can be proven that for stationary noise the MF maximises the signal-to-noise ratio (S/N) of a source that is optimally represented by the template (e.g. Schwartz & Shaw 1975; Das 1991; Zackay & Ofek 2017; Vio & Andreani 2016). In the second step, the MF-transformed image is segmented into objects via thresholding, that is, each pixel in the threshold mask is set to 1 if the MF-transformed value is above the threshold, and 0 otherwise. Connected 1-valued pixels then define the objects on which further measurements (e.g. centroid coordinates, brightnesses, ellipticities etc.) can be performed. Other image transformations (e.g. multi-scale methods) and detection strategies (e.g. histogram-based methods) exist, but the “MF + thresholding”-approach is most frequently employed, especially in optical/near-infrared imaging surveys for faint extragalactic objects. This widespread preference is certainly attributable to the conceptual simplicity and robustness of the method, despite known limitations (see e.g. Akhlaghi & Ichikawa 2015). But it is also due to the availability of a stable and user-friendly implementation of a software based on this approach (Shore 2009): SExtractor (Bertin & Arnouts 1996).

The detection and cataloguing of astronomical sources in 3D datasets has so far mostly been of interest in the domain of radio astronomy. Similar to integral-field spectroscopy (IFS), these observations result in 3D datacubes containing intensity values with two spatial axes and one frequency axis. Here, especially surveys for extragalactic 21 cm H I emission are faced with the challenge to discover faint line emission-only sources in such datacubes. The current generation of such surveys utilises a variety of custom-made software for this task, also relying heavily on manual inspection of the datacubes. Notably, the approach of Saintonge (2007) tries to minimise such error-prone interactivity by employing a search technique based on matched filtering, although only in spectral direction. More recently, driven mainly by the huge data volumes expected from future generations of large radio surveys with the Square Kilometre
Array, development and testing of new 3D source-finding tech-
niques has started (e.g. Koribalski 2012; Popping et al. 2012; 
Serra et al. 2012; Jurek 2012). Currently, two software pack-
ages implementing some of these techniques are available to the 
community: DUCHAMP (Whiting 2012) and SoFiA (Serra et al. 
2015). While in principle these programs could be adopted for 
source detection purposes in optical integral-field spectroscopic 
datasets, in practice there are limitations that necessitate the de-
velopment of a dedicated IFS source detector. For example, the 
noise properties of long exposure IFS datacubes are dominated by 
telluric line- and continuum emission and are therefore vary-
ing with wavelength, in contrast to the more uniform noise prop-
erties of radio datacubes. Moreover, the search strategies imple-
mented in the radio 3D source finders are tuned to capture the 
large variety of signals expected. But, as we argue in this paper, 
the emission line signature from compact high-redshift sources 
in IFS data is well described by a simple template that, however, 
needs an IFS-specific parameterisation. Finally, the input data as 
well as the parameterisation of detected sources is different in 
the radio domain compared to the requirements in optical IFS: 
typically radio datacubes have their spectral axis expressed as 
frequency and flux densities measured in Jansky, while in IFS 
cubes the spectral axis is in wavelengths and flux densities are 
measured as \( f_\lambda \) with units of erg s\(^{-1}\) cm\(^{-2}\) Å\(^{-1}\).

LSDCat is part of a long-term effort, initially motivated by 
the construction of MUSE, to develop source detection algo-
rithms for wide-field IFS datasets (e.g. Bourguignon et al. 2012). 
As part of this effort, Meillier et al. (2016) recently released the 
Source Emission Line Finder (SELFII). This software is based on 
a Baysian scheme utilising a reversible jump Monte Carlo 
Markov chain algorithm. While this mathematically sophisti-
cated machinery is quite powerful in unrheeling faint emission 
line objects in a datacube, the execution time of the software is 
very long for practical use. In contrast, the algorithm of LSDCat 
is relatively simple and correspondingly fast in execution time on 
state-of-the art workstations. It is also robust, as it is based on 
the matched-filtering method that has long been successfully utilised 
for detecting sources in imaging data. LSDCat is therefore well 
suited for surveys exploiting even large numbers of wide-field 
IFS datacubes. Furthermore, the short execution time also per-
mits extensive fake source insertion experiments to empirically 
reconstruct the selection function of such surveys.

This article is structured as follows: in Sect. 2, we de-
scribe the mathematical basis and the algorithm implemented in 
LSDCat. In Sect. 3, we validate the correctness of the imple-
mentation in our software. We then provide guidelines for the 
LSDCat user for adjusting the free parameters governing the de-
tection procedure in Sect. 4 and conclude in Sect. 5 with a brief 
outlook on future improvements of LSDCat. A link to the soft-
ware repository is available from the Astrophysics Source Code 
Library\(^1\). In Appendix A, we provide a short example on how the 
user interacts with LSDCat routines. The public release of the 
software includes a detailed manual, to which we refer all poten-
tial users for details of installing and working with the software.

### 2. Method description and implementation

#### 2.1. Input data

The principal data product of an integral field unit (IFU) observ-
ing campaign is a datacube \( F \) (e.g. Allington-Smith 2006; Turner 
2010). The purpose of LSDCat is to detect and characterise 
emission-line sources in \( F \). We adopt the following notations 
and conventions: \( F \) is a set of volume pixels (voxels) \( F_{x,y,z} \) with 
intensity related values, for example, flux densities in units of 
erg s\(^{-1}\) cm\(^{-2}\) Å\(^{-1}\). The indices \( x, y \) index the spatial pixels (spax-
ells), and \( z \) indexes the spectral layers of the datacube. Mappings 
between \( x, y \) and sky position (right ascension and declination), 
as well as between \( z \) and wavelength \( \lambda \) can be included in the 
metadata (Greisen & Calabretta 2002; Greisen et al. 2006). For 
the new generation of wide-field IFUs based on image-slicers, 
the sky is sampled contiguously, and typical dimensions of a 
MUSE datacube are \( x_{\text{max}}, y_{\text{max}}, z_{\text{max}} \approx 3 \times 10^3, 3 \times 10^3, 4 \times 10^3 \), 
that is, a datacube consists of \( \sim 4 \times 10^8 \) voxels.

We make a number of assumptions regarding the data struc-
ture, guided by the output of the MUSE data reduction system 
(DRS; Weilbacher et al. 2012, 2014):

- We assume that atmospheric line and continuum emission 
  has been subtracted from \( F \) (Streicher et al. 2011; Soto et al. 
  2016); see Sect. 4.4 for a brief discussion on how to account 
  for sky subtraction residuals within LSDCat.
- LSDCat currently requires a rectilinear grid in \( x, y, z \). In 
  particular, the mapping between \( z \) and \( \lambda \) has to be linear with a 
  fixed increment \( \Delta \lambda \) per spectral layer, that is,

\[
\lambda = \lambda_{\text{c}0} + z \Delta \lambda, 
\]

where \( \lambda_{\text{c}0} \) designates the wavelength corresponding to the 
wavelength of the first spectral layer.

For MUSE, this is achieved by the DRS through resam-
pling the raw CCD data into the final datacube \( F \). We 
also demand a constant mapping between \( x, y \) and sky po-
sition for all spectral layers \( z \), which the MUSE pipeline 
accounts for in the resampling step by correcting for the 
wavelength-dependent lateral offset (differential atmospheric 
refraction) along the parallactic angle (e.g. Filippenko 1982; 
Roth 2006).

- Together with the flux datacube \( F \), LSDCat expects a second 
  cube \( \sigma^2 \) containing voxel-by-voxel variances. While such a 
  variance cube is provided by the MUSE DRS as formal prop-
  agation of the various detector-level noise terms through the 
data reduction steps, the pipeline currently neglects the co-
  variences between adjacent voxels introduced by the resam-
  pling process. We discuss this issue and some practical con-
  siderations further in Sect. 4.4; here we simply assume that a 
datacube \( \sigma^2 \) with appropriate variance estimates is available.

