AUTOMATIC EQUIVALENT WIDTH

INTRODUCTION

`autoeqw` is a python script which can be used to calculate the abundance of an element in a stellar photosphere which would produce a prescribed amount of equivalent width for a particular spectral line. This is used in conjunction with the code `SYNSPEC`. `SYNSPEC` simulates transfer of radiation through a given model photosphere. Among other things it calculates the equivalent linewidths for a given spectral line in the absorption spectrum that is expected to emerge from the photosphere.

This document explains how to use the autoeqw code to calculate the abundances. It will begin with a brief explanation of how `SYNSPEC` is to be operated, then tells how this program works, followed by how to operate this program (skip to the last section, if you are not interested in doing any modifications).

HOW TO USE SYNSPEC

For a detailed explanation of how to use `SYNSPEC` read `syn43guide.pdf`. Input/output is done with the help of a few files labeled as `fort.n`, where `n` is an integer. We shall discuss only the details `autoeqw` concerns with. These are `fort.8`, `fort.19`, `fort.55`, and `fort.56` for input and `fort.16` for output. There is another file which includes model elemental abundances and usually has a name of the form `*.5`. To run the program use (replace *`modelname`*`.5` with the appropriate name):

```
./synbaba < modelname.5
```

FORT.8

`fort.8` contains information about the model photosphere as generated by `TLUSTY` program. It is the output of `TLUSTY` stored in `fort.7`. This has to be renamed to `fort.8` when using it with `SYNSPEC`.

FORT.19

This file contains information about all the lines that we wish the program to consider. This file contains one spectral line in each line of the file. In the `FORTRAN` code this format is named `INLIN`. It looks like:

```
  425.3589 16.02  0.107  147146.000 2.0  170648.938 3.0    0.00   0.00   0.00 0
  428.4979 16.02 -0.233  146736.547 1.0  170067.313 2.0    0.00   0.00   0.00 0
  433.2692 16.02 -0.564  146696.188 0.0  169770.047 1.0    0.00   0.00   0.00 0
  435.4566 16.02 -0.959  147690.984 2.0  170648.938 3.0    0.00   0.00   0.00 0
  436.1527 16.02 -0.606  147146.000 2.0  170067.313 2.0    0.00   0.00   0.00 0
  436.4747 16.02 -0.805  147744.547 3.0  170648.938 3.0    0.00   0.00   0.00 0
  449.9245 16.02 -1.640  147550.313 1.0  169770.047 1.0    0.00   0.00   0.00 0
```

Here's an explanation of each component (with column numbers and description)

```
[ 0-10] ALAM - wavelength (in nm)
[11-16] ANUM - code of the element and ion (as in Kurucz-Peytremann)
               (eg. 2.00 = HeI; 26.00 = FeI; 26.01 = FeII; 6.03 = C IV)
[17-23] GF   - log gf
[24-35] EXCL - excitation potential of the lower level (in cm*-1)
[36-39] QL   - the J quantum number of the lower level
[40-51] EXCU - excitation potential of the upper level (in cm*-1)
```

```
[52-55] QU    - the J quantum number of the upper level
[57-63] AGAM  = 0. - radiation damping taken classical
              > 0. - the value of Gamma(rad)
[64-70] GS    = 0. - Stark broadening taken classical
              > 0. - value of log gamma(Stark)
[71-77] GW    = 0. - Van der Waals broadening taken classical
              > 0. - value of log gamma(VdW)
[78-79] INEXT = 0 - no other record necessary for a given line
              > 0 - next record is read, which contains:
```

For all the lines we use `INEXT = 0`. The data is demarked by columns indices.

FORT.55

This files contains various parameter values and switches that are required by `SYNSPEC`. These have to be set correctly and a better knowledge of the `SYNSPEC` program would let you know how to use this. Read the `SYNSPEC` documentation to know more. For the purpose of `autoeqw` we only need to look at the sixth line of this file. The first two numbers are the bounds (in Å) of the synthetic spectrum which will be generated. Equivalent widths will be calculated only within this bounds (even if a line is mentioned in `fort.19`). The last parameter is bin size (in units of approx. 10 nm).

