

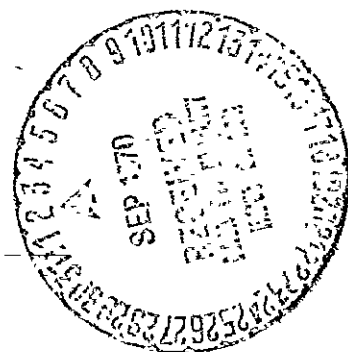
X-692-70-276

PREPRINT

NASA TM X-63997

IMPROVED SHOCK NORMALS OBTAINED FROM COMBINED MAGNETIC FIELD AND PLASMA DATA FROM A SINGLE SPACECRAFT

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JULY 1970



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GREENBELT, MARYLAND

FACILITY FORM 602	<u>N70-35 938</u>	(THRU)
	<u>103</u>	<u>1</u>
	(PAGES)	(CODE)
	<u>TMX 63997</u>	<u>25</u>
	(NASA CR OR TMX OR AD NUMBER)	(CATEGORY)

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AND PLASMA DATA FROM A SINGLE SPACECRAFT

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Space Plasma Physics Branch Preprint Series

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ABSTRACT

By assuming the validity of the Rankine-Hugoniot conservation relations for interplanetary type shocks in an isotropic medium it is demonstrated that improved shock normals can be calculated by employing a least squares technique to combined magnetic field and plasma data from a single spacecraft. The scheme uses only those conservation relations (six in number) which are devoid of pressure and temperature terms. Transforming these equations cast for a shock frame of reference into an arbitrary frame reduces the system to three independent "overdetermination" equations. These three equations constitute a three parameter redundancy among the eleven measured parameters of the system: \bar{B}_1 , \bar{B}_2 , \bar{W} ($\equiv \bar{V}_2 - \bar{V}_1$), ρ_1 , and ρ_2 , where subscripts 1 and 2 refer to before and after the shock respectively. By exploiting this redundancy in the cases of simulated shocks, whose basic noiseless characteristics are known exactly, it

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has been shown for many realistic examples, through the minimization of a least-squares loss function, that the normals are calculated with error improvements of factors of about 3 or so over calculations using the magnetic field alone.

↳ A corrected normal and improved shock parameters are then obtained for a real case: the August 29, 1966 (Pioneer 7) shock. An appendix provides a listing of the complete computer programs used in obtaining the best estimate shock parameters, the shock surface normals, and the associated error cones.

The scheme should prove useful in examining the shape of a shock surface whenever data for a shock event are available from two or more spacecraft widely separated in solar longitude.

IMPROVED SHOCK NORMALS
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AND PLASMA DATA FROM A SINGLE SPACECRAFT

I. INTRODUCTION

In space research there is increasing need for obtaining more accurate shock surface normals. This report presents a method of improving the calculation of oblique shock normals, over previous single spacecraft methods, by using combined magnetic field and plasma data from a lone spacecraft. One important reason for obtaining improved single spacecraft shock normals, which is of particular interest to the authors, lies in the observational study of the shape of interplanetary shock surfaces. For this type of study it is presently rare to obtain reliable data from two spacecraft widely separated in solar longitude, a situation necessary for this surface shape determination, much less from three or more spacecraft. If $N(N \geq 3)$ number of spacecraft useful for this sort of study do exist, that is, do reliably see the same shock surface, then one can be reasonably sure that $N - 1$ of them, or at best $N - 2$, will be located in the near earth region. And in no case in the foreseeable future will a situation exist whereby two spacecraft will be located far from the earth in solar longitude and at the same time remain in close proximity to each other. By close proximity we mean at least close enough to each other to see the same shock normal almost at the same time (i.e. with a time difference on the order tens or hundreds of minutes). Hence, we must be satisfied with reliably calculating the shock normal

from single spacecraft data, especially for the far-from-earth spacecraft. Figure 1 describes this situation where the far spacecraft shown is a Pioneer spacecraft (or could be considered any other solar orbiting probe), and the plane of the figure is approximately the ecliptic plane. The near-earth spacecraft could represent one or more of the Explorers or any other capable spacecraft in that region. If θ , the difference in solar longitude of the two spacecraft, is sufficiently large, then for around the time of the shock sighting the two calculated shock normals \bar{n}_P and \bar{n}_E should suffer a difference great enough to yield a respectable determination of the shock surface's curvature. In order to accomplish this the error angles associated with the estimates of the normals, represented in the figure as error cones of cone angles α_P and α_E respectively, should each be significantly smaller than $\theta/2$.

Previously when one wished to calculate the shock normal from the data of a single spacecraft the magnetic field alone was used in the expression

$$\bar{n} = \pm \frac{(\bar{B}_1 \times \bar{B}_2) \times (\bar{B}_2 - \bar{B}_1)}{|(\bar{B}_1 \times \bar{B}_2) \times (\bar{B}_2 - \bar{B}_1)|}, \quad (I - 1)$$

where \bar{B}_1 and \bar{B}_2 are the magnetic fields before and after the shock respectively. The plus or minus sign ambiguity is clarified once the sign of the plasma density change is ascertained, but quantitative knowledge of the density is not required. Expression (I - 1) rests on the so-called coplanarity theorem (Colburn and

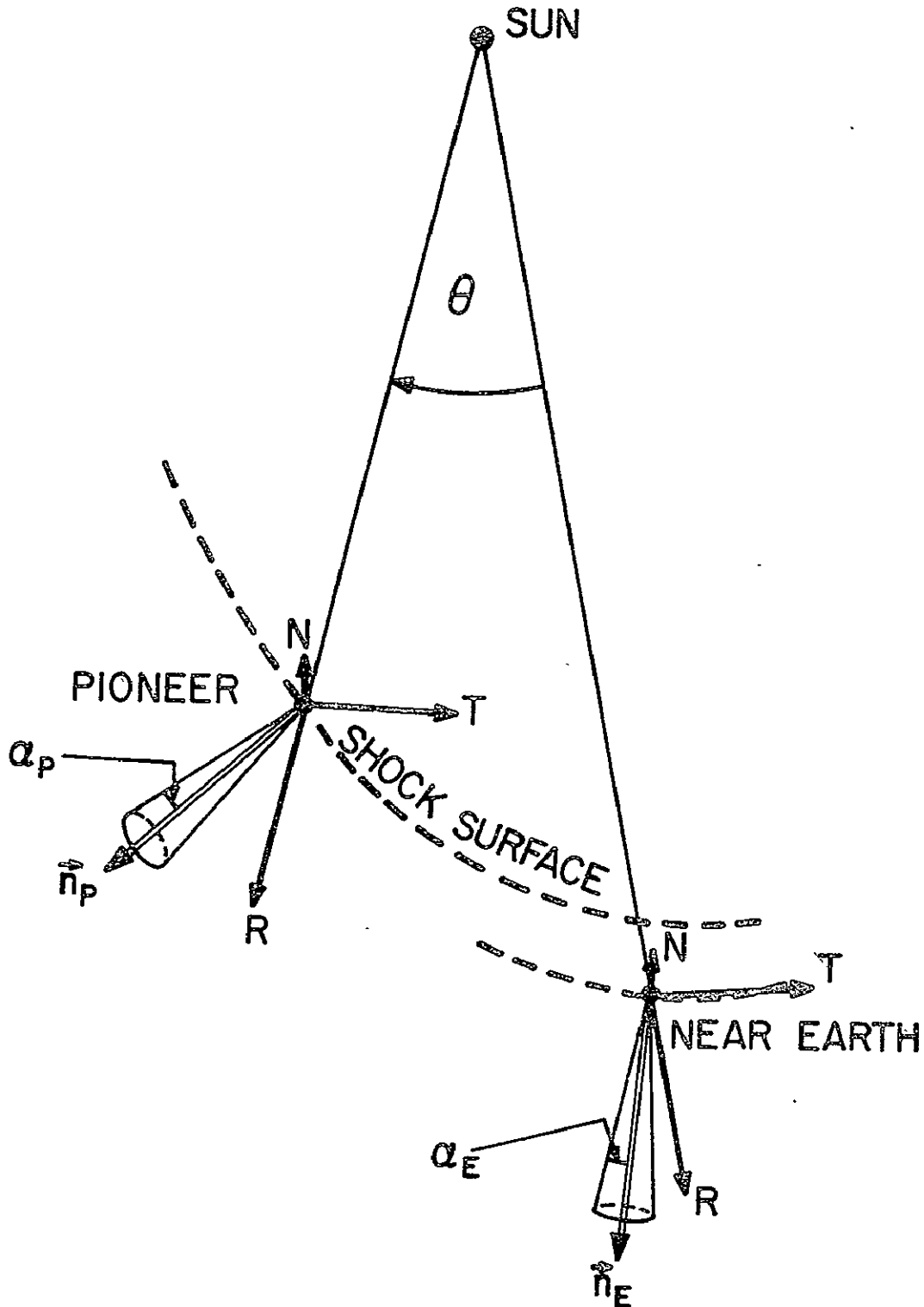


Figure 1. Two spacecraft, widely separated in solar longitude θ , each detecting different portions of the same shock surface. The plane of the Figure is approximately the ecliptic plane which contains the unit vectors R and T , orthogonal to each other and to N which is normal to the ecliptic. The quantities \hat{n} and α refer to the unit normal vector to the shock and its associated error cone angle, respectively.

Sonett, 1966) which in principle holds exactly. However, the values for the vectors \bar{B}_1 and \bar{B}_2 undergo fluctuations, and therefore straightforward average values are often used. If these averages are markedly different from the "actual" magnetic field values required by Expression (I - 1), then the effect of the errors in the \bar{B} 's will usually be magnified by the non-linear nature of the expression yielding a rather unreliable estimate of the normal. This is a particularly serious problem when the angle between \bar{B}_1 and \bar{B}_2 is small, say 10° or less, and the rms deviation of the field quantities is substantial, characteristically say 0.6γ for the components of \bar{B}_1 and perhaps 1.0γ or larger for the components of \bar{B}_2 , around the shock transition region. For this case, where \bar{B}_1 and \bar{B}_2 may be $\sim 6 \gamma$ and $\sim 11 \gamma$ respectively, the error cone angles for \bar{B}_1 and \bar{B}_2 themselves are each about as large as the average angle between them. These errors are then propagated by way of the two factors $\bar{B}_1 \times \bar{B}_2$ and $\bar{B}_2 - \bar{B}_1$ which join to increase the error in the final calculation (I - 1), leading often to a very inaccurate result. Conversely, a small increase in the accuracies of \bar{B}_1 and \bar{B}_2 should result in an even greater improvement in the accuracy of the shock normal's estimate. By utilizing the associated plasma data along with physical relationships connecting the plasma quantities to the magnetic field quantities we expect to obtain at least some improvement in the estimates of \bar{B}_1 and \bar{B}_2 . And this improvement, however small, will propagate its way through Equation (I - 1) to provide hopefully a significant improvement of the shock normal's estimate. It is expected, in most cases, that this improvement will occur even if the plasma data is acquired with poorer accuracy than the field data.

In Part III we describe this method of best fitting both plasma and magnetic field data which will be done by exactly satisfying the basic conservation relationships of the shock system. The best-fit magnetic field parameters are then used with Expression (I - 1) to obtain the so-called best estimate shock normal. Consistent with the proof of (I - 1) via the coplanarity theorem, which follows directly from the conservation equations, Part III uses these equations through a "best estimate" scheme to obtain the "proper" values to be used in (I - 1). It must be stressed that without such a scheme it is not at all clear what values for \bar{B}_1 and \bar{B}_2 are to be used in (I - 1). Surely shock parameters do not appear as simple step functions of time in the data, and by forcing step functions by a straightforward averaging of $\overline{B_1(t)}$ and $\overline{B_2(t)}$ to obtain $\langle \bar{B}_1 \rangle$ and $\langle \bar{B}_2 \rangle$ to be used in (I - 1) is usually inadequate and possibly very inaccurate, as was discussed above.

Part II discusses alternative methods, that is, multiple spacecraft methods, of obtaining accurate shock normals. It reviews established means by which our best estimate scheme can be tested, provided conditions are proper for the test. Part IV contains a short discussion of the use of the scheme in terms of simulated shock cases. And finally, the last section of Part IV deals with the actual calculation of a real shock normal previously studied by J. K. Chao (1970) and which serves as a test case of the overall scheme and associated computer programs (which appear in Appendix C).

