A hands-on lesson on classical spectroscopic methods

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22 September 2021



Stellar spectroscopy and Astrophysical parametrisation from Gaia to Large Spectroscopic surveys, 21-23 September 2021



Outline

- How to create a synthetic spectrum
- How to derive atmospheric parameters with spectral synthesis (T_{eff}, log g, [M/H], vmic, vmac, vsini)
- How to derive chemical abundances with spectral synthesis
- How to derive atmospheric parameters from the EW of iron (T_{eff}, log g, [Fe/H], vmic)
- Examples



What's on the market?

Synthesis (with EW analysis)	Equivalent Width	Machine Learning
iSpec (Blanco-Cuaresma+ 2014)	FAMA (Magrini+ 2013)	The Cannon (Ness+ 2015)
fasma (Tsantaki+ 2018)	ARES+MOOG (Sousa+ 2008)	The Payne (Ting+ 2019)
SME (Piskunov+ 2017)	GALA (Mucciarelli+ 2013)	NN for RAVE (Guiglion+ 2020)
BACCHUS (Masseron+ 2016)	StePar (Tabernero+ 2019)	ML for APOGEE (Garcia-Dias+ 2018)

There are also hybrid methods: e.g. SP_Ace (Boeche+ 2016), MATISSE (Recio-Blanco+ 2006)

Differences on:

- analysis methods
- model atmosphere physics
- time consumption
- atomic line data
- a few publicly available (and fewer user friendly)
- many, many more ...

Choose your package depending on the specific problem (e.g. spectral type, rotation, resolution)



1. How to create a synthetic spectrum



1. How to get the flux at the top of the photosphere



1. How to get the flux at the top of the photosphere

- Stellar atmospheric parameters (T_{eff} , log g, [M/H], vmic)
- Model atmosphere
 - MARCS (LTE, plane parallel/spherical geometry): cool stars
 - Kurucz (LTE, plane parallel): extended grid
 - TLUSTY (non-LTE, plane parallel): hot stars
- Line data: wavelengths, excitation potentials, oscillator strengths, broadening parameters
 - Vienna Atomic Line Database (VALD)
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- Radiative solver
 - MOOG
 - Turbospectrum
- Convolution with rotation kernels (vmac, vsini) & instrumental resolution



