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Europlanet Summer School 2023, Moletai, 8-18 Aug. 2023







# Machine Learning for stellar chemical composition Studies





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#### **Galactic Archaeology**

 $\rightarrow$  studying the formation and evolution of the Milky Way and it's local volume







 $\rightarrow\,$  Stellar chemistry in essential for Galactic Archaeology

 $\rightarrow$  Low-mass stars as fossil records of the interstellar medium



→ Chemical enrichment of the interstellar medium

#### → Stellar chemistry in essential for Galactic Archaeology

→ The Tinsley-Wallerstein diagram





Tinsley

George Wallerstein

#### → Stellar chemistry in essential for Galactic Archaeology

→ The Tinsley-Wallerstein diagram



#### Other types of elements:

- $\rightarrow \, \alpha$ -like: Ca, Ma, Ti, Si, O, Ne, S
- $\rightarrow$  Fe-peak: Z, Cu, Ni, Co, Fe, Mn, Cr, V
- $\rightarrow$  neutron-capture: Sr, Y, Zr, Ba, La, Ce, Pr, Sm, Eu, Gd, Dy, ...
- → Light: Li, B, Be, C, N
- $\rightarrow$  Odd-Z: Sc, K, Al, Na





#### The need for large spectroscopic surveys







>10<sup>4</sup> stars



10<sup>6</sup> stars



10<sup>5</sup> stars

>5x10<sup>5</sup> stars



>10<sup>6</sup> stars

>5x10<sup>6</sup> spec SDSS >10<sup>6</sup> stars



gaia

>10<sup>6</sup> stars



>5x10<sup>5</sup> stars



30x10<sup>6</sup> stars



>10<sup>6</sup> stars

Gaia: Gaia Collaboration, Vallenari et al. 2022 AMBRE/ESO: Guiglion et al. 2016 LAMOST: Zhang et al. 2021 Gaia-ESO: Romano et al. 2021 GALAH: Gao et al. 2020 APOGEE: Abdurro'uf et al. 2022 4MOST: de Jong et al. 2019 WEAVE: Jin et al. 2022 MSE: Bergemann et al. 2019 9 MOONS: Cirasuolo et al. 2020

- → Atmospheric parameters:
  - → Effective temperature T<sub>eff</sub>
  - → Surface gravity log(g)
  - → Overall metallicity [M/H]
- $\rightarrow$  Average abundance ratios
  - → For instance  $[\alpha/M]$  with  $\alpha$  goes for  $\alpha$ -elements (Mg, Si, Ca, O, Ti, Ne, S)
- → Individual chemical abundances
  - $\rightarrow$  [X/Fe] with X = {Mg, Si, Ti, Ni, Fe, Ba, Eu, ....}

Many other parameters, such as rotation, activity, mass, age ...

What type of stars are we interested in ?





→ Using stellar evolutionary models + magnitudes + parallaxes (distances)

- $\rightarrow$  Can measure T<sub>eff</sub>, log(g), [M/H]
- → StarHorse code: Queiroz et al (2018, 2020, 2023), Anders et al. (2019, 2022)

## How do we measure astrophysical quantities?

→ Using stellar spectra



## How do we form stellar absorption spectra ?



→ More on stellar spectroscopy:

- → D. F. Gray "The Observation and Analysis of Stellar Photospheres " (2021)
- $\rightarrow$  R. J. Rutten "Radiative Transfer in Stellar Atmospheres" (2003)

How do stellar spectra correlate with astrophysical parameters ?

