Bul. Astr. Soc. India (1986) 14, 25–33

Decomposition of data into a sum of nonlinear functions—Application to astronomical observations

B. G. Anandarao and Suhasini R. Rao
Physical Research Laboratory, Ahmedabad 380 009

Received 1985 September 11; accepted 1985 December 9

Abstract. In astronomical observations we often encounter spectra which are a result of superposition of individual contributions from phenomena of similar kind. We describe here a method together with its algorithm by which one can decompose a given set of data into a number of nonlinear functions and apply the method to a couple of astronomical data-sets. We discuss the modifications to be made in the algorithm, appropriate to the particular problem, in order to arrive at a solution. This method can be used in high-resolution spectroscopic and photometric data on astronomical objects to extract valuable information which otherwise is not apparent.

Key words : data reduction

1. Introduction

In many scientific problems, the data obtained are the resultant of a superposition of a number of functions of a similar type, but of different parametric values. The type or form of these functions depends upon the physical nature of the source. Therefore, the problem that we address ourselves to in this paper is to resolve or decompose into individual functions (with different parameters) from a given set of data, assuming the functional form.

One often encounters spectra in astronomical observation which are a result of superposition of several individual profiles which are not resolved unambiguously either due to a poor signal-noise ratio or due to closeness of the profiles, making the resolving power of the instrument insufficient. For instance, in the case of Seyfert galaxies, spectroscopic observations (of Wilson as referred to by Burbidge, Burbidge & Prendergasd 1959) showed partially resolved structured profile for several forbidden emission lines and the hydrogen-recombination line H_α. These structures are thought to represent the turbulent motions of several individual gas clouds. By resolving these structures into individual Gaussian profiles, one can obtain the density in each gas cloud from the peak intensity of each of these profiles, and the

turbulent velocities from the width of each of these profiles. In the case of a planetary nebula (Wilson 1950; Osterbrock, Miller & Weedman 1966) one expects the emission lines to give a double-peaked profile, indicating an expanding shell with respect to the central star in the nebula. However, in certain cases, even the high-resolution spectroscopic technique may not be able to resolve the double-peaked structure due to the reasons mentioned earlier. Furthermore, in the case of near- and far-infrared photometric data, sometimes one needs to fit a two- or multiple-temperature model (*i.e.* Planck's function with different temperatures and emissivities) representing different physical conditions of the emitting regions.

We describe here a numerical method using which we can resolve or decompose a set of data into a number of nonlinear (or linear) functions of assumed form. We consider two specific astronomical data-sets and apply the method to resolve the unresolved features.

2. Method

Mathematically, the problem under investigation is to fit the data with a model function which is a sum of a number of nonlinear functions of similar nature, having physically meaningful parameters of different magnitudes. The individual functions may be Gaussian, Lorentzian, exponential, Fourier, or Planckian.

The model function $F(X)$ which should represent the given data-set $P(X_1)$ is written as

$$F(X_1) = \sum_{k=1}^{M} f_k(X_1, \theta_1), \quad i = 1, 2, 3, \ldots, N; \qquad j = 1, 2, \ldots, l \qquad \ldots(1)$$

where $f_k(X_1, \theta_1)$ represent the individual functions that sum up to give $F(X_1)$; θ_1 are the physical parameters in each function that need be fixed so as to obtain a good fit; N is the number of data points; M the number of functions required to fit the data; and l the number of parameters (θ_1).

The deviation of the model from the data at each data point is defined as

$$D(X_1) = F(X_1) - P(X_1). \qquad \ldots(2)$$

Then the residual sum of squares ϕ can be written as

$$\phi(\theta_1, \theta_2, \ldots, \theta_L) = \frac{1}{N} \sum_{i=1}^{N} \left[D(X_1)^2 \right]; \quad N \geqslant L, \qquad \ldots(3)$$

where $L = l \times M$ represents the total number of parameters that need be evaluated.

Now the next step is to minimize the function with respect to $\theta_p (p = 1, 2, \ldots, L)$ for a good fit. Assuming that ϕ is differentiable, one can write these conditions as

$$\frac{\partial \phi(\theta)}{\partial \theta_p} = 0, \quad p = 1, 2, \ldots, L. \qquad \ldots(4)$$

These equations may be linear or nonlinear in θ depending upon the functional form. So, the problem reduces to determining the parameter set θ_p by solving these equations.

