

The Determination of Atmospheric Parameters of Curve-of-Growth by the Simulated Annealing Method

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疑似焼きなまし法による成長曲線からの大気パラメータの決定

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ABSTRACT

We made the program which determines the atmospheric parameters from the curve-of-growth by the Simulated Annealing Method. This program determines the four variables, Δx , Δy , θ_{ex} , and $\log_{10} 2\alpha$ as the best set of the four variables from the starting set of 5 points of the four variables, where Δx is a difference between an empirical curve-of-growth and a theoretical curve-of-growth in the direction parallel to the abscissa and Δy is a difference of the two curves in the direction parallel to the ordinate. The objective function is taken to be the variance of lines in curve-of-growth in the direction parallel to the abscissa. This program is a modification of the program of the Simulated Annealing method by Press et al. (1992), which uses a program of the Downhill Simplex Method.

The effectiveness of this program was tested by comparing the results by this program with those by the program of the method by Yoshioka and by the program of the Downhill Simplex Method by Yoshioka. The data used for the comparison are those for 86 lines of Fe I of HD187203. The following conclusions were drawn from the test.

- 1) This program is an effective method for the curve-of-growth analysis. In comparison with the program of the method by Yoshioka, this program reaches the four variables in quite short steps and in quite a short time. This program reaches the four variables in a similar time to that by the program of the Downhill Simplex Method.
- 2) In this program, the values of objective function corresponding to the best set is a little smaller than those by the program of the Downhill Simplex Method, when appropriate values of parameters of this program are selected.
- 3) The best set of the four variables, as well as the program by the Downhill Simplex Method, depends on the starting set. Judging on a standard of uncertainty in the curve-of-growth analysis, however, the uncertainty due to the starting set is small.

要 旨

われわれは、疑似焼きなまし法を適用して成長曲線から大気パラメータを求めるプログラムを作成した。本プログラムは、 Δx , Δy , θ_{ex} , and $\log_{10} 2\alpha$ の4つの変数をこの変数の5つの初期値の組から求めるものである。なお、 Δx は観測された成長曲線と理論成長曲線との横軸の差を意味し、 Δy は両成長曲線の縦軸の差を意味する。ここで目的関数は、成長曲線上にプロットされた吸収線のちらばりの分散値とした。本プログラムは、Press et al. (1992)の疑似焼きなまし法と吉岡が作成した滑降シンプレックス法を組み合わせ改良したものである。

われわれは、本プログラムと吉岡が作成した成長曲線法のプログラムと吉岡が作成した滑降シンプレックス法のプログラムの結果を比較することにより、本プログラムの有効性を調べた。比較に使われたデータは、HD187203のFe Iの吸収線86本である。そして、次の結論を得た。

- 1) 本プログラムは、吉岡の成長曲線法のプログラムとかなり短いステップとかなり短い時間で結果が得られるので、有効な方法である。吉岡の滑降シンプレックス法とは同程度の時間で結果が得られる。
- 2) パラメータを適当な範囲に選ぶならば、本プログラムで得られる評価関数は、吉岡の滑降シンプレックス法で得られる値よりも少し小さい値が得られる。
- 3) 吉岡の滑降シンプレックス法のプログラムと同様、本プログラムでも最終結果は初期値に依存する。しかし、それによる値の不定性は、成長曲線法での基準から言えば、小さい。

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I. Introduction

A curve-of-growth analysis is one of the methods which are used for the analysis of stellar photospheres. The other method which is mainly used is a model atmosphere analysis. Since detailed distribution of physical quantities such as temperature and pressure and so on are taken into account in a model atmosphere analysis, it is called a fine analysis. It is used when accurate observational data are available and the nature of stellar photosphere is known to a good approximation.

A curve-of-growth analysis is usually used when accurate observational data are not available or there is not enough knowledge about the nature of a stellar photosphere. In this analysis, one-layer approximation is made, i.e., it is assumed that there exists a specific value for a physical quantity of the photosphere such as temperature and pressure.