→ Example: effective temperature



## How do we measure chemical abundances ?

 $\rightarrow$  One popular method: spectral fitting



Challenges to face: 1D vs 3D LTE vs. NLTE (Lind of al. 2009, Wang of al. 2021)

Low-res vs. High-res

Blends Rotation, Turbulence



To create model spectra, we need: Model atmosphere

# Radiative transfer code

+



More details on chemical abundance derivation:  $\rightarrow$  Jofré, Heiter, and Soubiran (2019)

## The impact of spectral resolution on abundance determination



- → Lower spectral resolution:
  - → Less clean spectral features to rely on
  - $\rightarrow$  Less elements to be measured
  - → Lower precision

## A few examples of spectral analysis codes

#### $\rightarrow$ Ispec

(Blanco-Cuaresma et al. 2014) https://www.blancocuaresma.com/s/iSpec

Download	
If you use iSpec, we thank you to cite these two articles: A&A (2014) and MNRAS (2019). Installation and usage Ask to be informed about updatest	
iSpec	Anite     Anite     Anites     Anites
Ispec is a too tor the treatment and analysis of stellar spectra. Some of the main functionalities for spectra treatment are the following: Cosmic rays removal Continuum comailaation Resolution degradation Radial velocity determination and correction Telluric lines identification Re-sampling	

#### Atmospheric parameters and chemical abundances.

Epec is capable of determining atmospheric parameters (i.e effective temperature, surface gravity, metallicity, micro/macroturbulence, rotation) and individual chemical abundances for AFGKM stars by using two different approaches: synthetic spectra fitting technique or equivalent widths method. Spec integrates MARCS and ATLAS model atmospheres together with the following radial transfer codes:

- SPECTRUM R. O. Gray
- Turbospectrum Bertrand Plez
- SME Valenti & Piskunov
- MOOG Chris Sneden
   Synthe/WIDTH9 Kurucz/Atmos

Python 3 powered automatized analyses.

The user-friendly interface is perfect for learning and testing. However, to take advantage of the full potential, iSpec can be used from Python 3. This is the recommended way to use iSpec for complex scientific studies, it ensures reproducibility and give access to a wider range of functionalities and options.

#### → MOOG (Sneden et al. 2012) https://www.as.utexas.edu/~chris/moog.html

#### MOOG

HOME | TEACHING | HALOSTARS | DISKSTARS | LABDATA | MOOG | SPECTRE | MISC

MOOG is a code that performs a variety of LTE line analysis and spectrum synthesis tasks. The typical use of MOOG is to assist in the determination of the chemical composition of a star. The basic equations of LTE stellar line analysis are followed, in particular using the formulation of F. N. Edmonds, Jr. (1969, JQSRT, 9, 1427). Much of the MOOG code follows in a general way the WIDTH and SYNTHE codes of R. L. Kurucz (see his web site: http://kurucz.harvaf.edu/). Below are instructions on downloading MOOG. If you have truble grabing or decoding the code please email me at chris@verdia.atvareas.edu.

The coding is in various subroutines that are called from a few driver routines; these routines are written in standard FORTRAN. The standard MOOG version has been developed on unix, linux and macintosh computers.

One of the chief assets of MOOG is its ability to do on-line graphics. This means that the plotting commands are given within the FORTRAN code. MOOG uses the graphics package SM, chosen for its ease of implementation in FORTRAN codes. Plotting calls are concentrated in just a few routines, and it should be possible for users of other graphics packages to substitute other appropriate FORTRAN commands.

The current MOOG release (November 2019) is the only code that is actively supported. See below for downloading instructions of this code.

Finally, financial support from the US National Science Foundation and NASA for many years in development of this code is gratefully acknowledged.

#### → Spectroscopy Made Easy (SME)

(Valenti & Piskunov 1996, Piskunov & Valenti 2017) https://www.stsci.edu/~valenti/sme.html