In solving such problems (nonlinear least squares and optimization) the generalized Newton-Raphson method (Powell 1964, 1965) can be used very efficiently provided the initial approximations are properly chosen. The method essentially is an iterative procedure based on a Taylor series expansion about the current approximation to the required solution. In case the function to be minimized is a sum of squares and if each term in the sum of squares is relatively small at the minimum, further approximation can be made; and the procedure gains substantially because there is no need to explicitly evaluate the second derivatives.

Applying Taylor's series expansion in the neighbourhood of θ_p^0 (present approximation) and assuming that $\theta_p = \theta_p^0 + \delta_p$, is a later approximation, one can write equation (4) as

$$\frac{\partial \phi}{\partial \phi_p} = \frac{\partial \phi}{\partial \phi_p^0} + \delta_p \sum_{q=1}^{L} \frac{\partial^2 \phi}{\partial \theta_p^0 \partial_q^0} + O(\delta_q^2) = 0$$

$$\text{for } p = 1, 2, \ldots, L. \qquad \ldots(5)$$

Substituting equation (3) in equation (5), and neglecting $O(\delta_p^2)$ terms,

$$\sum_{i=1}^{N} \frac{\partial (D_i^2)}{\partial \theta_p^0} + \sum_{q=1}^{L} \left[\sum_{i=1}^{N} \frac{\partial (D_i^2)}{\partial \theta_p \, \partial \theta_q} \right]_{\theta=\theta^0} \delta_p = 0, \quad p = 1, 2, \ldots, L,$$

which is,

$$\sum_{i=1}^{N} \left[\frac{\partial D_i}{\partial \theta_p} D_i \right]_{\theta=\theta^0} + \sum_{q=1}^{L} \left[\sum_{i=1}^{N} \left\{ \frac{\partial^2 D_i}{\partial \theta_p \, \partial \theta_q} D_i + \frac{\partial D_i}{\partial \theta_p} \frac{\partial D_i}{\partial \theta_q} \right\} \right]_{\theta=\theta^0} \delta_p = 0. \qquad \ldots(6)$$

Near the minimum, if $D_i(\theta_p^0 + \delta_p) = 0$, then $D_i(\theta_p)$ is of the order of δ_p; thus the second derivative in the above equation turns out to be the order of δ_p^2 and can therefore be neglected. The equation (6) then reduces to

$$\sum_{i=1}^{N} \left[\frac{\partial D_i}{\partial \theta_p} D_i \right]_{\theta=\theta^0} + \sum_{q=1}^{L} \left[\sum_{i=1}^{N} \left\{ \frac{\partial D_i}{\partial \theta_p} \frac{\partial D_i}{\partial \theta_q} \right\} \right]_{\theta=\theta^0} \delta_p = 0. \qquad \ldots(7)$$

Defining the matrices

$$g = \sum_{i=1}^{N} \left[\frac{\partial D_i}{\partial \theta_p} D_i \right]_{\theta=\theta^0}; \quad p = 1, 2, \ldots, L,$$

$$G = \left[\sum_{i=1}^{N} \frac{\partial D_i}{\partial \theta_p} \frac{\partial D_i}{\partial \theta_q}\right]_{\theta=\theta^0}, \qquad \ldots(8)$$

one can write (7) as

$$\delta = -G^{-1} \cdot g \qquad \ldots(9)$$

which gives the solution for δ_p; and the next approximation $\theta_p = \theta_p^0 + \delta_p$ can be calculated.

3. Algorithm

The following are the steps we follow in solving equation (9) :

(i) Depending upon the nature of the source from which the data are obtained, we define the functional form of f_k in equation (1) and the number M of such functions which together will represent the data-set.

(ii) Then we choose a set of initial values for θ_p^0 based upon *a priori* knowledge of the source of the data. We comment on this aspect later.

(iii) We compute the deviations

$$D_i(\theta_p^0) = P_i - \sum_{k=1}^{N} f_{ki}(\theta_1^0, \theta_2^0, \ldots \theta_p^0, \ldots, \theta_L^0).$$

(iv) The column matrix elements

$$g_p = \sum_{i=1}^{N} \left[\frac{\partial D_i}{\partial \theta_p}(\theta^0)\, D_i(\theta^0)\right], \quad p = 1, 2, \ldots, L$$

are determined.

