An Hybrid Algorithm for Spectral Analysis Using Evolution Strategies and Standard Optimization Algorithms

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Abstract. In this paper we present a method that combines evolution strategies (ES) and standard optimization algorithms to solve the problem of fitting line profiles of stellar spectra. This method provides a reliable decomposition and a reduction in computing time over conventional algorithms. Using a stellar spectrum as input, we implemented an evolution strategy to find an approximation of the continuos spectrum and spectral lines. After a few generations, the parameters found by ES are given as starting search point to a standard optimization algorithm, which then finds the correct spectral decomposition. We used Gaussian functions to fit spectral lines and the Planck function to represent the continuos spectrum. Our experimental results present the application of this method to real spectra, showing that they can be approximated very accurately.

Keywords: Spectral Analysis, Evolution Strategies and Optimization

1 Introduction

An important task in the analysis of stellar spectra is to identify and measure the flux of emission and absorption lines in the spectra. These line profiles can be compared with the spectral profile of ionic and atomic transitions of known wavelengths. Sometimes, the observer biases these associations producing an incorrect interpretation of the data. The line flux in spectra may be measured by multiple techniques, including fitting individual lines. Standard spectral decomposition techniques using non-linear least squares fitting algorithms such as the Levenberg-Marquardt method [1, 2] or unconstrained optimization methods such as simplex search of Nelder and Mead [3] proved to be dependent on initial parameters provided by the user [4]. We propose an alternate solution for this problem, providing initial parameters to these algorithms using an evolution strategy to find them in a short

period time. ES are stable in the presence of noisy data [5], and they do not require the initialization of search parameters in contrast to other optimization algorithms.

In this work, spectral lines are fitted by a summation of Gaussian functions and the continuos spectrum by the Planck function. The free parameters of these functions are encoded in the ES, which initially assigns random values to them and after running for few generations finds a set of values for the parameters near the solution. Then, standard optimization algorithms (Simplex search and Levenberg-Marquardt algorithms) use these parameters to find the best set of values for fitting the model to the spectrum.

The remainder of this paper is organized as follows: Section 2 gives a brief overview of evolution strategies. Section 3 presents a brief description of stellar spectra. Section 4 presents the method used in our experiments, Section 5 presents experimental results and discussion and Section 6 presents conclusions and outlines directions for future work.

2 Evolution Strategies

Evolution Strategies (ES) are a class of probabilistic search algorithms loosely based on biological evolution. They work on a population of individuals, where each of them represents a search point in the space of potential solutions to a given problem. In evolution strategies, a vector of real numbers represents an individual. This is a good representation when the problem at hand deals with continuous parameters. Each individual is formed by a vector of elements called *object variables* x_i, and each variable has associated to it a standard deviation called *strategy parameter* s_i, as shown in figure 1.

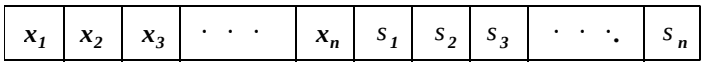

Fig. 1. Representation of individual

Initially, the algorithm randomly generates a population of individuals; subsequently this population is updated by means of randomized processes of recombination, mutation, and selection. Each individual is evaluated according to a fitness function that depends on the problem to be solved.

The selection process favors the fit individuals from the current population to reproduce in the next generation. In evolution strategies, this process is completely deterministic. In $(m+l)$-selection, the m best individuals from the union of m parents and l offspring are selected to form the next parent generation, and in (m, l)-selection this operator selects the m best individuals from the l offspring only; for this $m < l$ is required.

The recombination process allows to combine information from different members of a population, creating offspring from them. In [5] Bäck shows a variety of recombination mechanisms used in evolution strategies. Typical examples of them are: discrete recombination, which is a sexual operation that creates two offspring vectors from two parent vectors copying selected elements from each parent; and

intermediate recombination, which is commonly used as an arithmetic average with some variants. These operators can be used in sexual or panmictic form. In the sexual form, every element of an offspring is the result of recombination between two individuals randomly chosen from the parent population. In panmictic form, each element of an offspring may be the result of recombination among one individual and several other individuals randomly chosen from the parent population.

