TEMPO

THE ITERATIVE DETERMINATION OF MODEL PARAMETERS BY NEWTON'S METHOD

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THE ITERATIVE DETERMINATION OF MODEL PARAMETERS BY NEWTON'S METHOD

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The problem that we would like to solve is to determine numbers $a_1, a_2, \ldots, a_N$ and $\Delta_1, \Delta_2, \ldots, \Delta_N$ so that, with regard to an observation e(t) and for unknown N, the equation

$$e(t) = \sum_{K=1}^{N} a_K \; s(t-\Delta_K) \tag{1}$$

is satisfied.

Let us define

$$y(t;x) = \sum_{K=1}^{N} x_K \; s(t-x_{N+K}) - e(t). \tag{2}$$

In keeping with the spirit of Newton's method for finding the root of a function of one variable, we are looking for a vectorial increment δx such that

$$y(t;x+\delta x) = y(t;x) + \sum_{K=1}^{2N} \frac{\partial y}{\partial x_K} \delta x_K + \text{terms of higher order} = 0.$$

Thus we have an equation

$$\sum_{K=1}^{2N} \frac{\partial y}{\partial x_K} \delta x_K = -y(t;x) \tag{3}$$

from which to determine the incremental vector components δx_K. At this point it is important to recall that both members of Equation 3 are functions of t. In order to eliminate t and obtain 2N equation in 2N unknowns we could, for example, choose 2N values of t, $t_1, t_2, \ldots, t_{2N}$ and evaluate both members of Equation 3 at these t values. In a real situation this procedure has the drawback that the demands for accuracy placed on the values of y and its partial derivatives at the special t points would be too great. In the presence of noise (due to inaccuracies in measurement, in the model, round-off errors, etc.) the above method of creating 2N equations in the 2N unknowns should be rejected as being unstable.

Actually, however, this method is just one realization of a general method of deriving 2N equations in 2N unknowns from Equation 3. The general method postulates that 2N linear functionals be chosen $\gamma_1, \gamma_2, \ldots, \gamma_{2N}$ and applied to both members of Equation 3. The result is then

$$\sum_{\kappa=1}^{2N} \gamma_\iota \left(\frac{\partial y}{\partial x_\kappa} \right) \delta x_\kappa = -\gamma_\iota (y) . \quad (\iota = 1, 2, \ldots, 2N) . \tag{4}$$

We now have a non-homogeneous linear system of equations in the unknown δx_κ ($\kappa = 1, 2, \ldots, 2N$) and this system has a unique solution only if the matrix M with elements

$$M_{\iota\kappa} = \gamma_\iota \left(\frac{\partial y}{\partial x_\kappa} \right) \tag{5}$$

is non-singular and the vector g with elements

$$-\gamma_\iota (y) \tag{6}$$

does not vanish.

It is necessary to say a word about the notion of a linear functional γ. γ associates with each member f of a class of functions a number $\gamma(f)$ in such a way that if f and g are any two functions in the class, α and β are any two numbers, and that if the function $\alpha f + \beta g$ also belongs to the class, then

$$\gamma(\alpha f + \beta g) = \alpha \gamma(f) + \beta \gamma(g).$$

If the class of functions consists of all those which are square integrable over the real axis, then by the celebrated Riesz-Fischer theorem* every bounded functional γ has the representation

$$\gamma(f) = \int_{-\infty}^{\infty} f(x)\, \overline{h_\gamma(x)}\, dx ,$$

where h_γ is a square integrable function corresponding to the linear functional γ and the bar denotes complex conjugate.

