N84-26353

NASA

Technical Memorandum 86097

MODIFICATION TO SHOCK FITTING PROGRAM

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APRIL 1984

National Aeronautics and
Space Administration

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ABSTRACT

A modified form of the Lepping - Argentiero single spacecraft, shock normal determination procedure is presented. The modified method incorporates a simple predictor-corrector algorithm which allows a faster convergence rate and the use of average values of the parameters for the starting vector.

INTRODUCTION

A technique and associated computer program developed by Lepping and Argentiero (1971) to least-squares fit a sub-set of the Rankine-Hugoniot equations to shock-related plasma and magnetic field data, is modified in this note for the purpose of increasing the program's speed and efficiency and making unnecessary the need for multiple starting conditions in the iterative scheme. Originally the fitting scheme employed a standard Newton-Raphson numerical iterative procedure to solve simultaneously a set of eight nonlinear equations, denoted equations (36) in the original paper and equations (1) below. The iterative technique is described by Deutsch (1965). When convergence did not result, one was required to repeat the procedure using a different "starting vector" ($\vec{Z}_o$), the eight components of which constituted the independent plasma and field variables to be adjusted. The simple modification suggested here, as well as making the use of more than one starting vector unnecessary, in general speeds up convergence by eliminating occasional large "overshoots" in the iterative procedure.

Formulation

We denote $\hat{Z}$ as the exact solution of

$$\frac{\partial L(\vec{Z})}{\partial X_i} = 0 \qquad (i = 1,\ldots\ldots 8) \tag{1}$$

where

$$L(\vec{Z}) = \sum_{i=1}^{11} \sum_{j=1}^{N(i)} \left(\frac{X_i - Y_i^{(j)}}{\sigma_i} \right)^2 \tag{2}$$

with $\vec{Z} \equiv (X_1, X_2, \ldots X_8)$, and where $Y_i^{(j)}$ $(i = 1, .. 11;\ j = 1 .. N(i))$ are

the input data for the eleven physical quantities of interest, N(i) data points each, usually arranged in the following order:

B_{1x}, B_{1y}, B_{1z}, B_{2x}, B_{2y}, B_{2z}, $V_{2y} - V_{1y}$, $V_{2z} - V_{1z}$, N_1, N_2, and $V_{2x} - V_{1x}$

(i.e., components of the magnetic field, plasma velocity differences and densities, where the subscripts 1 and 2 represent pre-shock and post-shock states, respectively), and

$$\sigma_i \qquad (i = 1, .. 11)$$

are the "sigma noise parameters" used as weights in the least squares procedure and usually composed principally of the rms deviations of the measured physical quantities of interest (Y_i's), and finally

$$X_i \qquad (i = 1, ... 8)$$

are the independent variables (components of $\vec{Z}$) to be solved for, physically representing the first eight quantities of Y_i. Note that X_9 ($\equiv N_1$), X_{10} ($\equiv N_2$) and X_{11} ($\equiv V_{2x} - V_{1x}$) are related to X_i (i = 1, ... 8) by the three lowest order Rankine-Hugoniot equations, which play the key role of providing a constraint on the nonlinear least-squares process [see equations (18), (19), and (20) in Lepping and Argentiero (1971)].

We denote $\vec{Z}_n$ ($n = 1, ...n_{max}$) as an estimate of $\hat{Z}$ at iteration step n. The components of $\vec{Z}_o$, the starting vector, are commonly the <u>averages</u> of the first eight components, Y_i. Then at step n

$$\Delta\vec{Z}_n \equiv \vec{Z}_n - \vec{Z}_{n-1} \tag{3}$$

When a "best estimate" of $\hat{Z}$ is obtained, the magnetic field components, i.e., the first six components of that estimate of $\hat{Z}$, are used in the magnetic coplanarity formula (Colburn and Sonett, 1966) to obtain a "best estimate" of the shock normal.

The original computer program is described in the Appendix of Lepping and Argentiero (1970).

Modification of Scheme

At each step n the quantity L, given by equation (2) and referred to as the least squares "loss function", can be evaluated. Our basic purpose is to minimize $L(\vec{Z})$, as in equation (1). In order to avoid divergence of $|\Delta\vec{Z}_n|$ and $L(\vec{Z})$, we make a slight modification of the iteration procedure by allowing a choice of two branches in the fitting program, which are defined by the following:

First branch - If at step n $\quad L_n \leq L_{n-1}$, then

$$\Delta\vec{Z}_n = \vec{Z}_n - \vec{Z}_{n-1}, \tag{4}$$

as in the original scheme.