Mutation is an asexual operator that generates random changes to an individual and often provides new relevant information. The mutation operator is applied independently to each object variable of an individual. It is carried out as shown in equation 1. The strategy parameters may be mutated using a multiplicative, logarithmic normally distributed process as shown in equation 2.

$$x_i' = x_i + s_i' N(0,1) \quad (1)$$

$$s_i' = s_i \exp(N(0,1) + N_i(0,1)) \quad (2)$$

Where $N(0,1)$ is a normally distributed random variable having an expectation of zero and a standard deviation of one, $N_i(0,1)$ indicates that the random variable is sampled anew every time the index i changes.

Rechenberg proposed a deterministic adjustment of strategy parameters during evolution, called the 1/5-success rule [6], which reflects that, on average, one out of five mutations should cause an improvement in the objective function values to achieve best convergence rates. If more than 1/5 of the mutations are successful, σ is increased, otherwise it is decreased.

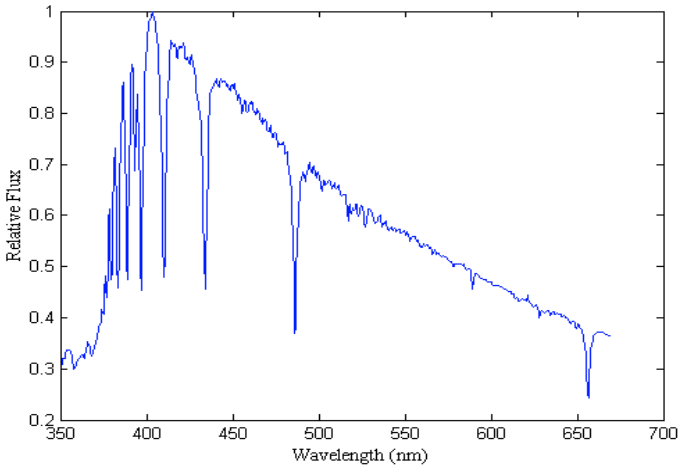

Fig. 2. Sample stellar spectrum

3 The Stellar Spectra

Astronomers can determine the chemical composition and physical nature of a star by analyzing its spectrum, which is a plot of flux density as a function of wavelength, as shown in figure 2. Stellar spectra consist of a continuous spectrum (background or continuum), with narrow discontinuities superimposed. These discontinuities are called absorption lines when the total flux is less than the continuum or emission lines when the total flux is greater than the continuum, and are caused by the presence of certain atoms in the star's atmosphere. Each absorption line appears as a valley, while each emission line appears as a peak in a stellar spectrum. The depth or height of each line indicates its strength. The width of each line indicates the range of wavelengths. Finally, each line has a specific shape. All of these characteristics convey information about the star. An expert astronomer can analyze these lines and estimate with good accuracy several of the most important properties of the star. In this paper we used the spectrum of a star of type A8V obtained from a digital optical stellar library [7]. It consists of fluxes covering 351.0 to 893.0 nm in wavelength with a resolution of 0.5 nm.

4 The methods

A disadvantage of standard optimization algorithms is that they are dependent on the initial values to find the optimal parameters, so these values must be near to the solution. A hybrid system as shown in figure 3, can overcome this problem, using ES to find these initial values and use them as inputs to standard optimization algorithm.