It should be pointed out that this scheme accomplishes a good deal more than simply yield, in some sense, best estimate shock normals. It also provides best estimate values for all the eleven relevant magnetic field and plasma parameters.

II. ALTERNATIVE METHODS

By alternative methods of obtaining shock normals we refer to multiple spacecraft methods. These methods apply when the two or more spacecraft lie in a small enough region (R) of space such that the two following basic assumptions apply:

1. The shock surface can be assumed plane as the shock traverses R.
2. The shock velocity remains constant over R.

These limiting assumptions are, of course, not imposed by our single spacecraft method described in Part III below. We now briefly describe three multiple spacecraft methods of obtaining shock normals.

A. Three Spacecraft Method

Ogilvie and Burlaga (1969) and Greenstadt et al. (1970) employ the three spacecraft method to obtain shock normals. This method requires the shock to be observed at three spacecraft located in region R such that the plane in which the three spacecraft lie has a substantial shock normal component perpendicular to it. Where R_{12} and τ_{12} are the relative displacement vector and the shock time delay, respectively, between the first and second sightings etc., it is easy to show from simple geometrical arguments that, for the shock speed V_s ,

$$\tau_{12} V_s = \left(\bar{n} \cdot \bar{R}_{12} \right) ,$$

$$\tau_{13} V_s = \left(\bar{n} \cdot \bar{R}_{13} \right) ,$$

and

$$\tau_{23} V_s = \left(\bar{n} \cdot \bar{R}_{23} \right), \quad (\text{II} - 1)$$

where

$$\bar{n} = \left(n_x, n_y, n_z \right),$$

such that

$$n_x^2 + n_y^2 + n_z^2 = 1. \quad (\text{II} - 2)$$

With these four equations the four unknowns n_x , n_y , n_z and V_s can easily be calculated. If the delay times are much longer than the uncertainties in the time measurements, then this method is usually a very reliable one.

B. Olbert Method

Professor S. Olbert* of M. I. T. has devised a method that requires only two spacecraft observations, one of which needs only to record time of shock onset and no other information (it could be the earth at sudden commencement). The other, however, must obtain magnetic field and plasma data as well as the shock onset time. By using the continuity of mass equation [See Equation (III-A-1)]

*Private communication.

and the coplanarity theorem (Colburn and Sonett, 1966) Olbert shows that the shock normal is given by

$$\bar{n} = \frac{(\bar{B}_1 \times \bar{W}) \times \bar{U}}{|(\bar{B}_1 \times \bar{W}) \times \bar{U}|}, \quad (\text{II} - 3)$$

where \bar{B}_1 is the magnetic field before the shock, $\bar{W} (= \bar{V}_2 - \bar{V}_1)$ is the plasma velocity difference, and \bar{U} is defined as

$$\bar{U} = \frac{\bar{R}}{\tau} - \frac{\rho_2 \bar{V}_2 - \rho_1 \bar{V}_1}{\rho_2 - \rho_1}, \quad (\text{II} - 4)$$

where \bar{R} is the vector displacement and τ the time delay between the two spacecraft, and ρ_1 and ρ_2 are the plasma densities before and after the shock measured at one of the spacecraft (at which \bar{B}_1 , \bar{V}_1 , and \bar{V}_2 are measured).

This method is useful when reliable plasma data is available and when the magnetic field after the shock has relatively large fluctuations so that Equation (I - 1) can not be used.

C. The Two Spacecraft Test

If through some other method \bar{n} is estimated, then the first of Equations (II - 1) constitutes a two spacecraft test of that estimate, provided V_s can also be reliably calculated. This will not be a conclusive check but can serve as a means of "filtering out" some bad normal estimates and adding strength to the estimates of others. We will make use of this straightforward check in Section IV-C.

III. IMPROVED SINGLE SPACECRAFT METHOD FOR OBLIQUE SHOCK NORMALS

A. Theoretical Basis and Conservation Equations

The shock normal improvement scheme described here rests on the following assumptions:

1. The Rankin-Hugoniot conservation relations expressed for an isotropic medium are applicable to interplanetary type shocks (Ogilvie and Burlaga, 1969 and J. K. Chao, 1970).
2. A shock can be represented as a "noised-up" step function increase in time as described in Section III-C.
3. Magnetic field and plasma (proton) bulk velocity and density data provide adequate observational information for our purpose. That is, temperature, pressure, electron-data etc. are not necessary for significant normal improvement even though they might be necessary to strictly identify the shock in the first place.

Only oblique shocks are considered in the scheme. That is, the special cases of the normal being either parallel with or perpendicular to the magnetic field are not treated here.

We now begin by stating the basic equations of our system.

The conservation equations in the shock (*) frame of reference for an isotropic medium are

$$\left[\rho V_n^* \right]_1^2 = 0, \quad (\text{III A - 1})$$

$$\left[\rho V_n^* V_t^* - B_n B_t / 4\pi \right]_1^2 = 0, \quad (\text{III A - 2, 3})$$

$$\left[V_n^* B_t - V_t^* B_n \right]_1^2 = 0, \quad (\text{III A - 4,5})$$

where $t = t_1$ or t_2

$$\left[B_n \right]_1^2 = 0, \quad (\text{III A - 6})$$

$$\left[P + (B^2 - B_n^2) / 8\pi + \rho V_n^{*2} \right]_1^2 = 0, \quad (\text{III A - 7})$$

and

$$\left[\frac{V^{*2}}{2} + \frac{\gamma}{\gamma-1} \frac{P}{\rho} + \frac{B^2}{4\pi\rho} - \frac{(\bar{B} \cdot \bar{n})(\bar{V}^* \cdot \bar{B})}{4\pi\rho(\bar{V}^* \cdot \bar{n})} \right]_1^2 = 0, \quad (\text{III A - 8})$$

where ρ is the plasma mass density, V_n^* is the plasma bulk velocity component normal to the shock surface, V_t^* ($t = t_1$ or t_2) are the components tangential to the shock surface, B_n and B_t ($t = t_1$ or t_2) are the associated normal and tangential components of the magnetic field, P is the total kinetic pressure, \bar{n} is

a unit vector normal to the shock surface, and γ is the usual ratio of specific heats for the plasma. The symbol $[\quad]_1^2$ means that the quantity within the brackets is to be evaluated before ("1") and after ("2") the shock transition zone and then the quantities subtracted. Equation (III A - 1) is the mass continuity equation, Equations (III A - 2 and 3) are the momentum conservation equations for the tangential components, Equations (III A - 4 and 5) are the tangential electric field continuity equations, Equation (III A - 6) is the normal magnetic field continuity equation, Equation (III A - 7) is the momentum conservation equation for the normal component, and finally Equation (III A - 8) is the energy conservation equation. According to assumption #3 above only the first six of these eight equations will be used in the normal improvement scheme.

One sees that these equations can not be used directly without knowledge of \bar{n} and the shock speed. Conversely then these equations may be viewed as constraints on the allowable values of \bar{n} for a given set of relevant shock data. It is in this indirect sense that these equations will be used.

B. Overdetermination Equations in Arbitrary Reference System

The first six conservation equations, (III A - 1 to III A - 6), can be separated into two sets, three equations in each. We call these sets the shock velocity set and the overdetermination equations set. Appendix A demonstrates how this separation is made and provides a proof of the overdetermination equations.

The shock velocity set is

$$\bar{V}_s = V_s \bar{n} \quad (3 \text{ equations}), \quad (\text{III B - 1})$$

where

$$\bar{V}_s \equiv \frac{(\rho_2 \bar{V}_2 - \rho_1 \bar{V}_1) \cdot \bar{n}}{\rho_2 - \rho_1}, \quad (\text{III B - 2})$$

$$\bar{n} \equiv \frac{\Delta \bar{B} \times (\bar{B}_1 \times \bar{B}_2)}{|\Delta \bar{B} \times (\bar{B}_1 \times \bar{B}_2)|}, \quad (\text{III B - 3})$$

$$\Delta \bar{B} \equiv \bar{B}_2 - \bar{B}_1, \quad (\text{III B - 4})$$

and where the transformation equation

$$\bar{V}_i = \bar{V}_i^* + \bar{V}_s \quad (i = 1, 2) \quad (\text{III B - 5})$$

was used.

And the second set, constituting the remaining (three) overdetermination equations, is

$$\bar{W} \cdot (\bar{B}_1 \times \bar{B}_2) = 0, \quad (\text{III B - 6})$$

$$\left(\frac{\rho_2}{\rho_1} \bar{B}_1 - \bar{B}_2 \right) \cdot \left[\bar{W} \times (\bar{B}_1 \times \bar{B}_2) \right] = 0, \quad (\text{III B - 7})$$

and

$$\left[\frac{\rho_1 \rho_2}{\rho_2 - \rho_1} (\bar{W} \cdot \Delta \bar{B}) \bar{W} + \frac{|\Delta \bar{B}|^2}{4\pi} \bar{B}_1 \right] \cdot \left[\Delta \bar{B} \times (\bar{B}_1 \times \bar{B}_2) \right] = 0 \quad (\text{III B - 8})$$

where

$$\bar{W} \equiv \bar{V}_2 - \bar{V}_1 . \quad (\text{III B - 9})$$

Firstly, we notice that Equations (III B - 6, -7, -8) are rendered in general vector form and are independent of the shock (*) frame of reference. Therefore they can conveniently be used in association with whatever coordinate frame the experimenter wishes. Their simplest use then will be for a frame fixed to and moving with the measuring spacecraft and oriented in some physically meaningful way. The arbitrary system will have x - y - z axes by our terminology, where for instance the x axis might be along a direction radially away from the sun and the z axis normal to the ecliptic plane etc. According to this format any three dependent variables can be isolated through the use of the three equations. Choosing these to be ρ_1, ρ_2 , and W_x the overdetermination equations become

$$N_1 = \frac{\rho_1}{m_p} = 5979.14 \left(\frac{r-1}{r} \right) R , \quad (\text{III B - 10})$$

$$N_2 = \frac{\rho_2}{m_p} = 5979.14 (r - 1) R , \quad (\text{III B - 11})$$

and

$$W_x = E , \quad (\text{III B - 12})$$

where m_p is the mass of the proton, N_1 and N_2 are in units of number of protons per cm^3 , all velocities are in km/sec , and magnetic fields are in γ , and where

$$r = \left(\frac{B_{2x} S_x + B_{2y} S_y + B_{2z} S_z}{B_{1x} S_x + B_{1y} S_y + B_{1z} S_z} \right), \quad (\text{III B - 13})$$

$$R = - \frac{FG}{TD} , \quad (\text{III B - 14})$$

$$E = - \left(\frac{W_y Q_y + W_z Q_z}{Q_x} \right), \quad (\text{III B - 15})$$

$$S_x = W_y Q_z - W_z Q_y , \quad (\text{III B - 16})$$

$$S_y = W_z Q_x - E Q_z , \quad (\text{III B - 17})$$

$$S_z = E Q_y - W_y Q_x , \quad (\text{III B - 18})$$

$$T \equiv E X_0 + W_y Y_0 + W_z Z_0 , \quad (\text{III B - 19})$$

$$D \equiv E M_x + W_y M_y + W_z M_z , \quad (\text{III B - 20})$$

$$G \equiv B_{1x} M_x + B_{1y} M_y + B_{1z} M_z , \quad (\text{III B - 21})$$

$$M_x \equiv Q_z Y_0 - Q_y Z_0 , \quad (\text{III B - 22})$$

$$M_y \equiv Q_z Z_0 - Q_x X_0 , \quad (\text{III B - 23})$$

$$M_z \equiv Q_y X_0 - Q_x Y_0 , \quad (\text{III B - 24})$$

$$Q_x \equiv B_{1y} B_{2z} - B_{1z} B_{2y} , \quad (\text{III B - 25})$$

$$Q_y \equiv B_{1z} B_{2x} - B_{1x} B_{2z} , \quad (\text{III B - 26})$$

$$Q_z \equiv B_{1x} B_{2y} - B_{1y} B_{2x} , \quad (\text{III B - 27})$$

$$F \equiv (X_0^2 + Y_0^2 + Z_0^2)/4\pi . \quad (\text{III B} - 28)$$

$$X_0 \equiv B_{2x} - B_{1x} , \quad (\text{III B} - 29)$$

$$Y_0 \equiv B_{2y} - B_{1y} , \quad (\text{III B} - 30)$$

and

$$Z_0 \equiv B_{2z} - B_{1z} , \quad (\text{III B} - 31)$$

and also from Equation (III B - 9)

$$W_y \equiv V_{2y} - V_{1y} , \quad (\text{III B} - 32)$$

and

$$W_z \equiv V_{2z} - V_{1z} , \quad (\text{III B} - 33)$$

That is, once eight parameters are fixed the remaining three, N_1 , N_2 and W_x , are constrained to take the values dictated by Equations (III B - 10, -11, -12).