Home SME IDL				Jeff Valenti		
Spectroscopy Made Easy (SME) is IDL software and a compiled external library that fits an observed high-resolution stellar spectrum with a synthetic spectrum to determine stellar parameters. The original paper describing SME is Valenti & Piskunov (1996). Subsequent enhancements of the package are described in Piskunov & Valenti (2016).						
SME Releases						
	Version	Size	<b>Release Date</b>			
	574	1276 MB	2020-Feb-22			
	522	414 MB	2016-Jul-15			
	423	294 MB	2014-May-15			
	412	294 MB	2014-Mar-04			
	342	102 MB	2013-Mar-25			
	312	81 MB	2012-Oct-26			
Release 574 introduced a serious bug that caused SME to overestimate the concentration of several negative ions. This resulted in underestimated electron concentration, H <sup>-</sup> concentration, and H <sup>-</sup> opacity. This error is particularly serious for M dwarfs. A new version will be released soon. Release 574 includes automatic continuum matching, more non-LTE grids, improved UV continuous opacities, and additional methods for extracting information from the external library.						
Each release includes the <u>SME User Handbook</u> and an <u>SME tutorial</u> . Version 412 and later include a <u>technical note</u> that describes major changes to the way model atmosphere information is stored in SME structures. Each release includes the SME external library, compiled for Linux, OSX, and Windows systems.						

Atomic and molecular line data formatted for SME may be obtained from <u>VALD3</u>, which supersedes the <u>previous version</u> of VALD. SME understands extended van der Waals encoding, which is enabled in the VALD3 <u>unit selection configuration page</u>. SME can solve for empirical log(gf) and damping parameters, using an observed spectrum of a star (usually the Sun) as a constraint.

Using empirical line data for wavelength ranges 5164-5190 (Mg b triplet) and 6000-6180 Å, <u>Valenti & Fischer (2005)</u> obtained spectroscopic parameters for 1040 cool stars. Damping wings of the Mg b lines are a useful gravity constraint for dwarfs cooler than about 6200 K. Mass, radius, gravity, and especially age in Table 9 were revised shortly after publication when a software bug was fixed.

Take home messages:

- Chemical abundances and kinematics are essential for Galactic Archaeology studies

- The analysis of stellar spectra is the only way to get detailed and precise chemical abundances

- Large spectroscopic surveys are required (many stars, many Galactic components surveyed, as many elements as possible)

- Standard spectroscopic pipelines are essential algorithms but can be slow (few tens of spectra analysed per second)

- Data analysis challenge for on-going and future surveys (>10<sup>7</sup> stars)

A fantastic machine for Galactic Archaeology: The ESA *Gaia* space mission



 $\bigstar$ 



https://www.esa.int/Enabling\_Support/Operations/Gaia\_s\_biggest\_operation\_since\_launch

#### **Useful link:**

https://www.esa.int/Science\_Exploration/Space\_Science/Gaia



https://www.cosmos.esa.int/web/gaia/instruments



104.26cm Blue Photometer CCDs **Red Photometer CCDs** Wave Front Sensor Wave Front Sensor 42.35 cm **Radial-Velocity Spectrometer** Basic Angle Monito **CCDs** Basic Angle Star motion in 10 s **Sky Mapper Astrometric Field CCDs CCDs** Low-resolution Intermediate-**Position & Spectra** resolution **Brightness** (Blue & Red) spectra (abundances :))

## Focal Plane

#### **Useful link:**

https://www.cosmos.esa.int/web/gaia/payload-module





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→ 2 million stars per hours are measured !!

#### Content of Gaia DR3: tremendous amount of data

	# sources in Gaia DR3	# sources in Gaia DR2	# sources in Gaia DR1
Total number of sources	1,811,709,771	1,692,919,135	1,142,679,769
	Gaia Early Data Release 3		
Number of sources with full astrometry	1,467,744,818	1,331,909,727	2,057,050
Number of 5-parameter sources	585,416,709		
Number of 6-parameter sources	882,328,109		
Number of 2-parameter sources	343,964,953	361,009,408	1,140,622,719
Gaia-CRF sources	1,614,173	556,869	2191
Sources with mean G magnitude	1,806,254,432	1,692,919,135	1,142,679,769
Sources with mean G <sub>BP</sub> -band photometry	1,542,033,472	1,381,964,755	-
Sources with mean G <sub>RP</sub> -band photometry	1,554,997,939	1,383,551,713	-
	New in Gaia Data Release 3	Gaia DR2	Gaia DR1
Sources with radial velocities	33,812,183	7,224,631	-
Sources with mean G <sub>RVS</sub> -band magnitudes	32,232,187	2	
Sources with rotational velocities	3,524,677	-	-
Mean BP/RP spectra	219,197,643	-	-
Mean RVS spectra	999,645	-	-
Variable-source analysis	10,509,536	550,737	3,194

