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Monte Carlo method for calculating oxygen abundances and their uncertainties from strong-line flux measurements[☆]

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ABSTRACT

We present the open-source Python code pyMCZ that determines oxygen abundance and its distribution from strong emission lines in the standard metallicity calibrators, based on the original IDL code of Kewley and Dopita (2002) with updates from Kewley and Ellison (2008), and expanded to include more recently developed calibrators. The standard strong-line diagnostics have been used to estimate the oxygen abundance in the interstellar medium through various emission line ratios (referred to as indicators) in many areas of astrophysics, including galaxy evolution and supernova host galaxy studies. We introduce a Python implementation of these methods that, through Monte Carlo sampling, better characterizes the statistical oxygen abundance confidence region including the effect due to the propagation of observational uncertainties. These uncertainties are likely to dominate the error budget in the case of distant galaxies, hosts of cosmic explosions. Given line flux measurements and their uncertainties, our code produces synthetic distributions for the oxygen abundance in up to 15 metallicity calibrators simultaneously, as well as for $E(B–V)$, and estimates their median values and their 68% confidence regions. We provide the option of outputting the full Monte Carlo distributions, and their Kernel Density estimates. We test our code on emission line measurements from a sample of nearby supernova host galaxies ($z < 0.15$) and compare our metallicity results with those from previous methods. We show that our metallicity estimates are consistent with previous methods but yield smaller statistical uncertainties. It should be noted that systematic uncertainties are not taken into account. We also offer visualization tools to assess the spread of the oxygen abundance in the different calibrators, as well as the shape of the estimated oxygen abundance distribution in each calibrator, and develop robust metrics for determining the appropriate Monte Carlo sample size. The code is open access and open source and can be found at https://github.com/nyusngroup/pyMCZ.

1. Introduction

Small amounts of carbon, oxygen, nitrogen, sulfur, iron and other elements provide a splash of color to the otherwise dominating grayscape of hydrogen and helium in the stars and gas of galaxies. Nevertheless, even this minute presence of heavy elements is important for many areas of astrophysics. For example, Johnson and Li (2012) suggest that if it were not for the relatively high metallicity level in our Solar System, planet formation may not have been possible. With Z representing the mass fraction of metals, all elements heavier than He (also collectively called metallicity), for our own Sun the value is measured to be $Z = 0.0153$ (Caffau et al., 2011), though there are suggestions of a lower Solar metallicity of $Z = 0.0134$ (Andrae et al., 2010; Grevesse et al., 2010). When properly observed and estimated, metallicity measurements of galaxies can tightly constrain models of galaxy formation and evolution (e.g., Kewley and Ellison, 2008 and references therein), and shed light on the metallicity dependence and production conditions for different types of supernovae (SNe)

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and long-duration gamma-ray bursts (GRBs) (e.g., Modjaz et al., 2008, 2011; Levesque et al., 2010; Anderson et al., 2010; Kelly and Kirshner, 2012; Sanders et al., 2012; Leloudas et al., 2015; Lunnan et al., 2014; Pan et al., 2014).

Metals are produced in the cores of massive stars during their fusion life cycle but also during the extreme conditions of stellar explosions. For example, the majority of iron is synthesized in thermonuclear explosions (SNe Ia) while nearly all oxygen and other α-elements[1] are released in various kinds of core-collapse SNe (SNe II and stripped-envelope core-collapse SNe).

However, for almost all astronomical objects, metallicity cannot be measured directly. The oxygen abundance in the gas-phase is the canonical choice of metallicity indicator for interstellar medium (ISM) studies. After Hydrogen, Oxygen lines are the strongest emission lines in optical wavelengths. Oxygen is the most abundant metal and it is only weakly depleted onto dust grains, in contrast to refractory elements such as magnesium, silicon, or iron (iron for example is depleted by more than a factor of 10 in Orion; see Simón-Díaz and Stasińska, 2011). The oxygen abundance is expressed as $12 + \log_{10}(\mathrm{O/H})$, where O and H represent the number of oxygen and hydrogen atoms, respectively. For example: (Caffau et al., 2011) measure a Solar oxygen abundance of $12 + \log_{10}(\mathrm{O/H}) = 8.76 \pm 0.07$, while Andrae et al. (2010) suggest $12 + \log_{10}(\mathrm{O/H}) = 8.69$.[2] While oxygen abundance is used to gauge metallicity, in many cases in the literature, including here, the terms metallicity and oxygen abundance are used interchangeably. Importantly, oxygen exhibits very strong nebular lines in the optical wavelength range in spectra of HII regions (e.g., Pagel et al., 1979; Osterbrock, 1989; Tremonti et al., 2004), which can be measured. Thus, many different diagnostic techniques relying on different lines of oxygen, hydrogen and other elements, have been developed (e.g., Kewley and Dopita, 2002 – hereafter KD02, Pettini and Pagel, 2004 – PP04, Kobulnicky and Kewley, 2004 – KK04, Kewley and Ellison, 2008 – KE08), and are discussed in the next section.