A curve-of-growth is a graphical representation of the relation between the logarithm of an equivalent width of an absorption line, $\log_{10}W$, and the logarithm of a number density of absorbing atoms, N , times an oscillator strength, f , times a statistical weight, g , $\log_{10}gfN$. The equivalent width of an absorption line is the width of the rectangular profile for which the height is equal to the continuum level near the absorption line. The equivalent width divided by the wavelength of the absorption line, W/λ is often used instead of W , and some multiplicative factor C , is often added to gfN . We obtain by this method the representative quantities of a photosphere, for example, electron pressure, gas pressure, micro-turbulent velocity, ionization temperature, and excitation temperature, T_{ex} , together with chemical composition. This analysis is also called coarse analysis.

In cases where accurate values for oscillator strength are not known, the values of the abscissa of the curve-of-growth, $\log_{10}X$, for a standard star are plotted instead of $\log_{10}gfN$ or $\log_{10}gfNC$. The standard star is the star for which the physical quantities and the chemical composition of the photosphere are already obtained. In this case, the relative values to the standard star for the physical quantities and the chemical composition are obtained instead of the absolute values. This analysis is called a differential curve-of-growth analysis or a differential coarse analysis.

II. Procedure by Using a Computer Done to Date

The curve-of-growth analysis has conventionally

been done by eye measure. There is a fear that the results obtained by eye measure depend on the subjectivity of an analyzer. Moreover, an objective estimate of an error cannot be made by eye measure. The curve-of-growth by using a computer have been applied in order to overcome the above weak points.

For example, Tech (1971)¹⁾ has made a differential curve-of-growth analysis for Ba II star ζ Cap, using ϵ Vir as a standard star, he determined the differential reciprocal temperature, $\Delta\theta_{\text{ex}}$ ($\theta_{\text{ex}} \equiv 5040/T_{\text{ex}}$) relative to the standard star by the minimum-sigma method, using a computer. Powell (1971)²⁾ has made a computer program for a differential curve-of-growth analysis of solar-type stars.

The detailed explanations for these methods are described in the original papers or in the paper by Yoshioka (2008)³⁾. We describe in this paper an outline and strong and weak points of these methods.

In the minimum-sigma method, several values of $\Delta\theta_{\text{ex}}$ are chosen and the abscissa of curve-of-growth, $\log_{10}X_{\text{rel}}$ is taken according to the following expression,

$$\log_{10}X_{\text{rel}} = \log_{10}X_s - \Delta\theta_{\text{ex}}\chi_1, \quad (1)$$

where $\log_{10}X_s$ is the abscissa of a curve-of-growth of a standard star and χ_1 is the excitation potential of the lower levels of a absorption line. Then, a theoretical curve-of-growth is fitted to the above empirical curve-of-growth, and the standard deviation σ of the empirical curve-of-growth from the theoretical curve-of-growth in the direction parallel to the abscissa is calculated. By repeating the above procedure for several values of $\Delta\theta_{\text{ex}}$, a correlation between σ and $\Delta\theta_{\text{ex}}$ is obtained. A graph of this correlation is generally a smooth curve with a unique minimum. The adopted value of $\Delta\theta_{\text{ex}}$ is taken to be the value for which σ takes the minimum value. Using this value of $\Delta\theta_{\text{ex}}$, the empirical curve-of-growth is constructed by plotting for each line $\log_{10}X_{\text{rel}}$ along the abscissa and $\log_{10}W/\lambda$ along the ordinate. This empirical curve-of-growth is used to obtain the other representative quantities of a photosphere.

The strong points of this procedure, which is the reversal of the weak points of the conventional procedure, are as follows : 1) Each line is treated separately and separate weight can be applied to each line ; 2) Correct excitation potential rather than mean values of excitation potential are taken into account ; 3) It gives dispassionately reproducible results and objective estimates of error. On the other hand, this procedure has the following weak points : 1) Great care must be exercised in assuring that no widely discordant lines are used ; 2) Since lines on the flat part or on the damping part of a curve-of-growth will dominate the value of σ and mask the variation due to

the variation of $\Delta\theta_{\text{ex}}$, such lines are excluded in this analysis, which brings about ambiguity to the results ; 3) There is not a guarantee that a theoretical curve-of-growth from which the value σ is calculated really represents the distribution of points adequately.