- Stellar atmospheric parameters (5777, 4.44, 0.0, 1.0)
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.5													
= 577	7	log	g=	4.44									
J		72											
879326)65E	-04	37	784.6	1.51	1E+01	2.44	6E+09	2.	514E-0	4 7	7.508E-02	1.000E+05
43583	47E	-04	38	306.3	1.97	7E+01	3.15	7E+09	2.	912E-0	4 7	7.989E-02	1.000E+05
70011	04E	-04	38	327.9	2.51	6E+01	3.96	8E+09	З.	352E-0	48	B.275E-02	1.000E+05
21146)53E	-03	38	351.2	3.14	2E+01	4.90	1E+09	З.	842E-0	48	B.394E-02	1.000E+05
82776	17E	-03	38	375.6	3.87	0E+01	5.98	1E+09	4.	386E-0	48	B.400E-02	1.000E+05
89003	24E	-03	39	900.3	4.72	1E+01	7.23	4E+09	4.	997E-0	48	8.346E-02	1.000E+05
48215	57E	-03	39	925.3	5.71	9E+01	8.69	2E+09	5.	679E-0	48	B.253E-02	1.000E+05
70034	18E	-03	39	949.9	6.89	0E+01	1.03	8E+10	6.	458E-0	48	B.133E-02	1.000E+05
65031	63E	-03	39	974.2	8.26	2E+01	1.23	6E+10	7.	349E-0	48	B.009E-02	1.000E+05
645495	90E	-03	39	98.0	9.86	7E+01	1.46	5E+10	8.	366E-0	4 3	7.892E-02	1.000E+05
26168	72E	-03	46	921.5	1.17	5E+02	1.73	0E+10	9.	519E-0	4 7	7.791E-02	1.000E+05
23756)22E	-03	46	944.4	1.39	6E+02	2.04	0E+10	1.	084E-0	3 7	7.737E-02	1.000E+05
56919	99E	-03	46	967.1	1.65	4E+02	2.39	8E+10	1.	237E-0	3 7	7.732E-02	1.000E+05
48509	82E	-03	46	989.7	1.95	6E+02	2.81	3E+10	1.	410E-0	3 7	7.757E-02	1.000E+05
26856)37E	-03	43	L12.5	2.30	9E+02	3.29	6E+10	1.	606E-0	3 7	7.792E-02	1.000E+05
323701	18E	-03	43	L35.5	2.72	2E+02	3.85	6E+10	1.	831E-0	3 7	7.845E-02	1.000E+05
57547	59E	-02	43	L59.1	3.20	5E+02	4.50	9E+10	2.	086E-0	3 7	7.901E-02	1.000E+05
62552	02E	-02	43	L83.3	3.77	1E+02	5.26	7E+10	2.	378E-0	3 7	7.961E-02	1.000E+05
02294	45E	-02	42	208.0	4.43	3E+02	6.14	8E+10	2.	713E-0	38	B.042E-02	1.000E+05
82386	05E	-02	42	233.4	5.20	5E+02	7.17	2E+10	З.	098E-0	38	B.141E-02	1.000E+05
09362	11E	-02	42	259.5	6.10	8E+02	8.36	2E+10	З.	541E-0	38	B.256E-02	1.000E+05
91253	42E	-02	42	286.4	7.16	1E+02	9.74	8E+10	4.	041E-0	38	B.357E-02	1.000E+05
37614	32E	-02	43	313.9	8.39	1E+02	1.13	6E+11	4.	612E-0	38	B.454E-02	1.000E+05
59246	53E	-02	43	342.2	9.83	0E+02	1.32	3E+11	5.	264E-0	38	B.543E-02	1.000E+05
68925	57E	-02	43	370.9	1.15	1E+03	1.54	0E+11	6.	005E-0	38	8.627E-02	1.000E+05
81283	82E	-02	43	399.9	1.34	7E+03	1.79	4E+11	6.	856E-0	38	8.738E-02	1.000E+05
13011	26E	-02	44	129.1	1.57	7E+03	2.08	7E+11	7.	832E-0	38	8.883E-02	1.000E+05
683545	90E	-02	44	158.4	1.84	4E+03	2.42	9E+11	8.	953E-0	3 9	9.065E-02	1.000E+05
816446	39E	-02	44	187.8	2.15	6E+03	2.82	4E+11	1.	022E-0	2 9	9.268E-02	1.000E+05
39401	25E	-02	45	517.2	2.52	1E+03	3.28	4E+11	1.	168E-0	2 9	9.520E-02	1.000E+05
68397	51E	-01	45	546.4	2.94	6E+03	3.81	8E+11	1.	334E-0	2 9	9.809E-02	1.000E+05
48819	81E	-01	45	575.8	3.44	3E+03	4.43	7E+11	1.	522E-0	2 3	1.014E-01	1.000E+05
59625	45E	-01	46	504.8	4.02	5E+03	5.15	6E+11	1.	738E-0	2 3	1.056E-01	1.000E+05
	5 = 577 79326 779326 779321 21146 839092 26166 839092 265691 448592 2665691 26856 223776 223760 225760 225760 225760 225760 225760 225760 225760 225760 2257	5 = 5777 7932065E 4358347E 7001104E 2114053E 8277017E 83900324E 4451557E 7003418E 65031632 44549509E 2375022E 5601939E 23761432E 2375022E 5601939E 235022E 5601939E 4850982E 23761432E 823865E 9125342E 3761432E 5924653E 6892557E 8128862E 813865E 81381258 8138	5 5 777 732:0652 7432:0652 7432:0652 7432:0652 7432:0652 7432:0652 7432:0652 7432:0752 7432:0752 7432:0752 7432:0752 7442:0557 7442:0557 7442:0557 7547:052 7547	S = 5777 100 g= 727 37052 37052 37051455347E - 64 33 37001146E - 64 33 37001146E - 64 33 38277017E - 63 33 4821507E - 63 33 2616872F - 63 34 4825992E - 63 44 45591992E - 63 44 45591992E - 63 44 45591992E - 63 44 45591992E - 63 44 2685037E - 63 44 2685037E - 63 44 2685037E - 63 44 2685037E - 63 44 3754759E - 62	S 3 9 5 9777 log g = 4.44 7820652 3784.6 12531475-04 3784.6 32531475-04 3875.2 82770176-03 3875.2 82770176-03 3875.2 82770176-03 3875.2 82770176-03 3974.9 9003246-03 3949.9 903346-03 3949.9 903346-03 3949.9 261687276-03 3949.9 25150276-03 3949.9 25150276-03 4087.1 25150276-03 4087.1 2616037276-03 4082.7 2616037276-03 4125.5 57547595-02 4133.3 27244516-02 4208.0 20360516-02 4234.9 9352116-02 4319.2 9352456-02 4319.2 93602126-02 4370.9 93602126-02 4370.9 93602126-02 4370.9 93602126-02 4370.9 936025576-02 4370.9	S = 5777 log g= 4.44 /732.0652 /732.0652 /732.0652 /732.0652 /732.0652 /732.0652 /732.0652 /732.0652 /732.0652 /732.0652 /732.072 /73	S 5 5777 log g= 4.44 727 727 728 744.6 747 3286.3 747 3286.3 748 386.3 747 3287.7 7214035 3851.2 747 3287.6 747 3285.2 747 3285.2 747 3285.2 747 3285.2 747 3285.2 7421 3285.2 7421 3285.2 74421 3285.2 744421 3275.2 744421 3394.9 744421 3275.2 7547598 4424.1 7547598-92 4489.1 7547598-92 4183.3 7547598-92 4183.3 7547598-92 4283.4 7547598-92 4283.4 7547598-92 4283.4 7547598-92 4283.4 7547598-92 4283.4 7547598-92 4283	S = 5777 100 g = 4.44 72 100 100 100 100 100 100 100 10	S = 9777 log g = 4.44 7820052 784 7820052 3784 7820052 3784 7821052 3805 7821052 3805 7821052 3871 7821052 3871 7821052 3871 7821052 3871 82770176-03 3871 39903 34 39903 990324 39349 990324 39349 990324 39349 97041186-03 39349 9704128 39349 9705128 39349 9705218 39349 9705218 39349 9705218 39349 9705218 39349 9705218 39349 9705218 39349 97052218 39349 97052218 39349 97052218 30441 97052218 30441 980534 40421 9705116103	S = 5777 10g g= 4.44 72 72 72 72 72 72 72 72 72 72	⁵ = 7777 log g = 4.44 78230652 782 78230652 7824 7824 7824 7824 7824 7824 7824 7824 7825 7	S 5 5777 log g= 4.44 7000 720 7200 720 7200 720 7200 720 7200 720 7200 720 7200 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7200 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 7201 720 <	⁵ = 7777 log g = 4.44 7300552 14553476 44 14553476 44 1455476 145548 14554876 1