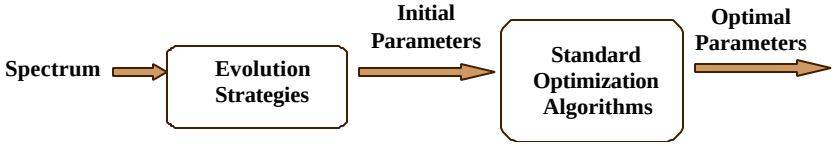

Fig. 3. Hybrid System

The model used to fit the stellar spectra is defined by P(λ) in equation 3, where *F(l)* is the background and the summation of $G_i(\lambda)$ is a set of Gaussian functions superimposed on background representing the stellar lines. The first function *F(l)* used in our model is the Planck function presented by equation 4, which approximates a blackbody emission [8]. This equation has two free parameters: the Temperature of the star *T*, and Adjustment constant *Cy*.

$$P(l) = F(l) + \sum_{i=1}^{N} G_i(l) \quad \textbf{(3)}$$

$$F(l) = Cy \cdot \frac{2hc^2}{l^5} \cdot \frac{1}{\exp\left(\frac{hc}{l\,kT}\right) - 1} \quad \textbf{(4)}$$

where

h = Planck Constant
k = Boltzmann Constant
c = Speed of Light
T = Temperature of the Star
Cy = Adjustment constante

Each Gaussian function is described by three parameters: a center point (l_o), a variance (**s**) and an amplitude (**A**), as defined by equation 5. These functions must be spread over the range of the evaluation data and each one must be assigned with an appropriate variance and central point in order to cause the best fitting to the spectral lines.

$$G(x) = A\exp\left(\frac{-(x - l_0)^2}{2s^2}\right) \quad \textbf{(5)}$$

The free parameters of $F(l)$ and $G(x)$ are encoded as object variables into the individual of the ES. The representation of the object variables into an individual for this problem has the form shown in figure 4.

n_g	T	Cy	l_{o1}	A_1	W_1	...	l_{oN}	A_N	W_M

Fig. 4. Representation of the object variables into an Individual

Where n_g corresponds to the number of Gaussian functions, and T, Cy, l_{oi}, A_i, W_i are the free parameters of $P(l)$.

In our evolution strategy implementation called *GaES-Planck*, we added an operator called intelligent-mutation. This procedure checks for the position of the greatest difference between data generated by the fitting model and the original data, and adds a Gaussian function in this position with the same amplitude as the error size and a random variance value, as shown in figure 5.

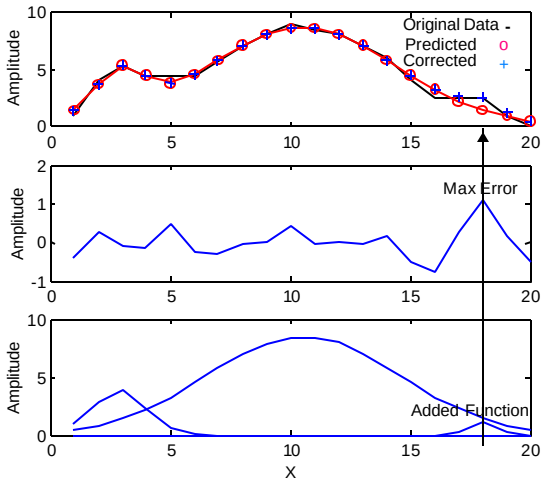

Fig. 5. Added function by Intelligent Mutation

Also, we added another procedure called elimination-mutation, which carries out the opposite function. It suppresses the Gaussian function that produces the smallest reduction in the error.

The fitness function of ES is shown in equation 6, where n_d is the number of points in the digital spectrum, $P(l_i)$ is a point generated by the model at l_i, $f(l_i)$ is a point in the original data, n_g is the number of Gaussian functions, and α is a constant. The first term of the fitness function corresponds to the root mean squared error and the second term is a penalty, which favors individuals with fewer Gaussian functions.

$$Fitness = \sqrt{\frac{\sum_{i=1}^{n_d} (P(l_i) - f(l_i))^2}{nd}} + a \cdot n_g \quad (6)$$

If these initial parameters achieved by ES are near the solution, the standard optimization algorithms will be fast, and it will find the optimal values of our model.

In our experimental results we shown that the ES can find a good model by itself, but it is achieved in a large generation number. Also, we show that the combination of both techniques decreases the computation time and achieves a good accuracy.