FORT.56

This file is used to set the abundances for elements for which we want the abundance to be different from what is given in the model file. The first line of this file contains the number of elements which would be entered. The following lines contain information about each element. We need to specify the atomic number and abundance relative to Helium. A sample file would look like:

```
1
14 3.45-05
```

If the value is set as zero, it takes the solar abundance; for negative values it takes the negative value times the solar abundance. If no information is provided it takes the default value from the model file. To test for zero abundance, use a very small value like 10^{-10}.

FORT.16

This output file tells the equivalent linewidth in for each wavelength. The program divides the wavelength space into a large number of bins (the size of these bins is specified in `fort.55`). The output has information about each bin on one line. The first two numbers are the bounds of the bin and the third number is the equivalent width (in mÅ). All the bins near a particular spectral line can be summated to calculate the synthetic equivalent linewidth of the line. Here's a sample file

```
    4494.200    4495.367          0.0          0.0          0.0          0.0
    4495.367    4496.533          0.0          0.0          0.0          0.0
    4496.533    4497.700          0.0          0.0          0.0          0.0
    4497.700    4498.866          0.1          0.1          0.1          0.1
    4498.866    4500.034         15.9         15.9         15.9         15.9
    4500.034    4501.203          0.0          0.0          0.0          0.0
    4501.203    4502.372          0.0          0.0          0.0          0.0
    4502.372    4503.541          0.0          0.0          0.0          0.0
    4503.541    4504.200          0.0          0.0          0.0          0.0
```

HOW AUTOEQW FUNCTIONS

autoeqw calculates abundances by a method of trial and error (you could call it estimated guesses). It simply writes a guess abundance in fort.56, runs the SYNSPEC program and then reads the equivalent width from fort.16. Then it refines its guess and reiterates till it gets a value of equivalent width close enough to the target value. It also automates the job for a large number of lines. The following lines explain how it works.

1. All the parameters from fort.55 are read. This is so that the program is able to write to it later.
2. The input file aeqw.in is read. The first line contains a few parameters. The following lines contain information about all the spectral lines to be tested and the target equivalent widths. Some lines which are too close to each other can be grouped and a common equivalent width be given (See the specifications in the next section to know how to enter input in this file). The data is stores as an array of sets of lines. Each set contains lines which need to be evaluated together. Most sets will contain single lines.
3. It is checked if fort.8 and the model file have the same temperature and specific gravity. If not a warning is displayed. However, the execution is not interrupted.
4. All lines are written to fort.19.
5. The following steps are taken for each set of lines:
    a. The bounds of the synthetic spectrum are set. This is simply:
    (smallest wavelength – RANGE, largest wavelength + RANGE)
    where RANGE is a parameter that can be set in aeqw.in (5.0 is preferred)
    This is written to fort.55.
    b. The equivalent width is calculated (using the method in steps d. to f.) for an abundance of 10e-10 (settable by modifying NULLABUN in autoeqw.py). This is used as a zero baseline for future calculations.
    c. An initial value of abundance is assumed. (settable by modifying INITABUN in autoeqw.py, default 1e-4).
    d. The assumed value of abundance is written into fort.56. The atomic number is inferred from the specification of the line.
    e. SYNSPEC is run.
    f. fort.16 is read. The equivalent width is calculated. Only bins which are up to a distance specified by the parameter BROAD (a value of 2.0 is preferred) from the spectral line are considered. If the edge of the considered range is inside a bin, the bin is considered partially.
    g. It is checked if the value of equivalent width is acceptable (using the parameter EPSILON in aeqw.in). If not a new estimate for abundance is made and the steps d. to f. are repeated. The new estimate is arrived by assuming the equivalent width to be a linear function of abundance. It is also checked if the line is too weak or if we see emission.
6. The output is written to aeqw.out. See specifications in next section to interpret it.

HOW TO USE `AUTOEQW`

INSTALLATION AND RUNNING

Have the files `autoeqw.py` and `isynspec.py` in the `SYNSPEC` directory. `Autoeqw.py` should be executable. If it is not use the following command to set it:

```
chmod u+x autoeqw.py
```

To run the program simply type the following in the shell:

```
./autoeqw.py
```

BEFORE RUNNING

Set up `fort.8` and `fort.55` as per your liking. Also have the model file in the `SYNSPEC` directory. Ensure that the files have the correct temperature and specific gravity. Edit `aeqw.in` file as required.

