DESCRIPTION OF THE PROGRAM FOR SELECTING THE THEORETICAL ISOCHRONE

February 14, 2024

1 Overview

The program is designed for the analysis of integrated-light (IL) spectra of globular clusters (GC) and originally described in the paper by [Sharina et al.(2024)]. This program allows ones to estimate the age, Y, and the approximate value of [Fe/H], determined from the isochrone parameter Z. The program is written in the Python language v3.8.8[1] using the Numpy and Scipy[2] packages. The spectra resolution for the application of the program in is recent state (see Sec. 2) is FWHM = 5.5 Å and the spectral range is 3900 - 5500 Å. To implement the algorithm, a grid of the synthetic spectra is calculated using the method described in the paper by [Sharina et al.(2024)] (Section 4) using the isochrones by [Bertelli et al.(2008)]. The resolution of the original model spectra is FWHM = 0.00166 Å. These model spectra are smoothed to the resolution of the observed spectra (FWHM = 5.5 Å in our case). The pixel size in the model and observed spectra should be 0.05 Å in order to the program works correctly. The model spectra were calculated with the element abundances given in Table 1 and the metallicity of the [Bertelli et al.(2008)] isochrones and atmospheric models indicated in Table 2. For each parameter Z of the isochrone, two values of [Fe/H] were used in the calculations of the atmospheric models. The estimates of the logarithm of the [Bertelli et al.(2008)] isochrone age for calculating the grid of the model spectra were chosen as follows: from 9.7 to 10.15 in 0.05 increments. The Y values were: 0.23, 0.26, and 0.30. The set of synthetic spectra computed with the [Bertelli et al.(2008)] isochrones and the fixed chemical composition (Table 1) are available on reasonable request to Sharina M.E.(sme@sao.ru). For the IL spectrum of the cluster obtained from telescope observations and reduced as described in the paper by [Sharina et al.(2024)] (Section 3), the error spectrum is calculated using the formula: $\sqrt{(obj + sky)Gain \cdot npix + Ron^2 npix}$, where obj+sky is the one-dimensional spectrum of the object before the sky subtraction, obtained in the same aperture as the analysed cluster spectrum and converted into the wavelength scale using the same dispersion relation; Gain is the gain factor of the CCD in [e-/ADU]; npix is the FWHM of the cluster in observations; Ron is the CCD readout noise in electrons. The spectrum of the object after reducing and subtracting the sky is also converted into electrons by multiplying by Gain.

At the first stage of the algorithm, a synthetic spectrum is searched for from the pre-calculated grid ones with a minimum deviation from the observed one, according to the parameter:

$$\chi = \sum_{i=0}^{N} \left(\frac{obj_i - theor_i[q_1, q_2, q_3, q_4]}{err_i} \right)^2$$

where obj_i and err_i are the elements of the cluster observed spectrum and error spectrum, theori is a synthetic spectrum set by the isochrone parameters q1, q2, q3, and q4 (Y, the logarithm of age, the metallicity of the isochrone Z_{B08}, and the metallicity of model atmospheres $[\mathrm{Fe/H}]_{atm}$). Before calculating χ, the continuum level of the observed spectrum is normalised to the level of the synthetic continuum. The parameters of the found synthetic spectrum are used as an initial approximation at the next stage of the program. At the next stage, a non-linear least-squares problem is solved with the given limitations of the parameters. To do this, the built-in function of the *scipy* library was used: scipy.optimize.least_squares[3] which finds the local minimum of the function F(x):

[1] http//www.python.org/
[2] https://scipy.org
[3] https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.least_squares.html

Table 1: Abundances of [X/Fe] elements for calculating the grid of the synthetic spectra.

$[X/Fe]$	Value
$[C/Fe]$	-0.2
$[N/Fe]$	0.3
$[O/Fe]$	0.2
$[Na/Fe]$	0.2
$[Mg/Fe]$	0.2
$[Si/Fe]$	0.1
$[Ca/Fe]$	0.1
$[Cr/Fe]$	0.0
$[Ti/Fe]$	0.1
$[Mn/Fe]$	0.0
$[Sr/Fe]$	0.15
$[Ba/Fe]$	0.15

Table 2: Parameters of the isochrones used to calculate the grid of the synthetic spectra.

