Evaluation of data compression techniques for the inference of stellar atmospheric parameters from high resolution spectra

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ABSTRACT

We evaluate the utility of several data compression techniques for alleviating the curseof-dimensionality problem in regression tasks where the objective is to estimate stellar atmospheric parameters from high resolution spectra in the 4000-8000 K range. We conclude that Independent Component Analysis (ICA) performs better than the rest of the techniques evaluated for all compression ratios. We also assess the necessity to adapt the signal-to-noise ratio (SNR) of the training set examples to the SNR of each evaluation spectrum and conclude that within the conditions of our experiments, at most only two such models are needed (in the case of regression models for effective temperatures, those corresponding to SNR=50 and 10) to cover the entire range. Finally, we also compare the prediction accuracy of effective temperature regression models for increasing values of the training grid density and the same compression techniques.

Key words: methods: statistical – methods: data analysis – stars: fundamental parameters – methods: data compression

INTRODUCTION

The rapid evolution of astronomical instrumentation and the implementation of extensive surveys have permitted the acquisition of vast amounts of spectral data. The reduction and management of large spectral databases collected by largearea or all-sky surveys like Gaia/Gaia-ESO (Jordi et al. 2006; Gilmore et al. 2012), RAVE (Steinmetz et al. 2006), or APOGEE (Eisenstein et al. 2011) require the use of automatic techniques for the consistent, homogeneous, and efficient extraction of physical parameters from spectra. The 10 availability of these huge databases opens new possibilities to better understand the stellar, Galactic, and extra-galactic astrophysics. Of special importance is the determination of intrinsic stellar physical parameters, such as effective temperature (T_{eff}) , surface gravity (log g), metallicity ([M/H]) and alpha to iron ratio ($[\alpha/Fe]$). However, the difficulty that atmospheric parameter estimation poses comes from the inherent size and dimensionality of the data. That is, the number of measured wavelengths in a single spectrum, which is the number of variables or dimensions of a dataset, is high as compared to the number of spectra or set of instances in the dataset. Thus, regression from stellar spectra suffers the so-called curse of dimensionality problem because the number of variables is much higher than the number of instances used to fit a regression model.

The curse of dimensionality (Bellman 1961) relates to the problem caused by the exponential increase in volume associated with adding extra dimensions to a mathematical space. When the number of data instances (set of spectra) is finite and the dimensionality (number of measured wavelengths in a single spectrum) increases, the volume of the space of independent variables increases so fast that it is not possible to ensure that there are several instances (spectra) with each combination of possible values that each dimension (measured wavelength) could have. That is, the density of data instances in the space decreases exponentially as the dimensionality increases. In other words, the available data become sparse. Because this sparsity is problematic for any method that requires statistical

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significance, the amount of data instances needed to support
the result often grows exponentially with the dimensionality
in order to obtain a statistically sound and reliable outcome.

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Furthermore, typical spectra obtained in many surveys 107 do not regularly reach the high signal-to-noise ratios (SNR) 108 —about 100 or greater — needed to obtain robust estimates, 109 which increases the difficulty to accurately estimate the 110 physical parameters of spectra. In summary, stellar spectra are high dimensional noisy vectors of real numbers and 112 thus, regression models must be both computationally efficient and robust to noise.

There are several ways to alleviate this so-called curse of 115 dimensionality. It is evident that not all wavelength bins in 116 an observed spectrum carry the same amount of information 117 about the physical parameters of the stellar atmosphere. One 118 way to reduce the dimensionality of the space of indepen- 119 dent variables is to concentrate on certain wavelength ranges 120 that contain spectral lines that are sensitive to changes in 121 the physical parameters. Before large-scale spectroscopic 122 surveys and the fast computers needed to analyse 123 them became available, astronomers derived physical pa- 124 rameters by interactively synthesizing spectra until a subjec- 125 tive best fit of the observed spectrum in certain spectral lines 126 was found. But the number of spectra made available to the 127 community in the past decades have made this manual and 128 subjective (thus irreproducible) fitting procedure impractical. Automatic regression techniques have therefore become a necessity.

The next step consisted in using derived features of the 132 spectrum such as fluxes, flux ratios or equivalent widths to infer the parameters via multivariate regression techniques 134 (see Allende Prieto et al. 2006; Rojas-Ayala et al. 2010, 2012; 135 Bruntt et al. 2010; or Mishenina et al. 2006). That way, 136 we significantly reduce the full spectrum to a much smaller 137 number of independent variables, at the expense of introducing a feature extraction process: defining a continuum 139 level and normalizing the observed spectrum in the wavelength region that contains the sensitive spectral feature. 141 The normalization process effectively consists in dividing two random variables: the observed flux and the estimated continuum level. The simplest hypoth- 144 esis consists in assuming that both quantities are 145 Gaussian distributed. Under these conditions, the 146 normalized spectrum will be a collection of random 147 variables (one per wavelength) each one distributed 148 according to the ratio distribution (see e.g. Geary 149 1930; Marsaglia 1965). Even in the best case that the 150 continuum flux is Gaussian distributed around a value significantly different from zero, the ratio distribution is asymmetric (thus systematically biasing the result) and has a heavy right tail (meaning that values significantly larger than the mode of the distribution can occur with non-negligible probabilities). In the cases of low signal-to-noise spectra, the situation can be catastrophic.

The potential dangers associated with the feature extraction in restricted wavelength ranges via continuum normalisation can be mitigated by projecting the observed spectra onto bases of functions spaces such as in the wavelet or Fourier decompositions (see Manteiga et al. 2010; Lu 62 & Li 2015; or Li et al. 2015, for examples of the two approaches). In essence, the goal is to change the representation of the spectra, originally involving a large

number of variables (measured wavelengths), into a low-dimensional description using only a small number of variables (dimensions). The new representation should preserve essentially all of the useful information within the high dimensional space. Thus, by retaining only the most significant variables (dimensions) to represent the spectra, we achieve a data compression that can be of great benefit for estimating atmospheric parameters as it reduces the dimensionality of the space required to describe the data.

The most popular data compression technique applied to stellar spectra is Principal Component Analysis (PCA). It has been widely applied in spectral classification combined with artificial neural networks (ANN) (Singh et al. 1998) or support vector machines (SVM) (Re Fiorentin et al. 2008a). For continuum emission, PCA has a proven record in representing the variation in the spectral properties of galaxies. However, it does not perform well when reconstructing high-frequency structure within a spectrum (Vanderplas & Connolly 2009). To overcome this difficulty, other methods have been used in the spectral feature extraction procedure. Locally linear embedding (LLE) (Roweis & Saul 2000) and Isometric feature map (Isomap) (Tenenbaum et al. 2000) are two widely used nonlinear data compression techniques. Some studies found that LLE is efficient in classifying galaxy spectra (Vanderplas & Connolly 2009) and stellar spectra (Daniel et al. 2011). Other authors concluded that Isomap performs better than PCA, except on spectra with low SNR (between 5 and 10) (Bu et al. 2014).

A detailed study of data compression techniques has to include the analysis of their stability properties against noise. In order to improve the overall generalisation performance of the atmospheric parameters estimators, experience shows that it is advantageous to match the noise properties of the synthetic training sample to that of the real sample because it acts as a regulariser in the training phase (Re Fiorentin et al. 2008b). The impact of the SNR on the parameter estimation ($T_{\rm eff}$, log g and [Fe/H]) with ANN is explored in Snider et al. (2001). They found that reasonably accurate estimates can be obtained when networks are trained with spectra –not derived parameters– with similar SNR as those of the unlabelled data, for SNR as low as 13.

Recio-Blanco et al. (2006) determined three atmospheric parameters (T_{eff} , log g and [M/H]) and individual chemical abundances from stellar spectra using the MA-TISSE (MATrix Inversion for Spectral SynthEsis) algorithm. They introduced Gaussian white noise to yield five values of SNR between 25 and 200 and found that errors increased considerably for SNR lower than ~ 25. In Navarro et al. (2012) authors present a system based on ANN trained with a set of line-strength indices selected among the spectral lines more sensitive to temperature and the best luminosity tracers. They generated spectra with a range of SNR between 6 and 200 by adding Poissonian noise to each spectrum. Their scheme allows classification of spectra of SNR as low as 20 with an accuracy better than two spectral subtypes. For SNR ~ 10 , classification is still possible but at a lower precision.