This constraint is the physical basis for the best-estimate scheme to be described in Section III - D.

It should be pointed out here that if Equation (III A - 7) were written in the notation given above, it would become

$$\Delta P \equiv P_2 - P_1 = \frac{D^2 R}{M^2} - \frac{A}{8\pi}, \quad (\text{III B - 34})$$

where the change in pressure across the shock surface, ΔP , is in units of 10^{-10} dynes per cm^2 and where

$$M^2 = M_x^2 + M_y^2 + M_z^2 \quad (\text{III B - 35})$$

and

$$A = B_{2x}^2 + B_{2y}^2 + B_{2z}^2 - B_{1x}^2 - B_{1y}^2 - B_{1z}^2. \quad (\text{III B - 36})$$

Equation (III B - 34) does not play a direct role in the estimation scheme but it can be used to calculate ΔP from the best-estimate parameters resulting from the scheme. Then the value of ΔP can be compared directly to pressure data (obviously the electron pressure cannot be ignored if this comparison is made).

Since $\bar{W} = \bar{V}_2 - \bar{V}_1$, it is easy to see that Equation (III B - 2) can be written

as

$$V_s = \frac{N_2 \bar{W} \cdot \bar{n}}{N_2 - N_1} + \bar{V}_1 \cdot \bar{n}, \quad (\text{III B - 37})$$

where $N_i = \rho_i/m_p$ ($i = 1, 2$) was used. In Equation (III B - 37) the first term and the factor \bar{n} in the second term (from Equation (III B - 3)) can be readily calculated from the best-estimate results. Then, in general, the calculation of the shock speed V_s will be only as reliable as the value of \bar{V}_1 , the undisturbed pre-shock plasma velocity. However, using a straightforward average to obtain \bar{V}_1 should give an adequate result, because the rms deviation on the magnitude of the pre-shock velocity is usually only a small fraction of the magnitude itself and its direction fluctuates very little (differing from the radial only slightly). This depends somewhat on the provision that a proper averaging interval is chosen. Experience shows that a proper interval might characteristically be anywhere between 5 and 25 minutes. Finally, Equation (III B - 1) is used to obtain the vector shock velocity.

C. The Noise Problem

The usual conceptual model of an observation of an interplanetary type shock consists of a step function increase in time of the magnitudes of the shock quantities \bar{B} , \bar{V} , P (or T), and N as one goes from the upstream to the downstream positions. [For a so-called slow shock $|\bar{B}|$ must decrease (J. K. Chao, 1970)]. The transition zone thickness is usually on the order of seconds, unless the probe

is observing the shock surface traveling edge-on. Indeed, for each physical entity the conservation relations accept only two values (a "before" and an "after" transition value). We retain this exceedingly simple concept of a shock but with the addition of stationary, uncorrelated, zero mean, noise to each of the basic shock quantities. That is, the noise is mathematically represented by a stationary, uncorrelated, zero-mean, random process. In most cases, however, we will find it necessary to restrict the before and after time zones to about 15 and 10 minutes respectively. Other cases might require longer time zones. Figure 2 describes the shock model used in this work. Pressure (P) and temperature (T) are not shown because they are not used as part of the estimation scheme.

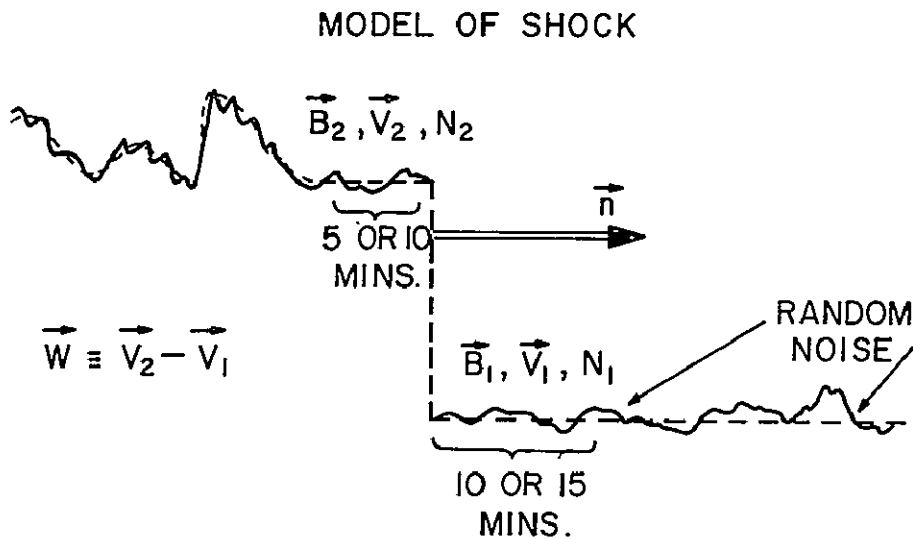


Figure 2. The conceptual model of an observation of an interplanetary type shock treated in this report. The straight line segments (i.e. the step function part) of the dashed curve refer to the basic ("true"), underlying values of the magnitude changes of the shock parameters shown. For a slow shock $|\vec{B}|$ changes in the opposite direction to that shown. Time intervals are only approximate.

D. Least-Squares Loss-Function Procedure

Guided by Section III - B we split the eleven basic parameters of our system into two groups: the 8-parameter independent set and the 3-parameter dependent set. The eight independent parameters then are chosen for convenience to be: \bar{B}_{1x} , B_{1y} , B_{1z} , B_{2x} , B_{2y} , B_{2z} , W_y , and W_z . Therefore, the three dependent parameters are N_1 , N_2 , and W_x . The coordinate system x-y-z is an arbitrary orthogonal system and therefore in a R-T-N system (See Figure 1), for instance, W_x may be W_R or W_T or W_N etc. provided one is consistent with the use of \bar{B}_1 and \bar{B}_2 .

In our mathematical scheme it will be convenient to define two vectors \bar{Y} and \bar{X} in the following fashion. The \bar{Y} vector is the vector of observations, the so-called data array. If a total of N observations (including all data types: B_{1x} , W_y , etc) is to be used in the scheme, then \bar{Y} will have dimension N. We have eleven basic data types and we impose on these types an order so that it becomes meaningful to speak of the first data type, the second data type, etc. Define $N(i)$, $i = 1, 2, \dots, 11$, as the number of observations of the i-th data type. Then the first $N(1)$ elements of \bar{Y} are to be the observations of the first data type, no particular order being necessary within the type, the elements of \bar{Y} from $N(1) + 1$ to $N(1) + N(2)$ are to be the observations of the second type, in any order within that type, etc. In symbolic form we write the N dimensional vector \bar{Y} as

$$\bar{Y} \equiv \left(Y_1^{(1)}, Y_1^{(2)}, \dots, Y_1^{(N(1))}, Y_2^{(1)}, \dots, Y_2^{(N(2))}, \dots, Y_{11}^{(1)}, \dots, Y_{11}^{(N(11))} \right) \quad (\text{III D - 1})$$

where, of course,

$$N = \sum_{i=1}^{11} N(i) . \quad (\text{III D - 2})$$

Now we define the scalar symbol X_i , a variable, to be the "best estimate" of the shock parameter measured by the observations in the i -th data type. The definition of what constitutes a best estimate will be provided below, and from this definition a mode of calculating a numerical value for X_i , $i = 1, 2, \dots, 11$, will be evident. Define an N dimensional vector \bar{X} by permitting each of the first $N(1)$ elements of \bar{X} to be X_1 identically, the next $N(1) + 1$ to $N(1) + N(2)$ elements each to be X_2 identically, etc. Symbolically we write

$$\bar{X} \equiv \left(\underbrace{X_1, \dots, X_1}_{\text{repeated } N(1) \text{ times}}, \underbrace{X_2, \dots, X_2}_{N(2) \text{ times}}, \dots, \underbrace{X_{11}, \dots, X_{11}}_{N(11) \text{ times}} \right) . \quad (\text{III D - 3})$$

The \bar{X} and \bar{Y} arrays must be compatible component for component with respect to the parameter types, i.e., by the i -groupings. Notice for later reference that any component of \bar{Y} can be expressed as $Y_i^{(j(i))}$ where $j(i)$ refers to the j -th

observation (or j-th point) of the i-th data type. Now for definiteness we make the following identification:

Table 1

Parameter Type	Data Array Component Symbol	Best estimate Array Component Symbol	
independent	B_{1x}	$Y_1^{(j(1))}, j(1) = 1, 2, \dots N(1)$	X_1 repeated $N(1)$ times
	B_{1y}	$Y_2^{(j(2))}, j(2) = 1, 2, \dots N(2)$	X_2 repeated $N(2)$ times
	B_{1z}	$Y_3^{(j(3))}, j(3) = 1, 2, \dots N(3)$	X_3 repeated $N(3)$ times
	B_{2x}	$Y_4^{(j(4))}, j(4) = 1, 2, \dots N(4)$	X_4 repeated $N(4)$ times
	B_{2y}	$Y_5^{(j(5))}, j(5) = 1, 2, \dots N(5)$	X_5 repeated $N(5)$ times
	B_{2z}	$Y_6^{(j(6))}, j(6) = 1, 2, \dots N(6)$	X_6 repeated $N(6)$ times
	W_y	$Y_7^{(j(7))}, j(7) = 1, 2, \dots N(7)$	X_7 repeated $N(7)$ times
	W_z	$Y_8^{(j(8))}, j(8) = 1, 2, \dots N(8)$	X_8 repeated $N(8)$ times
dependent	N_1	$Y_9^{(j(9))}, j(9) = 1, 2, \dots N(9)$	X_9 repeated $N(9)$ times
	N_2	$Y_{10}^{(j(10))}, j(10) = 1, 2, \dots N(10)$	X_{10} repeated $N(10)$ times
	W_x	$Y_{11}^{(j(11))}, j(11) = 1, 2, \dots N(11)$	X_{11} repeated $N(11)$ times

This scheme will be used throughout the remainder of this work.

The dependent parameters are related to the independent parameters through the overdetermination equations given by Equations (III B -10, -11, -12). In the new notation these equations are formally expressed by the following:

$$X_9 = X_9(\bar{Z}),$$

$$X_{10} = X_{10}(\bar{Z}),$$

$$X_{11} = X_{11}(\bar{Z}), \quad (\text{III D - 4})$$

where

$$\bar{Z} \equiv (X_1, X_2, \dots, X_8). \quad (\text{III D - 5})$$

That is, X_9 , X_{10} , and X_{11} are functions of X_1, X_2, \dots, X_8 only, rendering \bar{X} , given by Equation (III D - 3); in terms of eight implicit variables, which must yet be determined.

Also we define, the "sigma noise parameters" σ_i 's to be:

$$\sigma_i = \sigma_i' + \Delta\sigma \quad (i = 1, 2, \dots, 11) \quad (\text{III D - 6})$$

where

$$\sigma_i' = \left[\frac{\sum_{j=1}^{N(i)} (Y_i^{(j)} - \langle Y_i \rangle)^2}{N(i) - 1} \right]^{1/2} \quad (\text{III D - 7})$$

the unbiased rms deviation of the i th parameter-type observations, and

$$\langle Y_i \rangle = \frac{\sum_{j=1}^{N(i)} Y_i^{(j)}}{N(i)} , \quad (\text{III D - 8})$$

the average of the i th parameter-type observations, and where

$$\Delta\sigma_i (\geq 0) \quad (\text{III D - 9})$$

is additional weight given to σ_i' to account for instrumental noise.