As a very useful preparatory step for LSDCat, we recommend 
that galaxies and stars with bright continuum emission (i.e. 
sources with significant signal in the majority of spectral bins) 
are subtracted from \( F \). While the presence of such sources does 
not render the detection and cataloguing algorithm unusable, 
continuum bright sources may lead to (possibly many) catalogue 
entries unrelated to actual emission-line objects. We give some 
guidance for the subtraction of continuum bright sources prior to 
running LSDCat in Sect. 4.1.

Figure 1 depicts, as a flowchart, all the main processing steps 
of LSDCat, leading from the input datacube \( F \) and its associ-
ated variances \( \sigma^2 \) to a catalogue of emission lines. Each pro-
cessing step is implemented as a stand-alone Python\(^2\) program. 
The file format of the input data and variance cubes has to con-
form to the FITS standard (Pence et al. 2010). LSDCat requires

\(^1\) http://ascl.net/1612.002

\(^2\) Python Software Foundation. Python Language Reference, ver-
sion 2.7. Available at http://www.python.org
Table 1. Routines of LSDCat with the required input parameters.

<table>
<thead>
<tr>
<th>Processing step</th>
<th>LSDCat Routine</th>
<th>Input parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spatial filtering</td>
<td>lsd_cc_spatial.py</td>
<td>– PSF functional form: Moffat or Gaussian</td>
</tr>
<tr>
<td></td>
<td></td>
<td>– ( p_0, p_1, p_2 ) and ( \lambda_0 ) for</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( FWHM(\lambda)^{\prime} = p_0 + p_1(\lambda - \lambda_0) + p_2(\lambda - \lambda_0)^2 )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Moffat ( \beta ), if Moffat PSF)</td>
</tr>
<tr>
<td>Spectral filtering</td>
<td>lsd_cc_spectral.py</td>
<td>– FWHM of Gaussian profile: ( \nu_{\text{FWHM}} ) [km s(^{-1})]</td>
</tr>
<tr>
<td>Thresholding</td>
<td>lsd_cat.py</td>
<td>– Detection threshold: ( S/N_{\text{det}} )</td>
</tr>
<tr>
<td>Measurements</td>
<td>lsd_cat_measure.py</td>
<td>– Analysis threshold: ( S/N_{\text{ana}} )</td>
</tr>
</tbody>
</table>

For performing its operations, LSDCat needs up to four databases loaded simultaneously. Hence, for typical MUSE datacubes that contain \(10^8 - 10^9\) 32-bit floating point numbers, a computer with at least 16 GB of random access memory is recommended. Table 1 lists the names of the individual LSDCat routines implementing the various processing steps, together with the main input parameters that govern the detection and cataloguing process. In the following we describe each of the processing steps with its routines in more detail. A practical example of using the LSDCat routines is provided in Appendix A.

2.2. 3D matched filtering

The optimal detection statistic of an isolated signal in a dataset with additive white Gaussian noise is given by the matched filter transform of the dataset (e.g. Schwartz & Shaw 1975; Das 1991; Bertin 2001; Zackay & Ofek 2017; Vio & Andreani 2016). This transform cross-correlates the dataset with a template that matches the properties of the signal to be detected.

We utilise the matched filtering approach in LSDCat to obtain a robust detection statistic for isolated emission line sources in wide-field IFS datacubes. For a symmetric 3D template \( T \), this is equivalent to a convolution of \( F \) with \( T \):

\[
\tilde{F} = F * T.
\]  

(2)

Here \( * \) denotes the (discrete) convolution operation, that is, every voxel of \( \tilde{F} \) is given by

\[
\tilde{F}_{x,y,z} = \sum_{i,j,k} F_{i,j,k} T_{x-i,y-j,z-k} = \sum_{i,j,k} T_{i,j,k} F_{x-i,y-j,z-k}.
\]  

(3)

In principle, the summation runs over all dimensions of the datacube, but in practice, terms where \( T_{i,j,k} \approx 0 \) can be neglected. Propagating the variances from \( \sigma^2 \) through Eq. (3) yields the voxels of \( \tilde{\sigma}^2 \):

\[
\tilde{\sigma}^2_{x,y,z} = \sum_{i,j,k} T_{i,j,k}^2 \sigma^2_{x-i,y-j,z-k}.
\]  

(4)

The template \( T \) must be chosen such that its spectral and spatial properties match those of a compact expected emission-line source in \( F \). LSDCat is primarily intended to search for faint compact emission-line sources. For such sources it is a reasonable assumption that their spatial and spectral properties are independent of one another. We can therefore write \( T \) as a product

\[
T = T^{\text{spec}} T^{\text{spat}},
\]  

(5)

where \( T^{\text{spat}} \) is the expected spatial profile and \( T^{\text{spec}} \) is the expected spectral profile. The voxels of \( T \) are thus given by

\[
T_{x,y,z} = T^{\text{spat}}_{x,y} T^{\text{spec}}_{z}.
\]  

(6)
Fig. 2. Example of the effect of matched filtering on the detectability of a faint emission-line source in the MUSE datacube of the Hubble Deep Field South (Bacon et al. 2015). Shown is a Lyman $\alpha$ emitting galaxy at redshift $z = 3.278$ with flux $F_{Ly\alpha} = 1.3 \times 10^{-18}$ erg s$^{-1}$ (ID #162 in Bacon et al. 2015). The panels in the first row display four different spectral layers of the continuum-subtracted datacube $F$. The second row shows the same spectral layers, but for the filtered S/N cube (Eq. (9)) that was used to build the catalogue of emission line sources via thresholding (Eq. (18)). The leftmost panels show a layer significantly away from the emission line peak, the other panels show layers at spectral coordinates $z_{\text{peak}} - 1$, $z_{\text{peak}}$, and $z_{\text{peak}} + 1$, respectively, where $z_{\text{peak}}$ designates the layer containing the maximum S/N value of the source. The third row shows the flux density spectrum in the spaxels at ($x_{\text{peak}}, y_{\text{peak}}$) and ($x_{\text{peak}} + 1, y_{\text{peak}} + 1$), where $x_{\text{peak}}$ and $y_{\text{peak}}$ are the spatial coordinates of the highest S/N value. The bottom row shows a S/N spectrum extracted from the S/N cube at $x_{\text{peak}}$ and $y_{\text{peak}}$.

Of course, spatially extended sources with a velocity profile along the line of sight are not optimally captured by separating the filter into the spectral and spatial domain. However, as we detail in Sects. 4.2 and 4.3, moderate template mismatches do not result in a major reduction of the maximum detectability that could be achieved with an exactly matching template.

Now with Eq. (6), the 3D convolution of Eq. (3) yielding $\tilde{F}$ can be performed as a succession of two separate convolutions, in no particular order: a spatial convolution with the appropriate $T_{\text{spat}}$ in each spectral layer $z$, and a spectral convolution with $T_{\text{spec}}$ in each spaxel $x, y$:

\[
\tilde{F}_{x,y,z} = \sum_k T_k^\text{spec} \left( \sum_{i,j} T_{i,j}^\text{spat} F_{x-i,y-j,z-k} \right) = \sum_{i,j} T_{i,j}^\text{spat} \left( \sum_k T_k^\text{spec} F_{x-i,y-j,z-k} \right).
\]

Note that since every spectral layer $z$ of the datacube is convolved with a different spatial template, and since the width of the spectral template also changes with $z$ (see Sect. 2.3), the equivalence between Eqs. (7) and (8), mathematically speaking, is not strictly correct. However, the variations of the templates with $\lambda$ are much slower than the typical line widths of the spectral templates, meaning that we can approximate the convolution by using a locally invariant template.