In recent years, there seems to be a tendency to use the spectrum rather than fluxes or equivalent widths derived from it (see e.g. Torres et al. 2012; Recio-Blanco et al.

2014 and references therein; Ness et al. 2015; Walker et al. 2015; or Recio-Blanco et al. 2015). In this work we focus in this latter approach, and attempt to assess the relative merits of various techniques to serve as a guide for future applications of machine learning techniques for regression of stellar atmospheric physical parameters.

This paper presents a comparative study of the most popular data compression technique applied to stellar spectra (PCA) and five alternatives (two linear and three nonlinear techniques). The aims of the paper are (1) to investigate to what extent novel data compression techniques outperform the traditional PCA on stellar spectra datasets, (2) to test the robustness of these techniques and their performance in atmospheric parameters estimation for different SNRs, (3) to investigate the number of regression models of different SNRs needed to obtain the best generalisation performance for any reasonable SNR of the evaluation dataset, and (4) to analyse the effect of the grid density over the regression performance in atmospheric parameters estimation. The investigation is performed by an empirical evaluation of the selected techniques on specifically designed synthetic datasets. In Sect. 2 we describe the datasets used in our experiments. In Sect. 3 we review the data compression techniques evaluated in this work and their properties. Sect. 4 presents our results when comparing the compression techniques and compression rates in terms of the atmospheric 230 parameter estimation errors. In Sect. 5 we evaluate the optimal match between the SNR of the training set examples 232 to the SNR of the evaluation set, and in Sect. 6 we present $\,\,^{233}$ the main results from the analysis of the effect of the train- 234 ing set grid density over the regression performance. Finally, 235 in Sect. 7 we summarize the most relevant findings from the 236 experiments and discuss their validity and limitations.

THE DATASET

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Spectra used in our experiments are divided into two groups:

- ullet The training set, which refers to the portion $_{245}$ of spectra used to fit the atmospheric parameters models.
- $\bullet\,$ The evaluation set, which refers to that portion $_{248}$ of the spectra used only at the end of the model $_{249}$ building to assess how well each final model might $_{250}$ perform on additional spectra.

The synthetic spectra that form the basis of our study have been computed from MARCS model atmospheres (Gustafsson et al. 2008) and the turbospectrum code (Alvarez & Plez 1998; Plez 2012) together with atomic & molecular line lists. These spectra were kindly provided by the Gaia-ESO team in charge of producing the physical parameters for the survey (see de Laverny et al. 2012, for further details). More specifically, our analyses were performed using spectra simulated with two different 257 setups from the high-resolution (HR) mode of the 258 GIRAFFE spectrograph, which was used to carry out the observations of the survey: the HR10 setup (534-562 nm) and the HR21 setup (848-900 nm).

The complete dataset (including training and 262 evaluation data) contains a grid of 8780 synthetic high- 263

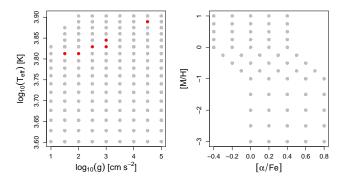


Figure 1. Coverage in parameter space of the dataset. Gray circles represent spectra available in the original collection provided by the Gaia-ESO collaboration. Red circles correspond to missing spectra that were linearly interpolated as described in the text.

resolution spectra (R = 19800) between 5339 and 5619 Å (the nominal GIRAFFE HR10 setup) with effective temperatures between 4000 and 8000 K (step 250 K), logarithmic surface gravities between 1.0 and 5.0 (step 0.5), mean metallicities between -3.0 and 1.0 (with a variable step of 0.5 or 0.25 dex) and $[\alpha/Fe]$ values varying between -0.4 and +0.4 dex (step 0.2 dex) around the standard relation with the following α enhancements: $[\alpha/Fe] = +0.0$ dex for $[M/H] \geqslant$ 0, $\left[\alpha/Fe\right] = +0.4$ dex for $\left[M/H\right] = \leq -1.0$ and $\left[\alpha/Fe\right] =$ $-0.4[\mathrm{M/H}]$ for $[\mathrm{M/H}]$ between -1.0 and +0.0 (Fig. 1). Elements considered to be α -elements are O, Ne, Mg, Si, S, Ar, Ca and Ti. The adopted solar abundances are those used by (Gustafsson et al. 2008). Fig. 2 (left) shows some example spectra from this dataset.

The sample size of our dataset (8780 spectra) is relatively small compared to the input dimension (2798 flux measurements per spectrum). With the rule of thumb of a minimum of 10 samples per dimension (Jain et al. 2000), our dataset should contain at least 10²⁷⁹⁸ spectra. In most real case applications in astronomy, the ratio of sample size to input dimensions is much lower and thus, the curse of dimensionality problem is expected to affect even more severely the inference process.

With a view to analyze the dependence of the validity of the results obtained with the selected dataset, we used a second dataset which is based on the same grid of atmospheric parameters but covering a different wavelength range. This new dataset contains high-resolution spectra (R = 16200) between 8484 and 9001 Å (the nominal GIRAFFE HR21 setup). Fig. 2 (right) shows some example spectra from this dataset. In this validity analysis, efforts were focused on the effective temperature.

DATA COMPRESSION

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In a dynamic environment, a complete rerun of a data compression algorithm becomes prohibitively time and memory consuming. For the sake of computational efficiency, the selection of the data compression techniques tested in our experiments was done amongst those capable of projecting new data onto the reduced dimensional space defined by the

Figure 2. Example spectra from the nominal GIRAFFE HR10 setup (left) and the nominal GIRAFFE HR21 setup (right).

training set without having to re-apply the algorithm (process also known as out-of-sample extension). Thus, in this work, we investigated three linear data compression techniques such as PCA, independent component analysis (ICA) and discriminative locality alignment can be generalised to new data: wavelets, Kernel PCA and diffusion maps (DM). We aimed at minimizing the regression error in estimating stellar atmospheric parameters with no consideration of the physicality of the compression coefficients. Physicality of the coefficients is sometimes required, for example, when trying to interpret galactic spectra as a combination of non-negative components, which closely resembles the physical process of emission in the mid-infrared.

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Other linear and nonlinear techniques could be used 297 for data compression, such as linear discriminant analysis 298 (LDA), locally linear embedding (LLE), Isomap, etc. When 299 the number of variables is much higher than that of training samples, classical LDA cannot be directly applied be- 301

cause all scatter matrices are singular and this method requires the non-singularity of the scatter matrices involved. Isomap's performance exceeds the performance of LLE, specially when the data is sparse. However, in presence of noise or when the data is sparsely sampled, short-circuit edges pose a threat to both Isomaps and LLE algorithms (Saxena et al. 2004). Short-circuit edges can lead to low-dimensional embeddings that do not preserve a manifold's true topology (Balasubramanian et al. 2002). Furthermore, Isomap and LLE cannot be extended out-of-sample.

3.1 Principal Component Analysis (PCA)

PCA (Hotelling 1933; Pearson 1901) is by far the most popular linear technique for data compression. The aim of the method is to reduce the dimensionality of multivariate data whilst preserving as much of the relevant information (assumed to be related to the variance in the data) as possible. This is done by finding a linear basis of reduced dimensionality for the data, in which the amount of variance in the data

is maximal. It is important to remark that PCA is based on 359 the assumption that variance is tantamount to relevance for the regression task.

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PCA transforms the original set of variables into a 362 new set of uncorrelated variables, the principal components, which are linear combinations of the original variables. The new uncorrelated variables are sorted in decreasing order of variance explained. The first new variable shows the maximum amount of variance; the second new variable contains the maximum amount of variation unexplained by the first one, and is orthogonal to it, and so on. This is achieved by 369 computing the covariance matrix for the full data set. Next, 370 the eigenvectors and eigenvalues of the covariance matrix are 371 computed, and sorted according to decreasing eigenvalue.

3.2Independent Component Analysis (ICA)

ICA (Comon 1994) is very closely related to the method 376 called blind source separation (BSS) or blind signal separa- 377 tion (Jutten & Hérault 1991). It is the identification and separation of mixtures of sources with little prior information. 379 The goal of the method is to find a linear representation of non-Gaussian data so that the components are statistically independent, or as independent as possible (Hyvärinen & Oia 2000).

