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A NONLINEAR HARMONIC ANALYZER *COMPAL*

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Abstract

A nonlinear method of least squares has been developed. The combination of the solution of the normal equations, the variational method, and the method of successive approximation, is used to give a compact approximation formula of sequential data. The method is superior to the usual method of nonlinear programming in that not only parameters but the number and form of basic functions are optimized. The method has been realized in COMPAL, the FORTRAN program for nonlinear harmonic analysis. Numerical tests show its merits to be as follows;

1) data are reproduced at any precision one likes as a linear combination of cosine waves with optimal amplitudes, frequencies and phases,
2) a high resolution is assured through a wide frequency range,
3) the variance of estimated frequency is evaluated as well as those for other estimates,
4) waves with different orders of magnitudes are detached,
5) it can handle waves whose wavelength is longer than the data length,
6) it works whether random noise is included in the data or not,
7) trend is determined simultaneously with other parameters,
8) the optimal number of terms of approximation formula is effectively determined.

Key Words: method of least squares—nonlinear programming—spectral analysis—multi-periodic phenomena

1. Introduction

The method of least squares has been a powerful tool in data processing. However two things are always troublesome to the user. One is what to choose as bases and the other is how many bases to choose. If groundless form or surplus number of bases are taken, the coefficient matrix of the normal equations will become singular and the method will come to a dead end. In order to avoid the above situation, bases are usually taken as a complete orthonormal system. The expansion in Fourier series is a typical case of that (Cheney, 1966). Though such expansion is easy and stable to be calculated, it would demand a number of terms to reproduce the data.

Why does such a trouble occur? The reason is that the choice of bases is inappropriate. If one can take necessary and sufficient number of bases so as to represent data well, the normal equations will be solvable even though bases are not orthogonal each other. Then how should such bases be determined? One of the answer is to represent each basis not as a function but as a sequential vector. The methods based on this idea include the method of spline functions (piecewise approximating polynomials) and the finite element

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method as well as the factor analysis (Hino, 1977). However such methods have two disadvantages. One is that the result is often difficult to be interpreted physically. The other is that the larger the data become, the more memories the methods demand. The latter may be a fatal one when one reproduces data and predicts the future tendency.

Another answer to the question above is to introduce some parameters into bases and optimize them. We will develop this idea in the present paper. In general, any smooth function can be represented by a set of some discrete and continuous parameters. This assertion can be proved by the existence of the Taylor expansion. For example, it is expressed by an integer parameter wheter a function is a cosine type or an exponential type, while it is expressed by two real parameters what frequency and phase a cosine function has. From the view of the the principle of least squares, the optimizing function would be a square sum of the residue. The parameters above are usually nonlinear so that the problem turns out to be a nonlinear programming both with discrete and continuous parameters. As for the number of such parameters and bases, the method of successive approximation will be utilized as will be stated in the next section.

From the view point to predict the future motion of observable quantities, there is another way which is slightly different from ours. That is to find a system of equations governing the observed phenomena. This typical example is the method of auto regression (Akaike, 1969) which is equivalent to the maximal entropy method (Burg, 1967). Our method may be equivalent to solve the equations above. Because, for example, to approximate data $f(t)$ as a linear combination of $\cos \omega t$ and $\sin \omega t$ is equivalent to give the equation governing data as $\ddot{f}+\omega^2 f=0$ and solve it. Clearly the way here is inferior to ours in the sense that it is difficult to reproduce data at any desired time.

We will state a general treatment for the nonlinear method of least squares in the following section. Then based on the treatment, a practical program whose name is COMPAL (COMPact Approximation by Least squares) is constructed in the case of harmonic analysis in Section 3. Using COMPAL, a variety of artificial data are analyzed in Section 4. In the final section, we summarize a number of excellent properties of COMPAL. As for the results of analysis by COMPAL for the natural complicated phenomena, the readers will refer to the paper of the author (1981) which analyzed the ephemerides of planets in the same volume of this report.