(v) We determine the matrix elements

$$G_{pq} = \left[\sum_{i=1}^{N} \left\{\frac{\partial D_i}{\partial \theta_p} \frac{\partial D_i}{\partial \theta_q}\right\}\right]_{\theta=\theta^0}; \quad p = 1, 2, \ldots, L, \quad q = 1, 2, \ldots, L.$$

(vi) We then solve the equations

$$\delta = -G^{-1} g.$$

(vii) We check whether $\underset{P}{\text{Max}} \left|\frac{\delta_p}{\theta_p^0}\right| \leqq \eta,$

where η is a pre-assigned accuracy limit. If this inequality is satisfied then we go to the following step, or else we start all over again from the step (iii) above.

(viii) We calculate $\epsilon \left(= \frac{1}{N} \sum_{i=1}^{N} D_i^2\right)$, the residual sum of squares, with the

new $\theta_p = \theta_p^0 + \delta_p$ and check whether $\epsilon \leqq \gamma$, a limit given to the standard deviation based on the amplitude of the errors in the data. If this inequality is satisfied then we stop the iteration or else we start from step (iii) above with new θ_p.

The following remarks on the nature of the solution are in order. In general, the solution to the problem discussed here is not unique because of its nonlinearity. Therefore, care should be taken in accepting a particular solution and rejecting several others. The method that we have adopted here searches for a solution in the neighbourhood of the initial choice θ_p^0. Thus, unless the initial choice is properly made, the method either diverges giving no solution, or even if it converges, does so to a solution which may be numerically correct but has no physical meaning. The first two steps in the algorithm as given above, namely, (i) choosing the functional form and the number of such functions, and (ii) assuming a set of initial values θ_p^0, require a prior knowledge as to the nature of the source from which the data have been observed.

Even after choosing the functional form and the number of functions, one needs enough prior knowledge regarding the object in order to judge whether or not a solution is meaningful. Sometimes the stability of the parameters also causes problems in convergence of the method. In such a case the iteration need not be done simultaneously for all the parameters. One can estimate a subset of parameters which are stable, and substituting these, the other parameters can be estimated. The whole iteration process is repeated once or twice to get the full set of parameters. The matrix G which consists of partial derivatives at data points gives an indication of the order in which the parameters to be iterated.

We have used Gauss-Seidel iterative method for solving the matrix equation given in (vi) above. In general, we have found that the method leads to fairly fast convergence, provided that the matrix G is well-conditioned.

4. Examples

We now give two examples of the type of functions that we have used for two astronomical data-sets

(a) *Gaussian decomposition of spectroscopic data*

It is fairly reasonable to assume that the emission-lines from astronomical sources have Gaussian profiles. This is because in most of such cases the line broadening is caused by the motion of particles in thermodynamic equilibrium or by the random turbulent motion of the gas. In such a situation, the resulting spectral line intensity distribution can be best approximated by a Gaussian. The data we have used for the decomposition are the hydrogen Balmer-alpha line observations made by Anandarao, Sahu & Desai (1985) on the peculiar Mira variable star R Agr by using a high-resolution Fabry-Perot spectrometer. The model function F_i in equation (1) is

$$F_i = \sum_{k=1}^{M} f_{ki}(\theta_j); \quad i = 1, 2, \ldots, N; \qquad j = 1, 2, \ldots, 1$$

$$f_{kl} = A_k \exp\left\{-\frac{(\lambda_{ok} - \lambda_i)^2}{2\sigma_k^2}\right\}.$$

The parameter A_k represents the maximum amplitude; λ_{ok} the wavelength of maximum amplitude; and σ_k the width of the profile number K. We have chosen $M = 4$ so that the observed profile represents two expanding shells with respect to the central star—each shell represented by two Gaussian profiles, one approaching edge and the other receding edge.