We now define a scalar quantity known as a loss function, which is a measure of how well \bar{Z} "fits" the data array \bar{Y} . The smaller the loss function the better the fit. For this function we choose a standard σ -weighted least squares loss function:

$$L(\bar{Z}) \equiv \sum_{i=1}^{11} \sum_{j=1}^{N(i)} \left(\frac{X_i - Y_i^{(j)}}{\sigma_i} \right)^2 . \quad (\text{III D - 10})$$

Notice that L is a function of \bar{Z} only, i.e. a function of only X_1, X_2, \dots, X_8 . Other functional forms for the loss function could be used provided they are positive definite. The exact structure of L is, of course, somewhat arbitrary. We define

the best estimate of \bar{Z} to be the value of \bar{Z} which minimizes the loss function (III D - 10).

In order to minimize $L(\bar{Z})$ its gradient with respect to X_1, X_2, \dots, X_8 must be zero. Hence, we set

$$\frac{\partial L(\bar{Z})}{\partial X_i} = 0 \quad (i = 1, 2, \dots, 8) \quad (\text{III D - 11})$$

for a necessary condition of solution. Because of the nonlinearity of Equations (III D - 4), the eight equations given by Equations (III D - 11) represent a non-linear set to be solved simultaneously for the eight unknowns, the components of \bar{Z} . Strictly speaking it is the solution of these equations which yields the components of the best estimate array. Expression (III D - 3) is more precisely a variable state vector whose all eleven components become, with the help of the overdetermination equations, the best fit array upon imposing condition (III D - 11).

An iterative procedure will be used to solve the eight equation set (III D - 11). The numerical technique used is the Newton-Raphson method. See Appendix B.1 for a more detailed development of the overall statistical methods and the numerical technique in use here. We outline below the numerical procedure.

We define \hat{Z} as the exact solution of Equations (III D - 11) when an absolute minimum is attained. Then \bar{Z}_0 is defined as the first estimate (i.e. the "starting

vector" for the iteration procedure) of \hat{Z} .* The vector \bar{Z}_0 could be, for instance, the average of the first eight data channels of \bar{Y} , i.e. its components could be $\langle Y_1 \rangle, \langle Y_2 \rangle, \dots, \langle Y_8 \rangle$.

For $\bar{\Delta Z}_n$ defined as

$$\bar{\Delta Z}_n \equiv \bar{Z}_n - \bar{Z}_{n-1} , \quad (\text{III D - 12})$$

Equation (B - 10) of Appendix B.1 shows $\bar{\Delta Z}_n$ in explicit terms to be

$$\bar{\Delta Z}_n \cong \left[\underline{\underline{B}} \underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} (\bar{Y} - \bar{X}) \right] \Big|_{\bar{Z}_{n-1}} \quad (\text{III D - 13})$$

where

$$\underline{\underline{A}}(\bar{Z}) \equiv \frac{\partial \bar{X}(\bar{Z})}{\partial \bar{Z}} , \quad (\text{III D - 14})$$

whose elements are $A_{ij} = \partial X_i / \partial X_j$, $i = 1, 2, \dots, N$ [N is given by Equation (III D - 2)] and $j = 1, 2, \dots, 8$.

$$\underline{\underline{B}}(\bar{Z}) \equiv \left(\underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} \underline{\underline{A}} \right)^{-1} , \quad (\text{III D - 15})$$

*In the strictest sense this should be \tilde{Z} defined in Appendix B.1. But the statement is still correct, in a relative sense, as it stands.

and where.

$$\mathbb{Q} \equiv \left(\begin{array}{c} \sigma_1^2 \\ \sigma_1^2 \dots \sigma_1^2 \\ \cdot \\ \sigma_2^2 \dots \sigma_{11}^2 \end{array} \right) \quad (\text{III D - 16})$$

The diagram shows a large pair of parentheses containing a matrix structure. On the left side, there are two circles. On the right side, there are two circles. A dotted line connects the top-left circle to the top-right circle, with the label σ_1^2 above it. Another dotted line connects the bottom-left circle to the bottom-right circle, with the label σ_2^2 above it. The matrix is labeled \mathbb{Q} on the left and (III D - 16) on the right.

such that σ_1^2 is repeated $N(1)$ times, σ_2^2 repeated $N(2)$ times, etc. By repeated application of Equation (III D - 13) with

$$\bar{Z}_n = \bar{Z}_{n-1} + \bar{\Delta Z}_n \quad (\text{III D - 17})$$

for $n = 1, 2, 3, \dots$, provided \bar{Z}_0 is carefully chosen to insure convergence of L to its absolute minimum, \bar{Z}_n should tend toward \hat{Z} , the exact solution of Equations (III D - 11). This iterative procedure can be discontinued after a fixed number of steps or when $|\bar{\Delta Z}_n|$ becomes sufficiently small, i. e. when

$$\frac{|\bar{\Delta Z}_n|}{|\bar{Z}_{n-1}|} \leq \epsilon \quad (\text{III D - 18})$$

for some sufficiently small $\epsilon > 0$. We fix ϵ at 0.01 and set n_{max} , the total number of iterations allowed, equal to 15. The iterative procedure continues

from $n = 1$ through $n = 15$ unless criterion (III D - 18) is satisfied. If a poor choice of \bar{Z}_0 is made the process may diverge. In this case, except under very unusual circumstances, (III D - 18) will not be satisfied, and the process stops at $n = 15$. Then a new \bar{Z}_0 must be chosen. Since the loss function can be calculated at each iteration step, then, even for a diverging case, that \bar{Z}_n associated with the smallest loss function is the one nearest to some acceptable starting vector \bar{Z}_0 in a least squares sense. It must then be slightly changed in usually only a few components to provide an adequate \bar{Z}_0 . Because of the nonlinearity of Equations (III D - 4), and hence the nonlinearity of Equations (III D - 11), the iterative process may converge to a false minimum, i.e. to one other than the absolute minimum sought. It is obvious when this occurs, because it leads to the "best estimate" values of N_1 , N_2 , and W_x differing greatly from the average values of these quantities, i. e. by more than 2σ for one or more of the three. Other hints of a false convergence are results leading to $N_1 > N_2$ or $P_1 > P_2$ when the seventh conservation equation, in the form of Equation (III B - 34), is used. This false convergence also requires trying a new \bar{Z}_0 to bring about true convergence.

In this connection it is useful to define a quality index, q , by the following

$$q \equiv \sqrt{\frac{N}{L(\bar{Z}_c)}} \quad (\text{III D - 19})$$

where \bar{Z}_c is that value of \bar{Z} which leads to convergence within some ϵ , and N , given by Equation (III D - 2), is the total number of data points for all eleven parameter-types. Obviously the nearer \bar{Z}_c is to \hat{Z} the larger q will be. The quantity q should be near, or slightly greater than, unity for common cases of interplanetary shocks. For too small a q , say $q = 1/2$ or so, the convergence may be a false one .

IV. TEST OF METHOD AND EXAMPLES OF ITS USE

A. Error Cones and Simulation

The preceding section outlined a method of utilizing plasma data to obtain "good" estimates of the before and after magnetic fields. Another and far simpler method of estimating these fields is to take straightforward averages of the observations of the fields as the estimate. The justification for utilizing the more complicated weighted least squares estimation procedure instead of the mean value method has been that the more complicated method yields a more accurate estimate of the before and after fields in general. And any small increase in the accuracy of these estimates because of the form of Equation (III B - 3) can yield substantial improvements in the estimate of the shock normal.

But, of course, this is an assumption which must be tested and proved, at least within some reasonable basic set of assumptions. In short, it is necessary to show that the weighted least squares estimation procedure leads to significantly better estimates of the shock normal than the mean value procedure within the limiting assumptions stated in Section III - A. In Section IV-B we do this by applying both estimation methods to simulated observations of a shock and associating with each method an error cone about the true normal to the shock surface. The comparison of these error cones will indicate the degree of improvement to be expected from the weighted least squares technique.

The meaning of these error cones and the means by which they are calculated will now be described. First, simulated shock observations are generated by

assuming a simple underlying step function model of a shock (See Section III-C) and associating with such a shock the eight independent parameters which constitute the components of the vector \bar{Z} . These parameters are chosen to be consistent with previous studies of shock properties. Then the remaining three dependent parameters are obtained from the overdetermination equations of Section III-B. These eleven parameters constitute the "true" shock parameters of the simulated shock. Zero mean (i.e. unbiased), stationary, uncorrelated, normally distributed noise is then imposed on all of the eleven measurable parameters. The number of observations of each measurable parameter and the variance figures on the noise are again chosen to be typical of what one should expect of shock observations. Both the weighted least squares and the mean value techniques are then utilized to obtain estimates of the before and after magnetic fields (and estimates of the plasma parameters). It is possible to obtain covariance matrices for both these estimation procedures. The manner by which this is done for the least squares method, along with general mathematical details of error cone construction, is given in Appendix B.2. The covariance matrix of the mean value estimate can be easily obtained by recalling that the variance of an estimate obtained by a mean value is just the variance of the underlying population divided by the sample size. This provides us with the diagonal elements of the desired covariance matrix. And since the noise on each data type is assumed to be independent of the noise on other data types, the off diagonal elements are zero.

These matrices are measures of the statistical dispersions of the estimates about the true values. What interests us now is how these statistical dispersions propagate their way through the non-linear function of Expression (III B - 3) into angular errors in the estimates of the true shock normal. Specifically we shall obtain, for each estimation procedure, a 95% critical angular error value α , that is, an angle for which the probability of the angular error (caused by the use of a particular estimation procedure) being smaller than α is 0.95. A Monte Carlo process is necessary to obtain these critical angles. Essentially this Monte Carlo procedure represents a method, indeed the only method, of propagating the statistical dispersion of the magnetic field estimates, as measured by a covariance matrix, through the highly non-linear function (III B - 3). The resulting critical error angle is related to the statistical dispersion of the estimate of the shock normal. The Monte Carlo procedure is also described in Appendix B.2.

These critical angular error values have an obvious geometric interpretation, namely, a 95% critical error angle α can be represented by the defining angle of a right circular cone with its axis being the true shock normal.

In Section IV-C error cone angles associated with a real shock will be calculated. True normals are not available in the cases of real shocks, of course. Hence, in these cases the two methods of obtaining error cones, the mean value and least squares methods, must have error cones defined in a slightly modified way from those of the simulated cases. In the mean value case the axis of the error cone will be the normal obtained from taking straightforward averages of

the field, and the cone is generated with respect to this average normal. In the best estimate (least squares) case the axis of the error cone is the best estimate normal, and the cone is generated with respect to that normal. It must be emphasized that these real shock associated error cones can not enjoy the same rigorous interpretation as those of the simulated shocks. But since the cone angles are expected to depend strongly on the σ_i 's ($i = 1, 2 \dots 11$), defined by Equation (III D - 6), and only weakly on the actual shock parameters in most cases, then the real cones, for practical purposes, should have interpretations analogous to the cones of the simulated cases. That is, the probability of the true shock normal lying within the 95% critical error cone for real cases is approximately 0.95. As in simulated cases of shocks the best estimate error cone for a real case will have a cone angle smaller, and sometimes very substantially smaller, than the mean value cone angle.

B. Study of a Simulated Case

As described in Section IV-A and Appendix B.2 realistic simulated shocks were generated in order to test the degree of success of the improvement scheme and to provide a check on the associated computer programs. The program has the capability (See the XMONTE subroutine in Appendix C.1) of generating a simulated \bar{Y} data array using preassigned values of σ_i , $N(i)$ ($i = 1, 2, \dots 11$), and X_i ($i = 1, 2, \dots 8$), the latter being components of what we refer to as the \bar{Z}_{true} vector*. The "true" components X_9, X_{10} , and X_{11} (dependent parameters) are

*This is called \tilde{Z} in Appendix B.

obtained from the overdetermination equations of Section III-B. The eleven true X_i 's are "noised-up" by adding the output from a random number generator, according to the values of the σ_i 's and the $N(i)$'s, yielding the vector \bar{Y} . Consistent with our previously described model the random number generator provides, for all practical purposes, samples of an unbiased, stationary, uncorrelated, normally distributed random variable. By calculating the mean values of the first eight data types, using \bar{Y} as if it were real data, gives $X_i(\text{mean})$ $i = 1, 2, \dots, 8$, or \bar{Z}_M in vector notation. The \bar{Z}_M vector should, in most cases, provide an acceptable starting vector for the iteration procedure of Section III-D. We then set $\bar{Z}_0 = \bar{Z}_M$ for all simulated shocks. Hence, we enter the simulation problem with all of the information that would be necessary to employ the improvement scheme to a real shock with the important difference that here \bar{Z}_{true} is known. And by design, the simulated data does satisfy the statistical model.