#### Gaia DR3 content:

https://www.cosmos.esa.int/web/gaia/dr3

#### Gaia DR3 papers:

https://www.cosmos.esa.int/web/gaia/dr3-papers

## Map of stellar magnitudes from Gaia's Early Data Release 3

GC



LMC SMC

https://www.esa.int/Science\_Exploration/Space\_Science/Gaia

**One major output of Gaia: parallaxes (and distances)** 



 $\rightarrow$  distance  $\approx$  1 / parallax

#### One major output of Gaia: parallaxes (and distances)

#### Estimating Distances from Parallaxes. V. Geometric and Photogeometric Distances to 1.47 Billion Stars in Gaia Early Data Release 3

C. A. L. Bailer-Jones<sup>1</sup>, J. Rybizki<sup>1</sup>, M. Fouesneau<sup>1</sup>, M. Demleitner<sup>2</sup>, and R. Andrae<sup>1</sup>

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<sup>2</sup> Astronomisches Rechen-Institut, Zentrum für Astronomie der Universität Heidelberg, Germany Received 2020 December 9; revised 2020 December 30; accepted 2020 December 31; published 2021 February 25



#### Gaia Rp, Rp spectra

 $\rightarrow$  220 millions spectra available

R~30-100 (De Angeli et al. 2022)



#### **Useful link:**

https://www.cosmos.esa.int/web/gaia/dr3-what-colour-do-they-have

Gaia RVS spectra → 1 million spectra available, R~11500 (Katz et al. 2022)



ESA/Gaia/DPAC/Observatoire de Paris-Meudon/Olivier Marchal & David Katz

Can we exploit in a homogeneous way Gaia spectra (RVS + BP/RP) magnitudes (G, Bp, Rp) and parallaxes for supercharged stellar parametrization?

→ Answer after 3 minutes break

→ Spoiler: yes. Method: modern techniques

# Modern == Machine techniques Learning

## The world of machine-learning

Supervised Learning			Unsupervised Learning		
Regression	Classification	Neural networks	Clustering	Dimensionality Reduction	
Linear Regression	Logistic Regression	Convolutional Neural Networks (CNN)	K-means	t-Distributed Stochastic Neighbor Embedding (t-SNE)	
K-Nearest Neighbors Regression (KNN)	K-Nearest Neighbors Classification (KNN)	Generative Adversarial Networks (GAN)	Gaussian Mixture Models (GMM)	Locally Linear Embedding (LLE)	
Random Forest Regression	Random Forest Classification	Long Short Term Memory Networks (LSTM)	Hierarchical Agglomerative Clustering (HAC)	Uniform Manifold Approximation and Projection (UMAP)	
Decision Tree Regression (CART)	Decision Tree classification (CART)	Gated Recurrent Units (GRU)	Density-Based spatial Clustering of Applications with Noise (DBSCAN)	Multidimensional Scaling (MDS)	
Support Vector Regression (SVR)	Support Vector Machines (SVM)	Feedforward Neural Networks (FFNN)		Principal Component Analysis (PCA)	
Multivariate Adaptive regression Splines (MARS)	Extreme Gradient Boosting (XGBoost)		<i>.</i>	Isomap Embedding	
	Gradient Boosted Trees				
	Naive Bayes	]			

Webb & Good 2023

#### $\rightarrow$ In the current talk, I will discuss only on Convolutional Neural-Networks

Why are we interested in Convolutional Neural Networks?

- Very versatile
- Allow to combine large datasets of different types
- Adapted for large datasets
- Allows to provide fast parametrization
- Able to learn from the noise in the data

## Basic concepts of Convolutional Neural-Networks (CNN)

 $\rightarrow\,$  Practical example: Cat and dog classification







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 $\rightarrow$  Practical example: Cat and dog classification





#### **Basic concepts of Convolutional-Neural Networks**



LeCun & Bengio 1995 Ciresan et al. 2011

#### **Basic concepts of Convolutional-Neural Networks**



LeCun & Bengio 1995 Ciresan et al. 2011

#### **Basic concepts of Convolutional-Neural Networks**

What is a neuron?