Second branch - If at step n $\quad L_n > L_{n-1}$, then

$$\Delta\vec{Z}_n = (L_{n-1}/L_n)\ (\vec{Z}_n - \vec{Z}_{n-1}). \tag{5}$$

This continues step by step until n equals a pre-chosen integer, M say, or until

$$(|\Delta\vec{Z}_n|/|\vec{Z}_{n-1}|) \leq \varepsilon \tag{6}$$

for some sufficiently small $\varepsilon > 0$. Notice that the second branch differs from the unmodified first branch only in that the length of each step along $\Delta\vec{Z}_n$(unmodified) is shortened according to the ratio of the new to the old loss function.

We have found in numerous cases that this simple modification has decreased, and sometimes significantly, the time needed to run the fitting program and/or the operator's efforts in finding a proper starting vector. In

extreme cases, for a given $\vec{Z}_o$, the original program would occasionally wander around the neighborhood of L_{min} with there being no apparent hope of satisfying (6) for a reasonable ε, especially when the gradient of $L(\vec{Z})$ was shallow near L_{min}, i.e., for poorly conditioned cases. This modification should eliminate that problem. Although not a unique solution to the convergence problem, this type of modification is attractively simple.

Example

Here we show the benefit of using the modified program by comparing its results with those of the unmodified program for a somewhat poorly behaved case; we have encountered much worse cases but they are not typical and therefore not good examples.

We examine a shock observed on Pioneer 6 at 2058 U.T. on March 22, 1966, which was first studied by Chao (1970); he graphically displays and discusses the data, which are from the Goddard magnetometer and the MIT plasma probe onboard the spacecraft. The right side ("DATA") of Table 1 shows the tabulated data points constituting 12.5 minutes of upstream field data, 14 minutes of downstream field data (partially decimated), and ±22.5 minutes of all plasma quantities. The analysis intervals were chosen on the basis of apparent steadiness of the data. All data are given in an R-T-N coordinate system, centered at the spacecraft, where $\hat{R}$ is positive radially away from the sun, $\hat{T}$ is perpendicular to $\hat{R}$, parallel to the ecliptic plane and positive in the direction of the earth's motion about the sun, and $\hat{N} = \hat{R} \times \hat{T}$. On the left side of the table are best estimate (B.E.) values from both the modified and unmodified programs, straight averages (AVG) of the quantities, and the associated sigma noise parameters (SIG), which in this case were simply rms deviations of the data values. The modified program converged to the B.E. value in 3 iterations where the AVG's were used for the components of the starting vector. By contrast the unmodified program required 11 steps when again the AVG starting vector was used. In the unmodified program the loss function L had the undersirable feature of oscillating in value, as shown in Table 2; the table also shows the monotonically decreasing values of L that the modified program produced, as expected. The table also gives a related quality factor defined below the table. We stress the case where AVG's were

used for the starting vector, $\vec{Z}o$, since that is obviously the easiest and most commonly used choice, as stated above. However, for this shock several other apparently reasonable $\vec{Z}_o$'s were attempted using the unmodified version of the program, and some did not give convergence after 15 interation steps; the program was set to stop at the 15th step.

It must also be emphasized that the selection of an optimum fitting coordinate reference frame is important in assuring proper and speedy convergence. The implementation of the modified and unmodified procedures have included interactive facilities to conveniently rotate the data into one of three orthogonal alignments such as to assure the optimum selection of dependent and independent variables in the fitting procedure. In general, the quantities exhibiting the greatest variability or uncertainty should be selected as the dependent variables to be least-squares estimated.

The best estimate shock normal, based on the B.E. values in Table 1, is

$$\hat{n}_{B.E.} = (n_R, n_T, n_N) = (0.94, -0.15, 0.31),$$

and the associated 95% certainty error cone half-angle was 7.7° (Lepping and Argentiero, 1971). [If AVG value fields had been used, the error cone half-angle would have been 3.3 times larger!]. By comparison Chao's estimate of the shock normal was

$$\hat{n}_{CHAO} = (0.84, -0.10, 0.54),$$

differing by 13.6° from our estimated direction. The shock was a rather typical oblique one (at 1 AU), whose B.E. normal was 59° from the upstream field direction $\vec{B}^{(1)}{}_{BE}$ and whose magnitude ratio across the shock was

$$|B^{(2)}{}_{BE}|/|B^{(1)}{}_{BE}| = 1.80.$$

We stress how different the velocity difference vector $\vec{W}$ = (WR, WT, WN) is between the B.E. and AVG values, especially in the WN component, as Table 1 shows. The angle between $\vec{W}_{BE}$ and $\vec{W}_{AVE}$ is 17.1°. If one were to use "velocity

coplanarity" (Abraham-Shrauner, 1972) and AVG values, the resulting shock normal would be