After this brief digression let us return to Equation 4 to see how it can be used to approach a solution by iteration. Suppose at the R^{TH} step an approximate solution Z^R has been calculated. To determine the next, hopefully improved, approximant Z^R, we set

$$\delta x^R = Z^{R+1} - Z^R$$

and let

$$M_{LK}^R \equiv \gamma_L^R \left(\frac{\partial y}{\partial x_K} \right)^R \text{ and} \tag{7}$$

$$g_L^R \equiv - \gamma_L^R (y^R) . \tag{8}$$

Then

$$M^R Z^{R+1} = M^R Z^R - g^R \tag{9}$$

and if M^R has an inverse, then

$$Z^{R+1} = Z^R - (M^R)^{-1} g^R . \tag{10}$$

It can be shown† that if the initial guess Z^0 is sufficiently close to a solution, then the sequence of approximants $Z^0, Z^1, Z^2, \ldots$ converges to the solution.

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* Halmos, Paul P., Introduction to Hilbert Space, Chelsea Publishing Company, New York, 1951, p 31.

† Stern, M. L., "Sufficient conditions for the convergence of Newton's Method in complex Banach spaces", Proc. Amer. Math. Soc., vol 3, (1952) pp 858-863.

It is apparent that one of the major problems with the method is the selection of a good initial approximant Z°. Two methods have been been devised to obtain approximate solutions for Equation 1. The first will be called the Fourier method. Taking the Fourier transform of both members of Equation 1, the result is

$$E(f) = \left(\sum_{\kappa=1}^{N} a_{\kappa} e^{-2\pi i f \Delta_{\kappa}} \right) S(f). \tag{11}$$

This expression is, however, valid only for those frequencies for which S(f) and E(f) do not vanish, that is, only for the frequencies that lie in the common band in case s and consequently e are bandlimited. If in Equation 11 we divide both members by S(f) and then take the inverse Fourier transform of the result, we obtain

$$d(t) = \sum_{\kappa=1}^{N} a_{\kappa} \int_{\Omega} e^{2\pi i f(t-\Delta_{\kappa})} df , \tag{12}$$

where Ω represents the pertinent band of frequencies.

If $\Omega = \left| f - \frac{w}{2} \leq f \leq \frac{w}{2} \right|$, then

$$d(t) = \sum_{\kappa=1}^{N} a_{\kappa} \frac{\sin \pi w(t-\Delta_{\kappa})}{\pi(t-\Delta_{\kappa})} \tag{13}$$

and the values of $\Delta_1, \Delta_2, \ldots, \Delta_N$ can be estimated as the position of the maxima of d(t). The values of $a_1, a_2, \ldots, a_N$ are approximated by the magnitudes of d(t) at the observed maxima. The limit of resolution of this method is about 1/w, i.e., if $\Delta_i - \Delta_{i+1} < 1/w$, then the corresponding two maxima will have moved together so as to yield only one maximum.

If $\Omega = \left\{ f \,\middle|\, -\frac{w}{4} - w_c \leq f \leq -w_c + \frac{w}{4} , w_c - \frac{w}{4} \leq f \leq w_c + \frac{w}{4} \right\}$, then

$$d(t) = \sum_{K=1}^{N} a_K \left\{ \frac{\sin \pi (2w_c + w/2)(t-\Delta_K) - \sin \pi (2w_c - w/2)(t-\Delta_K)}{\pi (t-\Delta_K)} \right\} \quad (14)$$

or

$$d(t) = 2 \sum_{K=1}^{N} a_K \cos 2\pi w_c (t-\Delta_K) \frac{\sin \pi w/2 (t-\Delta_K)}{\pi (t-\Delta_K)} . \quad (15)$$

Again the same method for estimating the Δ's and a's can be used.

If $\Omega = \left\{ f \mid w_c - \frac{w}{2} \leq f \leq w_c + \frac{w}{2} \right\}$,

then

$$d(t) = \sum_{K=1}^{N} a_K e^{2\pi i w_c (t-\Delta_K)} \frac{\sin \pi w (t-\Delta_K)}{\pi (t-\Delta_K)} \quad (16)$$

and the real part will again have maxima near the points $t=\Delta$ and the magnitudes of these maxima will be close to a_K.

