

# SPECTRAL ANALYSIS USING EVOLUTION STRATEGIES

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## ABSTRACT

In this paper we show how evolution strategies (ES) are successfully applied to the problem of fitting line profiles of stellar spectra, which provides a reliable decomposition. Using a stellar spectrum as input, we implemented an evolution strategy to find its components: continuous spectrum and spectral lines. In our experiments we used Gaussian functions to match spectral lines and three different equations to represent the continuous spectrum. We applied this method to simulated and real spectra.

Keywords: Spectral Analysis, Evolution Strategies, and Optimization

## 1. INTRODUCTION

A 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 unstable with noisy data and dependent on initial parameters provided by the user [4].

In this paper we use a summation of Gaussian functions for fitting line profiles and an evolution strategy as optimization method to find the parameters of the model. ES are stable in the presence of noisy data, and can be applied to non-linear systems [5]. Another advantage of this technique is that ES does not require the initialization of search parameters in contrast to other optimization algorithms.

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*  $\sigma_i$ , as shown in figure 1.

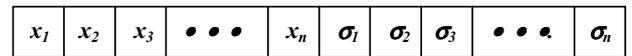


Figure 1. Representation of individual

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  $(\mu+\lambda)$ -selection, the  $\mu$  best individuals from the union of  $\mu$  parents and  $\lambda$  offspring are selected to form the next parent generation, and in  $(\mu, \lambda)$ -selection this operator selects the  $\mu$  best individuals from the  $\lambda$  offspring only; for this  $\mu < \lambda$  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.

$$x'_i = x_i + \sigma'_i N(0,1) \quad (1)$$

$$\sigma'_i = \sigma_i \exp(N(0,1) + N_i(0,1)) \quad (2)$$

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,  $\sigma$  is increased, otherwise it is decreased.

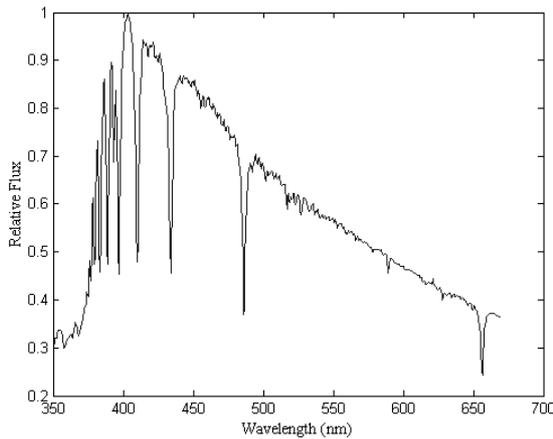


Figure 2. Sample stellar spectrum

### 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

We can define a Gaussian function with three parameters: a center point ( $\lambda_0$ ), a variance ( $\sigma$ ) and an amplitude ( $A$ ), as shown in figure 3. This function is defined by equation 3. The variance determines the shape of the Gaussian function. Two or more Gaussian functions can be combined to fit data as shown in figure 4.

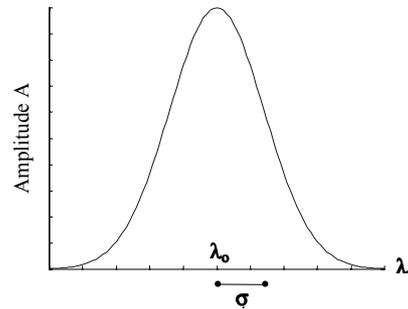


Figure 3. Standard Gaussian Function

$$G(x) = A \exp\left(\frac{-(x - \lambda_0)^2}{2\sigma^2}\right) \quad (3)$$

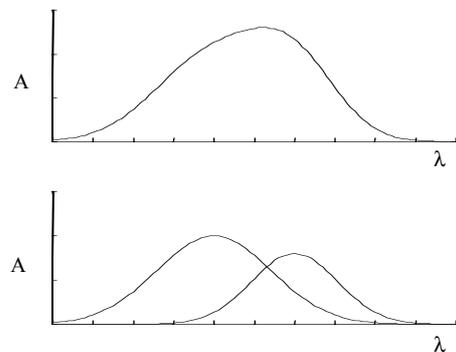


Figure 4. Combination of Gaussian Functions

We can represent a stellar spectrum with a function defining the background and a set of Gaussian functions representing the stellar lines. The first function may be a quadratic equation, another Gaussian function covering the entire spectrum or the Planck function, which approximates a blackbody emission [8]. Equation 4 shows the function used for this purpose.