In figure 1, we have given the emission-line profile data alongwith the model-fit with four Gaussians. One can see that the fit was remarkably good giving physically meaningful parameters. We have found that a model with three Gaussians also fits well enough with the data. However, the case of three Gaussians is rather less meaningful because if there were to be two expanding shells, then, these should necessarily be represented by four profiles. Supposing that there was only one shell then it should be represented by two profiles. We tried to fit two profiles to the data. However, the result was not satisfactory and the right-hand side of the observed profile could only be accounted by assuming that the profile with

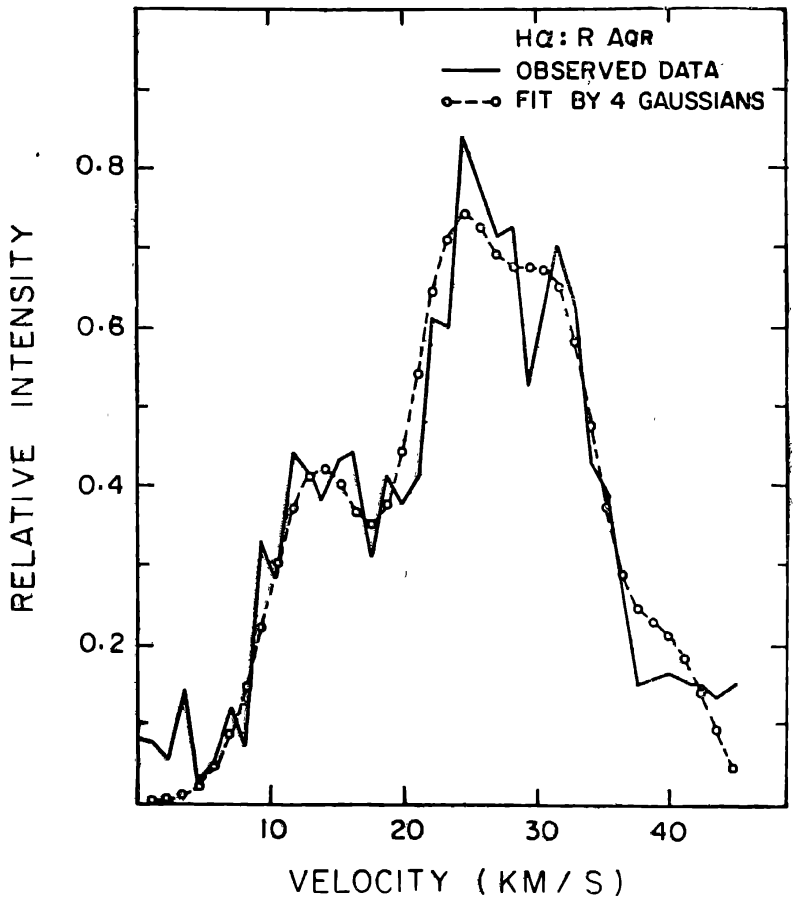

Figure 1. H-alpha line profile in the peculiar variable star R Aqr. Observed profile fitted with a Combination of four Gaussian profiles (after Anandarao, Sahu & Desai 1985)

the maximum amplitude in the data was actually composed of two profiles representing a single shell.

We have solved equation (9) by taking a set of similar parameters each time. That is, we first keep widths and position of the Gaussians fixed, and find out the amplitudes; then keep amplitudes and widths fixed and compute the positions; and finally, keep amplitudes and positions fixed and obtain widths. In doing this, it is of course necessary that we first keep the best known and stable parameters fixed and vary the least known ones. Thus the solutions depend to a considerable extent upon the initial values. We had to do this kind of piece-wise computation, because as we can see, in the matrices $[G]_{pq}$ and $[g]_q$, the elements corresponding to different parameters are different by orders of magnitude. It is felt that this way of solving the problem in a piece-wise manner reduces the risks involved in wild-goose chase. The reason is that when we know *a priori* the values of certain parameters, it is better to fix them first and solve for the unknown parameters, in the end making only slight changes in the parameters assumed *a priori*.

(b) *Multiple source model for far-infrared data*

There are a number of sources in the sky which are very strong emitters of far-infrared radiation: molecular clouds in our galaxy; external galaxies; protostars; and stars with circumstellar shells. In general, each of these sources can be approximated to be emitting like a blackbody at a certain temperature, with emissivity characteristic of the nature of the source. However, there are a number of sources for which we cannot make this simple approximation. Most often, the far-infrared emission is reradiation from dust grains heated by energetic photons from a hot source embedded in a dusty molecular cloud. The same is the case of a star with a circumstellar envelope. In such cases the far-infrared emission comes from two or more sources, namely, one stellar component and one (or more) dust component. What we observe is the sum of the radiation from those sources. The problem, therefore, is to decompose the observed far-infrared flux into the fluxes from two or more individual sources.