The second method, based on correlation, can also be used for obtaining first estimates. Let us multiply both members of Equation 1 by s(t-z) and integrate over all values of the variable t . We can then write

$$R_{s,\varepsilon}(z) = \sum_{K=1}^{N} a_K R_{s,s}(z-\Delta_K) , \quad (17)$$

where

$$R_{f,g}(z) \equiv \int_{-\infty}^{\infty} f(t-z)\, g(t)\, dt . \quad (18)$$

If the Δ_K are sufficiently separated, i.e., by more than 1/w, then the position of the maxima of $R_{s,\varepsilon}(z)$ provides first estimates for $\Delta_1, \Delta_2, \ldots \Delta_N$ and the magnitudes of the maxima divided by $R_{s,s}(o)$ provide estimates for $a_1, a_2, \ldots, a_N$.

Having found first estimates of $\Delta_1, \Delta_2, \ldots, \Delta_N$ and $a_1, a_2, \ldots, a_N$, we must now seek to improve them by iteration. The requirements for a good iterative method are:

1. Improvement of resolution. If one maximum actually corresponds to two separate components, the method should be able to resolve the two components.

2. If some secondary maxima have been confounded with primary maxima the iterative method should be capable of eliminating them.

3. Finally, an improvement in accuracy in the evaluation of $\Delta_1, \ldots, \Delta_N$ should result from the application of the method.

Once the initial estimates have been made we turn to Newton's method for their improvement. To this end we must choose functionals $\gamma_1, \ldots, \gamma_{2N}$.

Let

$$\gamma_i(f) = \int_{-\infty}^{\infty} f(t)\, s(t-x_{i+N})\, dt$$

and

$$\gamma_{i+N}(f) = \int_{-\infty}^{\infty} f(t)\, \{-x_i\, s'(t-x_{i+N})\}\, dt ,$$

where s' denotes the derivative of s. The matrix M^R, defined by Equation 7, takes the form

$$M_{LK}^{R} = \int_{-\infty}^{\infty} s(t-x_{K+N}^{R})\; s(t-x_{L+N}^{R})\; dt$$

$$M_{L+NK}^{R} = \int_{-\infty}^{\infty} s(t-x_{K+N}^{R})\; \{-x_L^R\; s'(t-x_{L+N}^{R})\}\; dt$$

$$M^R_{L,K+N} = \int_{-\infty}^{\infty} \{-x^R_K \, s'(t-x^R_{K+N})\} \, s(t-x^R_{L+N}) \, dt$$

$$M^R_{L+N,K+N} = \int_{-\infty}^{\infty} \{-x^R_K \, s'(t-x^R_{K+N})\} \{-x^R_L \, s'(t-x^R_{L+N})\} \, dt$$

for $L = 1, 2, \ldots, N$ and $K = 1, 2, \ldots, N$.

By using the notion of convolution or correlation we can write the above matrix elements more conveniently as

$$M^R_{L,K} = R_{s,s}(x^R_{K+N} - x^R_{L+N})$$

$$M^R_{L+N,K} = -x^R_L \, R_{s,s'}(x^R_{K+N} - x^R_{L+N})$$

$$M^R_{L,K+N} = -x^R_K \, R_{s',s}(x^R_{K+N} - x^R_{L+N})$$

$$M^R_{L+N,K+N} = x^R_K x^R_L \, R_{s',s'}(x^R_{K+N} - x^R_{L+N})$$

for $L = 1, 2, \ldots, N$ and $K = 1, 2, \ldots, N$.