As an indicator of the presence or absence of an emission line in $F$ at a position $x, y, z$ we then evaluate the statistic

\[
S/N_{x,y,z} = \frac{\tilde{F}_{x,y,z}}{\tilde{\sigma}_{x,y,z}},
\]

with $\tilde{F}_{x,y,z}$ from Eq. (3) and $\tilde{\sigma}_{x,y,z}$ as the square root of Eq. (4). The voxels $S/N_{x,y,z}$ constitute the signal-to-noise cube computed after the matched filtering has been performed. The values on the left side of Eq. (9) can be translated into a probability for rejecting the null-hypothesis of no source being present at position $x, y, z$ in $F$. This is commonly referred to as the detection significance of a source. However, in a strict mathematical sense this direct translation is only valid for sources that are exactly described by the adopted template $T$, in a dataset where the...
variance terms on the right-hand side of Eq. (4) are stationary and fully uncorrelated. Nevertheless, even if these strict requirements are not met by the IFS datacube, filtering with $T$ will always reduce high-frequency noise while enhancing the presence of sources that are similar in appearance with $T$. Thus Eq. (9) can still be used as a robust empirical measure of the significance of a source present in $F$ at a position $x, y, z$. We illustrate this for a faint high-redshift Lyman-$\alpha$ emitting galaxy observed with MUSE in Fig. 2; this source is detected with high significance for a faint high-redshift Lyman-$\alpha$ emitting galaxy observed with MUSE in Fig. 2; this source is detected with high significance.

In LSDCat, the spatial convolution is performed by the routine lsd_cc_spatial.py and the spectral convolution is performed by lsd_cc_spectral.py. The output of a subsequent run of those routines is a FITS file with two header and data units; one storing $F$ and the other one storing $\sigma^2$. Both routines are capable of fully leveraging multiple processor cores, if available, to process several datacube layers or spaxels simultaneously. Moreover, in lsd_cc_spatial.py the computational time is reduced by using the fast Fourier transform method provided by SciPy to convolve the individual layers. However, since the spectral kernel varies with wavelength we cannot utilise the same approach in lsd_cc_spectral.py, but the discrete 1D convolution operation can be written as a matrix-vector product with the convolution kernel given by a sparse banded matrix (Das 1991, Sect. 3.3.6). Hence here we achieve a substantial acceleration of the computational time by utilising the sparse matrix multiplication algorithm of SciPy. Typical execution times of lsd_cc_spatial.py and lsd_cc_spectral.py running in sequence on a full MUSE $300 \times 300 \times 4000$ datacube, including reading and writing of the data, are $\sim 5$ min on an Intel Core-i7 workstation with 8 cores, or $\sim 2$ min on a workstation with two AMD Opteron 6376 processors with 32 cores each.

2.3. Templates

In line with the approximate separation of spatial and spectral filtering described in the previous subsection, LSDCat requires two templates, a spatial and a spectral one.

For the spatial template $T^\text{spat}$ the user has currently the choice between a circular Gaussian profile,

$$T_{x,y} = \frac{1}{2\pi\sigma_G^2} \exp\left(-\frac{x^2 + y^2}{2\sigma_G^2}\right),$$

with the standard deviation $\sigma_G$, or a Moffat (1969) profile,

$$T_{x,y} = \frac{\beta - 1}{\pi \sigma_G^2} \left[1 + \frac{x^2 + y^2}{r_d^2}\right]^{-\beta},$$

with the width parameter $r_d$ and the kurtosis parameter $\beta$. Both functions are commonly used as approximation of the seeing induced point spread function (PSF) in ground-based optical and near-IR observations (Trujillo et al. 2001a,b) and therefore are well suited as spatial templates for compact emission line sources. Of course it is also possible to adopt a spatial template more extended than the PSF by choosing a correspondingly large value of $\sigma_G$ or $r_d$. As discussed in Sects. 4.2 and 4.3 below, the maximum S/N delivered by the matched filter behaves very benignly with respect to modest template mismatch, and the application of LSDCat is thus by no means limited to search for point sources.

6 In the limiting case $\beta \to \infty$ Eq. (12) is equal to Eq. (11); cf. Trujillo et al. (2001b).

Typically the parameter used to characterise the atmospheric seeing is the full width at half maximum (FWHM) of the PSF. For Eq. (11) this is

$$\text{FWHM} = 2 \sqrt{2\ln 2} \sigma,$$

and for the Moffat in Eq. (12) it is

$$\text{FWHM} = 2 \sqrt{2}\frac{1}{\beta} r_d.$$
that are spurious, that is, that do not correspond to real emission line objects. We give guidelines on the choice of the detection threshold based on our experience with MUSE data in Sect. 4 below.

For each detection, LSDCat records the coordinates $x_{\text{peak}}, y_{\text{peak}}, z_{\text{peak}}$ of the local maximum in the S/N-cube, its value $F_{\text{peak}}$, and the number of voxels $N_{\text{det}}$ constituting the detection. These values constitute an intermediate catalogue of detections. Each entry is assigned a unique running integer number $i$. Moreover, LSDCat also assigns an integer object identifier $i_{\text{Obj}}$ to detection clusters occurring at different wavelengths but similar spatial positions within a small search radius to account for sources with multiple significantly detectable emission lines. This intermediate catalogue is created by the routine 1sd_cat.py, utilising routines from the SciPy ndimage.measurements package. The intermediate catalogue is written to disk as a FITS binary table. The actual execution time is generally much shorter than the previous step of applying the matched filter, but it depends on the detection threshold that determines the number of objects.

### 2.5. Measurements

LSDCat provides a set of basic measurement parameters for each detection of the intermediate catalogue. These parameters are determined using the datacubes $F$, $\sigma^2$, $\tilde{F}$ and S/N. The set of parameters is chosen to be robust and independent from a specific scientific application. For more complex measurements involving, for example, fitting of flux distributions, the LSDCat measurement capability can serve as a starting point.

In Table 2 we list the various output parameters that are generated for each detection. This parameterisation of the detected sources and their emission lines constitutes the final processing step of LSDCat. The routine 1sd_cat_measure.py performs the parameterisation task and writes out the final catalogue. Running 1sd_cat_measure.py on an intermediate catalogue with $\sim 10^6$ entries takes typically 100 s on the two machines mentioned above in Sect. 2.2, with most of the time spent on reading the four input datacubes.

### 2.5.1. Centroids

The coordinates of each detections local maximum in the S/N-cube (Sect. 2.4) serve only as a first approximation of its spatial and spectral position. As a refinement lsd_cat_measure.py can calculate several different sets of centroid positions for each detected line cluster. For example, the 3D S/N-weighted centroid is given by the first moments

$$
\left( x_{\text{com}}, y_{\text{com}}, z_{\text{com}} \right) = \left( \frac{\sum_{x,y,z} x \cdot S/N_{x,y,z} \cdot \tilde{F}_{x,y,z} }{\sum_{x,y,z} S/N_{x,y,z}}, \frac{\sum_{x,y,z} y \cdot S/N_{x,y,z} \cdot \tilde{F}_{x,y,z} }{\sum_{x,y,z} S/N_{x,y,z}}, \frac{\sum_{x,y,z} z \cdot S/N_{x,y,z} \cdot \tilde{F}_{x,y,z} }{\sum_{x,y,z} S/N_{x,y,z}} \right).
$$

Here, for each detection, the summation runs over all non-zero ($x_{\text{peak}}, y_{\text{peak}}, z_{\text{peak}}$)-neighbouring voxels in a thresholded datacube similar to $L$ (Eq. (18)), but with voxels set to one if they are above an analysis threshold $S/N_{\text{ana}}$. This additional threshold, which must be smaller or equal to $S/N_{\text{det}}$, is the required input parameter for 1sd_cat_measure.py. Guidelines for choosing $S/N_{\text{ana}}$ are discussed in Sect. 4.5. Similarly, LSDCat can measure 3D centroid coordinates with the original flux cube $F$ and with the filtered flux cube $\tilde{F}$ as weights. In these cases, Eq. (19) is applied again, but with $S/N_{x,y,z}$ being substituted by $F_{x,y,z}$ and $\tilde{F}_{x,y,z}$, respectively.