5 Experimental Results

In this section we detail the results of combinnig GaES-Planck with the Levenberg-Marquardt algorithm and with the Simplex search algorithm. This method was applied to a real digital optical spectrum obtained from Davis' database [7]. We used for our experiments the real digital optical spectrum of a star of type A8V in the 380 - 500 nm wavelength range.

In a first experiment we used the Simplex direct search and Levenberg-Marqurad algorithms from the MatLab Optimization Toolbox giving the initial parameters as shown in figure 6. After 166,900 evaluations of objective function, the Simplex algorithm achieved an rms error of 0.0236 as shown in figure 7, and the Leverbeg-Marquard algorithm achieved an rms error of 0.0586 as shown in figure 8 after 18,255 evaluations of objective function. The last algorithm stops early due to the gradient in the search direction was quite small.

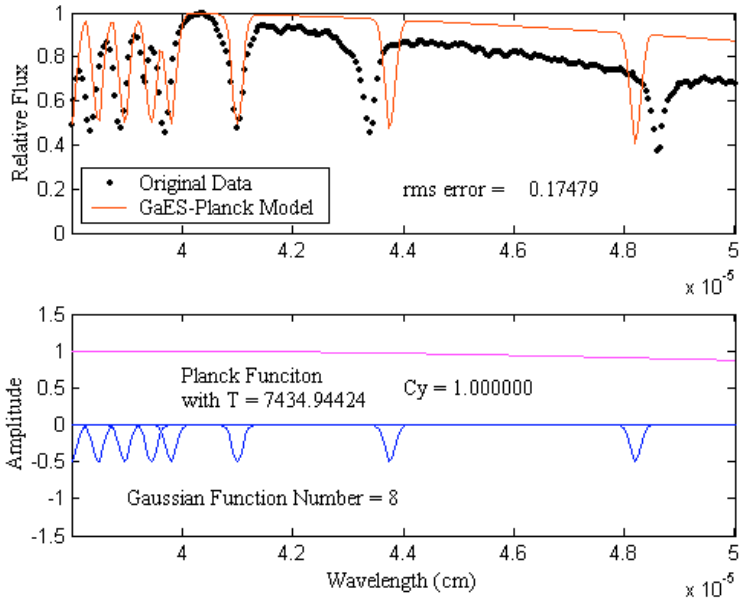

Fig. 6. Digital spectrum of a star of type A8V and Simplex-Planck initial fit model.

In the figure 9, we show the result of a second experiment using only the *GaES-Planck* model. In this case we achieved an rms error of 0.0199, finding 8 Gaussian functions after 3,338 generations. The population used in this experiment was 50 individuals for each generation, which gives a total of 166,900 evaluations of the objective function. The parameters used in our GaES-planck implementation were the following: discrete recombination on 10% of the parent population and intermediate recombination on another 10% of the parent population; mutation on 68% of the parent population; elimination-mutation on 10% and intelligent-mutation on 2% of the parent population.

In a third experiment we combined the Simplex and Levenberg Marquardt algorithms with the GaES-planck. The last algorithm ran until it had not improved upon its fitness function for 20 generations, after that it passed the parameters to the standard optimization algorithm. The figure 10 shows the initial parameters achieved by GaES-planck with an rms error of 0.05121 after 296 generations. Figure 11 shows the best fitting achieved by the Simplex method with these initial parameters after 24,181 evaluations of objective function, and it reached an rms error of 0.0197. The rms error and computing time of this hybrid algorithm are better than the results of the

two last experiments. Figure 12 shows the results of the Levenberg Marquardt algorithm after 519 evaluations of the objective function. It achieved a good fitting accuracy with an rms error of 0.0196 and a less computing time than all the algorithms mentioned previously.

Table 1. Comparison of the different methods to the spectral analysis.