According to the computer program made by Powell (1971)²⁾ the $\Delta\theta_{\text{ex}}$ value and the vertical and the horizontal shifts which fit an empirical curve-of-growth to a theoretical one are first determined, and then the shape of the theoretical curve, i.e. the damping parameter of the curve is determined. In the determination of the $\Delta\theta_{\text{ex}}$ value and the vertical and the horizontal shifts, only the lines which are on the linear part or on the knee of the flat part of the curve-of-growth are used, because the $\Delta\theta_{\text{ex}}$ value which is determined from these lines depends only slightly on the shape of the theoretical curve and is not affected much by the vertical shift adopted in the fitting. The determination of the $\Delta\theta_{\text{ex}}$ value and the vertical and the horizontal shifts is done in the following iterative way. First, the empirical curve-of-growth is constructed adopting the $\Delta\theta_{\text{ex}}$ value. Secondly, the empirical curve is fitted to the theoretical curve. Thirdly, this theoretical curve is shifted horizontally in order to normalize it so that the value of abscissa, $\log_{10}X$, and the value of ordinate, $\log_{10}W/\lambda$, agrees for weak lines. Then, the value of $\log_{10}X$ corresponding to $\log_{10}W/\lambda$ for the star analyzed is read off for each absorption line from this normalized theoretical curve. Lastly, a new $\Delta\theta_{\text{ex}}$ value is found from a least squares solution to the relation,

$$[X] = [A] - \Delta\theta_{\text{ex}}\chi, \quad (2)$$

where square bracket represents the logarithmic difference of the denoted quantity between the star analyzed and the standard star ; A is the number ratio of a relevant element and to hydrogen uncorrected for ionization. The above iterative process is repeated until a difference between successive estimate of $\Delta\theta_{\text{ex}}$ becomes less than the convergence tolerance ($=0.005$). Adopting the values of $\Delta\theta_{\text{ex}}$, and of the vertical and the horizontal shifts thus determined, the final value of damping parameter of the curve-of-growth is determined by obtaining the best fit of the empirical curve on the condition for a least-squares fit in a direction parallel to the ordinate. If the difference between this value of damping parameter and the previous value of the theoretical curve which is used to determine the $\Delta\theta_{\text{ex}}$ value and the vertical and the horizontal shifts, the whole process is repeated using the new value of damping parameter.

The strong points of this procedure are the same as described for the minimum-sigma method. The weak points of this procedure also are the same as the minimum-sigma method, except for the third point. There

are, however, other two weak points : 1) There is a fear of divergence in the iterative process ; 2) The determination of the values of $\Delta\theta_{\text{ex}}$, and of the vertical and the horizontal shifts is done on the condition for a least-squares fit in a direction parallel to the abscissa, while the determination of the value of damping parameter is done on the condition for a least-squares fit in a direction parallel to the ordinate, which lacks consistency.

Yoshioka (1987)⁴⁾ developed a new procedure. In the new procedure, the determination of the four values of $\Delta\theta_{\text{ex}}$, damping parameter, and vertical and horizontal shifts is done in the following way. First, the value of damping parameter is given for a theoretical curve-of-growth. Secondary, the theoretical curve is fitted to the empirical curve and the values $\Delta\theta_{\text{ex}}$, and horizontal shift are determined as least-squares solution in the direction parallel to abscissa for various values of vertical shift. Thirdly, the value of vertical shift and the corresponding values of $\Delta\theta_{\text{ex}}$ and horizontal shift which gives a minimum value of standard deviation, σ_{temp} , of the $\Delta\theta_{\text{ex}}$ value are selected. The above process is repeated for various values of damping parameter, and the four values for which the σ_{temp} value takes the minimum value are adopted as the final values. In the above process, a gradient of the theoretical curve-of-growth for the ordinate of a line is taken into account as a weight for the least-squares solution so that the lines on the linear and damping parts of the curve-of-growth are given heavier weight than those on the flat part of the curve, because the former lines gives a larger difference between theoretical and empirical curve-of-growths for the same value of error in the ordinate.

The strong points of this procedure are the same as those of the minimum-sigma method and of the procedure by Powell (1971)²⁾. The weak points of both of these procedures, i.e., the ambiguity in the use of lines and the inconsistency in the use of curve-of-growth are overcome in the procedure by Yoshioka (1987)⁴⁾, because this procedure uses all the lines which belong to those on the flat and damping parts of curve-of-growth as well as on the linear part and the same theoretical curve-of-growth are used for the determination of the four values of $\Delta\theta_{\text{ex}}$, damping parameter, and vertical and horizontal shifts.