Realistic input parameters σ_i , $N(i)$, ($i = 1, 2, \dots, 11$) and \bar{Z}_{true} were used to test the program. Table 2 gives an example of input values used in such a test. The shock computer program is listed in Appendix C.1. Appendix D.1 shows an example of a printed output of the results of using the input values given in Table 2. It represents only one 140-number sample from the random number generator, where 140 is the sum of the $N(i)$'s. Any number of samples from the generator, each giving a different \bar{Y} , are available where, of course, each \bar{Y} represents just a single data sample of the true shock of Table 2. The preface of Appendix C.1 explains what switches have to be set, and to what

Table 2

Example of Input Values for Simulated Shock Test.

Parameter	i	N(i)	σ_i (in units of X_i)	X_i (true)
B_{1x}	1	20	0.35	4.0 γ
B_{1y}	2	20	0.50	5.0 γ
B_{1z}	3	20	0.35	-1.0 γ
B_{2x}	4	10	0.60	3.5 γ
B_{2y}	5	10	1.10	9.0 γ
B_{2z}	6	10	1.30	-3.0 γ
W_y	7	10	10.0	10.0 km/sec
W_z	8	10	10.0	20.0 km/sec
N_1	9	10	0.7	(7.26 #/cm ³)
N_2	10	10	1.0	(13.86 #/cm ³)
W_x	11	10	10.0	(75.83 km/sec)

independent

dependent*

*Strictly speaking the three values in parenthesis are not input parameters.

values, in order to run a simulated shock program (and also for a real shock program). In the particular case of this simulated example the switches were set to the following values:

I PRO = 1

ISWTCH = 1

ICASE = 2

ISAMPL = 5

IPRO equal to 1 means simulated shocks being processed, and ISWTCH equal to 1 means that XSTART (which is the same as input \bar{Z}_{true} for a simulated shock) is replaced by XMEAN as the starting vector for the iteration process. ICASE of 2 simply means that two basic input shocks (or two cases) are being studied, where here Table 2 gives the values for only one of the two cases. ISAMPL equal to 5 means that five samples of noise are to be imposed in each of the two cases creating ten \bar{Y} 's. The input arrangement is such that the same basic shock is associated with each of the five samples, for both cases; that is, for each of the first five noise samples the same values of Table 2, say, are used as input to the random number generator and for the second five samples the same values of some other table (not shown) are used as input to the generator. Our sample output, Appendix D.1, is then the result of one of the ten \bar{Y} 's. Below we describe the shock program output sample.

From what has been said above the first eight lines are self evident (where SIG is σ_i and NN is $N(i)$). INPUT XSTART is just Z_{true} . The so-called G values are the values of the quantities available from the overdetermination equations, Equation (III B - 3), and Equation (III B - 34) all of Section III-B (See the CON subroutine in Appendix C.1). These are the three dependent shock parameters N_1 , N_2 , and W_x , the x-, y-, and z- components of \bar{n} , and the total kinetic pressure change ΔP . "Corresponding G values" then refer to those G values corresponding to \bar{Z}_{true} . The best estimate independent parameter matrix is a two dimensional array whose columns are the eight independent shock parameters, the components of \bar{Z} , and whose rows correspond to the iteration steps. The top, or "M - row"

(see far right for label), is composed of the mean values of \bar{Z} , and immediately below that is the starting vector \bar{Z}_0 in the zeroth-row. Notice the Mth and zeroth rows have the same values because XSTART is replaced by XMEAN (which is not the case for a real shock). The process went the full 15 steps because $Z = |\Delta\bar{Z}_n|/|\bar{Z}_{n-1}|$ did not become ≤ 0.01 as Expression (III D - 18) requires for a number of iterations (L) less than 15. The Z ratio is printed out at the far right, and the value of the loss function also, at each iteration step. Below that the quality, defined by Equation (III D - 19), is printed out for each step. Below the independent parameter matrix is the associated dependent parameter matrix whose columns are the values of the G-parameters described above; the rows again correspond to the iteration steps. The \underline{B} matrix is the evaluation of \underline{B} , given by Equation (III D - 15), for $\bar{Z} = \hat{Z}$, shown as the last step of the independent parameter matrix (i.e. the best estimate step). The contracted derivative matrix \underline{A} is a contraction of \underline{A} , given by Equation (III D - 14), evaluated for $\bar{Z} = \hat{Z}$. By contracting \underline{A} no information is essentially lost (See the \underline{C} matrix of the AA subroutine in Appendix C.1); the statement just below Equation (III D - 14) concerning the elements of \underline{A} , along with Equation (III D - 3), explains why this is so. The three numbers at the very bottom of the printed output refer to angles in degrees. These are:

AAVE is the angle between \bar{n} (true) and \bar{n} (Mean),

ABE is the angle between \bar{n} (true) and \bar{n} (B. E.),

and

AVE, ABE is the angle between \bar{n} (Mean) and \bar{n} (B. E.).

Note: In the real shock output \bar{n} (true) is replaced by \bar{n} calculated from \bar{Z}_0 , i. e., from XSTART. Hence, of the three angles only AVE, ABE has any relevant meaning in a real case .

The top or M-th row of the independent parameter matrix contains all eleven mean values of the shock parameters, the last three of which are, strictly speaking, not part of the matrix. The first eight parameters are the ones used to obtain what below are called the MEAN's G's, which are self explanatory. Notice that the mean values N_1 , N_2 , and W_x are distinctly different from those same quantities derived from the MEAN's G's, and this is most important (especially in real shock cases). When this difference is very great it indicates the low quality of using straightforward mean values as final estimates for the shock parameters. In fact, the mean quality parameter, $QUALITY M = 0.127$, is quite low compared to unity or so, which is expected for a least squares best estimate.

Notice that after only about 4 or 5 steps the calculation is essentially completed, and little is gained after those steps. The choice of $\epsilon = 0.01$ in expression (III D - 18) is obviously a conservative one since this sample output is rather typical. A comparison of the true shock parameters (i. e. XSTART and corresponding G's) with those from the mean value and best estimate calculations shows for this case, or rather for this sample of a case, how valuable the scheme can be. But the true test of improvement lies in a comparison of the two methods

of obtaining error cones as described in Section IV-A; below this is discussed. Notice that the best estimate normal lies only 3° away from $\bar{n}(\text{true})$ but $\bar{n}(\text{Mean})$ is almost 9° away. In some cases (i.e. for other $X_i(\text{true})$'s, etc.) the improvement might be much more dramatic and yet in others the improvement is insignificant. It is even possible that ABE turn out to be larger than AAVE, as one should expect in a statistical problem of this type, but it must occur infrequently.

Appendix D.2 shows a sample of the printed output of the cone computer program listed in Appendix C.2. This example corresponds exactly to the shock case described by Table 2, and, of course, gives the cone angles associated with the example program output of Appendix D.1 (and all other samples of this same case). The so-called "FI 1 RESULTS" refers to cone angles found by using the least squares technique, and the "FI 2 RESULTS" refers to the mean value method. All angles are given in degrees. The designations 15-, 30-, and 150- VALUE refer to 99.5%, 99%, and 95% error cone angles, respectively, where a Monte Carlo sample size of 3,000 was used. For example, consider the 150 VALUE case: 3,000 - 150 (= 2,850) refers to 95% of 3,000, and designates the cone within which 95% of the normal estimates lie. We will not be concerned with the 99.5% and the 99% error cones in this study. Notice then that, in this case, the angles $\alpha(\text{Mean})$ and $\alpha(\text{Best Estimate})$ are 10.6° and 5.2° , respectively. This represents an error cone angle improvement of better than a factor of 2, and is characteristic of realistic cases in general or perhaps is somewhat conservative. Sometimes the improvement factor is more dramatic (i.e. values of 3 and 4) for

realistically simulated shocks, and in no realistic case will it turn out that $\alpha(\text{Mean}) \lesssim \alpha(\text{Best Estimate})$.

C. Example of Actual Case: The August 29, 1966 (Pioneer 7) Shock

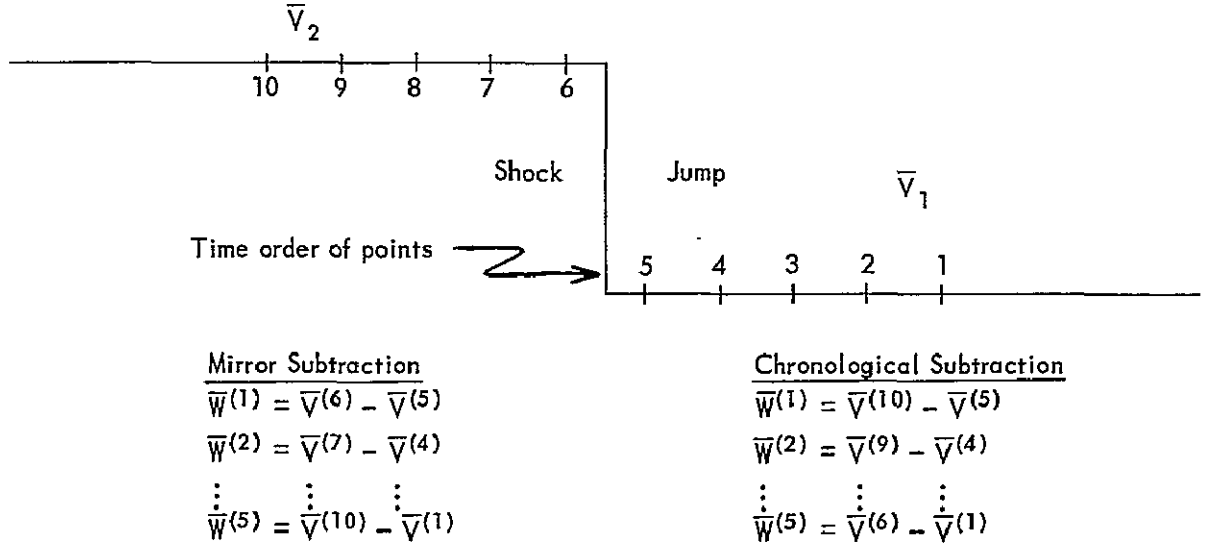
The August 29, 1966 shock, as observed in Pioneer 7 data, was first studied by J. K. Chao (1970) and is reexamined here as an example of the use of the least-square technique described in this report. Taylor (1968) also observed this shock in the magnetic field data of Explorer 28, but the associated plasma data was not existent for that spacecraft.

In applying the least-squares scheme, 25 alternate data points, representing 12.5 minutes, were used for the \bar{B}_1 field in the \bar{Y} array of Equation (III D - 1), and 18 points, representing 9 minutes, for the \bar{B}_2 field, and 5 points, representing ≈ 8 minutes, for each plasma parameter, before and after the shock, were used. The quality index for the best estimate convergence value, as defined by Equation (III D - 19), was 1.03, which is a common sort of value for interplanetary type shocks. For the total 154 data points this corresponds to a loss function value of 145. Table 3 gives the values of the shock's relevant parameters, as well as the observed onset time. The σ 's for the magnetic field were obtained directly from a calculation of the rms deviation in the data. The σ 's for the plasma parameters were found likewise with the addition of instrumental $\Delta\sigma$'s [See Equation (III D - 6)] to the statistical values. The values for the components of $\bar{W}(= \bar{V}_2 - \bar{V}_1)$

Table 3
Pioneer 7 Shock Event of
August 29, 1966 (14:16:57.4±.8 U.T.)

