Deep Learning application for stellar parameters determination: II- Application to observed spectra of AFGK stars

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Abstract: In this follow-up paper, we investigate the use of Convolutional Neural Network for deriving stellar parameters from observed spectra. Using hyperparameters determined previously, we have constructed a Neural Network architecture suitable for the derivation of $T_{\text{eff}}$, $\log g$, $[M/H]$, and $v_e \sin i$. The network was constrained by applying it to databases of AFGK synthetic spectra at different resolutions. Then, parameters of A stars from Polarbase, SOPHIE, and ELODIE databases are derived as well as FGK stars from the Spectroscopic Survey of Stars in the Solar Neighbourhood. The network model average accuracy on the stellar parameters are found to be as low as 80 K for $T_{\text{eff}}$, 0.06 dex for $\log g$, 0.08 dex for $[M/H]$, and 3 km/s for $v_e \sin i$ for AFGK stars.

Keywords: methods: data analysis, methods: statistical, methods: deep learning, techniques: spectroscopic, stars: fundamental parameters.

1 Introduction

Artificial Intelligence (AI) is becoming a vital tool in science due to its automation capabilities and its capacity to handle large amounts of data. In the context of astronomy, a subset of AI, Machine and Deep Learning (ML and DL) are used extensively for ground-based and sky surveys (Baron 2019). In our previous work, Gebran et al. (2022) (hereafter referred to as Paper I), we constructed a Deep Neural Network (DNN) in order to derive stellar parameters such as: effective temperature ($T_{\text{eff}}$), surface gravity ($\log g$), metallicity ($[M/H]$), and the projected equatorial rotational velocity ($v_e \sin i$) for B and A stars.

In Paper I, we constrained most of the hyperparameters utilized in the construction of the Neural Network (NN) in order to insure that the best accuracy for deriving stellar labels could be achieved. Many tools and techniques are being developed to derive the fundamental parameters of stars and most of them are either based on statistical or ML/DL approaches. A thorough list of the most updated studies can be found in the introduction of Paper I. Recently, Li et al. (2022b) used a combination of Least Absolute Shrinkage and Selection Operator (LASSO) and Multi-layer Perceptron (MLP) methods to estimate stellar atmospheric parameters from the Large Sky Area Multi-Object Fiber Spectroscopic Telescope (LAMOST) DR8 low-resolution spectra. Straumit et al. (2022) presented a spectral analysis algorithm, ZETA-PAYNE, developed to obtain stellar labels from SDSS-V spectra of stars of OBAF spectral types using machine learning tools. Li et al. (2022a) applied a ML technique, the Gaussian Process (GP) regression, to turn a sparse model grid into a continuous function. They also used the GP regression to determine the age and mass of stars. Kjaersgaard et al. (2021) presented a neural network autoencoder approach for extracting a telluric transmission spectrum from a large set of high-precision observed solar spectra from the The High Accuracy Radial Velocity Planet Searcher (HARPS-N) radial velocity spectrograph. Hu et al. (2022) presented a data-driven method based on long short-term memory (LSTM) neural networks to analyze spectral time series of Type Ia supernovae (SNe Ia). Their method allows for accurate reconstruction of the spectral sequence of an SN Ia based on a single observed spectrum around maximum light. More recently, Xiong et al. (2022) presented a Residual Recurrent Neural Network (RRNet) to extract spectral information, and estimate stellar atmospheric parameters.
along with 15 chemical element abundances for medium-resolution spectra from LAMOST.

Most of the automated techniques that are found in the literature deal with the derivation of the fundamental parameters \((T_{\text{eff}}, \log g, [M/H])\) without considering \(v_c \sin i\). Rotational profiles are usually found by applying transformations such as the Fourier Transform (FT, Zorec and Royer, 2012) or using rotational laws (Zorec et al., 2017). In our previous studies (Aydi et al., 2014; Gebran and Royer, 2012) or using rotational laws (Zorec et al., 2017), we have derived \(v_c \sin i\) using line profile fitting.

In this work, we complement the study of Paper I by using its best combination of hyperparameters to find the best NN architecture. The foremost purpose of our study is to develop a consistent model that is capable of predicting accurate and precise stellar parameters which is a guiding starting point to most stellar physics projects. Of course other sources of uncertainties can affect the predicted results when applied to real observations as will be discussed in this paper. Once the architecture and parameters are set, our technique is then applied to AFGK observed spectra (Gebran et al., 2016, 2014) and conclusion can be found in Sec. 6.