$$P(\lambda) = F(\lambda) + \sum_{i=1}^N G_i(\lambda) \quad (4)$$

$F(\lambda)$  represents the background or continuum, and  $G_i(\lambda)$ 's are the Gaussian functions superimposed on it. 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 required overlap among Gaussian functions.

$F(\lambda)$  can have one of the following forms:

$$F(\lambda) = \begin{cases} a\lambda^2 + b\lambda + c_1 & \text{quadratic equation} \\ A \exp\left(\frac{-(\lambda - \lambda_0)^2}{w^2}\right) & \text{Gaussian Function} \\ Cy \cdot \frac{2hc^2}{\lambda^5} \cdot \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right) - 1} & \text{Planck Function} \end{cases}$$

where

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

An evolution strategy is used to find the free parameters of  $P(\lambda)$ . The representation of the object variables into an individual for this problem has the form shown in figure 5.

$n_g$	Free Parameters of $F(\lambda)$	$\lambda_{o1}$	$A_1$	$W_1$	...	$\lambda_{oN}$	$A_N$	$W_M$
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Figure 5. Representation of the object variables into an Individual

Where  $n_g$  corresponds to the number of Gaussian functions. It means that individuals may have different sizes. The free parameters of  $F(\lambda)$  are  $a$ ,  $b$ , and  $c_1$  for the quadratic equation,  $Cy$  and  $T$  for Planck's function, and  $\lambda_0$ ,  $A$ ,  $w$  for the Gaussian function. Also, the free parameters of  $G_i(\lambda)$  are  $\lambda_{oi}$ ,  $A_i$ ,  $W_i$ .

In our evolution strategy implementation (hereafter *GaES*), 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 6.

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.

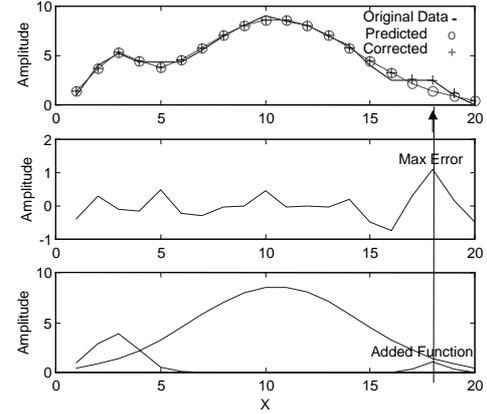


Figure 6 Added function by Intelligent Mutation

$$Fitness_{GaES} = \sqrt{\frac{\sum_{i=1}^{n_d} (P(\lambda_i) - f(\lambda_i))^2}{n_d}} + \alpha \cdot n_g \quad (5)$$

The fitness function is shown in equation 5, where  $n_d$  is the number of points in the digital spectrum,  $P(\lambda_i)$  is a point generated by the model,  $f(\lambda_i)$  is a point in the original data,  $n_g$  is the number of Gaussian functions, and  $\alpha$  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.

## 5. EXPERIMENTAL RESULTS

In this section we detail the result of applying *GaES* to a simulated spectrum and a real digital optical spectrum obtained from Davis' database [7]. We generate a simulated spectrum  $P(\lambda)$  with 5 spectral lines  $G_i(\lambda)$ 's with parameters  $[\lambda_{oi}, A_i, W_i] = [396.8 \times 10^{-5}, -0.30, 1.933 \times 10^{-7}, 407.6 \times 10^{-5}, -0.50, 1.504 \times 10^{-7}, 452.0 \times 10^{-5}, -0.28, 2.245 \times 10^{-7}, 477.2 \times 10^{-5}, -0.45, 0.997 \times 10^{-7}, 485.6 \times 10^{-5}, -0.37, 2.440 \times 10^{-7}]$  and using the Planck's function with a temperature of 6,500K for continuum approximation. *GaES-planck* found the temperature and simulated spectral lines with an rms error of  $4.38 \times 10^{-8}$  as shown in figure 7. The *GaES* ran for 5000 generations, but good fitness values were attained after about 1500 generations, as shown in figure 8.