Parameter	Average Value	σ	Best Estimate Value
B_{1R} (γ)	-2.3	0.57	-2.30
B_{1T}	0.9	0.65	0.68
B_{1N}	-2.3	0.35	-2.27
B_{2R}	-3.9	0.70	-3.70
B_{2T}	2.1	1.7	2.89
B_{2N}	-6.8	1.5	-6.98
W_R (km/sec)	79.4	6.90	78.9
W_T	25.2	10.2	27.9
W_N	-12.9(-166)	7.40	-17.8
N_1 (#/cm ³)	4.6(0.098)	0.46	4.88
N_2	14.9(0.206)	1.80	13.6
n_R	0.94		0.94 $\bar{5}$
n_T	-0.06		0.29 $\bar{6}$
n_N	-0.35		-0.14 $\bar{2}$
ΔP $\left(10^{-10} \frac{\text{dynes}}{\text{cm}^2}\right)$	2.2(-1.6)	0.5?	6.9
Error Cone Angle	25.3°		6.0°

were obtained by performing a mirror image subtraction about the shock transition time, of \bar{V}_1 from \bar{V}_2 , rather than a chronological one, as shown below:



This yielded the smallest σ 's for \bar{W} . [This variation of σ with the choice of the manner of subtracting \bar{V}_1 from \bar{V}_2 represents a slight violation of the ideal step model of the shock].

The average values taken directly from the data are given in the Table for a comparison with the best estimate results. The quantities in parentheses in the average value column are the values one obtains by using the average values of the eight independent parameters with the overdetermination equations of Section III-B. Notice that the average values of W_N , N_1 , and N_2 correspond poorly with those values calculated via the overdetermination equations. This is true even though the best estimate values, which satisfy the overdetermination equations exactly, and the average values do not differ very appreciably except perhaps in the case of the B_{2T} parameter. This demonstrates the sensitive

nature of these equations. In a similar manner Equation (III B - 34) is used to calculate ΔP . When average value parameters are used ΔP is seen to be negative which is impossible for an actual shock. The average value of 2.2×10^{-10} dynes/cm² corresponds to the change in proton pressure only but the best estimate value of 6.9×10^{-10} dynes/cm² refers to all particle species including, of course, electrons, and is expectedly larger. The angle between the \bar{n} -average and \bar{n} -best estimate is about 24°. Since great confidence is placed on the best estimate value owing to the large error cone angle decrease (25.3° to 6.0°) of a factor of about 4, then \bar{n} calculated via average magnetic field values only would have given an unacceptable result. Also J. K. Chao (1970) finds a value for \bar{n} ($n_R = 0.97$, $n_T = 0.25$, $n_N = -0.04$) which differs from our best estimate value by less than 7°. He also uses a best-fit technique (of trial-and-error fitting to the conservation equations) to obtain the normal.

Further evidence that \bar{n} -best estimate is a dramatic improvement over \bar{n} -average, in this case, lies in applying the two-spacecraft test described in Section II - C. This was done by utilizing the shock onset information obtained from Explorer 33 (See Figure 3), which also observed the August 29 shock. In an R-T-N coordinate system centered at the earth the position coordinates of Pioneer 7 and Explorer 33 were, respectively,

$$\bar{R}_7 = (257, 119, 7.7) R_E ,$$

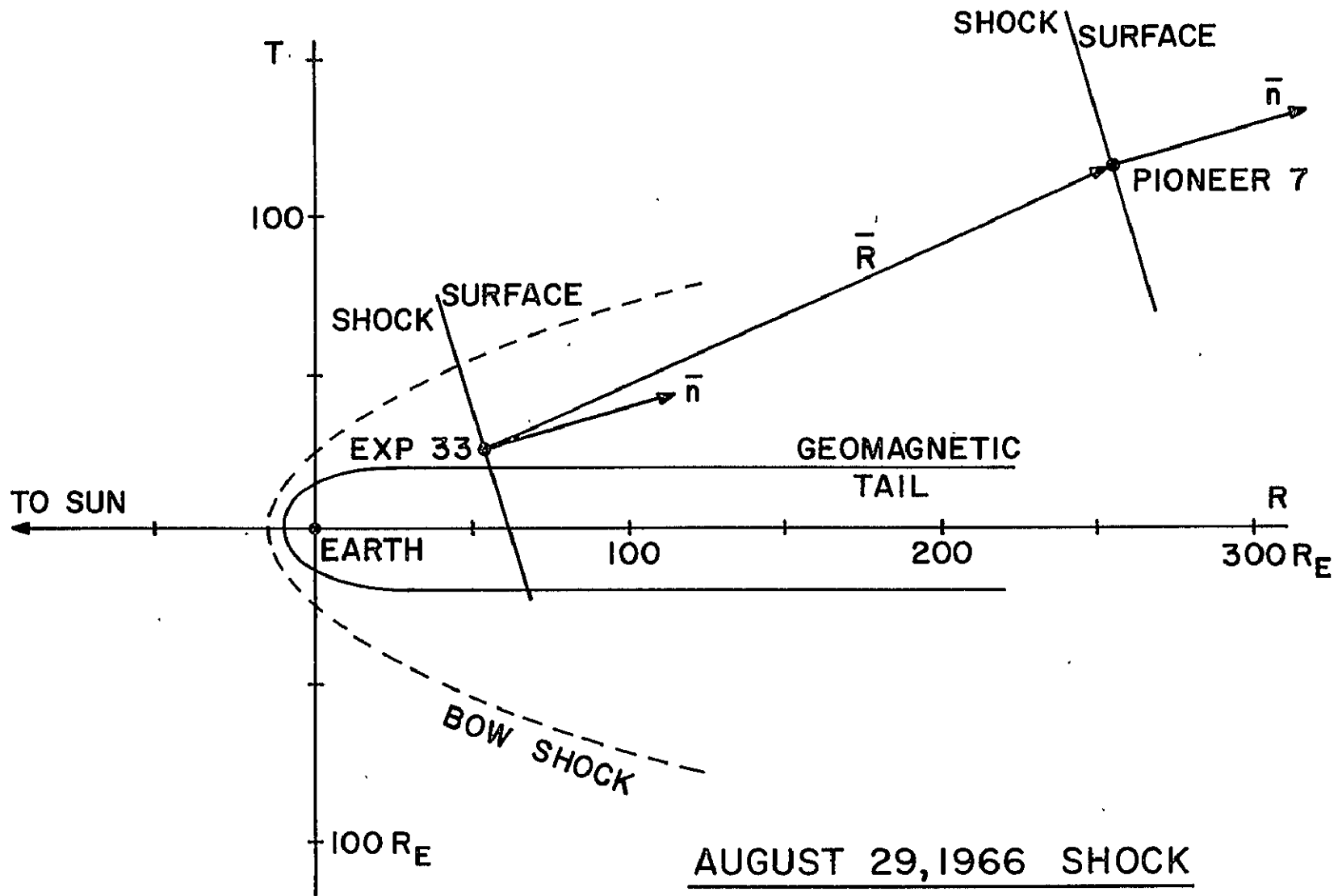


Figure 3. Explorer 33 and Pioneer 7 projected (onto ecliptic plane) positions during their observations of the August 29, 1966 shock. Theoretical locations of the unaberrated earth's bow shock and tail are shown, as well as the edge-on view of the local plane surface of the August shock with normal \vec{n} . \vec{R} is the relative position vector between the spacecraft.

and

$$\bar{R}_{33} = (54.9, 26.4, -17.0) R_E,$$

where R_E is the earth's radius. This yields a relative position displacement vector $\bar{R} = (1.29, 0.59, 0.16)$ in units of 10^6 km. Since the onset time at Explorer 33 was $13:28.5 \pm 0.7$ the delay time between sightings, τ , was 48.5 minutes. Using the first of Equations (II - 1), where the trial \bar{n} is our best estimate value, \hat{n} , we obtain an "observed" V_s , which is

$$\hat{V}_{s,obs} = \frac{\hat{n} \cdot \bar{R}}{\tau} = 471 \frac{\text{km}}{\text{sec}}.$$

For a "calculated" V_s we use Equation (III B - 37), where \bar{V}_1 will be simply the pre-shock average velocity and all other quantities best estimate ones from Table 3. This yields

$$V_{s,calc} = 467 \frac{\text{km}}{\text{sec}},$$

where

$$\bar{V}_1 = (353, 13.7, 24.8) \frac{\text{km}}{\text{sec}}.$$

We see that the observed and calculated values of V_s differ by less than 1%.

This fine correspondence is partly fortuitous since the second term in Equation (III B - 37) ($\bar{V}_1 \cdot \hat{n}$), the weak link in the argument, is probably in error by

slightly more than 1%. However, we believe that in this example, and in any case similar to it, the least squares method of calculating the shock normal leads to a significantly improved estimate of the normal as well as of the eleven relevant shock parameters.

V. ACKNOWLEDGMENT

We wish to thank the following: Mr. Eugene Lefferts for many helpful suggestions concerning the least squares technique in general and for the use of his G1NV2 computer subroutine in particular; Dr. L. F. Burlaga for his kind guidance and criticism throughout most of this work; Dr. N. F. Ness for the use of his Pioneer magnetic field data and Drs. A. J. Lazarus and Jih-Kwin Chao of M. I. T. for their Pioneer plasma data, used in the shock analysis; and Mr. Frank Ottens for his efficient and speedy support on all matters concerning the computer.

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APPENDIX A

DERIVATION OF THE OVERDETERMINATION EQUATIONS

Let Π denote the plane containing \bar{B}_1 and \bar{B}_2 and define the unit vectors

$$\bar{t}_1 \equiv \frac{\bar{\Delta B}}{|\bar{\Delta B}|} \quad (\text{A - 1})$$

$$\bar{t}_2 \equiv \frac{\bar{B}_1 \times \bar{B}_2}{|\bar{B}_1 \times \bar{B}_2|} , \quad (\text{A - 2})$$

and

$$\bar{n} \equiv \bar{t}_1 \times \bar{t}_2 \quad (\text{A - 3})$$

where

$$\bar{\Delta B} \equiv \bar{B}_2 - \bar{B}_1 . \quad (\text{A - 4})$$

Since

$$\bar{t}_1 \cdot \bar{t}_2 = 0 , \quad (\text{A - 5})$$

then

$$\bar{n} = \frac{\overline{\Delta B} \times (\bar{B}_1 \times \bar{B}_2)}{|\overline{\Delta B} \times (\bar{B}_1 \times \bar{B}_2)|} \quad (\text{A - 6})$$

We see that \bar{t}_2 is normal to the Π plane: Let Σ denote a plane perpendicular to Π and containing $\overline{\Delta B}$. Hence, both \bar{t}_1 and \bar{t}_2 must lie in the Σ plane. Then \bar{n} ($\equiv \bar{t}_1 \times \bar{t}_2$) is a unit vector normal to the Σ plane, provided neither \bar{t}_1 nor \bar{t}_2 is zero. It follows that \bar{n} lies in the Π plane. The coplanarity theorem (Colburn and Sonett, 1966) demands that the shock plane's normal lie in the Π plane.

[Notice that $\overline{\Delta B}$ (or \bar{t}_1) is common to both the Π and Σ planes]. One sees immediately, according to these definitions, that $\bar{B}_1 \cdot \bar{n}$ and $\bar{B}_2 \cdot \bar{n}$ are equal, as required by Equation (III A - 6) if \bar{n} represents the shock surface normal. We are then justified in uniquely identifying Σ with the shock surface, \bar{t}_1 and \bar{t}_2 as tangential to it while perpendicular to each other, and \bar{n} as normal to it. The situation is shown in Figure 4.