The construction of the training databases is explained in Sec. 2. The pre-processing steps are detailed in Sec. 3. The application of the method to AFGK stars is found in Secs. 4. The discussion and conclusion can be found in Sec. 6

2 Training Databases

A grid of 12 training databases was constructed for the purpose of this study. Other than modifying the stellar labels \((T_{\text{eff}}, \log g, [M/H], v_c \sin i)\), we have constructed a series of grids with the same range of stellar labels but at different resolving power. The purpose is to analyse the effect of resolution on the accuracy of the derived stellar label and to check the capability of our technique when applied to low, medium, and high resolution spectrometers.

We have followed the same strategy as in Paper I. We have first calculated a series of ATLAS9 (Kurucz, 1992) model atmospheres using the opacity distribution function of Castelli and Kurucz (2003) and with a mixing length parameter of 0.5 for 7000 K \(\leq T_{\text{eff}} \leq 8500\) K, and 1.25 for \(T_{\text{eff}} \leq 7000\) K (Smalley, 2004). Using SYNSPEC48 (Hubeny and Lanz, 1991), we have calculated synthetic spectra for AFGK stars. We ended up, for each resolving power, with a grid of 80,000 synthetic spectra with parameters ranging randomly between the values described in Tab. 1. We have used the same line list as the one used in Paper I. The wavelength range was selected to be between 4450 and 5400 Å. This wavelength range is indeed very sensitive to all stellar parameters in the spectral range of AFGK stars (Paletou et al., 2015; Gebran et al., 2016, 2014). A example of the calculated spectra for different resolving powers is displayed in Fig. 1

3 PCA for Pre-processing

Before applying the NN to the training database, a dimension reduction technique is applied. This step consists in reducing the size of the spectra from a sampling size of \(N_\lambda\) to \(n_k \times N_\lambda\). Depending on the resolving power, \(N_\lambda\) ranges between 4750 to 19000 data points. The \(n_k\) reduced data points are found by projecting the flux of each spectrum onto the first 50 Principal Components (PC). Technically, we apply this Principal Component Analysis (PCA) on the training database and we find the eigenvectors \(\phi_k(\lambda)\) of the variance-covariance matrix \(C\):

\[
C = (M - \bar{M})^T \cdot (M - \bar{M}),
\]

where the training database \(M\) is a \(N_{\text{spectra}} \times N_\lambda\) matrix containing the fluxes of the synthetic spectra. The value of \(n_k\) is found by analyzing the reconstructed error (Gebran et al., 2022). Having \(n_k=50\) reduces the mean reconstructed error to a value less than 0.5%. As a similar technique to PCA, one could also use the encoder part of an autoencoder in order to reduce the dimensionality of the database (Kjaersgaard et al., 2021). We have chosen PCA to be consistent with our previous findings in Gebran et al. (2016) and Gebran et al. (2022).

4 Deep Learning

We start by applying data augmentation as a regularization technique to all the training databases (see Sec. 4.1.1
Table 1. Ranges of the parameters used for the calculation of the training databases. The 3rd column displays the steps in the parameter range. Note that the steps in $T_{\text{eff}}$ and $\log g$ are the steps in ATLAS9 model atmospheres. Many databases were constructed for different resolving power ranging from 1000 to 115000. Random steps means that there is no restriction on the number selection.

| Parameters       | Range         | Step       |
|------------------|---------------|------------|
| $T_{\text{eff}}$ (K) | [4000,11000]  | 50         |
| $\log g$ (dex)   | [2.0,5.0]     | 0.05       |
| $[M/H]$ (dex)    | [-1.5,1.5]    | random     |
| $v_{e} \sin i$ (km s$^{-1}$) | [0,300] | random     |
| $\lambda$ (Å)   | 4450-5400     | $\lambda$ |
| Resolving Power  |               |            |

Fig. 1. Sample of synthetic spectra calculated with different stellar parameters and spectral resolutions. These noise free spectra are normalized to the local continuum.

of Paper I for technical explanations). This is done in order to take into account the noise in the real observed spectra as well as considering some modifications that could occur in the shape of the observed spectra due to a bad normalization or inappropriate data reduction. Every spectrum (including the augmented ones) in each database is represented by 50 data points and they correspond to a specific $T_{\text{eff}}$, $\log g$, $[M/H]$, and $v_{e} \sin i$. This is true at all resolving powers. A NN is then used to link these data points to their corresponding labels. Four different NNs were built, one for each stellar label ($T_{\text{eff}}$, $\log g$, $[M/H]$, $v_{e} \sin i$).
The initializers, optimizers, learning rates, dropout fraction, pooling layers, activation functions, loss functions, epochs, and batches are constrained according to the methodology of Paper I. These network parameters were derived for every network architecture tested in this work.