- Stellar atmospheric parameters (5777, 4.44, 0.0, 1.0)
- Model atmosphere
 - MARCS (LTE, plane parallel/spherical geometry): cool stars
- + optical depth at standard wavelengths
- + temperature in K
- + number density of free electrons
- + number density of all other particles
- = Calculate the radiative transfer equation \rightarrow Flux

MARCS						
Teff= 5777 log	g= 4.44					
NTAU 72						
5.37932065E-04	3784.6	1.511E+01	2.446E+09	2.514E-04	7.508E-02	1.000E+05
7.04358347E-04	3806.3	1.977E+01	3.157E+09	2.912E-04	7.989E-02	1.000E+05
8.97001104E-04	3827.9	2.516E+01	3.968E+09	3.352E-04	8.275E-02	1.000E+05
1.12114053E-03	3851.2	3.142E+01	4.901E+09	3.842E-04	8.394E-02	1.000E+05
1.38277017E-03	3875.6	3.870E+01	5.981E+09	4.386E-04	8.400E-02	1.000E+05
1.68900324E-03	3900.3	4.721E+01	7.234E+09	4.997E-04	8.346E-02	1.000E+05
2.04821557E-03	3925.3	5.719E+01	8.692E+09	5.679E-04	8.253E-02	1.000E+05
2.47003418E-03	3949.9	6.890E+01	1.038E+10	6.458E-04	8.133E-02	1.000E+05
2.96503163E-03	3974.2	8.262E+01	1.236E+10	7.349E-04	8.009E-02	1.000E+05
3.54549590E-03	3998.0	9.867E+01	1.465E+10	8.366E-04	7.892E-02	1.000E+05
4.22616872E-03	4021.5	1.175E+02	1.730E+10	9.519E-04	7.791E-02	1.000E+05
5.02375022E-03	4044.4	1.396E+02	2.040E+10	1.084E-03	7.737E-02	1.000E+05
5.95691999E-03	4067.1	1.654E+02	2.398E+10	1.237E-03	7.732E-02	1.000E+05
7.04850982E-03	4089.7	1.956E+02	2.813E+10	1.410E-03	7.757E-02	1.000E+05
8.32685037E-03	4112.5	2.309E+02	3.296E+10	1.606E-03	7.792E-02	1.000E+05
9.82370118E-03	4135.5	2.722E+02	3.856E+10	1.831E-03	7.845E-02	1.000E+05
1.15754759E-02	4159.1	3.205E+02	4.509E+10	2.086E-03	7.901E-02	1.000E+05
1.36255202E-02	4183.3	3.771E+02	5.267E+10	2.378E-03	7.961E-02	1.000E+05
1 600004455 00	4300.0	4 4335-03	6 1405-10	3 7135 03	0 0425 02	1 0005-05