III. Procedure by Using the Downhill Simplex Method

In the procedure by Yoshioka (1987)⁴⁾, as well as in the other procedure described above, the four values of $\Delta\theta_{\text{ex}}$, damping parameter, and vertical and horizon-

tal shifts are determined through some stages. Yoshioka (2008)⁵⁾ developed a new procedure using the downhill simplex Method. The procedure above described can be regarded as one of optimization problem where the optimal solution is the set of four variables, $\Delta\theta_{ex}$, damping parameter, and vertical and horizontal shifts. The objective function in our problem which is minimized by the optimal solution is selected according to the criterion of agreement between the empirical curve-of-growth and the theoretical one. The variance of absorption lines in the curve-of-growth in the direction parallel to the ordinate is selected as the objective function in the procedure by Powell (1971)²⁾. On the other hand, the variance of lines in the curve-of-growth in the direction parallel to the abscissa is selected as the objective function in the procedure of the minimum-sigma method and that by Yoshioka (1987)⁴⁾. Yoshioka (2008)⁵⁾ made a program which solves this optimization problem by the downhill simplex method due to Nelder and Mead (1965)⁶⁾ (hereafter referred to as DSM).

The detailed explanations of DSM is described in the paper by Yoshioka (2008)⁵⁾. We describe in this paper an outline of this method. In DSM, a simplex is the geometric figure consisting in N dimensions (N is the number of independent variables, and in our case, N is equal to 4) of $N + 1$ points (or vertices) and of all of their interconnecting line segments and of polygonal faces. In DSM, the determination of solution is done in the following iterative way. It starts with $N + 1$ points which define an initial simplex. The point of a simplex where the objective function takes the largest value, which is called the highest point, takes a series of the following four steps : 1) a reflection away from the highest point : 2) a reflection and expansion away from the highest point : 3) a contraction along one dimension from the highest point : 4) a contraction along all dimensions towards the lowest point. In the above steps, the lowest point is the point where the objective function takes the smallest value. The above steps repeat and they terminate when the vector distance moved in one of those steps is fractionally smaller in magnitude than some tolerance or, alternatively, the decrease in the objective function is fractionally smaller than some tolerance.

Yoshioka (2008)⁵⁾ obtained the four variables using the program made by him which determines these values by DSM as the values when the above steps terminate, whose values are hereafter called the best values. As described by Yoshioka (2008)⁵⁾, it was confirmed that this program is effective for the determination of the four values, i.e., in comparison with the

program by Yoshioka (1987)⁴⁾, this program reaches the best values in quite short steps and in quite short time. On the other hand, the following problems resulted.

- 1) The best values depend on the starting set of the four values. According to the starting set of the values, the four values of $\Delta\theta_{ex}$, damping parameter, $\log_{10}2\alpha$, horizontal shift, Δx , and vertical shift, Δy , differ by ± 0.01 , ± 0.09 , ± 0.05 , and ± 0.06 , respectively.
- 2) There are some starting sets of the four values which does not converge to the best values in the case where the tolerance of the decrease in the objective function for the termination of the iterative process is smaller than some value (in this case which is equal to 0.00007).

IV. New Procedure by Using the Simulated Annealing Method

In this paper, we have made the program which avoids the above problems for DSM. The objective function for the above determination of the four variables has many local minima, which causes the above problems. The simulated annealing method (hereafter referred to as SAM) is a method that is suitable for minimization problems of large scale where a desired global maximum is hidden among many local minima.

IV-1. The Approach of the Simulated Annealing Method

The heart of SAM is an analogy with the way that liquids freeze and crystallize. At high temperatures, the molecules of a liquids move freely due to the thermal motion. If the liquid is cooled slowly, thermal motion quietens down. The molecules form a crystal that is ordered over the distance which is long compared with the size of the molecules. This crystal is at the state of minimum energy for this system. For slowly cooled systems, nature is able to find this minimum energy state. If it is cooled quickly, it does not reach this state, but it ends up in a polycrystalline or amorphous state which has somewhat higher energy. The essence of this process is slow cooling, which requires ample time for redistribution of the molecules as they lose mobility. This is the technical definition of annealing, and it is essential for ensuring that a low energy state is achieved.