Several algorithms have been developed for performing ICA (Bell & Sejnowski 1995; Belouchrani et al. 1997; Ollila & Koivunen 2006; Li & Adali 2008). A large widely used one is the FastICA algorithm (Hyvärinen & Oja 2000) which has a number of desirable properties, including fast convergence, global convergence for kurtosis-based contrasts, and the lack of any step size parameter. RobustICA (Zarzoso & Comon 2010) represents a simple modification of FastICA, and is based on the normalised kurtosis contrast function, which is optimised by a computationally efficient iterative technique. It is more robust than FastICA and has a very high convergence speed. Another widely used ICA algorithm is the Joint Approximation Diagonalisation of Eigen-matrices (JADE) (Cardoso & Souloumiac 1993). This approach exploits the fourth-order moments in order to separate the source signals from mixed signals. In this work we selected the JADE algorithm for projecting the original spectra in the space of independent components.

3.3 Discriminative Locality Alignment (DLA)

DLA (Zhang et al. 2008) is a supervised manifold learning algorithm that performs data compression by utilizing the class label information of the data instances. A class is a collection of data instances with common characteristics and DLA uses this information to transform the dataset from a high dimensional space to a low dimensional space. In our case, the values that each atmosphere parameter $(T_{\text{eff}}, \log g,$ [M/H] and $[\alpha/Fe]$) could have are used as class labels. It is possible to apply this technique to our set of spectra because the number of possible val- 412 ues that each atmosphere parameter could have is limited.

The learning algorithm can be divided into three stages: 415 part optimisation, sample weighting and whole alignment. 416

In the first stage, for each spectrum a patch (region of the space of independent variables) is defined by the given spectrum and its nearest spectra based on a similarity (distance) measure. On each patch, DLA preserves the local discriminative information through integrating the two criteria that i) the distances between intra-class spectra are as small as possible and ii) the distance between the inter-class spectra is as large as possible. In the second stage, each part optimisation is weighted by the margin degree, a measure of the importance of a given spectrum for classification. Finally, DLA integrates all the weighted part optimisations to form a global subspace structure through an alignment operation (Zhang & Zha 2002). The projection matrix can be obtained by solving a standard eigendecomposition problem.

DLA requires the selection of the following two parameters:

- Neighbour samples from an identical class (k_1) : the number of nearest spectra with respect to x_i from spectra in the same class with x_i
- Neighbour samples from different classes (k_2) : the number of nearest spectra with respect to x_i from spectra in different classes with x_i

This method obtains robust classification performance under the condition of small sample size. Furthermore, it does not need to compute the inverse of a matrix, and thus it does not face the matrix singularity problem that makes LDA and quadratic discriminant analysis (QDA) not directly applicable to stellar spectral data.

Diffusion Maps (DM) 3.4

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DM (Coifman & Lafon 2006; Nadler et al. 2006) are a non linear data compression technique for finding the feature representation of the datasets even if observed samples are nonuniformly distributed, i.e., the density of data instances (set of spectra in our case) in the space of independent variables is not uniform. The non-uniform data distribution leads to a reduction in the performance of an algorithm.

DM are based on the assumption that there exist a low-dimensional manifold or topological space embedded in the high-dimension space of independent variables. Thus, this technique aims to uncover the manifold structure in the data. We conjecture that the spectra sharing the same atmospheric parameters must lie on some manifold. Therefore, we employ DM to discover the low-dimensional space that adequately represents such manifolds without loss of information.

Graph representation is an effective mechanism to represent complex relationships between data points (spectra). Thus, the DM embedding begins with the construction of a graph. Each data point (spectrum) is represented by a collection of numerical variables (measured wavelenghts), and the condition for two nodes to be connected in the graph is based on the proximity of the corresponding data points (spectra) in the space of independent variables. Subsequently, the data modeled as a graph is

combined with Markov chain techniques. In particular, random walks on the graph are used to obtain a measure for the proximity of the data points (diffusion distance), i.e., a measure of similarity between data points. The remarkable idea is that eigenvectors of Markov matrices can be thought of as coordinates. Thus, the data, originally modeled as a graph, can be represented (embedded) as a cloud of points in a Euclidean space. The hope is that this new representation will capture the main structures of the data in a few dimensions. In the low-dimensional representation of the data, DM attempt to retain the relationship between pairs of data points (spectra) as faithfully as possible.

In this work, the results were optimised by controlling ⁴⁹¹ the degree of locality in the diffusion weight matrix (referred ⁴⁹² to below with the parameter name *eps.val*).

Finally, the classical Nyström formula (Williams & Seeger 2001) was used to extend the diffusion coordinates computed on a subsample (the training set) to other spectra (the evaluation set).

3.5 Wavelets

Wavelets (Mallat 1998) are a set of mathematical functions used to approximate data and more complex functions by decomposing the signal in a hybrid space that incorporates both the original space where the data lie (which we will refer to as original space), and the transformed frequency domain. In our case, the original space will be the wavelength space, but in representing time series with wavelets the original space would be the time axis. The wavelet transform is a popular feature definition technique that has been developed to improve the shortcomings of the Fourier transform. Wavelets are considered better than Fourier analysis for modelling because they maintain the original space information while including information from the frequency domain.

Wavelets can be constructed from a function (named mother wavelet), which is confined to a finite interval in the original space. This function is used to generate a set of functions through the operation of scaling and dilation applied to the mother wavelet. The orthogonal or biorthogonal bases formed by this set allows the decomposition of any given signal using inner products, like in Fourier analysis. That is, wavelet and Fourier analyses are similar in the sense that both of them break a signal down into its constituent parts for analysis. However, whereas the Fourier transform decomposes a signal into a series of sine waves of different frequencies, the wavelets transform decomposes the signal into its wavelets (scaled and shifted versions of the mother wavelet).

In particular, wavelet transform breaks a spectrum into subsequences at different resolution scales, i.e., it decomposes a spectrum at different dilations to obtain (i) those approximation coefficients that represent the high-scale and low-frequency components of the spectrum and (ii) the detail coefficients that represent the low-scale and high-frequency components of the spectrum. Thus, wavelet analysis offers multi-resolution analysis in the original space and its frequency transformed domain, and it can satisfactory.

be useful to reveal trends, breakdown points or discontinuities.

Data compression with wavelets consists of keeping a reduced number of wavelet coefficients. There are two common ways of coefficient selection: (i) to eliminate the **detail** coefficients that are assumed to reflect only random noise, and (ii) to keep the k most statistically significant wavelet coefficients (which yields a representation of the signal with less variance) (Li et al. 2010). There are more sophisticated ways to further reduce the number of wavelet coefficients using standard machine learning techniques for feature selection, such as the LASSO (Least Absolute Shrinkage and Selection Operator) used in Lu & Li (2015), wrapper approaches, information theory measures, etc. A full analysis of all these alternatives is out of the scope of this paper and we will only apply the first reduction mentioned above.

3.6 Kernel PCA

Kernel PCA is the reformulation of traditional linear PCA in a high-dimensional space that is constructed using a kernel function (Schölkopf et al. 1998). This method computes the principal eigenvectors of the kernel matrix, rather than those of the covariance matrix. The reformulation of PCA in kernel space is straightforward, since a kernel matrix is similar to the inner product of the datapoints in the high-dimensional space that is constructed using the kernel function (the so-called kernel trick). The application of PCA in the kernel space allows for the construction of nonlinear mappings of the input space.

Since Kernel PCA is a kernel-based method, the mapping performed relies on the choice of the kernel function. Possible choices for the kernel function include the linear kernel (i.e., traditional PCA), the polynomial kernel, and the Gaussian kernel. An important weakness of Kernel PCA is that the size of the kernel matrix is proportional to the square of the number of instances in the dataset.

In this work we used the Gaussian kernel and optimized the predictive performance by fine tuning the inverse kernel width (σ) .

4 COMPARISON OF SPECTRUM COMPRESSION TECHNIQUES AND OPTIMAL RATES

We investigate the utility of six data compression techniques for feature extraction with a view to improving the performance of atmospheric parameters regression models. The robustness of these techniques against increasing SNR is evaluated, and the generalisation performance of training sets of varying SNRs is analysed.

Our set of experiments proceeds in three stages. In the first stage we aim at comparing the various compression techniques and compression rates **for different SNR regimes** in terms of the atmospheric parameter estimation errors. As a result of these experiments, we select an optimal compression approach and rate (dimensionality of the reduced space).