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# Wavelength	ele	EP	logg	f vdwa	als	Do
5339.188	20.1	8.44	-0.075	-7.196	nan	
5339.416	26.0	4.43	-2.146	-7.51	nan	
5339.526	27.0	4.23	-0.377	-7.51	nan	
5339.937	26.0	3.27	-0.609	-7.221	nan	
5340.189	26.0	4.29	-2.229	-7.52	nan	
5340.447	24.0	3.44	-0.724	-7.262	nan	
5340.666	22.0	0.82	-3.174	-7.65	nan	
5341.033	26.0	1.61	-1.717	-7.68	nan	
5341.053	25.0	2.11	-5.671	-7.74	nan	
5341.070	21.0	1.94	3.341	0	nan	
5341.327	27.0	4.15	-0.424	-7.51	nan	
5341.489	22.0	3.06	-0.760	-7.58	nan	
5341.524	58.1	0.67	-5.088	0	nan	
5342.701	27.0	4.02	0.578	-7.51	nan	
5342.958	21.0	0.00	-2.439	-6.11	nan	
5342.969	19.0	1.61	-1.795	0	nan	
5343.380	27.0	4.03	0.024	-7.51	nan	
5343.438	26.0	4.37	-0.806	-7.51	nan	



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Putting everything together



python-based spectral synthesis package: github.com/MariaTsantaki/FASMA-synthesis yalm configuration file

	*config1.yml ×	
1	star1:	
2	<pre>linelist: FASMA-synthesis/FASMA/rawLinelist/linelist.lst</pre>	
3	teff: 5777	
4	logg: 4.44	
5	feh: 0.00	
6	vt: 1.0	
7	vmac: 3.21	
8	vsini: 1.90	
9	model: marcs	Au
LΘ	save: False	MV
11	plot: True	
12	plot_res: False	
L3	<pre>intervals_file: FASMA-synthesis/FASMA/rawLinelist/intervals.lst</pre>	
14 15	snr: null resolution: 115000	



Questions?





Credit to M. Bergemann





Pre-process the observed spectrum

• input format (fits, dat)



- input format (fits, dat)
- cosmetic improvements



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- wavelength re-sampling



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- χ^2 minimization (mpfit, Levenberg-Marquardt)
- initial conditions
- refine minimization options



- clean for bad/missing lines
- vmic: T_{eff}, log g, [Fe/H] (Tsantaki+ 2013, Mortier+ 20)
- vmac: T_{eff} (Valenti+ 2005MW

Pre-process the observed spectrum

- input format (fits, dat)
- cosmetic improvements
- wavelength re-sampling
- (local) normalization

Minimization process

- χ^2 minimization (mpfit, Levenberg-Marquardt)
- initial conditions
- refine minimization options
- fixed parameters



- log g: seismic, trigonometric
- vmic: T_{eff}, log g, [Fe/H]

(Tsantaki+ 2013, Mortier+ 2013)

- vmac: T_{eff} (Valenti+ 2005

2. How to derive stellar parameters Error analysis



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Correlations in parameters with the benchmark values $(\ensuremath{\mathsf{Tsantaki+2014}})$

Putting everything together!

	*config2.yml
1	star1:
2	<pre>linelist: FASMA-synthesis/FASMA/rawLinelist/linelist.lst</pre>
3	teff: 5777
4	logg: 4.44
5	feh: 0.0
6	vt: 1.0
7	vmac: 3.21
8	vsini: 1.90
9	model: marcs
.Θ	save: False
.1	element: False
.2	fix teff: False
.3	fix logg: False
.4	fix feh: False
.5	fix vt: True
6	fix_vmac: True
.7	fix vsini: False
8	plot: True
.9	plot_res: False
Θ	damping: 1
1	minimize: True
2	refine: refine
3	observations: FASMA-synthesis/FASMA/spectra/Sun_HARPS.fits
:4	<pre>intervals_file: FASMA-synthesis/FASMA/rawLinelist/intervals.lst</pre>
:5	snr: null
6	resolution: 115000



Questions?



3. How to derive chemical abundances

- Overall metallicity ([M/H]) is derived from all the elements in a region
- Individual chemical abundances ([EI/H]) are derived for a specific element
- Create a synthetic spectrum of a known star (T_{eff}, log g, [M/H], vmic, vmac, vsini) of the specific species
- [EI/H] is the only free parameter
- χ^2 minimization \rightarrow best-fit value
- Select from: Li, Na, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, and Ni



3. How to derive chemical abundances

Putting all together!