4.1 Architecture

An infinite number of architectures could be applied to our purpose. The main goal is to find the most accurate transformation between the matrix of spectra coefficients (the 50 projected ones) and the labels. The best architecture will be selected according to its simplicity (size and calculation time) and to the accuracy of the results.

Fully dense NNs, Convolutional Neural Networks (CNN), and a combination of both were tested for each stellar label. In each case we have iterated on the number of layers, number of neurons in each layer, and the size of the filters in case of CNNs. As explained previously, network parameters were derived for each NN.

For every network and every resolving power, each augmented database was divided in 70% for training, 20% for validation, and 10% for testing. Gaussian signal to noise ratio (SNR) was selected randomly between 5 and 300 and applied to each spectrum of the 10% test spectra in order to check the accuracy of the technique on noisy data.

All our calculations are performed using the open-source programming language, Python, specifically with the Keras\(^4\) interface on the TensorFlow\(^3\). We have used the KerasTuner\(^5\) package (O’Malley et al., 2019), a scalable hyperparameter optimization framework that solves the pain points of hyperparameter search. It was used to derive the optimized number of layers as well as the filter sizes in case of CNNs. Linking the number of layers and dimension of the filters with the size of the database as well as the size of each spectrum in the database is not an easy task. In order to avoid over- and under-fitting, these two parameters should be optimized. KerasTuner helps in that regard and avoids the hassle of the time consuming trial and error phase.

After iterating the architecture shape and deriving the optimized parameters for each network, the result was a unique architecture that is applicable to all stellar parameters. Figure\(\^2\) shows the architecture of NN for deriving \(T_{\text{eff}}\). This architecture is similar for predicting \(\log g\), \([M/H]\), and \(v_e \sin i\). Although the four parameters are predicted with networks having similar architecture, these models differ in the activation function, the kernel initializer, the loss function, the optimizer, the dropout fraction, the epochs and the batches number (Gebran et al., 2022). The adopted values for the network parameters are derived using the technique explained in Paper I. These parameters are summarized in Tab.\(\^2\).

4.2 Resolution Effect

Spectroscopic surveys are based on instruments that have different resolving power. For that reason, we have applied our technique to different databases that are similar in parameter ranges (Tab.\(\^1\), except for the resolving power. Our tests contain spectra having a low resolution down to 1000 and a high resolution up to 115,000.

Once the networks are trained using the 70% of the data, we have derived the accuracy on the parameters for the validation, test, and noisy test data. The best accuracy reached as a function of the resolution are displayed in Fig.\(\^3\). For each stellar label, the derived accuracy for the noisy test data is representative of the error bar that should be assigned to observed spectra. For example, analyzing spectra at a resolving power of 50,000, the equatorial projected rotational velocity should be assigned and error \(\sigma_{v_e \sin i} \sim 2.5\) km/s. The subscript \(m\) corresponds to the fact that this is model related. For a resolving power larger than 5000, the accuracy’s are always in the same order and their average is 80 K for \(T_{\text{eff}}\), 0.06 dex for \(\log g\), 0.08 dex for \([M/H]\), and 3 km/s for \(v_e \sin i\).

5 Application to Observed Spectra

After the four networks were applied to synthetic data and the architecture and parameters found, we used them to predict the stellar parameters from observed spectra. We used well studied AFGK stars observed with different instruments at different resolution. Applying the predictions to observed spectra assumes that the radiative transfer code is able to produce synthetic spectra similar to the observed ones using the specific stellar parameters. We have shown in previous studies (Gebran et al., 2016; Kassounian et al., 2019) that SYNSPEC48 was able to reproduce spectra of AFGK stars with good accuracy but other reliable synthetic spectra codes could be used.
if needed. We can mention the PHOENIX models (Husser et al., 2013) that are well suited for stars having $T_{\text{eff}} \leq 12000$ K or TURBOSPECTRUM (Plez 2012) with all the molecular data that is used for giants and dwarfs stars.