Using Equations (A - 1 to 6) we can rewrite Equations (III A - 1 to 6), which become

$$(\rho_1 \bar{V}_1^* - \rho_2 \bar{V}_2^*) \cdot \bar{n} = 0, \quad (\text{A - 7})$$

$$\left[\rho_1 (\bar{V}_1^* \cdot \bar{n}) \overline{\Delta V}^* - \frac{\bar{B}_1 \cdot \bar{n}}{4\pi} \overline{\Delta B} \right] \cdot \overline{\Delta B} = 0, \quad (\text{A - 8})$$

$$\left[\rho_1 (\bar{V}_1^* \cdot \bar{n}) \bar{\Delta V}^* - \frac{\bar{B}_1 \cdot \bar{n}}{4\pi} \bar{\Delta B} \right] \cdot (\bar{B}_1 \times \bar{B}_2) = 0, \quad (\text{A} - 9)$$

$$\left(\bar{V}_1^* \times \bar{B}_1 - \bar{V}_2^* \times \bar{B}_2 \right) \cdot \bar{\Delta B} = 0, \quad (\text{A} - 10)$$

$$\left(\bar{V}_1^* \times \bar{B}_1 - \bar{V}_2^* \times \bar{B}_2 \right) \cdot (\bar{B}_1 \times \bar{B}_2) = 0, \quad (\text{A} - 11)$$

and

$$\bar{\Delta B} \cdot \bar{n} = 0, \quad (\text{A} - 12)$$

where

$$\bar{\Delta V}^* = \bar{V}_2^* - \bar{V}_1^*, \quad (\text{A} - 13)$$

and where Equations (A - 7 and - 12) aided in obtaining Equations (A - 8 and - 9).

We define a new velocity \bar{V} related to \bar{V}^* , the plasma velocity as measured in the shock frame of reference, by

$$\bar{V}_i = \bar{V}_i^* + V_s \bar{n} \quad (i = 1, 2) \quad (\text{A} - 14)$$

where V_s is the speed of the shock frame, fixed to the shock surface, measured with respect to whatever frame \bar{V} is measured in (which could be the spacecraft

the equation becomes

$$\bar{W} \cdot (\bar{B}_1 \times \bar{B}_2) = 0 \quad (\text{A} - 17)$$

where Equation (A - 14) was used.

Now consider Equation (A - 9), which is, upon expansion,

$$\rho_1 (\bar{V}_1^* \cdot \bar{n}) \left[\bar{W} \cdot (\bar{B}_1 \times \bar{B}_2) \right] - \frac{\bar{B}_1 \cdot \bar{n}}{4\pi} \left[\bar{\Delta B} \cdot (\bar{B}_1 \times \bar{B}_2) \right] = 0$$

where (A - 16) was used. From Equation (A - 17) this immediately reduces to $\bar{\Delta B} \cdot (\bar{B}_1 \times \bar{B}_2) = 0$ since $\bar{B}_1 \cdot \bar{n} \neq 0$ in the cases that we are considering. But this is already expressed by Equation (A - 5) and therefore reduces to another identity of no further use to us here.

Consider Equation (A - 11) now. By using Equation (A - 14) it becomes

$$\left[\bar{V}_1 \times \bar{B}_1 - \bar{V}_2 \times \bar{B}_2 + v_s (\bar{n} \times \bar{\Delta B}) \right] \cdot (\bar{B}_1 \times \bar{B}_2) = 0. \quad (\text{A} - 18)$$

The third term in the brackets, with the help of Equation (A - 15), is

$$\left[\frac{(\rho_2 \bar{V}_2 - \rho_1 \bar{V}_1) \cdot \bar{n}}{\rho_2 - \rho_1} \right] \bar{n} \times \bar{\Delta B}.$$

frame of reference). By using Equation (A - 14) together with Equation (A - 7)

V_s can be shown to be

$$V_s = \frac{(\rho_2 \bar{V}_2 - \rho_1 \bar{V}_1) \cdot \bar{n}}{\rho_2 - \rho_1}. \quad (A - 15)$$

We will now use Equations (A - 14 and - 15), with \bar{n} defined by either Equation (A - 3) or (A - 6), to render Equations (A - 8 to - 12) in terms of \bar{V} instead of \bar{V}^* .

Clearly Equation (A - 12) represents an identity when \bar{n} is replaced by the Expression (A - 6). In this sense it is not an "overdetermined equation" and can not be retained as such. Next we consider Equation (A - 10) which is, after expansion,

$$\bar{V}_1^* \times \bar{B}_1 \cdot \bar{B}_2 - \bar{V}_1^* \times \bar{B}_1 \cdot \bar{B}_1 - \bar{V}_2^* \times \bar{B}_2 \cdot \bar{B}_2 + \bar{V}_2^* \times \bar{B}_2 \cdot \bar{B}_1 = 0$$

or, by the operation exchange rule for triple scalar products (op rule), is

$$\bar{V}_1^* \cdot \bar{B}_1 \times \bar{B}_2 - \bar{V}_1^* \cdot \bar{B}_1 \times \bar{B}_1 - \bar{V}_2^* \cdot \bar{B}_2 \times \bar{B}_2 + \bar{V}_2^* \cdot \bar{B}_2 \times \bar{B}_1 = 0.$$

Noticing that the second and third terms are zero and defining

$$\bar{W} \equiv \bar{V}_2 - \bar{V}_1 \quad (A - 16)$$

Using Equations (A - 1), (A - 2), and (A - 3) and the op rule this becomes

$$\left[\left(\rho_2 \bar{V}_2 \times \bar{B}_2 - \rho_2 \bar{V}_2 \times \bar{B}_1 - \rho_1 \bar{V}_1 \times \bar{B}_2 + \rho_1 \bar{V}_1 \times \bar{B}_1 \right) \cdot \bar{t}_2 \right] \frac{\bar{t}_2}{\rho_2 - \rho_1} .$$

Replacing this back into Equation (A - 18) and noticing that $\bar{t}_2 \cdot (\bar{B}_1 \times \bar{B}_2) = |\bar{B}_1 \times \bar{B}_2|$; we finally obtain

$$\left(r \bar{B}_1 - \bar{B}_2 \right) \cdot \left[\bar{W} \times \left(\bar{B}_1 \times \bar{B}_2 \right) \right] = 0 \quad (\text{A - 19})$$

where r is defined as

$$r \equiv \frac{\rho_2}{\rho_1} \quad (\text{A - 20})$$

and where the op rule was again employed.

Only Equation (A - 8) remains to be reduced. By the usual substitutions it can be written

$$\rho_1 \left(\bar{V}_1 \cdot \bar{n} - v_s \right) \left(\bar{W} \cdot \Delta \bar{B} \right) - \frac{\bar{B}_1 \cdot \bar{n}}{4\pi} |\Delta \bar{B}|^2 = 0 .$$

Replacing v_s and \bar{n} by Equations (A - 15) and (A - 6) respectively this becomes

$$\left[\frac{\rho_1 \rho_2}{\rho_2 - \rho_1} \bar{W} (\bar{W} \cdot \Delta \bar{B}) + \frac{|\Delta \bar{B}|^2}{4\pi} \bar{B}_1 \right] \cdot \left[\Delta \bar{B} \times \left(\bar{B}_1 \times \bar{B}_2 \right) \right] = 0 . \quad (\text{A - 21})$$

We refer to Equations (A - 17, - 19, and - 21) as the Overdetermination Equations because, in the sense that all eleven shock parameters of the system are assumed measured, any three parameters are overdetermined by these equations using the other eight (independent) parameters. Notice that these equations do not depend on finding the directions \bar{t}_1 , \bar{t}_2 , or \bar{n} or on any parameter depending on the shock (*) frame of reference, such as \bar{V}^* , as Equations (III A - 1 to - 6) did, and even as Equations (A - 7 to - 12) did in part.

In review then we see that Equation (A - 7) provided V_s , Equation (A - 12) and Equation (A - 9) (through the coplanarity theorem) gave us the direction \bar{n} , and the remaining three Equations (A - 8, - 10, and - 11), properly transformed, yield the Overdetermination Equations.

APPENDIX B

THE LEAST SQUARES ESTIMATOR OF A

SHOCK NORMAL AND ITS ASSOCIATED ERROR CONE ANGLE

B.1 The Estimation Procedure

Below we develop in somewhat general terms the estimation procedure, necessary for a better understanding of the less statistically oriented Section III-D. The dimensionality of all vectors and matrices is evident from the discussions in Section III-D, and the notation used here is consistent with that Section.

Let the vector \tilde{Z} represent a state which is to be estimated.* Its components are to be conceptually identified with some (i. e. any eight) of the magnetic field and plasma quantities shown in Figure 2 as the shock's underlying step function (denoted by dashed straight lines) and discussed in Section III-C. Let the vector \tilde{Y} , of higher dimensionality (N) than \tilde{Z} , be another state functionally connected to \tilde{Z} by a known function \bar{X} . Thus, $\tilde{Y} = \bar{X}(\tilde{Z})$. Assume that the vector \bar{v} represents a multivariate normal distribution with mean zero and a known covariance matrix \underline{Q}_y defined by

$$\underline{Q}_y = \underline{\text{cov}}(\bar{Y}) = E \left[(\bar{Y} - E(\bar{Y})) (\bar{Y} - E(\bar{Y}))^T \right] \quad (\text{B} - 1)$$

where E is the expectation operator [E(\bar{Y}) then simply being the mean value of \bar{Y} , $\langle \bar{Y} \rangle$], and where the superscript T represents the transpose of the vector.

* \tilde{Z} represents \bar{Z}_{true} .

The problem to be solved is the following: given one sample \bar{Y} from the distribution $\tilde{Y} + \bar{\nu}$ obtain, in some sense to be discussed below, a "best" estimate of \tilde{Z} . In practice \tilde{Y} is considered a state which is directly observable and which has a known relationship to a state \tilde{Z} , the quantity to be estimated. The random variable $\bar{\nu}$ should be thought of as the noise on the observation of \tilde{Y} , caused by instrumental inaccuracies and natural but unexplained fluctuations in the values of the relevant parameters, i. e. unexplained in terms of the "known relationship" mentioned above. The assumption that $\bar{\nu}$ has normally distributed components with zero means is a valuable convenience from a mathematical point of view. But it has more to recommend it than mathematical convenience. Giving $\bar{\nu}$ a zero mean implies we have assumed that all systematic or modeling errors have been removed from the analysis. If significant modeling errors have not been removed, then no estimation procedure is likely to provide an acceptable estimate of \tilde{Z} . Hence, little appears to be lost in assuming a zero mean for $\bar{\nu}$. The justification for modeling the noise $\bar{\nu}$ as a normal random variable rests on the vague meta-statistical analogue to the law of large numbers which can be stated as follows: "If a large number of random variables are combined in a reasonably complicated fashion to form a single random variable, then it is likely that this random variable will have a nearly normal distribution." The assumptions of this meta-statistical principal are usually satisfied when one is making observations in nature. Thus, the assumption that $\bar{\nu}$ is normally distributed has at least some reasonable support.

It remains to be clarified in just what "best" sense \tilde{Z} is to be estimated. One such common estimation procedure insists that an estimator of \tilde{Z} be chosen such that the weighted sum of the squares of the differences between observed and expected observations is minimized. More specifically we define the so-called loss function L as

$$L(\bar{Z}) = (\bar{X}(\bar{Z}) - \bar{Y})^T \underline{W} (\bar{X}(\bar{Z}) - \bar{Y})$$

where the vector \bar{Z} is an independent variable which tends toward \hat{Z} , defined as the best estimate of \tilde{Z} , as L tends toward an absolute minimum, and \underline{W} is the so-called weighting matrix of the loss function. \underline{W} is generally set equal to \underline{Q}_y^{-1} or some slight modification of it. Then for our purposes the loss function, which is given as Equation (III D - 10), is

$$L = (\bar{X} - \bar{Y})^T \underline{Q}_y^{-1} (\bar{X} - \bar{Y}) \quad (B - 2)$$

where \underline{Q}_y is given formally by definition (B - 1).

We minimize L in the following way, known as the Newton-Raphson method:

The gradient, G, of Equation (B - 2) is

$$\bar{G}(\bar{Z}) = \frac{\partial L}{\partial \bar{Z}} = 2 \left(\frac{\partial \bar{X}}{\partial \bar{Z}} \right)^T \underline{Q}_y^{-1} (\bar{X} - \bar{Y}) . \quad (B - 3)$$

We define a matrix $\underline{\underline{A}}$ as the following

$$\underline{\underline{A}}(\bar{Z}) \equiv \frac{\partial \bar{X}(\bar{Z})}{\partial \bar{Z}} . \quad (\text{B - 4})$$

[Note that the elements of $\underline{\underline{A}}$ are $A_{ij} = \partial X_i / \partial X_j$, $i = 1, 2, \dots, N$ {N given by Equation (III D - 2)} and $j = 1, 2, \dots, 8$.]