So nature's minimization algorithms is based on the following procedure. The following Boltzmann probability distribution,

$$P(E) \propto \exp(-E/kT) \quad (2)$$

indicates that a system in thermal equilibrium at tem-

perature T has its energy probabilistically distributed among all different states with energy of E according to the expression (1), where P is the probability of distribution. According to the expression (1), there is a chance of a system being in a high state. Therefore, there is a corresponding chance for the system to get out of a local minimum in favor of finding a better and more global one. The system sometimes goes uphill of energy levels as well as downhill. The lower the temperature, the less likely is a significant uphill excursion.

SAM is a procedure for minimization which simulates the above procedure by nature. Metropolis and coworkers first made the program of SAM for combinatorial minimization which is known as the Metropolis algorithm. Afterwards, the programs of SAM for minimization with continuous variables were made by several researchers. We adopted the procedure by Press et al. (1992)⁸⁾, which uses a modification of DSM.

IV-II. The Procedure of Our Program

In our program, a simplex of $N + 1$ points moves in the same way as in DSM, i.e., which reflects or expands or contracts. A positive, logarithmically distributed random variable which is proportional to the temperature T is added to the four variables associated with every vertex of the simplex, and a similar random variable is subtracted from the four variables of every new point which is tried as a replacement point. This procedure almost accepts a downhill step, but sometimes accepts an uphill one. In the limit where T comes close to zero, this algorithm reduces DSM and converges to a local minimum. At a finite value of T , the simplex expands to a scale which approximates the size of the region that can be reached at this temperature, and then it executes a stochastic Brownian motion within that region, sampling new random points. The efficiency with which a region is explored is independent of the distribution of the value of the objective function around the region sampled, whereas the efficiency is dependent of the distribution in the majority of the other minimization method.

There are many annealing schedules which resemble the annealing by nature. Success or failure is often determined by the choice of annealing schedule. Our program adopts the following schedule where the value of T changes according to the value of the objective function, F .

[1] A starting points of a simplex in 4 dimension comprising of 5 points is given where each vertex consist of the four variables. Then, the F values

corresponding to each point are calculated, and the smallest F value, F_c , is determined.

- [2] A series of random movements of a simplex including contraction and expansion is executed according to a starting T value. Then, the smallest F value, F_s , is determined in the F values which are obtained in the above series of movements.
- [3] Next series of movements is executed and the corresponding F_s value is obtained. In the case where this F_s value is smaller than that obtained with the former step, the T value is multiplied or divided by the SS value which is smaller than 1 and is close to 1. In the above operation, the multiplication is executed when in the former step the multiplication is executed, and the division is executed when in the former step the division is executed. Then, we go to the step [2]. In the case where this F_s value is larger than that obtained with the former step, we go to the step [4].
- [4] In the case where this F_s value is smaller than F_c value, the F_s value of the former step is adopted. And the corresponding four variables is adopted as the best values. In the case where this F_s value is larger than F_c value, the T value is multiplied or divided by the SSS value which is much smaller than 1. In the above operation, the multiplication is executed when in the former step the division is executed, and the division is executed when in the former step the multiplication is executed. Then we go to the step [4].

IV-III. The Results

We have tested our program by comparing the results of our program with those of the program by Yoshioka (1987)⁴⁾ and of the program by Yoshioka (2008)⁵⁾. The data used for the comparison is that for Fe I lines of HD187203 which is a supergiant with F8 type. The number of Fe I lines is equal to 86.

An absolute curve-of-growth analysis is done for the above data with the program by Yoshioka (1987)⁴⁾ and the following set of the four variables Δx , Δy , θ_{ex} (instead of $\Delta\theta_{ex}$ in the case of an absolute curve-of-growth analysis) and $\log_{10}2\alpha$ is obtained; $\Delta x = -3.075$, $\Delta y = 4.63$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.85$. The corresponding F value is equal to 2.435970256.