- $\rightarrow$  Computer representation of human neuron
- → "Perceptron"
- → Linear threshold function
- → First implemented on machine by in 1958 by Frank Rosenblatt



https://teksands.ai/blog/evolution-of-design-of-artificial-neuron



 $\rightarrow$  Training a CNN consists in adjusting the weights and biases of neurons in all layers, to minimize the loss function (mean squared error between truth and prediction)

#### **CNNs for stellar spectroscopy**

→ Example: Measuring temperature of the star











#### **CNN for stellar spectroscopy:**

Bailer-Jones et al. 1997 Leung & Bovy 2019 Fabbro et al. 2018 Zhang et al. 2019 Bialek et al. 2020

#### Our experience with CNNs and Gaia-like spectra

- $\rightarrow$  1st application of CNNs combining RAVE spectra, Gaia magnitudes, and parallaxes
- $\rightarrow$  Training set: 4000\* with labels from APOGEE DR16 (R~22000)
- $\rightarrow$  Transfer high-quality labels to low-resolution RAVE spectra (R~7500)



 $\rightarrow$  Such particular combination of data allows to break the spectral degeneracies inherent to RAVE spectra (and likely to be present in Gaia RVS spectra)



#### Chemical evolution of lithium with CNN from stellar spectra

- $\rightarrow$  Why is lithium important ?
  - $\rightarrow$  Chemical evolution of Li in the Milky Way still unclear (e.g. Guiglion et al. 2019)





→ CNN learns efficiently from relevant spectral features !!
 → CNN well suited for Li derivation (good insigths for next surveys like 4MOST)





#### Are we sure that CNN is not measuring abundance correlations ?

- $\rightarrow$  [Al/Fe] and [Mg/Fe] ratios are anti-correlated in Globular Clusters (e.g. Pancino et al. 2017)
- → Training set: 14637 stars with Gaia-ESO spectra. Labels: T<sub>eff</sub>, log(g), [Fe/H], [AI/Fe], [Mg/Fe]



→ We know how to properly use CNNs for abundance measurements



M. Ambrosch

#### Analysis of the 1 million Gaia RVS-spectra with CNNs

# Beyond Gaia DR3: tracing the $[\alpha/M] - [M/H]$ bimodality from the Inner to the outer Milky Way disc with Gaia RVS and Convolutional Neural-Networks

G. Guiglion<sup>1</sup>, S. Nepal<sup>2,3</sup>, C. Chiappini<sup>2</sup>, S. Khoperskov<sup>2</sup>, G. Traven<sup>4</sup>, A. B. A. Queiroz<sup>2</sup>, M. Steinmetz<sup>2</sup>,
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R. Sordo<sup>5</sup>, S. Fabbro<sup>11</sup>, I. Minchev<sup>2</sup>, G. Tautvaišienė<sup>12</sup>, Š. Mikolaitis<sup>12</sup>, J. Montalbán<sup>13</sup>

#### Analysis of the 1 million Gaia RVS-spectra with CNNs

Motivations and goals:

- $\rightarrow\,$  Use homogeneously the full Gaia data product
- → Provide more precise and accurate atmospheric parameters and abundances than the standard Gaia spectroscopic pipeline (GSP-Spec)





 $\rightarrow$  Set the machine-learning path for Gaia data analysis (DR4 in 2025, DR5 in 2027)

→ Provide robust chemical estimates for low-S/N spectra (300000 spectra with 15<S/N<25 !!!!)