	Simplex	**Levenberg-Marquard (LM)**	**GaES-Planck**	**GaES-Planck-Simplex**	**GaES-Planck-LM**
Rms Error	0.0236	0.0586	0.0199	0.0197	0.0196
Evaluations Number	166,900	18,255	166,900	38,981	15,319

In the table 1, we show a comparison of the different methods used in our experiments. In this table we observe that using only GaES-planck by itself give a good result, but it requires a large computing time. If we combine this algorithm with a standard optimization algorithm in a hybrid method GaES-Planck-Standard-Optimization-Algorithm, it will give a better result.

6 Conclusions

In this paper we have presented an approach of an hybrid algorithm to fit a model of Gaussian functions and the Planck function to digital spectra in order to find spectral lines and background using ES and standard optimization algorithms. Our experimental results show that applying this method to a digital stellar spectrum provides the following advantages:

- It does not require user input regarding search parameter initialization nor the number of Gaussian functions.
- It decreases the computing time.
- It achieves better results than one algorithm by itself.

Future work will extend the experimental results to more spectra and compare the results with theoretical models.

7 References

1 Levenberg, K., "A Method for the Solution of Certain Problems in Last Squares," *Quart. Appl. Mat*h. Vol. 2, pp. 164-168, 1944.

2 Marquardt, D., "An Algorithm for Least Squares Estimation of Nonlinear Parameters," *SIAM J. Appl. Mat*h. Vol. 11, pp. 431-441, 1963.

3 Nelder, J.A. and R. Mead, "A Simplex Method for Function Minimization," *Computer J.*, Vol .7, pp. 308-313, 1965.

4 S. W. McIntosh, D. A. Diver, P. G. Judge, P. Charbonneau, J. Ireland, and J. C. Brown. Spectral decomposition by genetic forward modelling, Astronomy & Astrophysics Supplement Series, **132**, 1998, 145-153.

5 Tomas Bäck, *Evolutionary Algorithms in Theory and Practice*, Oxford University Press, 1996.

6 I. Rechenberg, *Evolutionsstrategie: Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*, (Stuttgart: Frommann-Holzboog Verlag), 1973.

7 D. R. Silva, *A New Library of Stellar Optical Spectra*, Astrophysical Journal Supplement Series Vol. 81, p.865 – 881, 1992

8 H. Karttunen, P. Kröger, H. Oja, M. Poutanen, K. J. Donner. Fundamental Astronomy: Second Enlarged Edition. Springer Verlag, 1993.

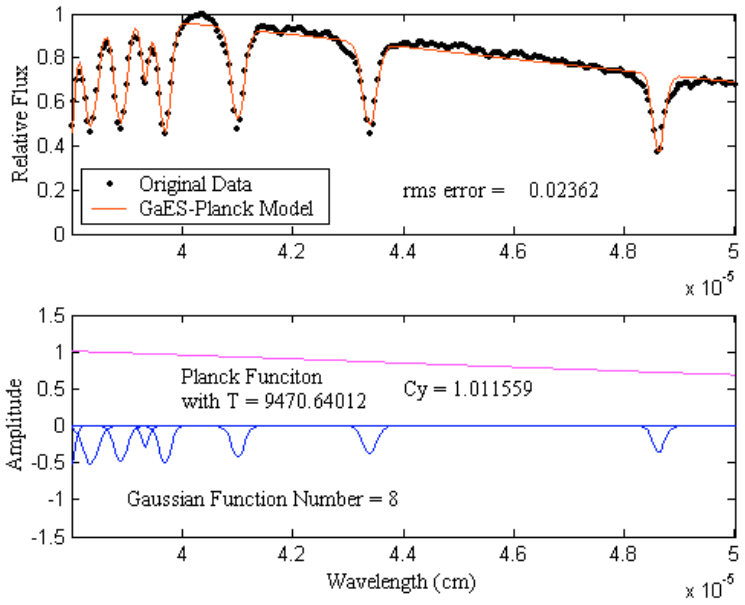

Fig. 7. Digital spectrum of a star of type A8V and Simplex-Planck final fit model.