For the A stars, we used the list of Gebran et al. (2016) and selected the ones that have the most values published in the literature. We ended up with 89 observed A stars with more than 9 values for $T_{\text{eff}}$ in the the Vizier catalog. These A stars were observed with NARVAL and ESPaDOnS high-resolution spectropolarimeters and having a spectral resolving power of 65000 in polarimetric mode and 76000 when used for spectroscopy. These spectra were retrieved from PolarBase (Petit et al., 2014), a high resolution spectropolarimetric stellar observations database. Another part of the A stars spectra were observed with ELODIE (Baranne et al., 1996) and SOPHIE (Perruchot et al., 2011) spectrographs with a resolving power of 42000 and 75000, respectively. Details about the observations can be found in Gebran et al. (2016) and Kassoumian et al. (2019). For the FGK stars, we have selected the ones that have more than 20 different parameters. To estimate the accuracy of our results, we used a weighted mean approach similar to the one described in Gebran et al. (2016). Quantitatively, and in order to give more weight to the catalogued values that have a large number of occurrence and a small spread in values, the dispersion and it corresponding standard deviation for a stellar parameter $X$ are calculated as follows:

$$\Delta X = \frac{\sum_i w_i (X_{\text{prediction}} - X_{\text{median}})}{\sum_i w_i}$$



### 5.1 AFGK Stars

Predicted stellar parameters are depicted in Tabs. 4 and 5 in the appendix. In these tables, the stellar parameters are represented with the median and closest values retrieved from Vizier catalogues using astroquery (Paletou and Zolotukhin 2014). Figure 4 shows the predicted effective temperature of a sample of stars as well as the range in the effective temperatures retrieved from the catalogues (box-plots) and the median. The selection of these stars was based on the number of values found in the literature. For A stars, we have selected the ones that have more than 20 different values in Vizier. As for FGK stars, we did the same with stars having more than 100 independent literature values for $T_{\text{eff}}$. Figures 5 to 7 are similar to Fig. 4 but for log $g$, $[M/H]$, and $v_\text{r} \sin i$. A stars in Fig. 5 have more than 10 catalogued values for log $g$ and F stars have more than 50. For $[M/H]$ and $v_\text{r} \sin i$, we have chosen the A stars that have more than 10 catalogued values for these two parameters. For FGK stars, we have selected the ones having more than 50 and 15 values for $[M/H]$ and $v_\text{r} \sin i$, respectively.

A large spread exists in the literature values for all parameters. To estimate the accuracy of our results, we used a weighted mean approach similar to the one described in Gebran et al. (2016). Quantitatively, and in order to give more weight to the catalogued values that have a large number of occurrence and a small spread in values, the dispersion and it corresponding standard deviation for a stellar parameter $X$ are calculated as follows:

$$\Delta X = \frac{\sum_i w_i (X_{\text{prediction}} - X_{\text{median}})}{\sum_i w_i}$$

#### Table 2. Set of parameters used for the 4 networks, for deriving $T_{\text{eff}}$, log $g$, $[M/H]$, and $v_\text{r} \sin i$. These parameters are derived using the technique explained in Paper I.

| Parameter          | $T_{\text{eff}}$ | log $g$ | $[M/H]$ | $v_\text{r} \sin i$ |
|--------------------|-----------------|---------|---------|-------------------|
| Kernel initializer | he_normal       | he_normal| Random Uniform | he_uniform           |
| Loss function      | mean squared logarithmic error | mean squared logarithmic error | Random Uniform | mean squared error |
| Optimizer          | Adam            | Adamax  | Adam    | Max                |
| Epochs             | 350             | 75      | 75      | 75                |
| Batch              | 128             | 128     | 32      | 64                |
| Activation function| Relu            | tanh    | tanh    | tanh              |
| Dropout fraction   | 0.3             | 0.3     | 0.2     | 0.3               |

6 [https://astroquery.readthedocs.io](https://astroquery.readthedocs.io)
7 [https://arxiv.org/abs/1408.7026](https://arxiv.org/abs/1408.7026)
Fig. 2. Neural Networks architecture used in this study. The parameters displayed in this model are the ones used for predicting $T_{\text{eff}}$, $\log g$, $[M/H]$, and $v_{\text{sini}}$ are predicted with networks having the same architecture but different parameters as shown in Tab. 2. Explanations about the kernel and bias dimensions can be found in Wu (2017).

where

\[ w_i = \frac{1}{\text{IQR}_i} \]

Fig. 3. Derived accuracy for $T_{\text{eff}}$, $\log g$, $[M/H]$, and $v_{\text{sini}}$ as a function of the resolving power. We present the accuracy’s for the training data (triangles), the validation (squares), test (triangles tilted right), and noisy test (circles) data.
Fig. 4. Comparison between our predicted effective temperatures (stars), and the values we obtained from available Vizier catalogues. The catalogued values are represented as classical boxplots. Objects we studied are listed along the horizontal axis. The horizontal bar inside each box indicates the median (Q2 value), while each box extends from first quartile, Q1, to third quartile Q3. Extreme values, still within a 1.5 times the interquartile range away from either Q1 or Q3, are connected to the box with dashed lines. Outliers are denoted by a “o” symbol.