On the other hand, we obtained by the program for DSM by Yoshioka (2008)⁵⁾ the following best set of the four variables; $\Delta x = -3.034$, $\Delta y = 4.67$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.87$, for the following starting set ①, $\Delta x_i = -2.90 - 0.05i$, $\Delta y_i = 4.80 - 0.05i$, $\theta_{exi} = 1.15 - 0.05i$, and $\log_{10}2\alpha_i = -2.00 + 0.05i$, where $i = 1, \dots, 5$, and for the tolerance of the decrease in the objective

function for the termination of the iterative process, $ftol = 1 \times 10^{-9}$. The corresponding F value is equal to 2.455285751.

We obtain by the program for SAM the following best set of the four variables ; $\Delta x = -3.034$, $\Delta y = 4.67$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.81$, which is obtained for the same starting set as ①. The corresponding F value is equal to 2.453717879. The above results are obtained for the following parameters, $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.0101$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$, where $IITER$ is the maximum execution number of iteration for the satisfaction of $ftol$ value ; $TEMPTR$ is the starting T value ; $IIDUM$ is a parameter for the program generating random number ; NM is the maximum number of iteration described in the former section. The above results little depend on $ftol$, SS , and SSS values. On the other hand, they depend on the $TEMPTR$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -3.023$, $\Delta y = 4.68$, $\theta_{ex} = 1.03$, and $\log_{10}2\alpha = -1.72$ for the following parameters ; $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.2$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$. The corresponding F value is equal to 2.692395486. The results also depend a little on the $IIDUM$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -3.037$, $\Delta y = 4.66$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.80$ for the following parameters ; $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.0101$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -4$, and $NM = 10$. The corresponding F value is equal to 2.468379893. In the case where $IIDUM = -4$, the F value takes the minimum value of 2.453411513. The corresponding best set of the four variables are as follows ; $\Delta x = -3.034$, $\Delta y = 4.67$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.80$.

These results depend on the starting set of the four variable. For example, we obtained by the program for DSM the following best set of the four variables ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.81$, for the following starting set ②, $\Delta x_i = -2.40 - 0.20i$, $\Delta y_i = 5.30 - 0.20i$, $\theta_{exi} = 1.60 - 0.20i$, and $\log_{10}2\alpha_i = -2.40 + 0.20i$, and for $ftol = 1 \times 10^{-9}$. The corresponding F value is equal to 2.646665165.

We obtain by the program for SAM the following best set of the four variables ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.69$, which is obtained for the same starting set as ②. The corresponding F value is equal to 2.623856010. The above results are obtained for the following parameters, $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.0112$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$. The above results little depend on $ftol$, SS , and SSS values also in this case. The above results also depend on $TEMPTR$ value. For example, the following best set of the four variables is obtained

; $\Delta x = -2.998$, $\Delta y = 4.70$, $\theta_{ex} = 1$, and $\log_{10}2\alpha = -1.80$, for the following parameters ; $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.2$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$. The corresponding F value is equal to 2.803163673. The results also depend a little on the $IIDUM$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$ for the following parameters ; $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.0112$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -4$, and $NM = 10$. The corresponding F value is equal to 2.642712278. In the case where $IIDUM = -4$, the F value takes the minimum value of 2.642042551. The corresponding best set of the four variables are as follows ; $\Delta x = -2.988$, $\Delta y = 4.67$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$.

We obtained by the program for DSM other best set of the four variables ; $\Delta x = -3.046$, $\Delta y = 4.65$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.82$, for the following starting set ③, $\Delta x_i = -2.90 - 0.05i$, $\Delta y_i = 4.80 - 0.05i$, $\theta_{exi} = 1.60 - 0.20i$, and $\log_{10}2\alpha_i = -2.40 + 0.20i$, and for $ftol = 1 \times 10^{-9}$. The corresponding F value is equal to 2.44151717739.