But

$$\frac{\partial R_{s,s}(\tau)}{\partial \tau} = -\int_{-\infty}^{\infty} s'(t-\tau)\, s(t)\, dt = -R_{s',s}(\tau)$$

and

$$\frac{\partial^2 R_{s,s}(\tau)}{\partial \tau^2} = \int_{-\infty}^{\infty} s'(t-\tau)\, s'(t)\, dt = R_{s',s'}(\tau).$$

Therefore,

$$
\begin{aligned}
M^R_{L,K} &= R_{s,s}(\tau)\Big|_{\tau = (x^R_{K+N} - x^R_{L+N})} \\
M^R_{L+N,K} &= x^R_L \frac{\partial R_{s,s}}{\partial \tau}\Big|_{\tau = (x^R_{K+N} - x^R_{L+N})} \\
M^R_{L,K+N} &= x^R_K \frac{\partial R_{s,s}}{\partial \tau}\Big|_{\tau = -(x^R_{K+N} - x^R_{L+N})} \\
M^R_{L+N,K+N} &= x^R_K x^R_L \frac{\partial^2 R_{s,s}}{\partial \tau^2}\Big|_{\tau = (x^R_{K+N} - x^R_{L+N})}
\end{aligned}
\qquad (19)
$$

for L = 1, 2, ..., N K = 1, 2, ..., N K = 1, 2, ..., N

The vector g^R whose components are given by Equation 8 takes the form

$$
\begin{aligned}
g^R_L &= \int_{-\infty}^{\infty} e(t)\, s(t - x^R_{L+N})\, dt = R_{s,\varepsilon}(x^R_{L+N}) \\
g^R_{L+N} &= \int_{-\infty}^{\infty} e(t) \{ -x_L\, s'(t - x^R_{L+N}) \}\, dt = x_L \frac{\partial R_{s,\varepsilon}}{\partial \tau}\Big|_{\tau = x^R_{L+N}} .
\end{aligned}
\qquad (20)
$$

Equations 19 and 20 show that the only data that we require for the application of Newton's method are the correlation functions $R_{s,s}$ and $R_{s,\varepsilon}$. If these are furnished by observation, numerical differentiation will yield the remaining matrix and vector elements.

In the course of iteration it is necessary to update the matrix M and the vector g at each step. This, however, is very easily done since it involves no more than a table look up of the values of functions and their derivatives at new values of their arguments.

To test the ideas presented above by means of an example, the choice was made of

$$S(t) = \frac{\sin(\pi t)}{(\pi t)} .$$

This choice is motivated not only by the desire to generate a test, but also by the notion that upon transformation by the Fourier method Equation 1 takes the form of Equation 13 which is the same as that of Equation 1 when the above choice is made. Therefore, with this choice we can proceed to solve Equation 13 directly by Newton's method.

To determine the matrix elements consider

$$R_{s,s}(\tau) = \int_{-\infty}^{\infty} \frac{\sin \pi (t-\tau)}{\pi (t-\tau)} \frac{\sin \pi t}{\pi t} dt$$

$$= \int_{-\infty}^{\infty} e^{2\pi i f \tau} \left| X(f) \right|^2 df = \frac{\sin \pi\tau}{\pi\tau} ,$$

where $X(f) = 1$ for $-1/2 \le f \le 1/2$ and $X(f) = 0$ for $|f| > 1/2$.

$$\frac{\partial R_{s,s}}{\partial \tau} = \pi \left. \frac{x\cos x - \sin x}{x^2} \right|_{x = \pi\tau}$$

$$\frac{\partial^2 R_{s,s}}{\partial \tau^2} = \frac{\pi^2}{x^4} \left[-2x^2 \cos x + x(2-x^2) \sin x \right]_{x = \pi\tau} .$$

A program (listed in the Appendix) was written to carry the calculations through numerically. Tests were performed on a weighted sum of delayed and truncated replicas of six πt/πt. Then tests showed that convergence, when it occurred, was rapid. We had numerical difficulties in high dimensions because of the many matrix inversions involved. The program was, however, able to resolve two pulses that were separated by 0.2, that is, by 0.2 of the normal resolution limit.

In order to facilitate decisions as to the best value of N, the mean square difference between the function **e** and its approximant was calculated and that solution was adopted as the final one which had a number of components yielding the smallest mean square difference.