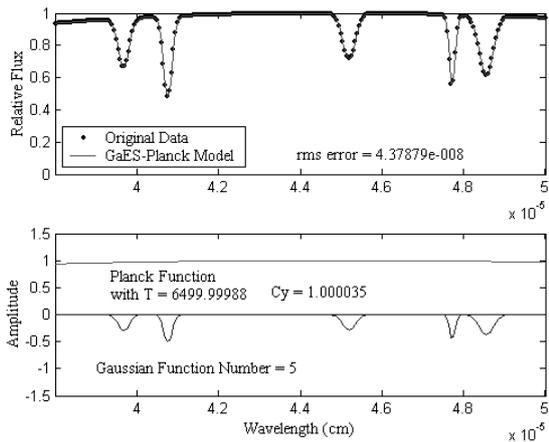


Figure 7. Simulated Spectrum and GaES-Planck fit model.

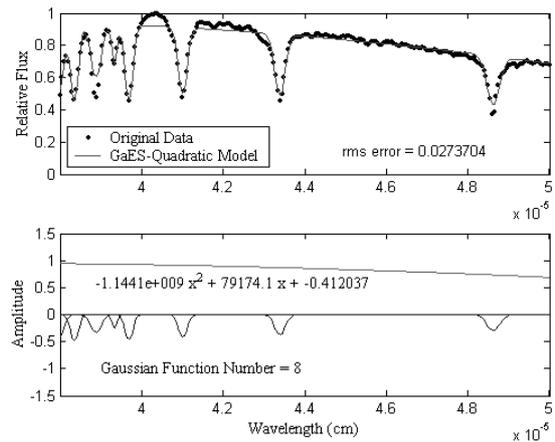


Figure 9. Digital spectrum of a star of type A8V and GaES-Quadratic fit model.

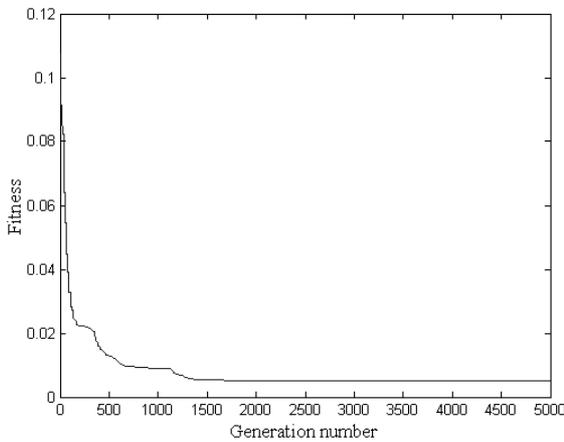


Figure 8. Fitness of GaES-Planck for a simulated spectrum.

Real data possess inherent noise, and this is a problem for traditional techniques, but ES have shown to be insensitive to noisy data. We applied our method to the analysis of a real digital optical spectrum of a star of type A8V in the 380 - 500 nm wavelength range. In the first experiment we used the *GaES-Quadratic* model, where it achieved to an rms error of 0.0274, finding 8 Gaussian functions as shown in figure 9. In the second experiment, we used the *GaES-Gaussian* model, where it achieved an rms error of 0.0207 and 8 Gaussian functions as shown in figure 10. In the last experiment we used the *GaES-Planck* model achieving an rms error of 0.0199 and finding 8 Gaussian functions as shown in figure 11.

The evolution strategy ran for 5000 generations. We used in all the experiments a population of 50 individuals, implying 250,000 evaluations of the objective function. Also, we used two different recombination methods: discrete recombination on 10% of the parent population and intermediate recombination on another 10% of the parent population. Mutation is the most important operator in ES and we used it on 68% of the parent population. We used elimination-mutation on 10% and intelligent-mutation on 2% of the parent population.