We obtain by the program for SAM the following best set of the four variables ; $\Delta x = -3.034$, $\Delta y = 4.67$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.78$, which is obtained for the same starting set as ③. The corresponding F value is equal to 2.453154568. The above results are obtained for the following parameters, $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.0129$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$. The above results little depend on $ftol$, but it depends a little on $IITER$, SS and SSS . For example, we obtain the following best set of the four variables ; $\Delta x = -2.999$, $\Delta y = 4.70$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.69$, for the following parameters ; $ftol = 0.05$, $IITER = 40$, $TEMPTR = 0.0129$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$. The corresponding F value is equal to 2.563514747. And we obtain the following best set of the four variables ; $\Delta x = -3.034$, $\Delta y = 4.67$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.78$, for the following parameters ; $ftol = 0.05$, $IITER = 40$, $TEMPTR = 0.0129$, $SS = 0.999$, $SSS = 0.001$, $IIDUM = -2$, and $NM = 10$. The corresponding F value is equal to 2.453154355. The above results depend on $TEMPTR$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -3.042$, $\Delta y = 4.66$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.81$, for the following parameters ; $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.001$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -2$, and $NM = 10$. The corresponding F value is equal to 2.440207523. The results also depend a little on the $IIDUM$ value, though in this case the effect is small. For example, the results for the parameters of $ftol = 0.05$, $IITER = 20$, $TEMPTR = 0.0129$, $SS = 0.99$, $SSS = 0.01$, $IIDUM = -4$, and $NM = 10$ are the same as those for

the parameters of $ftol=0.05$, $IITER=20$, $TEMPTR=0.0129$, $SS=0.99$, $SSS=0.01$, $IIDUM=-2$, and $NM=10$. And the following best set of the four variables is obtained ; $\Delta x = -3.032$, $\Delta y = 4.66$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.81$, for the following parameters ; $ftol=0.05$, $IITER=20$, $TEMPTR=0.001$, $SS=0.99$, $SSS=0.01$, $IIDUM=-1$, and $NM=10$. The corresponding F value is equal to 2.439946313 which is smallest in the F values obtained by our program for SAM.

We also obtained by the program for DSM other best set of the four variables ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$, for the following starting set ④, $\Delta x_i = -2.40 - 0.20i$, $\Delta y_i = 5.30 - 0.20i$, $\theta_{exi} = 1.60 - 0.20i$, and $\log_{10}2\alpha_i = -1.20 - 0.20i$, and for $ftol = 1 \times 10^{-9}$. The corresponding F value is equal to 2.642037475.

We obtain by the program for SAM the following best set of the four variables ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$, which is obtained for the same starting set as ④. The corresponding F value is equal to 2.642039632. The above results are obtained for the following parameters, $ftol=0.05$, $IITER=20$, $TEMPTR=0.01$, $SS=0.99$, $SSS=0.01$, $IIDUM=-2$, and $NM=10$. The above results little depend on $ftol$, SS , SSS , and NM values. For example, the following best set of the four variables is obtained ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$ for the following parameters ; $ftol=0.05$, $IITER=20$, $TEMPTR=0.01$, $SS=0.999$, $SSS=0.001$, $IIDUM=-2$, and $NM=20$. The corresponding F value is equal to 2.642115121. In this case, the same results are obtained independent of the $IIDUM$ value. The results depend a little on the $IITER$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -2.982$, $\Delta y = 4.72$, $\theta_{ex} = 1.02$, and $\log_{10}2\alpha = -1.78$ for the following parameters ; $ftol=0.05$, $IITER=40$, $TEMPTR=0.01$, $SS=0.99$, $SSS=0.01$, $IIDUM=-2$, and $NM=10$. The corresponding F value is equal to 2.702625811. The results also depend on the $TEMPTR$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -2.998$, $\Delta y = 4.70$, $\theta_{ex} = 1.00$, and $\log_{10}2\alpha = -1.80$ for the following parameters ; $ftol=0.05$, $IITER=20$, $TEMPTR=0.2$, $SS=0.99$, $SSS=0.01$, $IIDUM=-2$, and $NM=10$. The corresponding F value is equal to 2.803163673.

Furthermore, we obtained by the program for DSM other best set of the four variables ; $\Delta x = -2.989$, $\Delta y = 4.69$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$, for the following starting set ⑤, $\Delta x_i = -2.40 - 0.20i$, $\Delta y_i = 4.10 + 0.20i$, $\theta_{exi} = 1.60 - 0.20i$, and $\log_{10}2\alpha_i = -1.20 - 0.20i$, and for $ftol = 1 \times 10^{-9}$. The corresponding F value is equal to 2.542638882.