INPUT FILE: `AEQW.IN`

An example input file looks like:

```
ltv652her.5 11.54 2.0 5.0 0.1

C
C Silicon II lines
412.8054 14.01  0.359   79338.500 1.5  103556.156 2.5    9.44  -4.87   0.00 0 30.0
# The following two lines will be evaluated simultaneously
# with a combined eqw of 34.0
413.0872 14.01 -0.783   79355.023 2.5  103556.156 2.5    9.44  -4.87   0.00 0 0
413.0894 14.01  0.552   79355.023 2.5  103556.031 3.5    9.44  -4.87   0.00 0 34.0
504.1024 14.01  0.029   81191.344 0.5  101023.047 1.5    9.03  -4.70   0.00 0 35.0
505.5984 14.01  0.523   81251.320 1.5  101024.352 2.5    9.04  -4.70   0.00 0 44.0
C
C Sulphur III lines
425.3589 16.02  0.107  147146.000 2.0  170648.938 3.0    0.00   0.00   0.00 0 174.0
428.4979 16.02 -0.233  146736.547 1.0  170067.313 2.0    0.00   0.00   0.00 0 103.0
433.2692 16.02 -0.564  146696.188 0.0  169770.047 1.0    0.00   0.00   0.00 0 66.0
435.4566 16.02 -0.959  147690.984 2.0  170648.938 3.0    0.00   0.00   0.00 0 53.0
436.1527 16.02 -0.606  147146.000 2.0  170067.313 2.0    0.00   0.00   0.00 0 68.0
436.4747 16.02 -0.805  147744.547 3.0  170648.938 3.0    0.00   0.00   0.00 0 34.0
449.9245 16.02 -1.640  147550.313 1.0  169770.047 1.0    0.00   0.00   0.00 0 16.0
```

The first line stores the values of some parameters. These are

```
modelfilename LOGHE BROAD RANGE EPSILON
```

`modelfilename` is the name of the model file.
`LOGHE` is the logarithm of the absolute abundance of Helium. This is used to calculate the absolute abundance of all the elements in the output file.
`BROAD` is the width up to which the bins are considered, set it slightly more than half the expected width of a line.
`RANGE` specifies the extent of the synthetic spectrum.
`EPSILON` is the accuracy to which the program will try to match the equivalent width.

The following lines specify information about the spectral lines and their target equivalent width. Blank lines and lines which start with a # or a C are ignored. Whatever follows a C in a line which starts with a C is also copied as is in the output file.

The first part of each line uses the same format in `fort.19`. Following this information one can input the target equivalent width in mÅ. This can be entered as a zero in order to combine this line with the following line. This will force the program to calculate the equivalent width for both lines together with the value specified in the next line to be the combined equivalent width. If this number is left blank then nothing is evaluated for this line, but is still added to the `fort.19` file.

OUTPUT FILE: `AEQW.OUT`

Here is the output file that the example input file will generate.

```
26000.00 3.00
LAMBDANM  Z.Q  ABUN/He  LOGABUN

Silicon II lines
412.8054 14.01 1.09e-04 7.58
413.0872 14.01
413.0894 14.01 7.45e-05 7.41
504.1024 14.01 3.27e-04 8.05
505.5984 14.01 1.39e-04 7.68

Sulphur III lines
425.3589 16.02 4.15e-05 7.16
428.4979 16.02 2.06e-05 6.85
433.2692 16.02 1.97e-05 6.84
435.4566 16.02 3.74e-05 7.11
436.1527 16.02 2.23e-05 6.89
436.4747 16.02 1.46e-05 6.70
449.9245 16.02 4.15e-05 7.16
```

The first line contains the temperature and logarithm of specific gravity. The next line is just a header line. The blank lines and the lines which read like “Silicon II lines” are generated due to the lines in the input file which start with a C. The comments have been added as is to the output file. The other lines contain the output. Each line has the wavelength, the atomic number, the level of ionization (-1), the relative abundance to Helium, and the logarithm of the absolute abundance.