_	
1 st	arl:
2	linelist: FASMA-synthesis/FASMA/rawLinelist/linelist elements.lst
3	teff: 5777
4	logg: 4.44
5	feh: 0.0
6	vt: 1.0
7	vmac: 3.21
8	vsini: 1.90
9	model: marcs
10	save: False
11	element: Li
12	plot: True
13	plot res: False
14	damping: 1
15	minimize: True
16	observations: FASMA-synthesis/FASMA/spectra/Sun_HARPS.fits
17	<pre>intervals_file: FASMA-synthesis/FASMA/rawLinelist/intervals_elements.lst</pre>
18	snr: null
19	resolution: 115000



Questions?



- Line list of neutral (Fel) and ionized species (Fell)
- EW measurements (IRAF, daospec, ARES)
- Calculate [Fe/H] from the curve of growth
- Model atmospheres (MARCS, Kurucz)
- excitation balance of Fel lines → T_{eff} ionization balance of Fel and Fell lines → log g



Ingredients:

• Line list of Fe isolated lines



- EW measurements (IRAF, daospec, ARES)
- Calculate [Fe/H] from the curve of growth
- Model atmospheres (MARCS, Kurucz)
- excitation balance of Fel lines → T_{eff} ionization balance of Fel and Fell lines → log g



- Line list of Fe isolated lines
- EW measurements with ARES



- Calculate [Fe/H] from the curve of growth
- Model atmospheres (MARCS, Kurucz)
- excitation balance of Fel lines → T_{eff} ionization balance of Fel and Fell lines → log g



Ingredients:

- Line list of Fe isolated lines
- EW measurements with ARES
- Calculate [Fe/H] from the curve of growth: MOOG+MARCS



 excitation balance of Fel lines → T_{eff} ionization balance of Fel and Fell lines → log g



Ingredients:

- Line list of Fe isolated lines
- EW measurements with ARES
- Calculate [Fe/H] from the curve of growth: MOOG+MARCS
- excitation balance of Fel lines $\rightarrow T_{eff}$ *ionization* balance of Fel and Fell lines $\rightarrow \log g$



- Microturbulence: A(FeI) vs reduced EW (=log EW/λ)

- T_{eff} : Excitation Balance All abundances from Fe should agree for all excitation potentials

- log g: Ionization Balance Average $\log A$ obtained from differing ionization stages must fine agree



- EW measurements with ARES
- Calculate $[{\rm Fe}/{\rm H}]$ from the curve of growth: MOOG+MARCS
- excitation balance of Fel lines → T_{eff} ionization balance of Fel and Fell lines → log g





- EW measurements with ARES
- Calculate [Fe/H] from the curve of growth: MOOG+MARCS
- excitation balance of Fel lines → T_{eff} ionization balance of Fel and Fell lines → log g







www.iastro.pt/fasma



References

Books

 The Observation and Analysis of Stellar Photospheres, Gray D., Cambridge University Press, 2015

• Free packages for parameters

- SME (Valenti+ 1996)
- GALA (Mucciarelli+ 2013)
- FAMA (Magrini+ 2013)
- q2 (Ramirez+ 2014)
- iSpec (Blanco-Cuaresma+ 2014)
- fasma (Tsantaki+ 2018)
- StePar (Tabernero+ 2019)
- Radiative transfer codes
 - MOOG (Sneden+ 1973)
 - SYNTHE (Kurucz+ 1981)
 - SPECTRUM (Gray+ 1992)
 - Turbospectrum (Plez+ 2012)

- Model atmospheres
 - Kurucz (Kurucz+ 1999)
 - PHOENIX (Hauschildt+ 1997)
 - MARCS (Gustafsson+ 2008)
- Atomic data / Line lists
 - NIST (Kramida+ 2020)
 - VALD (Ryabchikova+ 2015)
 - Kurucz (Kurucz 1995)
 - Surveys: Gaia-ESO, ÁPOGEE
 - Specific for K-type (Tsantaki+ 2013)
 - Specific for M-type (Marfil+ 2021)
- Free packages for EWs
 - ARES (Sousa+ 2007)
 - DAOSPEC (Stenson+ 2008
 - VoigtFit (Krogager+ 201

Finally remarks

Things conviniently neglected:

- Non-LTE
- 3D hydrodynamics
- magnetic fields

- winds
- sphericity
- molecules

Don't use the codes as black boxes. Be patient... astronomers are not programers.







Your turn!