We obtain by the program for SAM the following

best set of the four variables ; $\Delta x = -2.969$, $\Delta y = 4.66$, $\theta_{ex} = 1.00$, and $\log_{10}2\alpha = -1.78$, which is obtained for the same starting set as ⑤. The corresponding F value is equal to 2.510111125. The above results are obtained for the following parameters, $ftol=0.05$, $IITER=40$, $TEMPTR=0.0001$, $SS=0.99$, $SSS=0.01$, $IIDUM=-3$, and $NM=10$. The above results little depend on $ftol$, SS , SSS , and NM values. The results depend on the $TEMPTR$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -2.988$, $\Delta y = 4.71$, $\theta_{ex} = 1.01$, and $\log_{10}2\alpha = -1.79$ for the following parameters ; $ftol=0.05$, $IITER=40$, $TEMPTR=0.01$, $SS=0.99$, $SSS=0.01$, $IIDUM=-3$, and $NM=10$. The corresponding F value is equal to 2.642039632. The results also depend on the $IITER$ value. For example, the following best set of the four variables is obtained ; $\Delta x = -2.999$, $\Delta y = 4.70$, $\theta_{ex} = 1.00$, and $\log_{10}2\alpha = -1.80$ for the following parameters ; $ftol=0.05$, $IITER=20$, $TEMPTR=0.0001$, $SS=0.99$, $SSS=0.01$, $IIDUM=-3$, and $NM=10$. The corresponding F value is equal to 2.852018285.

V. Conclusions and Discussion

The following conclusions are drawn from the above results.

- 1) The best set of the four variables depends on the starting set. According to the starting set with appropriate four values and parameters, the best set of Δx , Δy , θ_{ex} , and $\log_{10}2\alpha$ differ by ± 0.035 , ± 0.03 , ± 0.01 , and ± 0.09 . This result was also obtained by the program for DSM, though the uncertainties in Δx , Δy are small in this case. The best set differs according to the order of values of the four variables, even if the starting sets are equal as a set. The starting sets ②, ④, and ⑤ are equal as a set. This dependence appears also in the results by the program for DSM. Judging on a standard of uncertainty in the curve-of-growth analysis, these uncertainties are small.
- 2) The appropriate values of parameters are as follows ; $ftol=0.1 \sim 0.01$, $IITER=10 \sim 50$, $TEMPTR=0.0001 \sim 0.01$, $SS=0.99 \sim 0.999$, $SSS=0.01 \sim 0.001$, $IIDUM=-1 \sim -5$, and $NM=10 \sim 20$. In many cases, the best set depends little on the values of $ftol$, SS , SSS , and NM . On the other hand, the best set depends a little on the values of $IITER$ and $IIDUM$, and it depends on the $TEMPTR$ value.
- 3) Usually the corresponding F values obtained in our program of SAM is a little smaller than that obtained with the program of DSM with the same starting set of the four variables, though they are larger than that obtained with the program by

Yoshioka (1987)⁴⁾.

In addition to the problem described in Yoshioka (1987)⁴⁾, the following problems are left for a future study. Although our program obtains the best set of four variables with smaller F values than that obtained with the program of DSM, it gives, as well as the program of DSM, different sets according to the starting set. It is desirable to devise an algorithm to avoid converging in a local minimum before converging to the global minimum.

References

- 1) Tech, J. L. 1971, A High-Dispersion Spectral Analysis of the Ba II star HD204075 (ζ Capricorni), (U. S. Government Printing Office, Washington, D. C.)

- 2) Powell, A. L. T. 1971, Royal Observatory Bulletines, No.171, 3.
- 3) Yoshioka, K. 2009, Journal of the Open University of Japan, 2008, No.26, 119.
- 4) Yoshioka, K. 1987, Journal of the University of the Air, No.4, 65.
- 5) Yoshioka, K. 2008, Journal of the Open University of Japan, No.26, 119.
- 6) Nelder, J. A., and Mead, R. 1965, Computer Journal, Vol.7, 308.
- 7) Metropolis, N., Rosenbluth, A., Teller, A., and Teller, E. 1953, Journal of Chemical Physics, Vol.21, 1087.
- 8) Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P., 1992, Numerical Recipes in Fortran 77 : The Art of Scientific Computing, 2nd ed. (Cambridge University Press, New York).

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