3D centroids provide a non-parametric way of calculating spatial and spectral positions, making use of the full 3D information present in the datacube. While the calculation using the flux cube is unbiased against a particular choice of filter template, it is not very robust for low S/N detections. This shortcoming is alleviated for the centroids calculated on the filtered flux cube or the S/N-cube. The latter, however, could potentially be biased by local noise extrema, for example, at spectral layers near sky-lines.

### Table 2. Output parameters for each LSDCat detection.

<table>
<thead>
<tr>
<th>Output Parameter(s)</th>
<th>LSDCat Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
<td>I</td>
<td>Running ID; see Sect. 2.4</td>
</tr>
<tr>
<td>$i_{\text{Obj}}$</td>
<td>ID</td>
<td>Object identifier; see Sect. 2.4</td>
</tr>
<tr>
<td>$x_{\text{peak}}, y_{\text{peak}}, z_{\text{peak}}$</td>
<td>(x,y,z)_PEAK_SN</td>
<td>$S/N_{\text{peak}}$ coordinate; see Sect. 2.4</td>
</tr>
<tr>
<td>$N_{\text{det}}$</td>
<td>DETSN_MAX</td>
<td>Number of voxels above $S/N_{\text{det}}$, see Sect. 2.4</td>
</tr>
<tr>
<td>$x_{\text{com}}, y_{\text{com}}, z_{\text{com}}$</td>
<td>(x,y,z)_SN</td>
<td>$S/N$ value at $x_{\text{peak}}, y_{\text{peak}}, z_{\text{peak}}$; see Sect. 2.4</td>
</tr>
<tr>
<td>$F_{\text{com}}, y_{\text{com}}, z_{\text{com}}$</td>
<td>(x,y,z)_FLUX</td>
<td>$F$-weighted centroid; Eq. (19)</td>
</tr>
<tr>
<td>$x_{\text{com}}, y_{\text{com}}, z_{\text{com}}$</td>
<td>(x,y,z)_SFLUX</td>
<td>$F$-weighted centroid; Eq. (19) with $S/N_{x,y,z}$ substituted by $F_{x,y,z}$ from Eq. (3)</td>
</tr>
<tr>
<td>$x_{\text{com}}, y_{\text{com}}, z_{\text{com}}$</td>
<td>(x,y,z)_1MOM</td>
<td>2D moment-based centroid in NB, $\tilde{F}$ (Eqs. (20), (21))</td>
</tr>
<tr>
<td>$x_{\text{com}}, y_{\text{com}}, z_{\text{com}}$</td>
<td>(x,y,z)_2MOM</td>
<td>2D second central moments in NB, $\tilde{F}$ (Eqs. (22), (23), (24))</td>
</tr>
<tr>
<td>$R_\sigma$</td>
<td>R_SIGMA</td>
<td>$R_\sigma = \sqrt{(x^2+y^2)/2}$</td>
</tr>
<tr>
<td>$R_{\text{KRON}}$</td>
<td>R_KRON</td>
<td>Kron radius (Eq. (22))</td>
</tr>
<tr>
<td>$F(k \cdot R_{\text{KRON}})$</td>
<td>FLUX_(k)_KRON</td>
<td>Integrated flux in $k \times R_{\text{KRON}}$ aperture (Eq. (27))</td>
</tr>
<tr>
<td>$\sigma_F(k \cdot R_{\text{KRON}})$</td>
<td>ERR_FLUX_(k)_KRON</td>
<td>Uncertainty on $F(k \times R_{\text{KRON}})$</td>
</tr>
</tbody>
</table>

Notes. A comma separated list within brackets in the second column indicates the set of corresponding LSDCat output column names. For each $x, y$ coordinate there is also a corresponding right ascension and declination value available and for each $z$ coordinate a corresponding wavelength can be tabulated if a corresponding world coordinate system is specified.
As an alternative approach to 3D centroids, LSDCat can calculate 2D centroids on synthesised narrow-band images \( N_B(y, z) \) from the filtered flux cube \( F \):

\[
N_B(y, z) = \sum_{x=\min}^{\max} x \cdot y \cdot \frac{F(x, y, z)}{\sum_{x,y} y \cdot \frac{F(x, y, z)}{F}}.
\]

(20)

The boundary indices of each synthetic narrowband image \( N_B \) and \( z_{\min} \) are taken as the minimum and maximum \( z \) coordinate of all voxels of a detection above the analysis threshold \( S/N_{\text{ana}} \). Then the 2D weighted centroid coordinates follow from the first image moments:

\[
(x^{(1)}, y^{(1)}) = \left( \frac{\sum_{x,y} x \cdot y \cdot \frac{F(x, y, z)}{F}}{\sum_{x,y} y \cdot \frac{F(x, y, z)}{F}}, \frac{\sum_{x,y} y \cdot y \cdot \frac{F(x, y, z)}{F}}{\sum_{x,y} y \cdot \frac{F(x, y, z)}{F}} \right).
\]

(21)

In this equation the summation runs over all pixels \( x, y \) of \( N_B(x, y, z) \) that belong to the detection cluster and are above the analysis threshold \( S/N_{\text{ana}} \) in the \( z \)-peak layer of the \( S/N \)-cube.

The 2D narrowband images are furthermore used by \texttt{lsdcat\_measure.py} to derive basic shape information using the second central image moments of each detection. These are defined as

\[
x^{(2)} = \frac{\sum_{x,y} x^2 \cdot \frac{F(x, y, z)}{F}}{\sum_{x,y} \frac{F(x, y, z)}{F}} - (x^{(1)})^2,
\]

\[
y^{(2)} = \frac{\sum_{x,y} y^2 \cdot \frac{F(x, y, z)}{F}}{\sum_{x,y} \frac{F(x, y, z)}{F}} - (y^{(1)})^2,
\]

\[
[x'y']^2 = \frac{\sum_{x,y} x^2 \cdot y^2 \cdot \frac{F(x, y, z)}{F}}{\sum_{x,y} \frac{F(x, y, z)}{F}} - x^{(1)} \cdot y^{(1)},
\]

(22-24)

These values are simple indicators for the spatial extent and elongation of a detected emission line cluster. For example, \( [x'y']^2 \approx 0 \) for a circular symmetric distribution of the object in \( N_B(x, y, z) \). Moreover, in this case the radius

\[
R_{\text{Kron}} = \frac{\sum_{x,y} \frac{F(x, y, z)}{F}}{\sum_{x,y} \frac{F(x, y, z)}{F}} \sqrt{(x-x^{(1)})^2 + (y-y^{(1)})^2}.
\]

(26)

In order to avoid possibly unphysical small or large values of \( R_{\text{Kron}} \) caused by artefacts in the data, a minimal and a maximal value for \( R_{\text{Kron}} \) can be set by the user.

The factor \( k \) is also defined by the LSDCat user. Multiple values of \( k \) result in multiple columns of the output catalogue. The line flux \( F_{\text{line}}(k \cdot R_{\text{Kron}}) \) is then given by the sum

\[
F_{\text{line}}(k \cdot R_{\text{Kron}}) = \Delta \lambda \sum_{x,y} \sum_{z=\min}^{\max} \frac{F(x, y, z)}{F}.
\]

(27)

with the first sum running over all \( x, y \) that satisfy \( \sqrt{(x-x^{(1)})^2 + (y-y^{(1)})^2} \leq R_{\text{Kron}} \). The aperture thus has cylindrical shape, with its symmetry axis going through the 2D centroid position. The factor \( \Delta \lambda \) that denotes the increment per spectral layer is needed to convert the sum of voxel values into a proper integral over the line.