2. Method

We are concerned with finding an economical approximation of sequential data in the sense of least squares. In other words, we look for the function $g(\cdot)$ that can be evaluated fast, needs a few memories and minimizes the potential defined by

$$\phi=\frac{1}{2}(f-g, f-g)\equiv\frac{1}{2}\sum_{i=1}^{M}|f_i-g(t_i)|^2, \tag{1}$$

where f_i is a datum at $t=t_i$, inner product $(\cdot,\cdot)$ means product sum along sequence, and M denotes the number of data.

Generally an approximation function can be expressed as a linear combination of basic functions with some nonlinear parameters as follows,

$$g(t)=\sum_{j=1}^{N} c_j\ \phi_j(\{\omega_k\}\ ;t). \tag{2}$$

Here are four kinds of undefiniteness : the number of bases N, the form of bases $\{\phi_j(\cdot)\}$, linear coefficients $\{c_j\}$, and nonlinear parameters $\{\omega_k\}$. In this section we shall use the word 'coefficients' as linear coefficients and the word 'parameters' as nonlinear parameters. Note that the number of parameters K is not equal to that of bases. For simplicity we suppose that K is a function of N. Then the unknowns $\{c_j\}$, $\{\omega_k\}$, $\{\phi_j(\cdot)\}$ and N are determined as follows in the present method.

On the first stage, let all of them but coefficients be fixed. Then the problem reduces to find an usual least squares approximation and the optimal coefficients are determined by solving the normal equations

$$\sum_{j=1}^{N} c_j(\phi_j,\ \phi_i)=(f,\ \phi_i),\ i=1,\cdots\cdots,\ N. \tag{3}$$

In this sense the optimal coefficients are unique functions of parameters as long as the form and number of bases are fixed. Of course, the variance of estimated coefficients is easily obtained through the Gram matrix $G_{ij}=(\phi_i,\ \phi_j)$.

On the second stage, when the form and number of bases are fixed, parameters are determined by a sort of variational method since the normal equations for them are too complicated to be solved directly. The minimization algorythm of function with multivariables which was developed by Davidon (1959) and Fletcher and Powell (1960) is used for this purpose. This technique needs the minimization scheme on a line and the evaluation of the gradient vector at any point. As the former the combination of the regular falsi method and the parabolic interpolation method has been developed. The Newton-Raphson scheme and other methods using the gradient on a line often failed to reach the true minimum. Probably this is because the potential has a complicated structure and some spurious optima exist. The gradient vector of the potential is given as

$$\frac{\partial\phi}{\partial\omega_k}=\sum_{i=1}^{N}\sum_{j=1}^{N} c_i\ c_j\left(\phi_i,\ \frac{\partial\phi_i}{\partial\omega_k}\right)-\sum_{l=1}^{N} c_l\left(f,\ \frac{\partial\phi_l}{\partial\omega_k}\right), \tag{4}$$

where coefficients are optimal ones given by the normal equations. This combination of solving the normal equations and the variational method has been practically proved to be stably convergent and to save much computational time than the variational method only. This effect is remarkable in the case that the number of coefficients is greater than that of parameters. As the present minimization algorythm gives the inverse of the Hess matrix defined by

$$(H_{ij})^{-1}=\left(\frac{\partial^2\phi}{\partial\omega_i\ \partial\omega_j}\right)^{-1} \tag{5}$$

at minimal point. The variance of estimated parameters is easily obtained using this curvature matrix and the final decrement of potential.

On the third stage, the form of bases is determined as follows. We remark that the form of bases is identified by an integer as stated in the preceding section. Let coefficients and parameters be optimal under the given number and form of bases. Then the only way to

decrease the potential will be to add some new bases to the approximation function. We could find no elegant way to determine the number of bases to be added. We decided to add only one new basis in order not to introduce false components. As for the form of such a basis, our strategy is basically the rule of trial and error. It consists of the following five steps. On the first step, the residual data produced by old approximation function are fixed. On the second, some sets of parameters are supposed as the initial guesses for the new basis to be added. Not a single but multiple sets are selected in order to decrease the risk to extract spurious components. A sort of spectrum of the residue may be a great help for selecting them. Even though such tool is not available, the Monte Carlo method can be always used. Anyhow it is not much important how the initial guesses are generated. On the third, combinations with different form of functions are made for each obtained set of parameters. Of course the set of form of functions must be prepared before the method is applied. On the fourth, parameters of each combination are optimized to represent the residue as well as possible. This procedure is called the pre-minimization. Such decomposition of minimization procedure into a multi-stage scheme can be shown to save computational time since our minimization routine costs time in proportion to approximately the fourth powers of the number of indepedent variables. On the last, the best combination is determined so as to reduce the residue maximally. It is merged to the old bases after the independency of bases is checked by calculating the determinant of the Gram matrix. The non-zero Gram determinant assures the solvability of the normal equations.