Z_{B08}	$[Fe/H]$
0.0001	-2.5;-2.0
0.0004	-2.0;-1.5
0.001	-1.5;-1.0
0.002	-1.0;-0.5
0.004	-1.0;-0.5
0.008	-0.5;0.0

$F(x) = 0.5 \cdot \sum_{i=0}^{m-1}(\rho(f_i(x)^2))$, under the condition of lb $\leq$ x $\leq$ ub, where f(x) is the residual function $f_i(x) = (obj_i - theor_i(x))/err_i$, i is the spectrum element; and $\rho(s)$ is the loss function. This function uses the default value: $\rho(s) = s = f(x)^2$, where x are the required parameters: Y, log(Age), Z_{B08}, and $[\mathrm{Fe/H}]_{atm}$. Minimization is performed using the 'trf' (Trust Region Reflective) algorithm. At each iteration of the minimization algorithm, the model spectrum (theor(x)) is calculated as a linear interpolation of the grid spectra to the obtained parameters x. The observed cluster spectrum (obj) and the error spectrum (err) are normalised to the model interpolated spectrum (theor(x)) also at each iteration. The program calculates the 95% confidence interval for the obtained parameters, this procedure was taken from https://gist.github.com/81809e6f53c07a18cd12.git. The procedure for normalising the spectra to the theoretical continuum level is as follows. A list of wavelengths, in which the continuum is determined, was compiled in advance. The intensities of the observed spectrum at these points of the continuum are averaged over the range of ± 1 Å. To determine the continuum level of the model spectrum, the maximum intensity in the range of ± 1 Å is taken. The resulting continuum points are linearly interpolated over the whole length of the observed and model spectra. As a result, the observed spectrum is divided by the continuum of the observed spectrum and multiplied by the pseudo-continuum of the model spectrum.

2 Download and settings

The program for the automatic determination the parameters of a theoretical isochrone described here is provided primarily for informational purposes. Before using the program, we recommend contacting the authors.

The presented GitHub archive contains: chi_lsqnonline_4p.py - the program; models.zip - the grid of model synthetic spectra; contz001.dat - a list of wavelengths in which the continuum required for spectrum normalization is determined.

The algorithm is adapted to work with the IL spectra of GCs obtained at the 6-m BTA telescope using the SCORPIO-I instrument (please, see Sec. 2 of the paper by [Sharina et al.(2024)] for the description of observational data). Accordingly, the presented grid of model spectra is smoothed to a resolution of FWHM = 5.5Å, the spectral range is 3900-5900Å, the wavelength step is 0.05. Before starting calculations with the program, model spectra must be unzipped and placed in a separate

folder.

Before starting calculations with the program, it is necessary to create a working directory in which the observed spectrum, error spectrum and a list of lines in which the continuum contz001.dat is determined will be located. The observed spectrum and the error spectrum should be represented as an ascii table in the first column of which are the wavelengths, in the second the corresponding intensity values. The observed spectrum and the error spectrum must correspond to the model spectra, that is, have the same spectral resolution, initial wavelength (3900 Å) and wavelength step of 0.05.

The paths to the working directory and the directory in which the model spectra are located, as well as the names of the observed spectrum and the error spectrum, must be indicated directly in the body of the chi_lsqnonline_4p.py program (starting from line 94: "initialization of parameters"). The following parameters must be specified:

path_obj - the path to the working directory where the observed spectrum, the error spectrum, and contz001.dat are located.

path_theor - the path to the model grid.

obj - in quotes " indicate the name of the observed spectrum .

err - in quotes " indicate the name of the error spectrum.

n_elem - the number of elements in the spectrum that will be used, starting from the beginning of the spectrum.

At the end, the program creates an output file in the working directory with the results resultchi_nonline.dat. The file contains the following data: 1) the best fit among the grid spectra; 2) isochrone parameters determined at each iteration of the nonlinear minimization algorithm; 3) final parameter values obtained by nonlinear minimization (Y, logAge, Z, $[Fe/H]_{atm}$) and corresponding errors.

References

G. Bertelli, L. Girardi, P. Marigo and E. Nasi, Astronomy and Astrophysics, **484**, 815 (2008).

M. E. Sharina, M. I. Maricheba, A. Y. Kniazev, V. V. Shimansky and I. A. Acharova, MNRAS (in press).