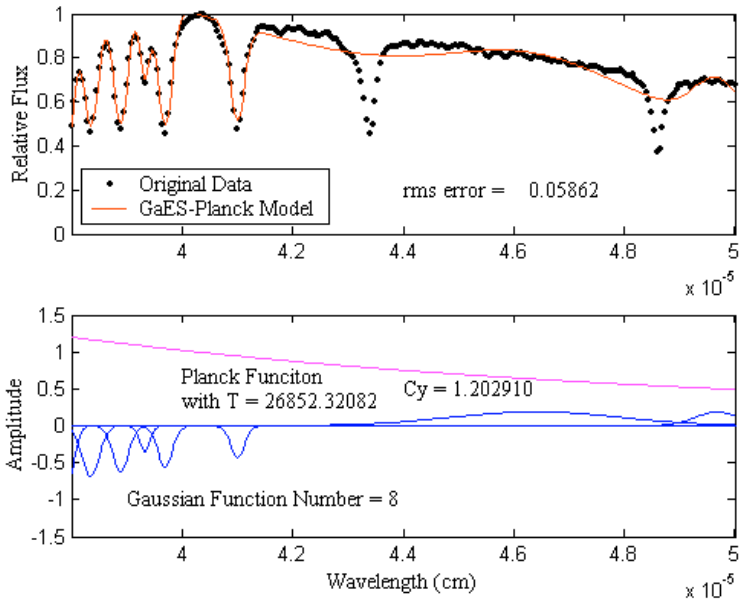

Fig. 8. Digital spectrum of a star of type A8V and Levenberg-M.-Planck final fit model.

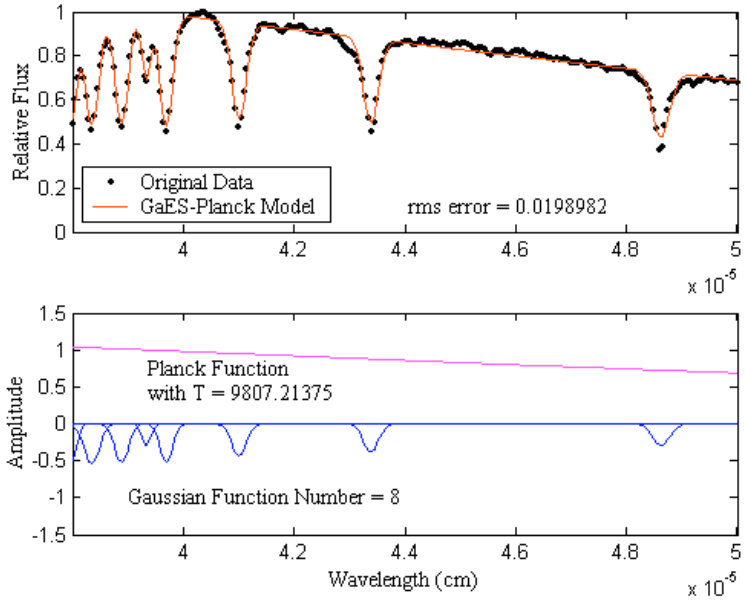

Fig. 9. Digital spectrum of a star of type A8V and GaES-Planck final fit model.