It can be shown that the 2.5 \( R_{\text{Kron}} \) aperture includes \( \geq 90\% \) of the total flux even for extended sources with relatively shallow profiles, as long as the determination of the Kron radius in Eq. (26) accounts for pixels at sufficiently large radii (Graham & Driver 2005). We follow a similar approach as adopted in \texttt{SEXtractor} (Bertin & Arnouts 1996) by summing over all \( x, y \) in Eq. (26) that satisfy

\[
\sqrt{(x-x^{(1)})^2 + (y-y^{(1)})^2} \leq 6 \cdot R_{\sigma},
\]

(28)

with \( R_{\sigma} \) as defined in Eq. (25). The uncertainty \( \sigma_F \) of this flux measurement is obtained by propagating the voxel variances \( \sigma_{x,y,z}^2 \), through Eq. (27).

3. Validation of the software

3.1. Creation of test datacubes

We now validate the correctness of the algorithms implemented in the LSDCat software. To this aim we produced a set of
datacubes that contain fake emission line sources at known positions with known fluxes and extents. Instead of utilising a completely artificial data set with ideal noise, we based our source insertion experiment on the MUSE HDF-S datacube (Bacon et al. 2015). Thereby we ensure that our test data is identical in noise and (potential systematics) with real observations. Furthermore, we self-calibrated the noise by calculating empirical variances as we recommend in Sect. 4.4.

We implanted the fake emission line sources into a continuum-subtracted version of the HDF-S datacube at a wavelength of 5000 Å. Continuum subtraction was performed with the median-filter subtraction method detailed in Sect. 4.1. The chosen insertion wavelength ensures a clean test environment which is not hampered by systematic sky-subtraction residuals that exist in the redder parts of the datacube. In total we created 23 test datacubes for the fake source emission line fluxes log F [erg s$^{-1}$ cm$^{-2}$] = $-16.2$ to $-18.5$ in steps of 0.1 dex. Each cube contains 51 fake sources with the same emission line flux. The spatial positions of the implanted sources are based on the pseudo-random Sobol sequence (Press et al. 1992, Sect. 7.7). The pseudo-random grid guarantees that all sources have different distances to the edges of the rectangular grid of MUSE slicer-stacks, thus possible systematic effects from localised noise properties within this slicer-stack grid are mitigated. As test sources we utilised Gaussian emission lines with a line width (FWHM) of 250 km s$^{-1}$. The sources were assumed to be PSF-like and we approximated the PSF blurring by a 2D Gaussian with 0.88 FWHM at 5000 Å, a value we obtained from averaging our empirical noise estimate across the whole data set that we consider here. Therefore Eq. (4) can be written as

$$\sigma_{\text{spec}}^{2} \approx \sum_{i,j} (T_{i,j}^{\text{spec}})^{2} \left( \frac{T_{k}^{\text{spec}}}{\sigma_{r}^{2}} \right)^{2}.$$  \hspace{1cm} (31)

Assuming that the dispersion $\sigma_{L}$ and $\sigma_{G}$ of the 1D and 2D Gaussian in Eqs. (11) and (21) are large enough to make sampling and aliasing effects of the profiles in the datacube negligible we can replace the sum with an integral, thus

$$\sum_{i,j} (T_{i,j}^{\text{spec}})^{2} \approx \int_{-\infty}^{\infty} \frac{1}{2\pi\sigma_{r}^{2}} \exp \left( -\frac{z^2}{\sigma_{r}^{2}} \right) dz = \frac{1}{2\sqrt{\pi} \sigma_{r}}.$$  \hspace{1cm} (32)

and

$$\sum_{i,j} (T_{i,j}^{\text{spec}})^{2} \approx \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{4\pi\sigma_{G}^{2}} \exp \left( -\frac{x^2+y^2}{\sigma_{G}^{2}} \right) dxdy = \frac{1}{4\pi\sigma_{G}^{2}}.$$  \hspace{1cm} (33)

With these expressions in Eqs. (30) and (31) we can write the peak detection significance of the line at position $x', y', z'$ via Eq. (9) as

$$S/N_{x',y',z'} \approx \frac{1}{8\pi^{1/4}\sigma_{G}\sigma_{r}} \times \frac{F_{\text{line}}}{\sigma_{\text{det}}}.$$  \hspace{1cm} (34)

With the expression given in Eq. (34) it is now possible to estimate the minimum recoverable line flux at a given detection threshold. For the artificial sources implanted in the MUSE HDF-S data we have $\sigma_{G} = 0.88'' = 1.84$ px. The spectral line width $\text{FWHM} = 250$ km s$^{-1}$ translates to $\sigma_{r} = 1.46$ px at 5000 Å and $\Delta l = 1.2$ Å. By averaging our empirical noise estimate around 5000 Å we find $\overline{\sigma} = 1.42 \times 10^{-20}$ erg s$^{-1}$ cm$^{-2}$ Å$^{-1}$. As we detailed in Sect. 4.5 for the MUSE HDF-S datacube, a detection threshold of $S/N_{\text{det}} \approx 8$ is a value found to be suitable for practical work. With the stated values inserted into Eq. (34) we calculate

$$\log F_{\text{line}} [\text{erg s}^{-1} \text{cm}^{-2}] \approx -17.83$$  \hspace{1cm} (35)

as the minimum line flux at which sources should be detectable at $S/N_{\text{det}} = 8$, if an exactly matching filter was chosen in the cross-correlation process. We now perform the recovery experiment utilising the test datacubes introduced in Sect. 3.1 to check whether LSDCat is indeed able to detect emission line sources with $S/N_{\text{det}} = 8$ at the estimated minimum line flux. Therefore we process all 23 test datacubes with LSDCat utilising the perfect matched filter, as well as setting $S/N_{\text{det}} = 8$. In the resulting catalogues we then

\[\text{http://muse-vlt.eu/science/hdfs-v1-0/}\]
search for positional cross-matches with the input source positions. From counting these cross-matches we produce the completeness curve $f_c(\log F[\text{erg s}^{-1}\text{cm}^{-2}\text{Å}^{-1}])$ displayed in Fig. 3. This curve displays the fraction of recovered sources as a function of input emission line flux. As vertical dashed and dotted lines, respectively, we show in this figure the analytically approximated minimum flux of Eq. (35) for detectability and 50% completeness estimate.

As can be seen in Fig. 3, the completeness curve starts to rise at the analytically estimated minimum flux for detectability. This validates the implementation of the detection algorithm in LSDCat. Nevertheless, it is also clear from Fig. 3 that the rise of the completeness curve is not from 0 to 1 at the estimated minimum, but it takes approximately 0.4 dex to recover all emission line sources at $\log F[\text{erg s}^{-1}\text{cm}^{-2}\text{Å}^{-1}] = -17.6$; slightly above the estimated minimum value. Overall, however, there is an excellent match between a simple analytic model of detectability and our realistic implementation of a detection experiment, especially given the fact that the noise in the real data is certainly not exactly Gaussian as assumed in the model.

### 3.3. Line flux measurements

Given the known input emission line fluxes of the implanted fake emission line sources $F_{\text{in}}$ we are equipped to validate the flux integration routine implemented in LSDCat. As detailed in Sect. 2.5.2, LSDCat integrates fluxes in circular apertures of radii $k \cdot R_{\text{Kron}}$ (Eqs. (26) and (27)). It has been shown that apertures with $k = 3$ are expected to contain >99% of the flux for Gaussian profiles (Graham & Driver 2005). Therefore we compare in this experiment $F_{\text{out}}$ to the LSDCat measured flux in three Kron-radii: $F_{\text{out}} = F(3 \cdot R_{\text{Kron}})$. In absence of noise we thus expect that for every source $F_{\text{out}} = F_{\text{in}}$.