On the last stage, the optimal number of bases is determined by the method of successive approximation. The approximation goes while increasing the number of bases one by one from zero. On every stage of approximation, parameters are optimized and a new basis introduced. Of course, *a priori* information on data may be utilized as the zeroth approximation. In the case of data without noise, the approximation is terminated when the desired precision is attained, i.e.

$$\underset{1 \leq i \leq M}{\mathrm{Max}} \, | f_i - g(t_i) | < \varepsilon, \qquad (6)$$

where ε denotes the permissible error. In the case of the data with noise, one can terminate the approximation when the potential becomes lower than a certain value. In the latter case, however, it is preferable to terminate when the residue becomes similar to white noise. This similarness can be measured by means of Fourier power spectrum since the power spectrum of ideal white noise is flat. Though this process is easy to be incorporated in an automatic routine, it is recommended for the user himself to see the spectrum and criticize.

Roughly speaking, our method goes as follows.

(0) Initial bases are supposed due to *a priori* knowledge. If such knowledge is not, go to (3).

(1) Parameters and coefficients are optimized to reduce the potential.

(2) It is criticized whether a further approximation is necessary or not.

(3) A new basis to be added is determined from the residual data.

(4) Return to (1).

Finally we show that it is easy to extend the method in a multi-dimensional case.

When one would like to analyze an I-dimensional data vector with a J-dimensional variable vector $\boldsymbol{f}(\boldsymbol{x})$, one only has to define an inner product $<\cdot,\cdot>$ and define the potential as

$$\phi\equiv\frac{1}{2}<\boldsymbol{f}-\boldsymbol{g},\ \boldsymbol{f}-\boldsymbol{g}>. \tag{7}$$

Then an I-dimensional approximation vector function $\boldsymbol{g}(\boldsymbol{x})$ is given by

$$\boldsymbol{g}(\boldsymbol{x})=\mathrm{C}\boldsymbol{\phi}(\boldsymbol{\omega}\,;\,\boldsymbol{x}), \tag{8}$$

where C denotes an $I\times L$ coefficient matrix, $\boldsymbol{\phi}(\cdot)$ an L-dimensional base vector function, and $\boldsymbol{\omega}$ a K-dimensional parameter vector. Note that all the dimension of vectors $\boldsymbol{g}$, $\boldsymbol{x}$, $\boldsymbol{\phi}$ and $\boldsymbol{\omega}$ are different each other in general. The normal equations and the gradient vector are easily obtained through differentiating the potential formally by coefficient matrix and parameter vector respectively.

3. Program COMPAL

The method of the preceding section has been realized in the FORTRAN program COMPAL, which was intended to be one dimensional harmonic analyzer. It seeks for a following approximation formula from the given data,

$$g(t)=c_0+c_1t+\sum_{j=1}^{J}(c_{2j}\cos\omega_jt+c_{2j+1}\sin\omega_jt)$$
$$+\sum_{k=J+1}^{K}(c_{2k}t\cos\omega_kt+c_{2k+1}t\sin\omega_kt), \tag{9}$$

where the amplitudes $\{c_j\}$, the frequencies $\{\omega_k\}$, and the number J and K are to be optimized.

The linear term t is added to cope with the data including a trend and/or waves with very low frequency. The mixed terms $t\cos\omega t$ and $t\sin\omega t$ are added by a different reason. Let the data consist of a pair of cosine waves with close frequencies ω and $\omega+\delta\omega$ where $|\delta\omega/\omega|\ll1$. If the approximation function has cosine type bases only, then the Gram matrix will be nearly singular as the optimization goes. The amplitudes of such waves will be enlarged by the order of $|\omega/\delta\omega|$ causing to loose a precision. The situation above is due to the inappropriate choice of basic functions and will be adjusted by choosing both $\cos\omega t$ and $t\cos\omega t$ as bases. Further mixed terms, t^2 or $t^2\cos\omega t$ for example, are not necessary since they can be represented well by the bases above. Of course, these linear and mixed terms can be excluded through an user's option.