$$\hat{n}_{vel} \approx \vec{W}_{AVG}/|\vec{W}_{AVG}| = (0.69,\ -0.20,\ 0.70),$$

which differs by 26.4° from our best estimate normal; the author warns that this method is an approximation. Our added warning is that using average values is often inadequate. For example, we see that by using the B.E. $\vec{W}$ and velocity coplanarity we obtain

$$\hat{n}'_{vel} \approx \vec{W}_{BE}/|\vec{W}_{BE}| = (0.86,\ -0.23,\ 0.46),$$

which is only 9.8° from $\hat{n}_{BE}$. Obviously in all of the above we have made the tacit assumption, argued in Lepping and Argentiero (1971), that $\hat{n}_{BE}$ is indeed generally the best estimated shock normal from data from a single spacecraft.

Many such examples can be found to show the desirability of using the modified version of the 'best-fit' technique.

Acknowledgement

We thank K. Behannon for reading and commenting on this note.

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TABLE 1

March 22, 1966 Pioneer 6 Event

B.E.	AVG	STG	Quantity*		DATA												
1.78	1.96	1.29	Y_1	B_1T	1.3	1.5	1.1	0.6	0.6	0.4	1.0	2.7	2.9	3.0	2.2	3.5	4.7
-3.40	-3.64	0.48	Y_2	B_1N	-4.2	-4.0	-4.5	-4.2	-3.8	-3.7	-3.5	-3.4	-3.2	-3.3	-2.9	-3.2	-3.4
4.72	4.82	0.43	Y_3	B_1R	4.2	4.4	4.1	4.6	5.2	5.2	5.3	5.1	4.9	4.9	5.5	4.8	4.5
4.07	4.00	0.80	Y_4	B_2T	3.0	4.8	3.1	4.6	4.6	4.0	3.9						
-7.82	-7.66	0.40	Y_5	B_2N	-7.2	-7.8	-7.2	-7.9	-7.8	-8.0	-7.7						
6.54	6.34	0.60	Y_6	B_2R	7.1	6.8	6.7	6.2	5.6	6.0	6.0						
31.6	56.6	25.0	Y_7	WN	65.0	12.3	88.1	65.2	64.9	34.5	66.0						
59.3	55.7	12.6	Y_8	WR	42.2	60.8	49.9	52.3	48.2	73.3	62.9						
4.30	3.97	0.34	Y_9	N1	4.4	4.0	4.3	3.8	3.8	3.8	3.7						
8.22	9.63	0.98	Y_{10}	N2	9.9	8.1	9.7	9.8	10.0	9.1	10.8						
-15.9	-16.2	10.6	Y_{11}	WT	-23.2	-6.5	-23.3	-21.0	-23.1	-13.4	-3.1						

*Note that $\vec{W} \equiv \vec{V}_2 - \vec{V}_1$.

TABLE 2

Loss Function Values

Iteration Step	L-unmodified (Q*)		L-modified (Q*)	
0 {Starting vector	1,095	(.295)	455	(.457)
1	19,360	(.070)	174	(.739)
2	2,985	(.178)	111	(.925)
3	2,749	(.186)	108	(.938)
4	7,336	(.114)		
5	805	(.344)		
6	5,013	(.138)		
7	1,156	(.287)		
8	1,639	(.241)		
9	127	(.865)		
10	139	(.826)		
11	108	(.938)		

*Q ≡ Quality = $(N_T/L)^{1/2}$, where N_T is the total number of data points, 95 in this case. Either two sucessive Q's of 0.85 or larger, or Q of 0.90 or larger, is usually considered a successful convergence, provided reasonable "sigma parameters" were used.

BIBLIOGRAPHIC DATA SHEET

1. Report No. TM 86097	2. Government Accession No.	3. Recipient's Catalog No.
4. Title and Subtitle Modification to Shock Fitting Program		5. Report Date 6. Performing Organization Code 695
7. Author(s) M. H. Acuna, R. P. Lepping		8. Performing Organization Report No.
9. Performing Organization Name and Address Planetary Magnetospheres Branch Laboratory for Extraterrestrial Physics Goddard Space Flight Center Greenbelt, Maryland 20771		10. Work Unit No. 11. Contract or Grant No.
12. Sponsoring Agency Name and Address		13. Type of Report and Period Covered 14. Sponsoring Agency Code

15. Supplementary Notes

16. Abstract

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17. Key Words (Selected by Author(s))	18. Distribution Statement		
19. Security Classif. (of this report) Unclassfied	20. Security Classif. (of this page) Unclassified	21. No. of Pages 11	22. Price*

*For sale by the National Technical Information Service, Springfield, Virginia

22161

GSFC 25-44 (10/77)