The result of the above comparison from our source insertion and recovery experiment is visualised in Fig. 4 where we plot, as a function of input flux, the difference between input and output flux for each individual emission line source detected by LSDCat. In addition to the individual differences we also show, again as a function of input flux, the mean and the standard deviation of the difference over all recovered sources (blue circles and red bars in Fig. 4). We can compare the latter with the expected spread in flux measurements. This expected spread is simply given by the average uncertainty on the flux measurement as tabulated by LSDCat for each input flux bin. As noted in Sect. 2.5.2, the flux measurement uncertainties follow from direct propagation of the voxel variances through Eq. (27).

As can be seen from Fig. 5, there is no bias in the recovered flux levels above input fluxes of $\log F_{\text{in}}[\text{erg s}^{-1}\text{cm}^{-2}\text{Å}^{-1}] = -17.5$. Even for lower flux levels, the systematic errors are small, with (on average) 90% of the total flux being recovered. Still, at the lowest flux levels, where the detection completeness is also below 100%, a handful of implanted emission line sources are recovered with fluxes that are only ∼50% ($\log(F_{\text{out}}/F_{\text{in}}) \leq -0.3$) of the input flux. We checked that the larger deviations for some of the faintest simulated sources are all due to imperfections in the HDFS datacube. This experiment thus demonstrates at the same time the robustness of the flux measurement procedure in LSDCat, but also the need to use real data in quantifying the true performance of a certain measurement approach.

### 3.4. Comparison to manual flux integration on spatially extended objects

To further demonstrate the robustness of the fluxes obtained with LSDCat, we compare the flux measurements from LSDCat with manually measured fluxes (Fig. 5). The sample on which we performed the test consists of 60 Lyman $\alpha$ emitting galaxies that were found by us in MUSE datacubes (Herenz et al., in prep.). As established recently by Wisotzki et al. (2016), such galaxies
show regularly extended but low-surface-brightness Lyman α haloes, thus constituting good test cases for the flux measurement in non-trivially shaped extended objects. We obtained the manual flux measurements by using a curve-of-growth approach on pseudo-narrow-band image created from the datacube. The width and central wavelength of those images were determined by eye in order to ensure that the complete emission line signal is encompassed within the band-pass. Therefore we utilised 1D spectra extracted in a circular aperture of three pixel radius centred on $x^{\text{com}}, y^{\text{com}}$. On these images we then constructed the growth curve by integrating the fluxes in concentric circular apertures with consecutively increasing radii. Finally, we visually inspected these curves to pin down the radius at which the curve saturates, and the total flux within this circular aperture was adopted as the final flux measurement.

The LSDCat measurements were obtained in apertures of $R = 2R_{\text{Kron}}$ and $R = 3R_{\text{Kron}}$ and applying Eq. (27). As can be seen in Fig. 5, the different measurement approaches agree very well globally. The LSDCat $R = 2R_{\text{Kron}}$ fluxes are systematically somewhat below the growth curve measurements, indicating that the $2R_{\text{Kron}}$ apertures still lose a small but significant fraction of the flux ($-2\%$ or $-6\%$ flux lost compared to the manual fluxes in the median or average of the sample, respectively); this is no longer the case for the $R = 3R_{\text{Kron}}$ apertures ($+10\%$ or $+8\%$ flux gained in the median or average, respectively). We conclude that LSDCat delivers reliable and robust flux measurements for emission lines with non-pathological spatial and spectral shapes.

4. Guidelines for the usage of LSDCat

We now provide some guidelines for using LSDCat on wide-field IFU datacubes. These are based on our experience with applying the code on MUSE datacubes, searching for faint emission lines from high-redshift galaxies (first results presented in Bacon et al. 2015; and Bina et al. 2016; more will be reported in Herenz et al. 2017). We intend these guidelines to be instructive for the potential LSDCat user, but they should not be understood as recipes.

4.1. Dealing with bright continuum sources in the datacube

Even in relatively empty regions in the sky, any blank-field exposure will contain objects that produce a detectable continuum signal within the datacube, and that correspondingly appear in a white-light image resulting from averaging over all layers in the datacube (e.g. Fig. 3 in Bacon et al. 2015). To detect such sources, conventional 2D source detection algorithms are clearly sufficient. Since in the detection process of LSDCat we implicitly assume any significant signal to be due to emission lines, it is advisable to either mask out or, better, subtract any significant continuum signal from the datacube before running LSDCat. This step is not strictly needed, and the presence of continuum sources in the datacube does not render the detection algorithm unusable as such. But the significance of a line detection would clearly change if the line sat on top of a continuum signal, while a very bright continuum-only object would even turn out a band of spurious detections.

To remove the continuum, we found it useful to create and subtract a “continuum-only” cube by median filtering the original flux datacube in spectral direction only. The width of the median filter should be much broader than the expected widths of the emission lines, and it should be narrow enough to approximately trace a slowly varying continuum. In our experience, filter radii of $\sim 150\,\text{Å} - 200\,\text{Å}$ serve these goals very well. The median filter-subtracted datacube can then be used as input $F$ for LSDCat.

4.2. Width of the spatial filter template

The matched filtering approach produces maximum significance if the shapes of the true signal and of the template exactly agree; any template mismatch leads to a reduced $S/N_{\text{peak}}$ value. Fortunately, this dependence of $S/N$ on the template shape parameters is relatively weak around the optimum. If both signal and template are of Gaussian shape and the template has an incorrect width of $FWHM_{\text{temp}} = \kappa \times FWHM_{\text{true}}$, it can be shown that $S/N_{\text{peak}}$ decreases only as $S/N_{\text{peak}} \propto 2\kappa/\kappa^2 + 1$, \hspace{1cm} (36)

(Zackay & Ofek 2017). Hence even a difference of 20% between the adopted and the correct FWHM will result in a reduction of $S/N$ by only $\sim 2\%$, entirely negligible for our purposes; this number is supported by our own numerical experiments.

When searching for compact emission line objects, a single spatial template modelling the light distribution of a point source (i.e. the PSF) will therefore be sufficient for many applications. Even neglecting the wavelength dependence of the seeing (i.e. setting the polynomial coefficient $p_0$ in Eq. (15) to the mean Gaussian seeing FWHM, and all other PSF parameters to zero) will result in only a very modest reduction of sensitivity at the lowest and highest wavelengths.

To go one step further in accuracy, one has to account for the seeing as a function of wavelength. In the framework of the
standard (Kolmogorov) turbulence model of the atmosphere, the seeing is expected to decrease with increasing wavelength as $\text{FWHM} \propto \lambda^{-5/3}$, where the constant of proportionality also depends on airmass (e.g. Hickson 2014). In reality, other effects also play a role, such as guiding errors, or the blurring induced by co-adding multiple differently exposed images of the same field.

When the observed field contains a point source of sufficient brightness, a direct measurement of $\text{FWHM}(\lambda)$ is possible from the datacube. As an example, we show in Fig. 6 the derived $\text{FWHM}(\lambda)$ relation from a Moffat fit to the brightest star in the MUSE HDFS datacube (Same data as Fig. 2 in Bacon et al. 2015). Here we overplot the polynomial fit according to Eq. (15) and the relative difference between this fit and the $\text{FWHM}$ values derived from the star, $(\text{FWHM}_\text{star} - \text{FWHM}_\text{fit})/\text{FWHM}_\text{star}$. This difference is less than 3%, thus totally negligible in our matched-filter application. For datacubes containing only faint stars, it may be advisable to bin over several spectral layers before modelling the PSF.