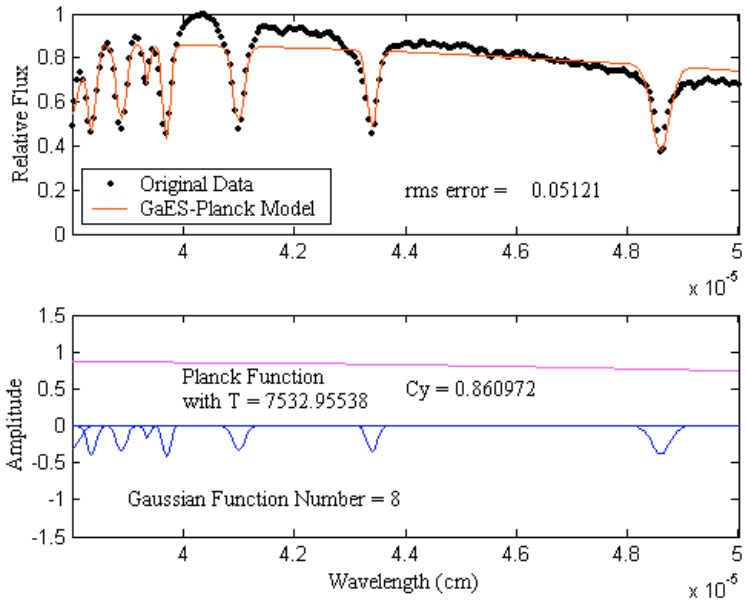

Fig. 10. Digital spectrum of a star of type A8V and initial point provided to standard optimization algorithm by GaES-Planck fit model.

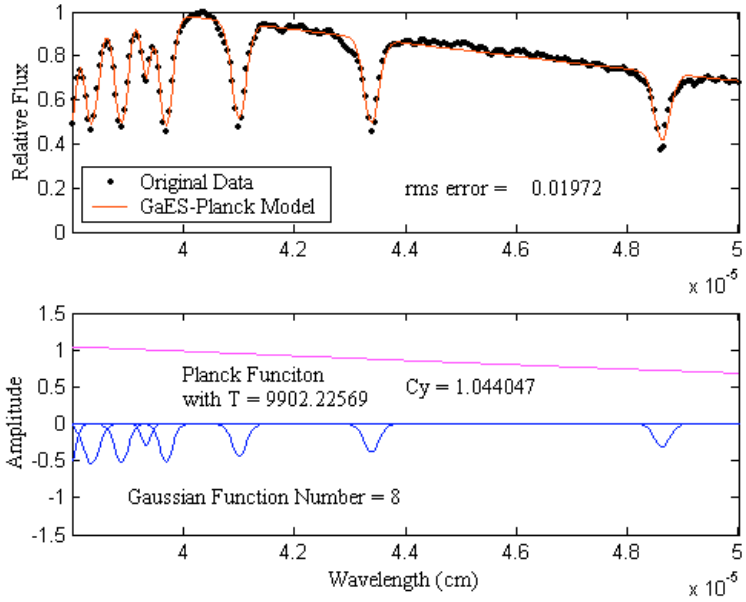

Fig. 11. Digital spectrum of a star of type A8V and GaES-Planck-Simplex final fit model.

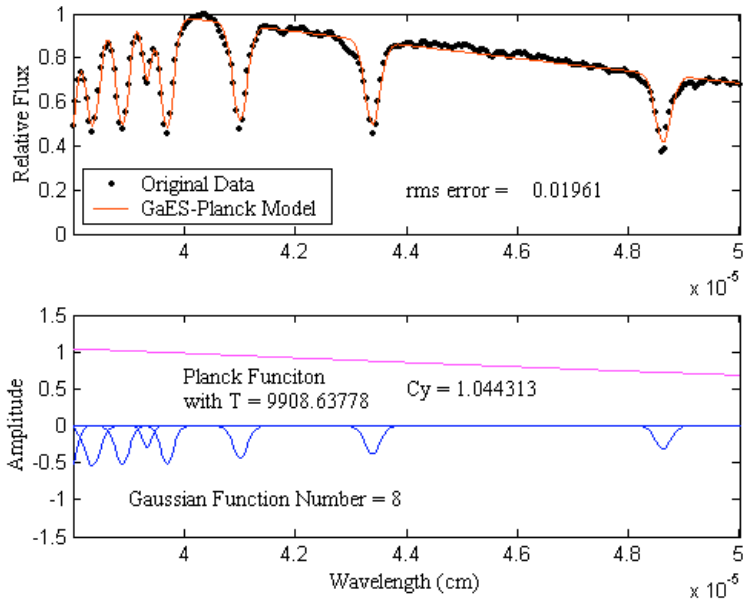

Fig. 12. Digital spectrum of a star of type A8V and GaES-Planck-Levenberg final fit model.