Analysis of the 1 million Gaia RVS-spectra with CNNs

- $\rightarrow$  Labels we aim at deriving: T<sub>eff</sub>, log(g), [M/H], [\alpha/M], [Fe/H]
- → Building a robust training set



Knowledge transfer from high-quality high-res APOGEE labels to intermediate-res RVS

(dex) v

log(g)

5

**gaia** R~11000



#### A hybrid Convolutional Neural-Network for Gaia-RVS analysis



 $\rightarrow$  CNN combines *Gaia* G, Bp, **Rp** magnitudes, Parallaxes, **RVS spectra, and XP data** 

 $\rightarrow$  Labels derived: T<sub>eff</sub>, log(g), [M/H], [α/M], [Fe/H]

 $\rightarrow$  Prediction time 4 labels in 3300 stars / second

 $\rightarrow$  Deep ensemble approach to derive uncertainties.

Layers

ů

#### Robust estimates of T<sub>eff</sub>, log(g), [M/H] for 690000 Gaia stars

Guiglion, Nepal et al. 2023



 $\rightarrow$  By adding magnitudes, parallaxes and XP data, CNN is able to break spectral degeneracies in Gaia RVS spectra.

#### Robust estimates of T<sub>eff</sub>, log(g), [M/H] for 690000 Gaia stars

Guiglion, Nepal et al. 2023



 $\rightarrow$  By adding magnitudes, parallaxes and XP data, CNN is able to break spectral degeneracies in Gaia RVS spectra.

 $\rightarrow$  CNN results are as good as the training set can be.

Are we really breaking the RVS degeneracies by using mag., parallaxes and XP data?

→ Test: Training CNN only using RVS spectra (no mags, no parallaxes, no XP)



Are we really breaking the RVS degeneracies by using mag., parallaxes and XP data?

→ Test: Training CNN only using RVS spectra (no mags, no parallaxes, no XP)



 $\rightarrow$  Hard for CNN to differentiate between cool dwarfs and cool giants (same for GSP-Spec)

 $\rightarrow$  Large uncertainties for >75% of the sample

 $\rightarrow$  Thus, combining spectra, magnitudes, parallaxes, and XP data is required for precise and accurate parametrization

#### How does CNN compare to Gaia GSP-Spec (standard spectroscopy) for halo stars ?



 $\rightarrow$  CNN provides precise and accurate labels down to [M/H]=-2.4 dex

# Guiglion, Nepal et al. 2023

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#### **CNN uncertainties**



→ We provide realistic uncertainties thanks to a deep ensemble approach

#### How does CNN gravities compare to precise asteroseismic ages ?

- → Asteroseismology relies on stellar oscillations (Chaplin & Miglio 2013)
- → Widely used for validation purposes (eg. in RAVE; Valentini et al. 2017)
- $\rightarrow$  We use here Zinn et al. (2022) asteroseismic data for validation



 $\rightarrow$  We selected giants, to probe large distances, and limit possible systematics  $\rightarrow$  147416 stars

→ Galactic radius and Height adopted from Nepal et al. In prep. (using StarHorse distances).



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 $\rightarrow$  Studying the chemical abundance pattern [ $\alpha$ /M] vs. [M/H] as function of R and Z





## Last take home messages:

- Convolutional Neural-Networks (CNN) are well suited for stellar parametrization
- CNN parametrization is mainly reliable within the training sample limits
- Modern techniques are essential for providing training sample labels
- CNN parametrization is fast and robust (several 10<sup>3</sup> stars per second)
- The training sample should be built in a pro-active way
- Future spectroscopic surveys will strongly benefit from such algorithms

#### An example of future spectroscopic survey: 4MOST

- → Survey description: de Jong et al. 2019
- $\rightarrow$  Survey strategy: Guiglion et al. 2019
- $\rightarrow$  MW Halo surveys: Helmi et al. 2019, Christlieb et al. 2019
- → **MW Disc and bulge surveys:** Chiappini et al. 2019, Bensby et al. 2019
- $\rightarrow$  Magellanic clouds: Cioni et al. 2019



>20 elements to be measured at R=5000



4MIDABLE-LR ESO proposal 2020

→ CNN is currently one of the tested ML algorithm for the 4MOST Galactic pipeline



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4MIDABLE-LR ESO proposal 2020