The power spectrum by Fourier transformation is utilized to select the initial guesses of frequencies for the pre-minimization in notations of the precedeng section. It has been empirically shown that good initial guesses are pointed by the peaks with high Q-value or high power in the spectrum. We note that the frequency derivative of the approximation function are calculated as simple as

$$\frac{\partial g}{\partial\omega_k}=-c_{2k}t\sin\omega_kt+c_{2k+1}\,t\cos\omega_kt\quad 1\leqq k\leqq J,$$
$$=-c_{2k}t^2\sin\omega_kt+c_{2k+1}t^2\cos\omega_kt\quad J+1\leqq k\leqq K. \tag{10}$$

The program COMPAL is written in about 2300 structured FORTRAN statements. It needs memories in double precision (two words per one real variable) as many as

$$\{19+(9K^2+39K+4M)/1024\}\ \textit{Kilo words}, \tag{11}$$

where K and M denote the number of frequencies and data, respectively.

4. Numerical tests

Using COMPAL we have analyzed a group of data generated by following functions :

$$f_1(t)=\cos 4t+\cos 64t+\cos 65t+\cos 124.5t+p, \tag{12 a}$$

$$f_2(t)=\cos t+0.2p, \tag{12 b}$$

$$f_3(t)=-\sin t+0.2p, \tag{12 c}$$

$$f_4(t)=\cos 0.6t+0.2p, \tag{12 d}$$

$$f_5(t)=0.5+t/2\pi+\cos 10t+0.1\cos(25t+0.1)+0.01\cos(45t+0.2)+0.001\cos(70t+0.3), \tag{12 e}$$

where p is a uniform random noise with a range $0\leqq p\leqq 1$. The number of each set of data is 257 and the sampling rate is constant. The range of independent variable t is $-\pi\leqq t\leqq\pi$. Therefore the Nyquist frequency ω_N and the basic frequency ω_B are given as

$$\omega_N\equiv\frac{\pi}{\Delta t}=128,\quad \omega_B\equiv\frac{2\pi}{T}=1 \tag{13}$$

where Δt is the sampling rate and T is the data length (Hino, 1977).

All calculations were done in double precision (18 decimals) by NEC System 700 at Hydrographic Department.

The first generating function is taken from the paper of Radoski *et, al.* (1975) in order to test the resolution and effective range of frequency. The result is shown in Table 1. Here the first column of the Tables shows the number of iteration, the second the number of potential evaluation n which amounts to a great part of computing time, the third the accumulated computing time in second, the fourth the maximal absolute error in the same unit of data, the fifth the fraction of the frequency area A where the power is greater than 1% of the maximum in the spectrum of residue, and the last shows the analyzed result. Though the approximation is terminated when A exceeds 50%, one more iteration is examined to convince the effectiveness of the termination condition. Final estimations of frequency are following : 64.02 ± 0.06, 4.001 ± 0.004, 124.48 ± 0.07, 65.02 ± 0.06, where the estimated errors are calculated from the obtained Hess matrix. Considering that the mean and standard deviation of noise are 0.5 and $1/\sqrt{12}=0.289$ respectively, the obtained result is much satisfactory.

In order to examine the effect of phase and data length, the second three functions are taken from the work of Ulrych (1972) though the number of samples is different. The results are shown in Tables 2 through 4. As Urlych said in his paper, the usual Fourier spectral analysis cannot identify the frequency lower than the basic frequency. The results here show that a direct method as COMPAL is apt to handle with very low frequency phenomena.

Finally in order to see the effect of trend and amplitudes, the last function is examined. The result is shown in Table 5. As noise is excluded, the generating function is completely reproduced after five iterations.