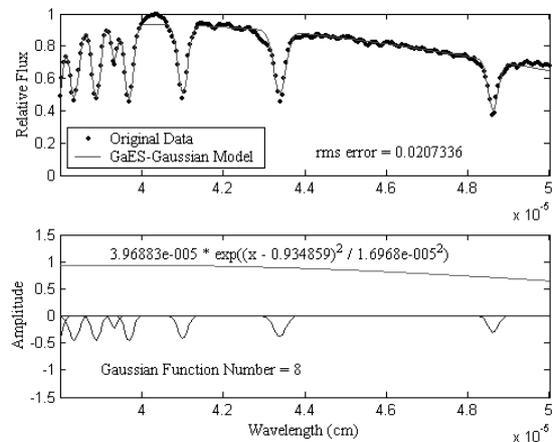


Figure 10. Digital spectrum of a star of type A8V and GaES-Gaussian fit model.

The behavior of each GaES is shown in figures 12, 13 and 14. As can be seen in the figures, good fitness values can be attained quickly after a few hundred iterations; after that, progress becomes slower. This behavior is typical of stochastic optimization algorithms.

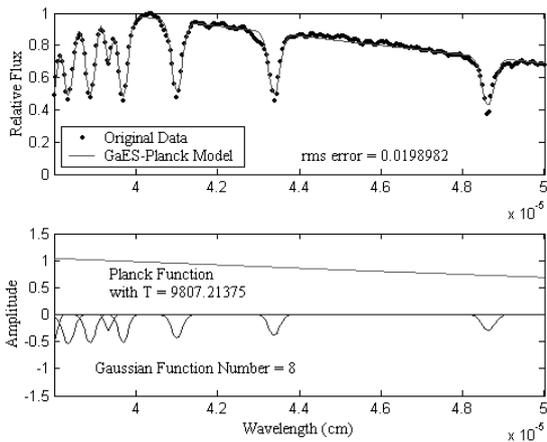


Figure 11. Digital spectrum of a star of type A8V and GaES-Planck fit model.

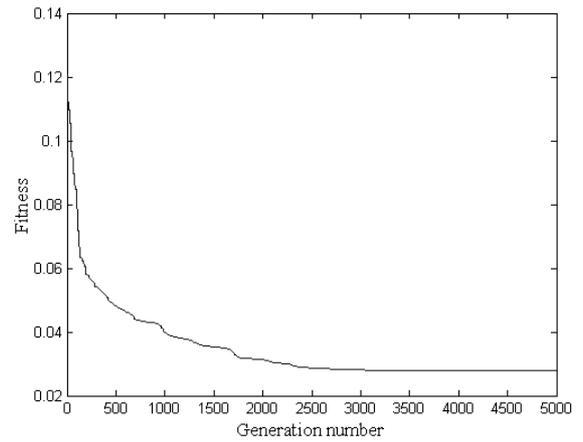


Figure 14. Fitness function of GaES-Planck.

For comparison we made an experiment using the Nelder-Mead Simplex direct search from the MatLab Optimization Toolbox giving the initial parameters as shown in figure 15. After 46,920 iterations and 250,000 evaluations of objective function, we achieved an rms error of 0.0379 as shown in figure 16. We use the same fitness function from ES to evaluate the objective function and its behavior is shown in figure 17. The run time was similar for both algorithms.

One disadvantage of this method is the dependence on initial search parameters, but a combination of this algorithm with the ES to find the initial search parameters may be an alternate solution to reduce the search time and to achieve a better accuracy.

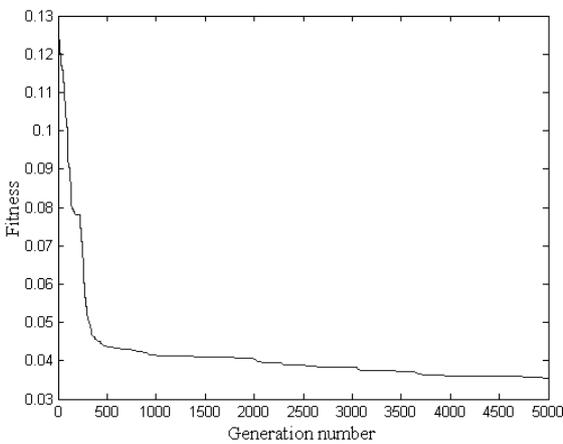


Figure 12. Fitness function of GaES-Quadratic.