A possible improvement might be had by evaluating the gradient of y, i.e., $\{ \partial y/\partial x_k \}$, at some point other than the last approximant to the zero. Work to realize this idea is going on at present and will be reported subsequently.

CONCLUSION

A method for solving the functional equation

$$e(t) = \sum_{K=1}^{N} a_K \, s(t-\Delta_K)$$

is presented. The method adapts the idea of Newton's method to the case at hand which differs from the classical situation in that the functions whose zeroes are sought are themselves elements of a function space. To illustrate the method a program was written that demonstrated a marked improvement in resolution for pulses of the form sin(πt) / (πt). One of the drawbacks of the method is that initial guesses have to be close to the actual solution. Another difficulty arises from the fact that since N is unknown, solution must be attempted with various values of N.

APPENDIX

```
IT-1       0:18   SB MON 09/05/67

1 FILE K-R
10 DIM E(256)
20 DIM M(20,20),W(20,20),F(20,1),Q(20,1),A(10),D(10)
25 READ T0,A0,B0,B
30 FOR I=1 TO T0\READ FILE 1,E(I)\NEXT I
40 P1=3.1415927
60 FOR S=1 TO 100\INPUT T1,L2
70 T=2*T1
110 FOR I=1 TO T1\INPUT A(I),D(I)\NEXT I
120 FOR L1 =1 TO L2
130 MAT M=ZER(T,T)
140 MAT W=ZER(T,T)
150 MAT Q=ZER(T,1)
200 MAT F=ZER(T,1)
210 FOR J=1 TO T1\FOR I=1 TO T0
220 A1=P1*(A0*I-B0-D(J))
230 IF ABS(A1)<=.000001 THEN 270
240 F(J,1)=F(J,1)+E(I)*SIN(A1)/(A1*B)
250 F(T1+J,1)=F(T1+J,1)-E(I)*P1*(A1*COS(A1)-SIN(A1))/(A1↑2)
260 GO TO 280
270 F(J,1)=F(J,1)+E(I)/B
280 NEXT I
285 F(T1+J,1)=A(J)*F(T1+J,1)
290 NEXT J
295 MAT F=(A0)*F
300 FOR I=1 TO T1
310 FOR J=1 TO T1
320 K=P1*(D(J)-D(I))
325 IF ABS(K)<=.00001 THEN 400
330 M(I,J)=SIN(K)/(K*B)
340 M(T1+I,T1+J)=A(I)*A(J)*(P1↑2)*B*(2*K*COS(K)+((K↑2)-2)*SIN(K))/(K↑3)
350 M(I,T1+J)=P1*A(J)*(K*COS(K)-SIN(K))/(K↑2)
360 GO TO 490
400 M(I,J)=1/B
410 M(T1+I,T1+J)=A(I)*A(J)*B*(P1↑2)/3
420 M(I,T1+J)=0
430 M(T1+I,J)=0
490 NEXT J\NEXT I
495 FOR I=1 TO T1\FOR J=1 TO T1\M(I+T1,J)=M(J,T1+I)
496 NEXT J\NEXT I
497 FOR I=1 TO T\FOR J=1 TO T\IF ABS(M(I,J))>=10 E-11 THEN 500
498 M(I,J)=0\NEXT J\NEXT I
500 MAT W=INV(M)
510 MAT Q=W*F
520 FOR J=1 TO T1
530 A(J)=Q(J,1)
540 D(J)=D(J)+Q(T1+J,1)
550 NEXT J
560 NEXT L1
600 FOR I=1 TO T1
610 PRINT I;A(I);D(I)
620 NEXT I
630 NEXT S
700 DATA 100,.1,5,1
9999 END
```

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The principle of Newton's method for determining a zero of a function has been adopted to the problem of determining parameters $a_1, a_2, \ldots, a_n$ such that $y(t; a_1, a_2, \ldots, a_n) = 0$ for almost all values of t. The method has been applied to the solution of a particular equation. Methods for determining initial guesses are also presented.

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