Different machine learning models have been used for the automatic estimation of atmospheric parameters from stellar spectra. Two of the most widely used techniques in practice are ANN and support vector machines (SVM). Unlike ANN, SVM does not need a choice of architecture before training, but there are some parameters to adjust in the kernel functions of the SVM. We use SVM with radial basis kernel functions and adjust the SVM parameters by maximizing the quality of the atmospheric parameter ($T_{\rm eff}$, log g, [M/H] or [α/Fe]) prediction as measured by the root mean squared error (RMSE, Eq. 1) in out-of-sample validation experiments.

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$$RMSE_k = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(\hat{\theta}_{k;i} - \theta_{k;i}\right)^2} \tag{1}$$

where k indexes the atmospheric parameter (θ_k is one of $T_{\rm eff}$, $\log g$, [M/H] or $[\alpha/Fe]$), $\hat{\theta}_{k;i}$ and $\theta_{k;i}$ are the predicted and target values of θ_k for the i-th sample spectrum, and n represents the total number of spectra in our evaluation set.

In order to study the dependency of the estimation performance on the noise level of the input spectra, Gaussian white noise of different variances (SNRs equal to 100, 50, 25 and 10) was added to the original synthetic spectra. Then, the datasets were randomly split into two subsets, one for training (66% of the available spectra) and one for evaluation (the remaining 34%). Since the goal of these first experiments is to compare the compression techniques rather than obtaining the best predictor, splitting the dataset into training and evaluation sets is considered a good scheme. In essence, the experimental procedure consists of the following steps illustrated in Fig. 3:

(i) Compute the low-dimensional representation of the data using the training set. Because some of the techniques used to reduce the dimensionality depend on the setting of one or more parameters, a tuning process was performed in order to determine the optimal parameter values (in the sense that minimize the RMSE; see below). Table 1 presents the ranges of values that were searched, as well as the best parameter value obtained in each case.

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- (ii) Construct SVM models using the training set, and 617 a varying number of dimensions (2, 5, 10, 15, 20, 25, 30 618 and 40) of the reduced space. The SVM parameters (kernel 619 size and soft-margin width) and the compression parameters (where applicable; see Table 1) are fine-tuned to minimize 621 the prediction error of the atmospheric parameter ($T_{\rm eff}$, log 622 g, [M/H] or [α/Fe]).
- (iii) Project the evaluation spectra onto the lowdimensional space computed in step (i).
- (iv) Obtain atmospheric parameter predictions by applying the SVM models trained in step (ii) to the evaluation set obtained in step (iii).
- (v) Calculate the performance of the predictor based on the RMSE obtained on the evaluation set.

4.1 Results

First, we compare the performance of the data compression 635 techniques described in section 3 using noise-free synthetic 636 spectra as well as degraded spectra with SNR levels of 100, 637 50, 25 and 10. Figures 4 to 7 show the RMSE obtained with 638 the evaluation set of the HR10 spectra (the 33% of the full 639

Table 1. Summary of the parameters analysed for the data compression techniques.

Technique	Parameter	Analysed range	Best value
DLA	k_1	[2 - 8]	2
	k_2	[2 - 8]	3
DM	eps.val	[0.01 - 700]	600
Kernel PCA	σ	[0.0001 - 0.01]	0.001

set of spectra that was not not used to define the compression transformation or to train SVM models) grouped by SNR. Equivalent figures grouped by compression technique are included in Appendix A to facilitate comparisons.

Inspection of the figures reveals that the best strategies to compress the spectra are kernel PCA and ICA, with ICA performing marginally better than kernel PCA in most of the parameter space, except sometimes for the lowest compression rate. RMSE errors increase only moderately down to a SNR of 10, which seems to indicate that most of the examined compression techniques serve well as noise filters.

The performance comparison of the analysed data compression techniques shows that although traditional PCA is not the most efficient method, it outperforms some of the nonlinear techniques used in this study, such as DM or wavelets. The lower performance of DM compared to that of PCA could be partially explained by the Nyström extension. Although this method results in diffusion coordinates very similar to those that would be obtained by including the new spectra in the diffusion map, it may lead to small losses of prediction accuracy. As an illustration, the RMSE obtained for the $T_{\rm eff}$ in the high SNR regime (SNR=100) is between 0.5–1.5% better if the diffusion coordinates were computed from the whole dataset, instead of applying the out-of-sample extension. In the case of wavelets, it seems clear that even at the lowest compression rates of 40 components we are eliminating spectral information that is relevant for the subsequent regression task.

Overall, wavelets combined with SVM models have the highest errors regardless of the number of retained dimensions, with the exception of the [M/H] estimation where DLA performed worse for noisy synthetic spectra. Then, DLA was outperformed by most other techniques (except wavelet compression) for almost any compression rate and SNR. However, it achieved the lowest prediction errors for the hardly useful scenarios of noise-free data (not shown here for the sake of conciseness) or the highest compression rates (two or five dimensions) when estimating $T_{\rm eff}$ and $\log g$. PCA and DM yield similar $T_{\rm eff}$ prediction errors in the high SNR regime, but DM are more robust against noise specially for the lowest compression rates examined.

It is interesting to note that compression techniques can be grouped into two categories: DLA, DM and Wavelets show a flat RMSE for target dimensions greater than ten, even for the lowest SNR explored in this Section (SNR=10); PCA, Kernel PCA and ICA show positive slopes in the RMSE curves for SNRs below 25 and target dimensionalities greater than 25, indicating that components beyond this limit are increasingly sensitive to noise.

The relative difference of DM with respect to the best performing compression techniques (ICA and kernel PCA) improves as the SNR diminishes until it becomes almost

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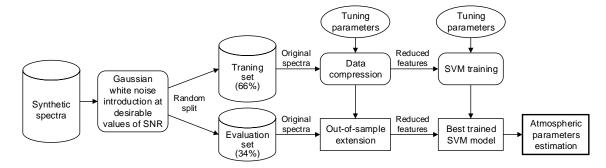


Figure 3. Process flow chart for investigating the performance of the selected data compression techniques.

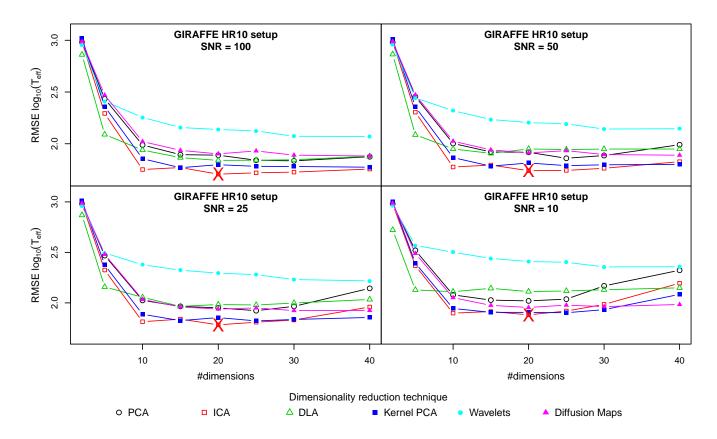


Figure 4. Temperature estimation errors as a function of the number of dimensions used for data compression, for noisy synthetic spectra from the nominal GIRAFFE HR10 setup.

comparable for SNR=10, while at the same time rendering 653 the SVM regression module insensitive to the introduction 654 of irrelevant features (as shown by the flat RMSE curves for increasing numbers of dimensions used).

Table 2 quantifies the prediction errors of the best models for each SNR. It is interesting that ICA compression with 657 20 independent components remains as the best option for any SNR, except for the unrealistic noise-free data. These 659 results evidence that for a given sample size (the number 660 spectra in the training set) there is an optimal number 661 features beyond which the performance of the predictor 662 will degrade rather than improve. On the other hand, as 663 expected, the quality of atmospheric parameter predictions 664

degrades for lower SNR. However, RMSE errors were relatively low even for low SNR (~ 10).

4.1.1 Applicability of the HR10 results to the HR21 setup

The same analysis was carried out on the HR21 dataset characterized by a much wider wavelength range (almost twice as wide as the HR10 setup). Figure 8 and Table 3 show the results obtained for the $T_{\rm eff}$ with the evaluation set.