If no point source is present within the datacube, the relations by Tokovinin (2002) can be used to get an idea of the dependence of $\text{FWHM}$ on $\lambda$. They predict $\text{FWHM}(\lambda)$ given a differential image motion monitor (DIMM) seeing $\text{FWHM}$, the airmass of the observation, and an additional parameter $\psi_0$ (called the wavefront outer scale length) that quantifies the maximum size of wavefront perturbations by the atmosphere (e.g. Martin et al. 1998). In Fig. 6 we also compare the $\text{FWHM}(\lambda)$ relation derived from this model to the actual measurement of the brightest star in the HDFS. For the plot, we adopted a DIMM seeing of 0.75'' at 5000 Å and an airmass of 1.41, both averages over all individual MUSE HDFS observations. We set $\psi_0$ to 22 m, which is the median of this for the Paranal observatory (Conan et al. 2000). As can be seen, this model provides a very good description of the measured $\text{FWHM}(\lambda)$ relation. Moreover, from this figure it is also clear that a second-order polynomial is a nearly perfect representation of the Tokovinin $\text{FWHM}(\lambda)$ prediction.

4.3. Width of the spectral filter template

As explained above, LSDCat assumes the spectral (Gaussian) template to have a fixed width in velocity space. We now briefly demonstrate the effect of template mismatch in the spectral domain. Similarly to the 2D case considered in the previous subsection (Eq. (36)), it can be shown that $S/N_{\text{peak}}$ decreases as

$$S/N_{\text{peak}} \propto \sqrt{2\kappa/(\kappa + 1)}$$

where $\kappa$ is the ratio between adopted and true template width. Even when the filter width is half or twice that of the actual object, the maximum reachable detection significance reduces by only ~10%. For the same reason, the achievable $S/N$ is very robust against moderate shape mismatches between real emission line profiles and the Gaussian template profile.

A good choice of the spectral filter width $\text{FWHM}_\lambda$ can be motivated by analysing the distribution of expected emission line widths (taking instrumental line broadening into account). If the distribution of observed line widths is relatively narrow it will be sufficient to adopt a single template with width close to the midpoint of the expected distribution. If however the expected distribution is very broad, for example, when searching both for star-forming galaxies and for AGN, it may be useful to generate two filtered datacubes with significantly different $\text{FWHM}$ values (the ratio should be at least a factor 3). This implies two LSDCat runs creating two catalogues that later have to be merged.

To demonstrate the impact of varying the template width $\text{FWHM}_\lambda$ on the detectability of a particular class of emission-line objects we show in Fig. 7 the dependence of the ratio $\xi \equiv (S/N)/(S/N_{\text{max}})$ for all Lyman $\alpha$ emitters in the MUSE Hubble Deep Field South datacube (Bacon et al. 2015). Here, $S/N_{\text{max}}$ denotes the maximum detection significance for a line, comparing all considered line widths. The plot shows that $\xi$ varies quite slowly with template width, confirming the theoretically expected behaviour (shown by the red curve). A good...
choice, at least for this object class, appears to be a filter width of $FWHM = 250 \text{ km} \text{s}^{-1}$, for which basically all the Lyman $\alpha$ emitters in the sample are detected with at least 90% of their maximum possible detection significance. The same template will capture even completely unresolved emission (i.e. with just the MUSE instrumental line width $FWHM$ of $\sim 100 \text{ km} \text{s}^{-1}$ at $\lambda = 7000 \text{ Å}$) at more than 80% of the value for a perfectly matching template.

4.4. Empirical noise calibration

Source detection is essentially a decision process based on a test statistic to either reject or accept features in the data as genuine astronomical source signals (e.g. Schwartz & Shaw 1975; Wall 1979; Hong et al. 2014; Zackay & Ofek 2017; Vio & Andreani 2016). This decision is usually based on a comparison with the noise statistics of the dataset under scrutiny. Consequently a good knowledge of the noise properties is required for deciding on meaningful thresholds, for example, in terms of false-alarm probability. In LSDCat we assume that $\sigma^2$ contains a good estimate of the variances. However, in reality this is often not so easy to obtain. In particular, resampling processes carried during the data reduction usually neglect the covariance terms; even if known, it would be computationally prohibitive to formally include them in a dataset of $4 \times 10^5$ voxels. In consequence, any direct noise property derived from $\sigma^2$ will underestimate the true noise, possibly by a very substantial factor, and the resulting detection significances will be biased towards overly high values that lose their probabilistic connotation.

A possibly remedy is self-calibration of the noise from the flux datacube. There are several ways to accomplish this, and here we simply provide a few insights from our own experience with MUSE cubes. It must be realised that the pixel-to-pixel noise in any given spectral layer will be as much affected by the resampling as the propagated variances, and therefore biased low in the same way. This is not so, however, for the variance of a typical aperture, for which the effects of resampling are much lower (basically acting only on the pixels at the circumference of the aperture). One can therefore estimate effective variances by evaluating the standard deviation between several identical apertures placed in different blank sky locations, separately for each spectral layer. This approach also implicitly accounts for additional noise-like effects due to imperfect flatfielding or sky subtraction.

Indeed, sky subtraction residuals can still be an issue in MUSE data, especially for the OH forest in the red part of the spectral range. If a dataset should be heavily affected and suffer from too many spurious detections that are just sky residuals (and even the new ZAP software by Soto et al. 2016, not providing sufficient improvement), it is still possible to increase the effective variances for the affected spectral layers to a level where only extremely bright sources at these wavelengths are detected by LSDCat.

4.5. Choosing the detection and analysis thresholds

A crucial quantity in each detection process is the incidence rate of false positives. If the noise properties are accurately known, the false-alarm probability can be directly calculated from the detection threshold $S/N_{\text{det}}$. Given the $\gtrsim 10^8$ voxels in a MUSE-like wide-field datacube it is obviously necessary to have a very low false-alarm probability. After matched filtering with a typical template the number of independent voxels gets reduced by a factor of $\sim 10^2$. (Here we consider as a typical template $FWHM = 300 \text{ km} \text{s}^{-1}$ and $p_0 = 0.8''$ (the default values in LSDCat), Given the spatial sampling of $0.2''$ per spatial pixel and spectral sampling of $1.25 \text{ Å}$ per datacube layer in MUSE, this corresponds to the central wavelength range of MUSE ($\sim 6980 \text{ Å}$) to a filter $FWHM$ of $\sim 10$ voxels.) Even assuming perfect Gaussian noise, a threshold of $S/N_{\text{det}} = 5$ would then already result in $\sim 10$ spurious detections per cube. However, the wings of the noise distribution are never perfectly Gaussian, to which also flatfielding and sky subtraction residuals have to be added; any such deviations from Gaussianity will directly inflate the false detection rate.

Instead of relying on theoretically expected false alarm probabilities, we recommend self-calibrating the rate of spurious detections using LSDCat on the negated cube $-F$. While obviously no real emission line object can be detected in such a dataset, it can probably be assumed that the effective noise properties are approximately the same in original and negated data. Running LSDCat on both versions then immediately allows us to estimate the ratio of real to spurious detections and adjust the final value of $S/N_{\text{det}}$ accordingly. A possible criterion could then be the point of diminishing returns, where lowering the detection threshold would produce a large increase in spurious detections with only a small compensatory increase of genuine emission lines.

In Fig. 8 we exemplarily present the result of such an analysis for the MUSE HDFS dataset. This datacube was processed according to the guidelines given in the previous subsections. In the figure, we show both the number of detections in the original and in the negated datacube at different thresholds. Moreover, in the bottom panel of Fig. 8 we show the ratio $R = (p - n)/p$, where $p$ and $n$ designate the number of detections in the original...
and negated datacube, respectively. Assuming a symmetric noise distribution around zero and no systematic negative holes in the data, the rate of genuine detections within a catalogue at a given threshold can be approximated by \( R \) (e.g. Serra et al. 2012). However, we find that the sky-subtraction residuals in the MUSE HDFS datacube appear to be systematically skewed to more negative values. In addition, since we subtracted continuum signal utilising the median filter approach (Sect. 4.1), absorption lines in some continuum bright objects created holes that mimic emission line signals in the negated datacube. Indeed, most of the detections in the negated cube at \( S/N_{\text{det}} \gtrsim 10 \) can be associated either with sky subtraction residuals or holes from over-subtracted absorption lines. Taking this into account, we notice in Fig. 8 a second strong increase of detections in the negated dataset that is not compensated by positive detections at \( S/N_{\text{det}} \lesssim 8 \). Hence, for this particular dataset a threshold below \( S/N_{\text{det}} \approx 8 \) would not be advisable.