Many fields rely on the determination of the metallicity environments to understand physical phenomena, such as SN and planetary formation, from a causal, and possibly mechanicistic point of view. However many of these fields, including SN studies, have used metallicity calibration techniques somewhat acritically, at times inferring from calibrators that are not comparable, as they rely on different assumptions, because of the scarcity of complete dataset that would allow consistent estimates, and often ignoring many sources of uncertainty.

The purpose of this paper is to present a public code that collects different abundance diagnostics to efficiently and rapidly compute metallicity from strong emission line fluxes as well as the associated statistical uncertainties due to the measured emission line flux uncertainties. This source of uncertainty is particularly relevant in the study of SN metallicity environments, since the host galaxies of these cosmics explosions are often at large distances. While in many other contexts the signal-to-noise (SNR) of the spectra themselves may contribute negligibly to the total uncertainty budget, compared for example to errors in the model parameters, it is often a substantial source of uncertainty for high Z galaxies that host SNe. The necessity to compute metallicity quickly, and systematically for large samples arises from the new availability of large samples, enabled by IMACS spectrographs for example, and collected by surveys such as MANGA (Bundy et al., 2015).

Our open-source Python package is named **pyMCZ**. This Python code allows the user to quickly produce metallicity values with sensible confidence regions for several metallicity calibrators at once, given an input set of spectral line measurements and their errors, and to obtain and visualize the distribution of metallicities. `pyMCZ` is structured in a modular way in order to allow the user to include other strong line metallicity calibration methods, and link to external code packages, with minimal modifications, and naturally extend the advantages of the Monte Carlo (MC) based propagation of the observational uncertainties to the newly included calibrators. While we do not mean to advocate for a particular metallicity calibrator to be adopted, the comparison of multiple calibrator outputs, and the shape of each metallicity distribution, can guide the user in understanding the reliability of a metallicity estimate, given a set of line fluxes. Below we describe the different oxygen abundance diagnostics, and our Python module implementation.

2. Oxygen abundance diagnostics and calibrators

In this section, we present a brief overview of the various observational methods for measuring the gas-phase oxygen abundance—however, for a detailed discussion, and to understand the many caveats, we encourage the reader to read the reviews by, e.g., Stasińska (2002), KE08, Moustakas et al. (2010), Stasińska and Stasińska (2002), López-Sánchez et al. (2012), Dopita et al. (2013), hereafter D13, and Blanc et al. (2015).

The so-called "classical" way to estimate oxygen abundances is the electron temperature (T_e) method, which estimates the electron temperature and density of a nebula using a number of oxygen lines in different ionization states, including the auroral [O III] λ4363 line, to then directly estimate the O II and O III abundances and finally, after correcting for the unseen stages of ionization, to obtain the total oxygen abundance. However, except for low-metallicity environments, the auroral [O III] λ4363 line is very weak, and it saturates at metallicities higher than solar (Stasińska, 2002), since at higher metallicities the cooling is dominated by the oxygen fine structure lines in the near-infrared (NIR). In addition, there are other caveats about the T_e-method, as fluctuations and gradients in temperature or in chemical composition may lead to underestimates of the oxygen abundance (see for example Peimbert, 1967, and López-Sánchez et al., 2012). Most recently, Berg et al. (2015) suggested that among the auroral lines [O II], [O III] and [N II], the [O III] λ4363 line, commonly used for T_e measurements, is the most problematic one, giving rise to temperature discrepancies. Thus, other methods have been developed that estimate the oxygen abundance from ratios of strong nebular lines in the spectra of HII regions, including amongst others [O III] $\lambda\lambda$ 4959, 5007, [O II] $\lambda\lambda$ 3726, 3729, [N II] λ 6584, [S II] $\lambda\lambda$ 6717, 6731, as well as Hα and Hβ. These are called *strong-line calibrations* and are the subject of this manuscript.[3]

Strong-line methods can be categorized into three types, depending on how they calibrate the observed emission line ratios:

- empirical methods, which calibrate line ratios on observed T_e-based metallicities (e.g., Pilyugin and Thuan, 2005 – hereafter P05; Pilyugin et al., 2010 – P10; Pilyugin et al., 2012 – P12; Marino et al., 2013 – M13),

[1] α-elements are element with even atomic number lower than 22, synthesized by α-capture.

[2] The ongoing debate about the value of the Solar oxygen abundance should be kept in mind when metallicities are expressed relative to solar metallicity.

[3] There is one more class of methods, for which the recombination lines of different metal ions are used (e.g., Stasińska, 2002; López-Sánchez et al., 2012). However, these lines are so weak (for O and C they are $\sim 10^{-4}$ of Hβ) that these methods can be used for HII regions in the Milky Way and in the Local Group, but not over large extragalactic distances, in which we are interested.