Some of our previous conclusions are confirmed by these results: i) Kernel PCA and ICA remain as the best compression techniques consistently for all SNRs, but at the lowest SNR (10), PCA and DM have comparable performances; ii) the SVM models trained with wavelet coefficients have

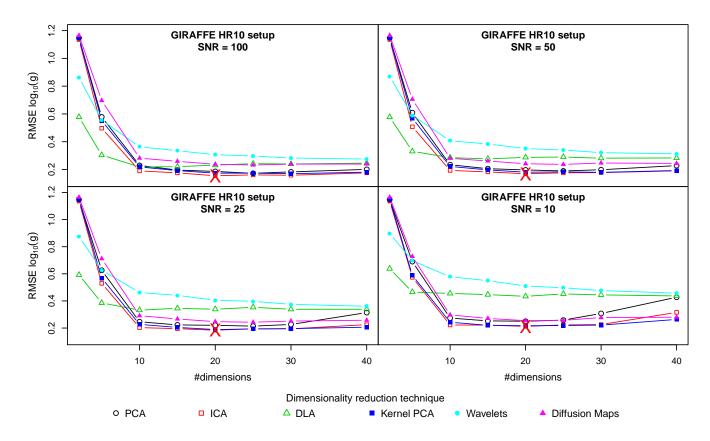


Figure 5. Surface gravity estimation errors as a function of the number of dimensions used for data compression, for noisy synthetic spectra from the nominal GIRAFFE HR10 setup.

Table 2. RMSE on the evaluation set of 2986 spectra for the best SVM trained models (HR10).

\mathbf{SNR}	Method	Nr. Dim.	$egin{aligned} \mathbf{RMSE} \ T_{\mathrm{eff}} \ \mathbf{(K)} \end{aligned}$	$egin{array}{c} \mathrm{RMSE} \ \log \ g \end{array}$	$\frac{\text{RMSE}}{[\text{M/H}] \text{ (dex)}}$	$\begin{array}{c} \mathbf{RMSE} \\ [\alpha/Fe] \text{ (dex)} \end{array}$
			en ()		[/] (/	. , , ,
∞	DLA / ICA^{1}	$40 / 30 / 20^{2}$	27.16	0.13	0.017	0.025
100	ICA	20	50.81	0.15	0.033	0.028
50	ICA	20	54.91	0.17	0.038	0.032
25	ICA	20	60.59	0.18	0.043	0.036
10	ICA	20	76.21	0.21	0.057	0.044

¹The best performance for T_{eff} , log g and [M/H] was obtained with DLA, while best performance for $[\alpha/F_{\text{eff}}]$ was obtained with ICA

the highest errors and are outperformed by PCA in most of the parameter space; and *iii*) DLA performed best for both noise-free data and the highest compression rates (two to five dimensions). However, there are also some differences. For low SNR data, the optimality criterion translates into retaining fewer components. This fact was first identified by Bailer-Jones et al. (1998) in the context of PCA compression of relatively low resolution spectra. We confirm this conclusion for other compression techniques in the HR21 setup where the wavelength coverage is greater than 300 Å, but not for the smaller coverage characteristic of the HR10 setup. Also, in the high SNR regimes the RMSE errors are lower with the HR21 setup than those obtained with the HR10 setup. However, the performance is considerably worsened for the lowest SNR explored in this work (SNR=10). This

Table 3. RMSE on the evaluation set of 2986 spectra for the best SVM trained models (HR21).

SNR	Method	Nr. Dim.	RMSE
			$T_{\rm eff}$ (K)
∞	DLA	15	12.58
100	ICA	20	32.69
50	ICA	20	49.18
25	ICA	15	82.36
10	ICA	10	202.39

clearly indicates that the spectral information relevant for the prediction of effective temperatures is less robust to noise than in the case of the HR10 setup.

performance for $[\alpha/Fe]$ was obtained with ICA. ²The best performance for $T_{\rm eff}$ and log g was obtained with 40 dimensions, while for [M/H] and $[\alpha/Fe]$, 30 and 20 dimensions were needed respectively.

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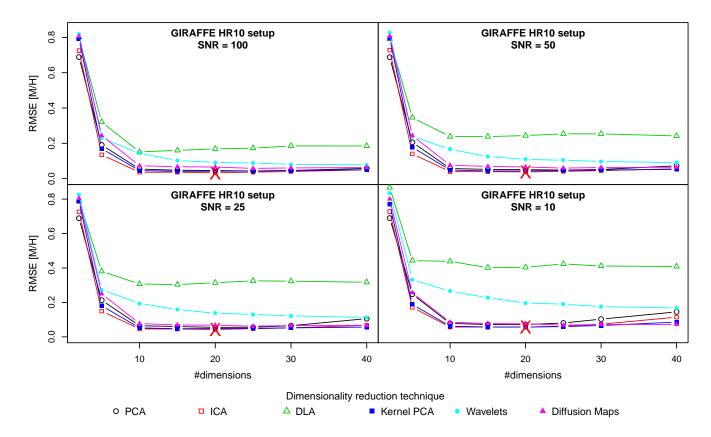


Figure 6. Metallicity estimation errors as a function of the number of dimensions used for data compression, for noisy synthetic spectra from the nominal GIRAFFE HR10 setup.

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OPTIMAL TRAINING SET SNR

In this Section we analyse the optimal match between the SNR of the training set and that of the spectra for which the atmospheric parameter predictions are needed (in the following, the evaluation set).

In order to analyse the dependence of the predicition accuracy with the training set SNR, we generate 25 realisations of the noise for each of the following 8 finite SNR levels: 150, 125, 100, 75, 50, 25, 10 and 5. We create the 25 noise realisation in order to estimate the variance of the results and the significance of the differences. This amounts to $25 \times 8 = 200$ datasets, plus the noiseless dataset, all of which are compressed using ICA. The 20 first independent components are retained for the subsequent regression stage. The choice of compression technique and target dimensionality was dictated by the results presented in the previous Section. For each of these datasets we trained an SVM model to estimate each of the atmospheric parameters ($T_{\rm eff}$, log g, [M/H] or $[\alpha/Fe]$), and to assess the consistency of the results as the evaluation set SNR degrades. The model performances were evaluated using 10-fold cross validation as follows:

(i) The noiseless dataset is replicated 25×8 times: 25 re- 731 alisations of Gaussian white noise for each of the following 732 SNRs: 150, 125, 100, 75, 50, 25, 10, and 5. These 200 replicates together with the original noiseless dataset forms the 734 basis for the next steps.

- (ii) Each spectrum in each dataset is projected onto 20 independent components (as suggested by the experiments described in Section 4).
- (iii) Each of the 201 compressed datasets is then split into 10 subsets or folds. The splitting is unique for the 201 datasets, which means that each spectrum belongs to the same fold across all 201 datasets.
- (iv) An SVM model is trained using 9 folds of each dataset (all characterized by the same SNR). This amounts to 201 models.
- (v) The model constructed in step (iv) is used to predict physical parameters for the tenth fold in all its 201 versions. The RMSE is calculated independently for each value of the SNR and noise realisation.
- (vi) Steps (iv) to (v) are repeated 10 times (using each time a different fold for evaluation) and the performance measure is calculated by averaging the values obtained in the loop.

Results 5.1

Fig. 9 shows the mean (averaged over the 25 noise realisations) RMSE results and the 95% confidence interval for the mean as a function of the SNR of the evaluation set. The nine different lines correspond to the SNR of the training set used to generate both the projector and the atmospheric parameters predictor. The main conclusions of the analysis can be summarised as follows.

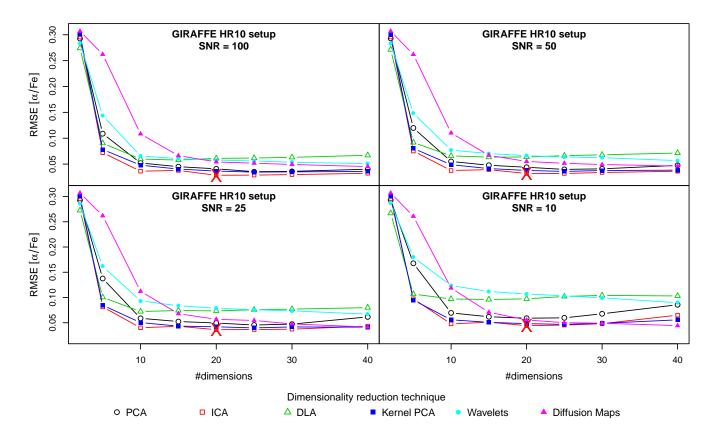


Figure 7. $[\alpha/Fe]$ estimation errors as a function of the number of dimensions used for data compression, for noisy synthetic spectra from the nominal GIRAFFE HR10 setup.