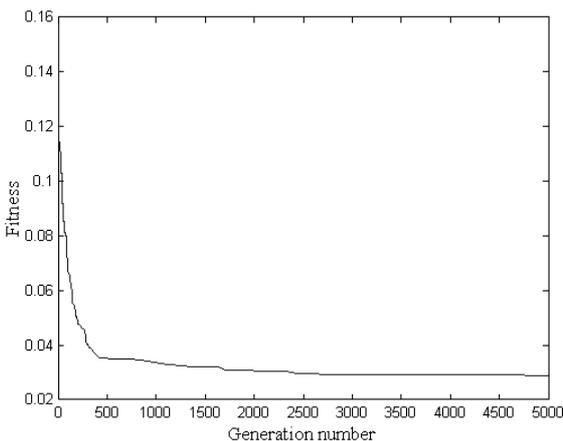


Figure 13. Fitness function of GaES-Gaussian.

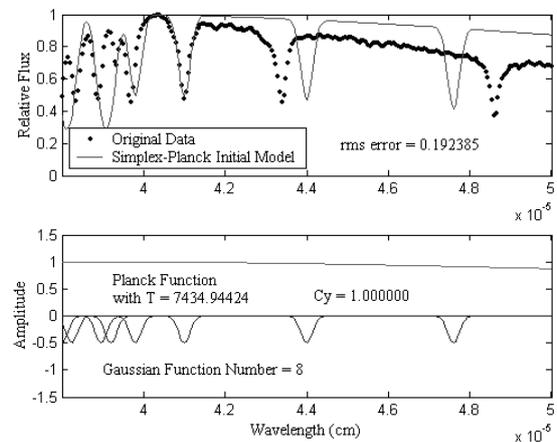


Figure 15. Digital spectrum of a star of type A8V and Simplex-Planck initial fit model.

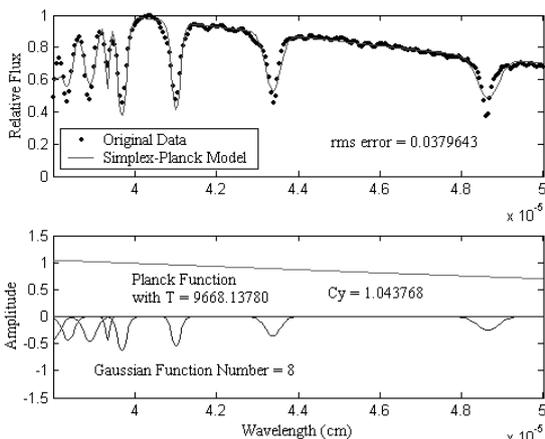


Figure 16. Digital spectrum of a star of type A8V and Simplex-Planck fit model.

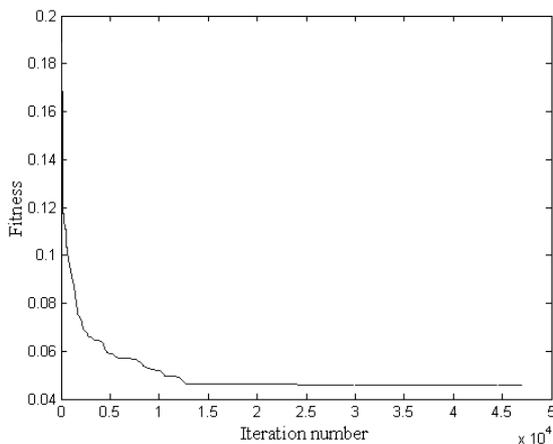


Figure 17. Fitness function of Simplex Method.

## 6. CONCLUSIONS

In this paper we have presented an approach to fit a model of Gaussian functions to digital spectra in order to find spectral lines and background using ES. 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 is stable in the presence of noisy data.
- It is less sensitive to local minima than gradient-based methods.

Future work will extend the experimental results to more spectra and compare the results with theoretical models. Also, we will attempt to combine ES with standard optimization methods to reduce the search time.

## 7. REFERENCES

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