Table 1 Data with noise : signal $= \cos 4t + \cos 64t + \cos 65t + \cos 124.5t$

Iter.	n	CPU (sec)	ε_{max}	A (%)	Result
1	1	7.5	4.04	8.0	0.502
2	1	15.2	2.87	11.3	0.497
					$+1.258 \cos(64.48t - 0.02)$
3	17	52.9	2.15	8.4	0.497
					$+1.250 \cos(64.48t - 0.01)$
					$+1.018 \cos(4.00t + 0.00)$
4	27	92.5	1.42	34.8	0.497
					$+1.251 \cos(64.48t + 0.00)$
					$+1.018 \cos(4.00t + 0.00)$
					$+1.003 \cos(124.48t - 0.02)$
5	96	193.5	0.60	93.0	0.502
					$+1.015 \cos(64.02t - 0.02)$
					$+1.027 \cos(4.00t + 0.00)$
					$+1.001 \cos(124.48t - 0.02)$
					$+0.934 \cos(65.02t + 0.01)$
6	32	258.0	0.53	92.8	0.502
					$+1.016 \cos(64.02t - 0.02)$
					$+1.027 \cos(4.00t + 0.00)$
					$+1.001 \cos(124.48t - 0.02)$
					$+0.933 \cos(65.02t + 0.01)$
					$+0.091 \cos(57.95t - 1.69)$

Table 2 Data with noise : signal $= \cos t$

Iter.	n	CPU (sec)	ε_{max}	A (%)	Result
1	1	7.3	1.09	3.3	0.096
2	22	46.1	0.11	93.8	0.102
					$+1.004 \cos(1.006t - 0.010)$
3	22	80.3	0.12	95.1	0.102
					$+1.004 \cos(1.006t - 0.010)$
					$+0.216t \cos(112.40t - 2.44)$

Table 3 Data with noise : signal $= -\sin t$

Iter.	n	CPU (sec)	ε_{max}	A (%)	Result
1	1	7.4	1.08	1.8	0.098
2	9	29.2	0.11	91.8	0.098
					$+0.993 \cos(1.000t + 1.570)$
3	34	65.9	0.12	94.1	0.098
					$+0.993 \cos(1.000t + 1.570)$
					$+0.019 \cos(15.635t - 1.785)$

Table 4 Data with noise : signal=cos 0.6 t

Iter.	n	CPU (sec)	ε_{max}	A (%)	Result
1	1	7.2	0.90	4.9	0.606
2	17	38.2	0.10	91.0	0.093
					+1.008 cos (0.597 t −0.013)
3	16	65.2	0.12	92.2	0.094
					+1.007 cos (0.597 t −0.013)
					+0.021 cos (111.56 t +2.99)

Table 5 Data without noise : signal=0.5+ $t/2\pi$+cos 10t+0.1 cos (25 t +0.1) +0.01 cos (45 t +0.2)+0.001 cos (70 t +0.3)

Iter.	n	CPU (sec)	ε_{max}	A (%)	Result
1	1	10.3	1.111	3.7	0.49997
					+1.01677 $t/2\pi$
2	11	32.4	0.111	3.5	0.49992
					+0.99329 $t/2\pi$
					+0.99998 cos (10.001 t +0.000)
3	22	63.8	0.011	3.5	0.50000
					+0.99958 $t/2\pi$
					+0.99999 cos (10.000 t +0.000)
					+0.09999 cos (24.999 t +0.100)
4	41	119.1	0.001	3.3	0.50000
					+1.00001 $t/2\pi$
					+1.00000 cos (10.000 t +0.000)
					+0.10000 cos (25.000 t +0.100)
					+0.01000 cos (45.000 t +0.200)
5	57	204.3	3.85E-11	—	exactly same as signal

5. Concluding remarks

The numerical tests in the preceding section show the effectiveness of COMPAL as follows : 1) the input signal is reproduced with high accuracy, 2) not only frequencies but also amplitudes and phases are determined from data, 3) a high resolution is achieved in a wide frequency range, 4) low frequency phenomena can be handled, 5) the variance of estimated quantities can be evaluated, 6) waves with different orders of amplitudes are detached, 7) it works well whether noise is included in the data or not, 8) trend is determined simultaneously with other parameters, 9) the optimal number of approximating terms is effectively determined.

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