The analysis yields the very important (albeit somehow 764 predictable) consequence that models trained with noise-free 765 spectra are the worst choice for spectra with SNRs up 50/75, 766 and are unnecessary for $T_{\rm eff},~\log~g$ and $[\alpha/Fe]$ in contexts 767 of higher SNRs. Only the [M/H] regression models slightly 768 benefit from training with noiseless spectra if the evaluation 769 spectra are in the SNR \geq 50 regime. The accuracy of the $_{770}$ model trained with noise-free spectra degrades exponentially for SNR<50.

There are no large discrepancies amongst the estimations obtained by applying the 25 models trained with a given SNR to different noise realisations, which translates into small confidence intervals and error bars in the plot. 776 This is so even for the lowest SNR tested (SNR=5).

For the effective temperature and metallicity estimation from evaluation spectra with SNR > 50, there are minimal differences in the precision achieved by models trained with spectra of SNR \geq 50, while for evaluation sets with 50 \geq SNR > 10, the best accuracy is obtained with the model constructed from spectra with SNR of 50. For SNR lower than 10, the model with best generalisation performance is that trained with SNR=10. Hence, two models suffice to obtain $_{783}$ the best performance across the entire SNR range explored in this set of experiments: one trained with SNR=50 examples for evaluation spectra of any SNR above 10, and one trained with SNR = 10 examples for lower SNRs.

Finally, only one ICA+SVM model trained with 788 SNR=25 examples would be enough to estimate the surface 789 gravity for spectra of all SNRs with the best performance (the SNR=50 model yielding similar although lower performances), and only one ICA+SVM model trained with SNR of 50 would be enough to estimate the alpha to iron ratio for spectra of all SNRs.

As a summary, models trained with noiseless spectra are either catastrophic choices or just equivalent to other models. Moreover, there is no need to match the SNR of the training set to that of the real spectra because only two ICA+SVM models would be enough to estimate $T_{\rm eff}$ and [M/H] in all SNR regimes, and a single model is needed for the optimal prediction of surface gravities and alpha to iron ratios.

5.1.1 Application to the HR21 setup spectra

The same evaluation procedure described above was applied to the HR21 setup spectra in order to check for the applicability of our conclusions in different wavelength ranges and coverages. Figure 10 shows the results obtained for the prediction of $T_{\rm eff}$.

Again, we observe that there is no need to match the SNR of the training set to that of the real spectra. Models trained with noise-free spectra are only adequate to estimate $T_{
m eff}$ of noise-free spectra, and completely useless in any other SNR regime. This effect is much more evident here than in the case of the HR10 setup.

It is also clear that again, if the evaluation spectra are

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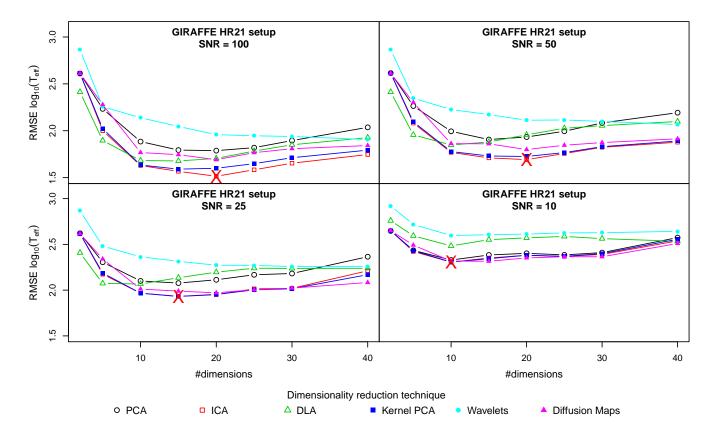


Figure 8. Temperature estimation errors as a function of the number of dimensions used for data compression, for noisy synthetic spectra from the nominal GIRAFFE HR21 setup.

in the SNR>25 regime, the $T_{\rm eff}$ regression models have to be trained with SNR≥50 examples. For evaluation spectra with SNR≥100, the differences in the precision achieved by models trained with spectra of SNR≤50 are easier to notice than in the HR10 setup. There, the best option is one ICA+SVM model trained with SNR of 125.

In summary, our conclusions for the HR10 setup remain valid, except that a third model a model trained with SNR=125 examples would be marginally better than the SNR=50 one in the highest SNR regime (that is, above 100).

Table 4. Size of the new datasets computed with different grid densities.

$T_{\rm eff}$ step-size (K)	Number of spectra
50	679
62.5	545
100	343
125	277
200	175
250	143

6 TRAINING SET DENSITY

In this Section we evaluate the dependence of the regression RMSE with the training set density. In order to simplify the interpretation of the results, we restrict the problem to solar metallicities and alpha abundace ratios. This simplification reduces the set of available spectra from 8780 to only 137 spectra in HR10 setup dataset with solar [M/H] and [alpha/Fe]. These 137 spectra are situated at the nodes of a regular grid except for a few gaps (see Fig. 1) that were interpolated as a weighted bilinear combination four nearest neighbours in the space of physical parameters. Thereafter, succesive grid refinements were obtained by recursively interpolating spectra at intermediate points between grid nodes. These interpolated spectra were obtained again as weighted linear combinations of the bracketing spectra, with

weights given by the inverse square of the normalized euclidean distance to the nearest neighbours.

A total of six grids of synthetic spectra with different grid densities were used to train SVM models. The $T_{\rm eff}$ values varied between 4000 and 8000 K with step-sizes equal to 50, 62.5, 100, 125, 200, and 250 K. The other grid parameters were established as follows: the log g were regularly sampled from 1 to 5 dex in steps of 0.5 dex and both [M/H] and $[\alpha/Fe]$ were set equal to zero. Table 4 presents the step-sizes used in this study as well as the number of synthetic spectra available in each grid. In addition to this, noisy replicates of these grids were generated for four different SNR levels (100, 50, 25, 10).

We evaluated the performance of the SVM regression models using 10-fold cross validation. Figures 11 and 12 present the $T_{\rm eff}$ estimation errors obtained with the different grid densities and the two optimal training set SNRs (50

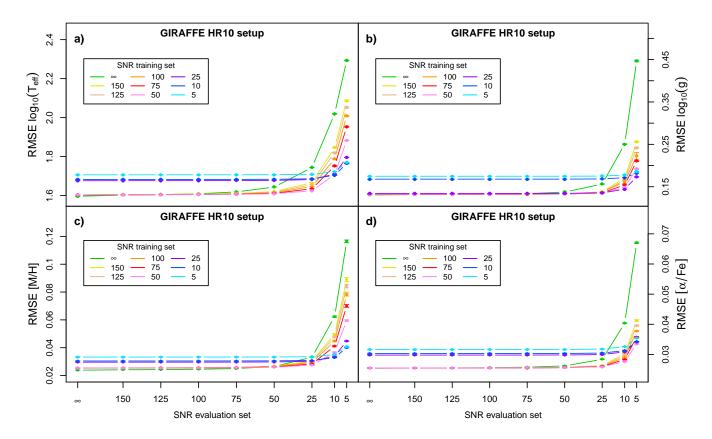


Figure 9. Estimation errors as a function of the SNR of the evaluation set for $T_{\rm eff}$ (a), $\log(g)$ (b) and [M/H] (c) and $[\alpha/Fe]$ (d). Each line corresponds to a model trained with a specific SNR (nominal GIRAFFE HR10 setup).