The choice of the analysis threshold \( S/N_{\text{thr}} \) used in the measurement routine (Sect. 2.5) again depends on the noise characteristics. Here it is useful to visually inspect the \( S/N \)-cubes. Considering for example the faint emission line source presented in Fig. 2, by comparing the left panel (where no source is present) to the right panel that includes the source, we find that non-source voxels rarely obtain \( S/N \) values higher than 3. Hence, in this dataset, voxels around a real detection above a threshold value of 3.5 are likely linked to the actual source and should be included in the measurement process.

5. Conclusion and outlook

Here we presented LSDCat, a conceptually simple but robust and efficient detection package for emission line objects in wide-field IFS datacubes. The detection utilises a 3D matched filtering approach to detect individual emission lines and sorts them into discrete objects. Furthermore, the software measures fluxes and the spatial extents of detected lines. LSDCat is implemented in Python, with a focus on fast processing of the large data volumes generated by instruments such as MUSE. In this paper we also provided some instructive guidelines for the prospective usage of LSDCat.

LSDCat is open-source. Following the example of Astropy Collaboration et al. (2013), we release it to the community under a 3-clause BSD style license. This license permits usage and modification of the code as long as notice on the copyright holders (E.C. Herenz & L. Wisotzki) is given. A link to download the software is provided on the MUSE Science Web Service, and it is also available via the Astrophysics Source Code Library (Herenz & Wisotzki 2016).

LSDCat is documented in two ways. First, each of the routines described in Sect. 2 is equipped with an online help. Secondly we provide an extensive README file describing all the routines and options in detail. Moreover, that README contains examples and scripts that help use LSDCat efficiently.

LSDCat is actively maintained as it is currently used by the MUSE consortium to search for high-\( z \) faint emission line galaxies (e.g. Bacon et al. 2015; Bina et al. 2016; Herenz et al., in prep.; Urrutia et al., in prep.). Development takes place within a git repository. Technically inclined members of the community are invited to contribute to the code. We also offer a bug tracker that allows users to report problems with the software.

While LSDCat is fully operational, we see a number of aspects where there is room for future improvement. For example, LSDCat currently does not perform a deblending of over-merged detections, nor does it automatically merge detections belonging to a single source unless their initial positions are within a predefined radius. Indeed, in our search for faint line emitters in MUSE datacubes we encountered a few cases of very extended line-emitting galaxies that fragmented into several “sources”. We aim at addressing this problem in a future version. Currently these sources have to be merged or deblended manually in the resulting output catalogue. Another improvement planned for a future release is an automatic object classification for objects where multiple lines are detected. To this aim, the combination of spectral lines found at the same position on the sky must match a known combination of redshifted galaxy emission line peaks (Garilli et al. 2010). Finally, while in principle the software could be used for any sort of astronomical datacubes (e.g. coming from radio observations, or other IFS instruments), we have so far focused our efforts in development and testing on MUSE datacubes. However, the code is independent of instrument specifications and requires only valid FITS files following the conventions stated in Sect. 2.1. Still, despite all these possible enhancements LSDCat is already a complete software package, and we hope that it will be of value to the community.

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8 https://www.w3.org/Consortium/Legal/2008/03-bsd-license.html
9 http://muse-vlt.eu/science/tools/
10 http://ascl.net/1612.002
11 http://git-scm.com

References

Allington-Smith, J. 2006, Astron. Rev., 50, 244
Annunziatella, M., Mercuro, A., Brescia, M., Cavuoti, S., & Longo, G. 2013, PASP, 125, 68
Bourguignon, S., Mary, D., & É. Slezak 2012, Statistical Methodology, 9, 32
Graham, A. W., & Driver, S. P. 2005, PASA, 22, 118
Jurek, R. 2012, PASA, 29, 251
Appendix A: Usage example

We provide a short example to demonstrate how the user interacts with the LSDCat routines to obtain an emission line catalogue from an IFS datacube (see also Fig. 1). For this example we use the MUSE HDFS datacube (Bacon et al. 2015) in version 1.34. This datacube can be downloaded from the MUSE consortium data release web page. For brevity, we refer to the MUSE HDFS datacube FITS file as datacube.fits. Moreover, in all following commands, the -o option specifies the output filename of a particular routine.

As detailed in Sect. 4.1 any detectable source continua should be removed from a datacube on which LSDCat is used. There we outlined, that it is often sufficient to subtract these continua by subtracting an in-spectral-direction median filtered version of the datacube from the original datacube. We package with LSDCat an additional routine median-filter-cube.py that performs this task via the following command:

```
median-filter-cube.py datacube.fits -o mf_datacube.fits
```

(Run with its default settings the full width of the running median is 180 Å.) The output file mf_datacube.fits contains suitable input datacubes $F$ and $\sigma^2$ for the matched-filtering procedure (Sect. 2.2).

The spatial convolution and corresponding error propagation can now be achieved by running the following command:

```
lsd_cc_spatial.py --gaussian -p0=0.65 -p1=-4.5e-5 --lambda0=7050 -i mf_datacube.fits -m mask.fits -o spac_datacube.fits
```

Here we specified with $-p0$, $-p1$ and $--\text{lambda0}=7050$ the coefficients and zero-point of the linear function $p(\lambda[\text{Å}]) = 0.65-4.5\times10^{-5}(\lambda[\text{Å}] - 7050\text{Å})$ which is an apt representation of the PSF FWHM wavelength dependency in this field. The switch $--\text{gaussian}$ models the PSF as a circular Gaussian (Eq. (11)). Here we also utilise a mask mask.fits that masks out imperfections in the HDFC datacube near the FoV borders and the brightest star in the field, as these features cause numerous unwanted detections in the datacube. In the LSDCat documentation, we detail how such a mask can be created. The output file is named spac_datacube.fits.

Next, the spectral convolution is run on spac_datacube.fits via

```
lsd_cc_spectral.py -i spac_datacube.fits --FWHM=300 -o 3d_filtered_datacube.fits
```

Here $--\text{FWHM}$ is used to specify a filter FWHM of 300 km s$^{-1}$. The output 3d_filtered_datacube.fits now contains the matched filter output $\tilde{F}$ and $\tilde{\sigma}^2$ from which we can compute the signal-to-noise cube $S/N$ (Eq. (10)) via:

```
s2n-cube.py -i 3d_filtered_datacube.fits -o sncube.fits
```

While optional, the above step reduces the execution time of the routines lsd_cat.py and lsd_cat_measure.py, as they normally would create the $S/N$ datacube on the fly.

We can now create an emission line source catalogue with $S/N_{\text{det}} > 10$ by typing:

```
lsd_cat.py -i sncube.fits -t 10 -c catalogue.cat.
```

Utilising the thresholding procedure described in Sect. 2.4, the above command creates an ASCII and FITS table catalogue.cat and catalogue.fits for 2456 emission line candidates from 225 potential individual objects. Finally, the basic measurements described in Sect. 2.5 are obtained for each of the emission line candidates with the command

```
```

At this stage we recommend the catalogue to be inspected with QtClassify, a graphical user interface that helps to classify emission line candidates in IFS data, and which is optimally suited to work with catalogues created by LSDCat (Kerutt 2017).

More complete and up-to-date documentation describing all the routines can be found in the LSDCat repository. Moreover, for all routines, on-line usage information can be displayed by calling them with the $-h$ switch.

13 In order to follow the example we provide a suitable mask for the HDFC datacube version 1.34 in the examples folder of the LSDCat repository.

14 https://bitbucket.org/Leviosa/qtclassify