\[ \text{IQR}_i = \text{Q3} - \text{Q1} \]

IQR\(_i\) being the interquartile range defined as the difference between the third and first quartile of each set of values. The standard deviation is calculated as:

\[ \sigma_X = \sqrt{\frac{\sum_i w_i (X_{\text{prediction}} - X_{\text{median}})^2}{\sum_i w_i}} \]

Stars having only one catalogued value for a specific parameter were not considered in the calculation of the dispersion. The results of the dispersion as well as the standard deviations are displayed in Tab. 3. Catalogued values are all coming from different sources and each author uses a different technique (photometry, spectroscopy, spectrophotometry, asteroseismology, ...). This leads to a
Table 3. Dispersion and standard deviation for the comparison between our predicted parameters and the catalogue values. The last two rows deal with a limited catalogued sample, the one used to plot Figs. 4 to 7.

| $T_{\text{eff}}$ (K) | $\log g$ (dex) | $[M/H]$ (dex) | $v_c \sin i$ (km/s) |
|---------------------|----------------|---------------|---------------------|
| $\Delta$            | 160            | 0.40          | 0.15               | 12                  |
| $\sigma$            | 300            | 0.55          | 0.35               | 15                  |
| $\Delta_{\text{lim}}$ | 150            | 0.01          | 0.04               | 3.0                 |
| $\sigma_{\text{lim}}$ | 250            | 0.15          | 0.14               | 5.5                 |

6 Discussion and Conclusion

Two sources of errors should be assigned to the predicted stellar parameters. One relates to the model (i.e., parameter_m, see Sec. 4.2) and the other relates to how close the radiative transfer code (i.e., SYNSPECTRE, parameter_rt) represents the observations. $\sigma_{\text{parameter_m}}$ can be derived using a list of well studied stars with well established stellar parameters over a wide range in the HR Diagram. It is beyond the scope of this study, but we should be aware that this source of error could be wavelength dependent as each radiative transfer code uses a different line list with different atomic data.

Model (i.e., NN) and radiative transfer errors are independent and can be added in quadratic manner to find the total accuracy that we found in Sec. 5.1:

$$\sigma_{\text{parameter, total}} = \left( \sigma_{\text{parameter_m}}^2 + \sigma_{\text{parameter_rt}}^2 \right)^{\frac{1}{2}}$$

While comparing with the median values from literature, we found that $T_{\text{eff}}$ is derived with an accuracy of 150 K, $\log g$ with 0.01 dex, $[M/H]$ with 0.04 dex, and $v_c \sin i$ with 3.0 km/s. Some of these deviations are smaller than the errors found in the model (80 K for $T_{\text{eff}}$, 0.06 dex for $\log g$, 0.08 dex for $[M/H]$, and 3.0 km/s for $v_c \sin i$), but one should consider the accuracy of the model as a minimum limit for the stellar parameters and then calculate the total accuracy depending on the radiative transfer code specificity.

We have used a large range of spectral type and found acceptable values for the accuracy. One could use a combination of stellar library with synthetic data adapted for each spectral type and luminosity range or a large database of observed stars with accurate stellar parameters. However, NN prove to be a fast (refer to Paper I for computational time) and accurate way to derive stellar parameters and can handle a large amount of data. These results are very promising as they are less than the accuracy that are usually found with photometric techniques or spectroscopic ones or a combination of both.

In a future work, we will be testing the effect of specific spectral region on the stellar parameters. This will be done through autoencoders, a type of unsupervised learning technique, leading to a more "intelligent" and compact database construction.

One straightforward application is the use of such a network in order to derive the stellar parameters of
Gaia spectra (Gaia Collaboration et al. 2016). The radial velocity spectrometer (RVS, Cropper et al. 2018) on board of Gaia will deliver medium resolution spectra (R~11000) in the CaII triplet region (λ ranging from 8470 to 8710 Å). Several millions of stars have their spectra available during the Data Release 3 (DR3, Gaia Collaboration et al. 2022; Frémat et al. 2022).

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Gaussian Process Regression: augmenting stellar model grid. 

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Table 4: Predicted values for $T_{\text{eff}}$, log $g$, [M/H], and $v_c \sin i$ for A stars with the median and closest values from Vizier catalogue.