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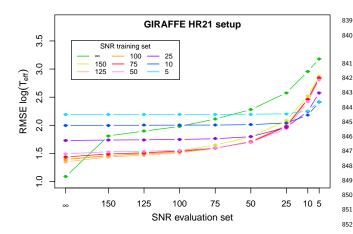


Figure 10. Estimation errors as a function of the SNR of the HR21 evaluation set for $T_{\rm eff}$. Each line corresponds to a model trained with a specific SNR.

and 10) found in the previous Section. Similar figures for $_{859}$ SNR=25 and 100 are shown in Appendix B. $_{860}$

As expected, the estimation errors increase when the $_{861}$ grid density decreases. We see how ICA remains as a win- $_{862}$ ning alternative in this second scenario (a simplified training set with no variation in metallicity or $[\alpha/Fe]$), where $_{864}$ kernel PCA becomes non optimal and another linear tech- $_{865}$

nique (PCA) takes its place amongst the best performing techniques.

The prevalence of our conclusion for ICA as a winning alternative regardless of the grid spacing is reassuring. However, the non linear version of PCA lost its place amongst the best performing compression techniques. It is evident from the comparison of Figs. A1 and 11 that it is only at the largest grid spacings (250 K) that the non linear version of PCA performs better than the linear version (consistent with the results declared in Section 4), because the latter improves faster due to the grid refinement. It remains to be tested whether this faster decrease in the RMSE is due to the reduction in the training set complexity brought about by the removal of the non solar metallicities and $[\alpha/Fe]$ ratios, or it is still present in the full space of four physical parameters. It is plausible that the simplification to solar abundances brings the distribution of examples in feature space closer to a gaussian distribution where indeed the first principal components are effectively more correlated with the effective temperature.

It is interesting to note that the (non linear) compression with Diffusion Maps benefits much less from the grid refinement than the linear compression techniques PCA and ICA. Given the high dimensionality of the input space, it may be the case that much finer grid spacings are needed for the benefits of Diffusion Maps to become apparent. More experiments are needed to confirm this hypothesis, but inso-

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far as the grid spacings are constrained to the values tested 925 here, Diffusion Maps remain suboptimal choices. 926

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7 CONCLUSIONS

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In this work we have carried out a complete set of experiments to guide users of spectral archives to overcome the problems associated with the curse-of-dimensionality, when inferring astrophysical parameters from stellar spectra using standard machine learning algorithms.

In Section 4 we demostrate that, taken globally (that is, including the four stellar atmospheric parameters, a range of SNRs, and a range of compression ratios), Independent Component Analysis outperforms all other techniques, followed by Kernel Principal Component Analysis. The comparative advantage of using ICA is clearer for the $T_{\rm eff}$ and $[\alpha/Fe]$ regression models, and less evident for $\log g$ and [M/H]. Furthermore, we prove that this advantage holds too for a completely different wavelength range and a wavelength coverage twice as large. This is not enough to recommend ICA compression of high resolution spectra for any spectrograph observations, but it is a good indication that our results are not strongly dependent on the actual characteristics of the spectra.

The conclusions drawn from the set of experiments described in Section 4 are tied to the restricted range of physical parameters, wavelengths, and the spectral resolution of the datasets adopted (the HR 10 and 21 setups), but we hope that they still hold for datasets of similar characteristics (different wavelength ranges but similar resolutions and parameter subspaces). In completely different scenarios such as the coolest regions of the Hertzsprung-Russell diagram, where spectra are dominated by molecular absoption bands, the validity of our results still remains to be proved.

In Section 5 we show that there is no need to match the SNR of unlabelled spectra (the spectra for which we want to predict astrophysical parameters) with a regression model trained with the same SNR. On the contrary, only two models are needed to achieve optimal performance in $T_{\rm eff}$ and $[\alpha/Fe]$ regression models (one trained with SNR=50 examples for SNR > 10 spectra and one trained with SNR=10 examples for the lowest SNR regime), and only one model is needed for the prediction of $\log g$ and $[{\rm M/H}]$ (trained with SNR=25 and 50 examples respectively). The $T_{\rm eff}$ result holds also for the HR21 setup regression, although the model trained with SNR=125 is marginally better than the SNR=50 one in the highest SNR regime above 100.

In Section 6 we demostrate in a very simplified setup with no metallicity or alpha-enhancement effects incorporated in the training set, the importance of dense training sets in reducing the cross-validation errors, even in the context of compressed data spaces. We emphasize that this is only applicable to cross-validation errors (that is, errors estimated from spectra entirely equivalent to those used for training). These cross-validation errors are often known as internal errors as they do not take into account systematic differences between the training and evaluation sets. In our case, we have used MARCS model atmospheres, not observed spectra of real stars. In practical applications of the results presented above, the mismatch between the training set and the observed spectra inevitably leads to additional

errors. It seems a reasonable working hypothesis to assume that there is a limit beyond which the total errors are dominated by this mismatch and further increasing the training grid density will not significantly decrease the total errors.

Again, ICA turns out to be the best performing compression technique in the simplified experiments described in Section 6. The underlying assumptions of ICA may not be fulfilled to their full extent in the context of stellar spectra, but certainly we have reasonable hints that they apply, even if approximately. Our working hypothesis is that the independent components reflect groupings of spectral lines of various atomic elements with similar behaviour, such that the strengths and shapes of the lines pertaining to a given component respond in the same way to changes in the atmospheric parameters. Any such component would certainly have a non gaussian distribution across our training set (assumption one), albeit the fulfillment of the statistical independence assumption is, however, less clear under our interpretation of the ICA components. JADE maximizes nongaussianity (rather than minimizing mutual information as in other flavours of ICA) via the fourth order moment of the distribution, and this turns out to result in the best projection amongst those tested in our regression models. This is certainly a result that holds for the synthetic spectra that constitute our working data set, but we have hints that this holds too for observed spectra (Sarro et al. 2013).

There are other reasons that may limit the applicability of the results presented in this work. Extending the applicability analysis to prove our conclusions universally valid is beyond the scope of this article.

In the first place, we have used the most standard or general versions of the techniques evaluated here. In the case of wavelet compression, for example, there are approaches to coefficient shrinkage other than simply removing the smallest spatial scales. The bibliography is endless and it would be impossible to test each and every proposed variation of the techniques presented here. In any case, it is important to note that the validity of our conclusions is limited to the standard versions tested here.

Another source of limitation is due to the use of a single regression model to assess the prediction errors. Again, Support Vector Machines and empirical risk minimization are very standard and robust statistical learning techniques amongst the top performing models for a very wide range of real life problems (van Gestel et al. 2004). Of course, the no-free-lunch theorem (see Igel & Toussaint 2005, and references therein for a formal statement of the theorem) always allows for the existence of algorithms that perform better than SVMs for this particular problem, but in the absence of free lunches, SVMs are a very reasonable choice and a good standard to measure the compression techniques.

Finally, we have focused our research in a battery of discriminative regression models where the *curse-of-dimensionality* may lead to severe problems. Forward models such as the *Cannon* (Ness et al. 2015) are not affected by this *curse-of-dimensionality* but would certainly benefit from a reduction of the more than 80000 parameters needed to model each and every flux in the spectrum.

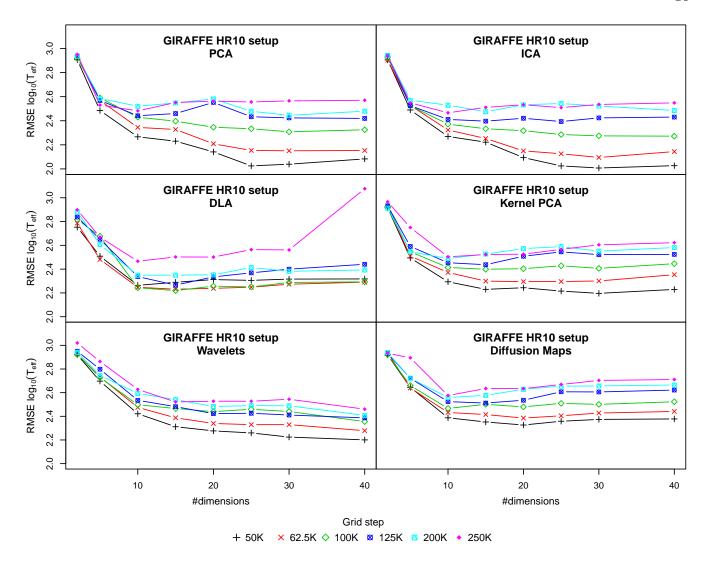


Figure 11. Temperature estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific grid step (SNR = 50)