Let us assume that $p(\lambda_l)$ is the observed data from a source. We use here a simplified version of radiative transfer problem (Jones & Merrill 1976). We write down the following equation for the model $F(\lambda_l)$:

$$F(\lambda_l) = a \cdot B(\lambda_l, T_*) + \sum_{k=1}^{M} b_k . B(\lambda_l, T_k) \{1 - \exp(-2 d_k Q_k(\lambda_l))\},$$

where a, b_k are constants which physically represent the source size in steradians; $B(\lambda, T)$ is the well-known Planck's function for blackbody radiation given by

$$B(\lambda, T) = \frac{2hc}{\lambda^3} \frac{1}{\{e^{hc/KT\lambda} - 1\}}.$$

Here d_k is a constant; $Q_k(\lambda_l)$ are the far-infrared absorption efficiencies of a particular type of grains that we assume; T_* is the effective temperature of the star.

The data used, given in table 1, were obtained by Epchtein *et al.* (1980) on the peculiar symbiotic star R Aquarii in the region 9–30 μm when the star was in phase $\phi = 0.35$. The field of view was 15 arcsec for all the photometric bands. The effective temperature of the star was taken to be $T_* = 2800$ K. We can find readily that the fluxes in the region 9–30 μm cannot be accounted for by the star alone. We also know from the nature of the star that it is surrounded by circumstellar dust shells which have formed due to shedding of matter from the star in its late stage. We have assumed that silicate grains constitute the dust in the circumstellar envelope. The infrared absorption efficiencies for silicate grains were taken from Pegourie & Papoular (1985). Models were generated for various sizes of the grain and it was found that the best fit required a grain size of 0.5 μm. As given in table 1, we were able to explain the infrared fluxes observed by the following source parameters : (i) The star with effective temperature $T_* = 2800$ K and the solid angle $a = 1.0 \times 10^{-15}$ Sr and (ii) a dust shell with temperature $T_d = 430$ K and the solid angle $b = 7.0 \times 10^{-13}$ Sr. We point out here that the observational errors in the data are more than 10%. These errors will reflect in the model parameters also.

Table 1. R Aqr mid-infrared data compared with a two-temperature model

Wavelength	Flux density, janskys	
μm	Observations*	Model
9.6	879	898.6
10.0	994	951.8
12.0	623	668.4
20.0	424	416.6
30.0	174	144.0

*Data from Epchtein *et al.* (1980).
Model parameters : $T_* = 2800$ K; $a = 1.0 \times 10^{-15}$ Sr
$T_d = 430$ K; $b = 7.0 \times 10^{-13}$ Sr
Silicate grains of 0.5 μm size are assumed to constitute the dust shell.

5. Conclusions

We have developed a method and its algorithm to decompose observational data into a given number of nonlinear (or linear) functions. We have given two examples to show that physically meaningful solutions for the functional parameters can be obtained. When prior knowledge of the source is available, our method yields a better physical insight into the nature of the source. Though the mathematical method described here is a standardized one, the details of the usage of its algorithm depend very much on the particulars of the given data. Thus the algorithm is data-dependent.

Acknowledgement

This work was supported by the Department of Space, Government of India.

References

Anandarao, B. G., Sahu, K. C. & Desai, J. N. (1985) *Ap. Sp. Sci.* **114**, 351.
Burbidge, E. M., Burbidge, G. R. & Prendergast, K. H. (1959) *Ap. J.* **130**, 26.
Epchtein, N., Guibert, J., Rieu, N. Q., Turon, P. & Wamstekar, W. (1980) *Astr. Ap.* **85**, L 1.
Jones, T. W. & Merrill, K. M. (1976) *Ap. J.* **209**, 509.
Osterbrock, D. E., Miller, J. S. & Weedman, D. W. (1966) *Ap. J.* **145**, 697.
Pegourie, R. & Papoular, R. (1985) *Astr. Ap.* **142**, 451.
Powell, M. J. D. (1964, 1965) *Comp. J.* **7**, 155; 303.
Wilson, D. C. (1950) *Ap. J.* **111**, 279.