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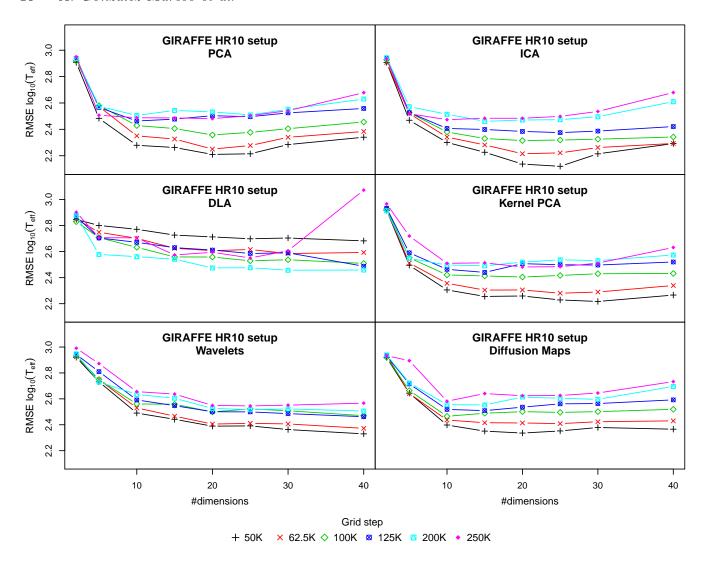


Figure 12. Temperature estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific grid step (SNR = 10)

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COMPRESSION TECHNIQUE FOR SNR=25

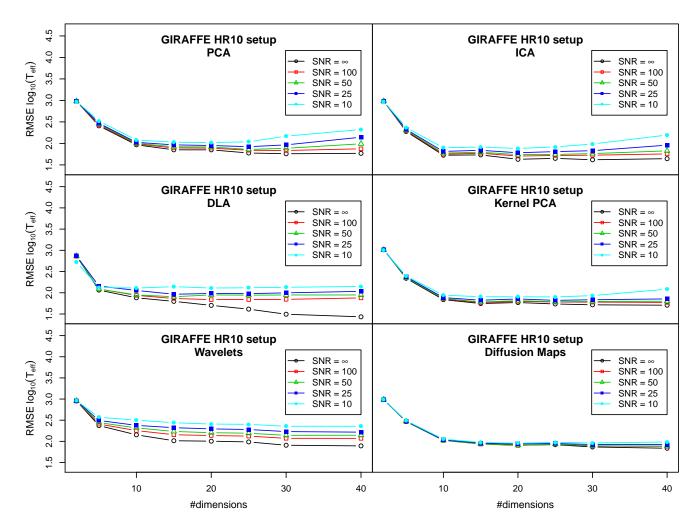


Figure A1. Temperature estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific SNR

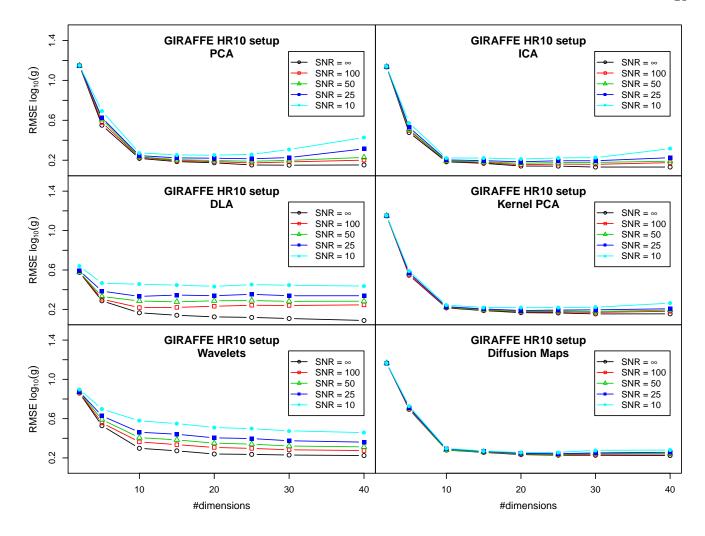


Figure A2. Surface gravity estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific SNR

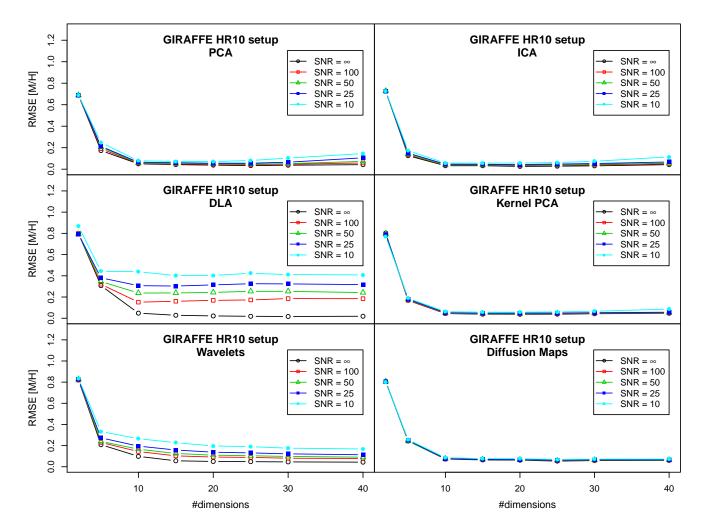


Figure A3. Metallicity estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific SNR

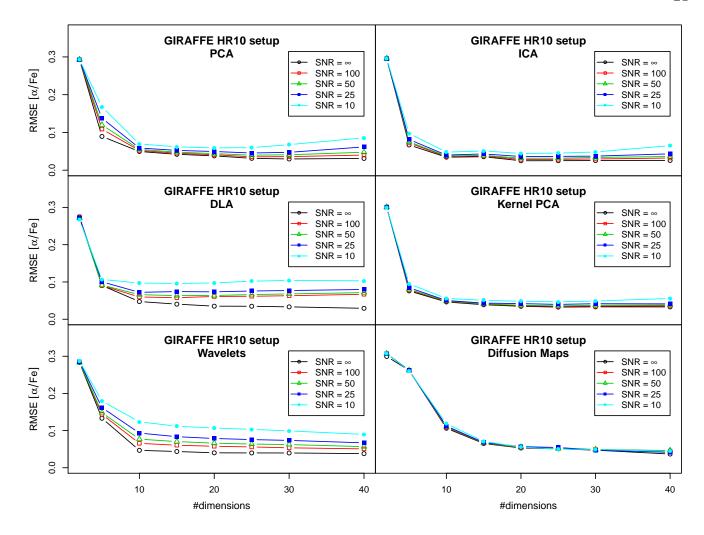


Figure A4. $[\alpha/Fe]$ estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific SNR

Figure B1. Temperature estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific grid step (SNR = 25)

Grid step

× 62.5K ♦ 100K

125K
200K ◆ 250K

#dimensions

#dimensions

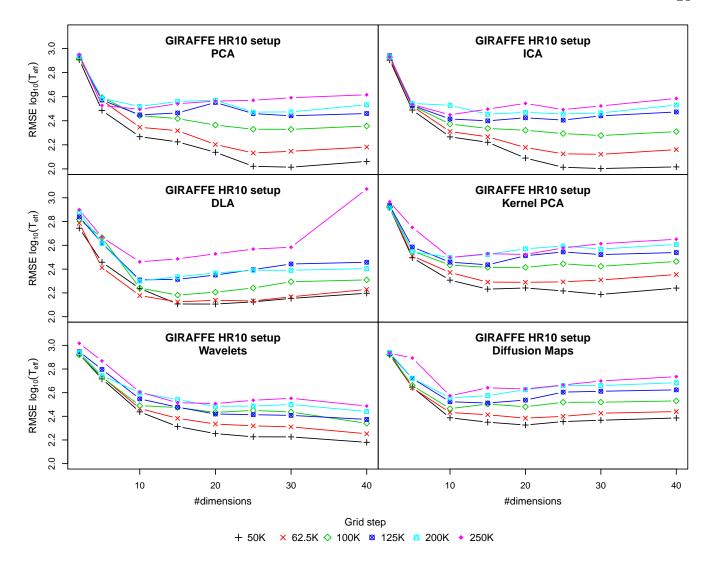


Figure B2. Temperature estimation error against the number of dimensions used for data compression. Each line corresponds to a model trained with a specific grid step (SNR = 100)