From Equations (B - 3) and (B - 4) the gradient of G is

$$\frac{\partial \bar{G}}{\partial \bar{Z}} = 2 \frac{\partial \underline{\underline{A}}^T}{\partial \bar{Z}} \underline{\underline{Q}}_y^{-1} (\bar{X} - \bar{Y}) + 2 \underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} \underline{\underline{A}} . \quad (\text{B - 5})$$

The first order Taylor's expansion of $G(\bar{Z})$ is

$$\bar{G}(\bar{Z}_n) \cong \bar{G}(\bar{Z}_{n-1}) + \left. \frac{\partial \bar{G}(\bar{Z})}{\partial \bar{Z}} \right|_{\bar{Z}_{n-1}} (\bar{Z}_n - \bar{Z}_{n-1}) . \quad (\text{B - 6})$$

Using Equations (B - 3) and (B - 5) and disregarding the latter's second order term Equation (B - 6) becomes

$$\bar{G}(\bar{Z}_n) \cong 2 \underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} (\bar{X} - \bar{Y}) \Big|_{\bar{Z}_{n-1}} + 2 \underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} \underline{\underline{A}} \Big|_{\bar{Z}_{n-1}} \bar{\Delta Z} , \quad (\text{B - 7})$$

where

$$\overline{\Delta Z}_n = \overline{Z}_n - \overline{Z}_{n-1} . \quad (\text{B} - 8)$$

For minimization of $L(\overline{Z})$, $\overline{G}(\overline{Z}_n)$ must be zero, as expressed by Equation (III D - 11). Then by defining the eight by eight matrix $\underline{\underline{B}}$ in the following way

$$\underline{\underline{B}} = \left(\underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} \underline{\underline{A}} \right)^{-1} \quad (\text{B} - 9)$$

Equation (B - 7), upon minimization, becomes

$$\overline{\Delta Z}_n \cong \left[\underline{\underline{B}} \underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} (\overline{Y} - \overline{X}) \right] \Big|_{\overline{Z}_{n-1}} . \quad (\text{B} - 10)$$

Combining Equations (B - 8) and (B - 10) yields

$$\overline{Z}_n \cong \left[\overline{Z} + \underline{\underline{B}}(\overline{Z}) \underline{\underline{A}}^T (\overline{Z}) \underline{\underline{Q}}_y^{-1} (\overline{Y} - \overline{X}(\overline{Z})) \right] \Big|_{\overline{Z}_{n-1}} \quad (n = 1, 2, \dots) . \quad (\text{B} - 11)$$

By repeated application of Equation (B - 11), provided \overline{Z}_0 is carefully chosen to insure convergence to the absolute minimum of L , \overline{Z}_n should tend toward \hat{Z} , the exact solution of Equation (III D - 11). This iterative process should converge rapidly to the correct value \hat{Z} , the best estimate of \tilde{Z} .

For different samples \bar{Y} of the random variable $\tilde{Y} + \bar{v}$ the iteration procedure will yield different values of \hat{Z} , representing samples of the associated distribution of a new random variable. This new entity will henceforth also be symbolically represented as \hat{Z} since there is little chance of confusing the random variable with one of its samples, i. e., the solution of $\bar{G}(\hat{Z}) = 0$ for a given \bar{Y} .

In evaluating the quality of an estimator \hat{Z} of \tilde{Z} , two factors are usually considered. One is the extent to which the estimator is biased. The bias of the estimator \hat{Z} of \tilde{Z} is defined as $E[\hat{Z} - \tilde{Z}]$. The other factor is the dispersion of the estimator \hat{Z} about \tilde{Z} . This is obtained by taking the second moment of \hat{Z} about \tilde{Z} defined as $E[(\hat{Z} - \tilde{Z})(\hat{Z} - \tilde{Z})^T]$. Of course, the smaller the bias and the dispersion the better the quality of the estimator. Neither the bias nor the dispersion of \hat{Z} can be conveniently calculated without the imposition of a certain linearity assumption. It must be assumed that \bar{X} can be represented by a linear expansion of itself about \tilde{Z} . From Equation (B - 4) this is

$$\bar{X}(\bar{Z}) - \bar{X}(\tilde{Z}) \cong \underline{A}(\tilde{Z})(\bar{Z} - \tilde{Z}). \quad (\text{B} - 12)$$

If one assumes that the vector root \hat{Z} of $\bar{G}(\hat{Z}) = 0$ is sufficiently close to \tilde{Z} to permit the use of Equation (B - 12), then $\bar{G}(\hat{Z}) = 0$ can be written as

$$\underline{A}^T(\tilde{Z})\underline{Q}_y^{-1}\bar{X}(\hat{Z}) + \underline{A}^T(\tilde{Z})\underline{Q}_y^{-1}\underline{A}(\tilde{Z})(\hat{Z} - \tilde{Z}) - \underline{A}^T(\tilde{Z})\underline{Q}_y^{-1}\bar{Y} \cong 0, \quad (\text{B} - 13)$$

with the help of Equation (B - 8). By applying the expectation operator to Equation (B - 13) one obtains

$$\underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} \bar{X}(\tilde{Z}) + \underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} \underline{\underline{A}}(\tilde{Z}) E[\hat{Z} - \tilde{Z}] - \underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} E[\bar{Y}] = 0 \quad (\text{B - 14})$$

Since \bar{Y} is a sample chosen from the distribution $\tilde{Y} + \bar{v} = \bar{X}(\tilde{Z}) + \bar{v}$ and since $E[\bar{v}] = 0$, as mentioned above, then it follows that $E[\bar{Y}] = \bar{X}(\tilde{Z})$. Therefore Equation (B - 14) yields:

$$E[\hat{Z} - \tilde{Z}] = 0 \quad (\text{B - 15})$$

and the estimator \hat{Z} has zero bias, i. e., it is unbiased. In the case of an unbiased estimator the covariance of the estimator is the same as the second moment of the estimator about the true value. Let $\text{cov}(\hat{Z})$ represent the covariance of \hat{Z} . By multiplying both sides of Equation (B - 13) by $\underline{\underline{B}}(\tilde{Z}) \left[\underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} \underline{\underline{A}}(\tilde{Z})^{-1} \right]$ one obtains

$$\hat{Z} = \tilde{Z} + \underline{\underline{B}}(\tilde{Z}) \underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} (\bar{Y} - \bar{X}(\tilde{Z})) \quad (\text{B - 16})$$

But $\tilde{Y} = \bar{X}(\tilde{Z})$ and $\bar{Y} - \tilde{Y} = \bar{v}$, therefore

$$\hat{Z} - \tilde{Z} = \underline{\underline{B}}(\tilde{Z}) \underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} \bar{v}, \quad (\text{B - 17})$$

and

$$\text{cov}(\bar{Y} - \bar{X}(\tilde{Z})) = \text{cov}(\bar{v}) = \underline{\underline{Q}}_y. \quad (\text{B - 18})$$

By applying the "cov" operator to both sides of Equation (B - 17) we obtain

$$\begin{aligned} \text{cov}(\hat{Z} - \tilde{Z}) &= \underline{\underline{B}}(\tilde{Z}) \underline{\underline{A}}^T(\tilde{Z}) \underline{\underline{Q}}_y^{-1} \underline{\underline{Q}}_y \underline{\underline{Q}}_y^{-1} \underline{\underline{A}}(\tilde{Z}) \underline{\underline{B}}(\tilde{Z}) \\ &= \underline{\underline{B}} \underline{\underline{A}}^T \underline{\underline{Q}}_y^{-1} \underline{\underline{A}} \underline{\underline{B}} \\ &= \underline{\underline{B}} \underline{\underline{B}}^{-1} \underline{\underline{B}} = \underline{\underline{B}}(\tilde{Z}). \end{aligned} \quad (\text{B - 19})$$

But

$$\begin{aligned} \text{cov}(\hat{Z} - \tilde{Z}) &= \mathbf{E} \left[\{(\hat{Z} - \tilde{Z}) - \mathbf{E}(\hat{Z} - \tilde{Z})\} \{(\hat{Z} - \tilde{Z}) - \mathbf{E}(\hat{Z} - \tilde{Z})\}^T \right] \\ &= \mathbf{E} \left[(\hat{Z} - \mathbf{E}(\hat{Z})) (\hat{Z} - \mathbf{E}(\hat{Z}))^T \right] \\ &= \text{cov}(\hat{Z}) \end{aligned}$$

by definition where Equation (B - 15) was used and $E(\tilde{Z}) = \tilde{Z}$ itself. Hence, Equation (B - 19) becomes

$$\text{cov}(\hat{Z}) = \underline{B}(\tilde{Z}) . \quad (\text{B} - 20)$$

According to Equation (B - 12) $\underline{A}(\tilde{Z}) \cong \underline{A}(\hat{Z})$. Using this approximation along with the definition of \underline{B} , from Equation (B - 9), Equation (B - 20) becomes

$$\text{cov}(\hat{Z}) \cong \left[\underline{A}^T(\hat{Z}) \underline{Q}_y^{-1} \underline{A}(\hat{Z}) \right]^{-1} = \underline{\underline{B}}(\hat{Z}) . \quad (\text{B} - 21)$$

We wish to strongly emphasize that the usual assumption of the unbiasedness of the least squares estimate and the assumption that Equation (B - 21) represents the covariance of the least squares estimate rest on the linearity condition given by Equation (B - 12). The validity of this linearity condition is influenced by the degree of nonlinearity of the function which relates the state \tilde{Z} to the state of observations \tilde{Y} and by the distance between \hat{Z} and \tilde{Z} . This last factor is highly correlated with \bar{v} , the noise on the observations.

Since $\underline{\underline{B}}(\tilde{Z})$ is available at each step of the iteration procedure described by Equation (B - 11), then for the final ("best") estimate giving $\underline{\underline{B}}(\hat{Z})$, assuming true convergence, Equation (B - 21) provides us with a means of calculating the covariance matrix of \hat{Z} . This will be used in the next section (Appendix B.2) to obtain the error cone angle associated with the best estimate array \hat{Z} .

For further detail concerning estimation theory in general see Deutsch (1965).

B.2 The Construction of Error Cone Angles

In Appendix B.1 we provided a computational procedure for obtaining \hat{Z} , the least squares estimate of a vector \tilde{Z} (and also \hat{X} after the overdetermination equations are employed using the components of \hat{Z} as the independent variables). We also established the mean and variance of \hat{Z} as a random variable by assuming unbiased measurements and a linearity condition. To generate error cones for \bar{n} what we require as well is the precise distribution of the least squares estimate of \tilde{B}_1 and \tilde{B}_2 . To obtain this, one further assumption, previously stated but not used until now, is needed. That is, the noise \bar{v} on the observations is assumed normally distributed. Notice that Equation (B - 17) gives the least squares estimate \hat{Z} as

$$\hat{Z} = \tilde{Z} + \left(\underline{A}^T(\tilde{Z}) \underline{Q}_y^{-1} \underline{A}(\tilde{Z}) \right)^{-1} \underline{A}^T(\tilde{Z}) \underline{Q}_y^{-1} \bar{v}$$

where \tilde{Z} is, of course, a constant. Thus, \hat{Z} is a linear function of \bar{v} . A linear function of a normal random variable is normal also. A convenient feature of the normal distribution is that it is completely determined by its mean and variance. The least squares estimator \hat{Z} is unbiased. Hence, its expectation is \tilde{Z} . Its covariance matrix is given by Equation (B - 21). Thus, under the assumption of normal noise on the observations, the distribution of \hat{Z} is completely

specified. However, our main interest now is focused on the distribution of the least squares estimates of the vectors \tilde{B}_1 and \tilde{B}_2 , i. e. on the first six components of \hat{Z} .

Let \hat{Z}' be the least squares estimate of \tilde{B}_1 and \tilde{B}_2 , i. e. $\hat{Z} = (\hat{Z}', W_y, W_z)$ [See Table 1 and Equation (III D - 5)]. Then, since \hat{Z} is normal, \hat{Z}' is also normally distributed with expectation the true values of \tilde{B}_1 and \tilde{B}_2 . The covariance matrix of \hat{Z}' can be obtained simply by deleting the last two rows and columns of the covariance matrix of \hat{Z} (Graybill, 1961). Using this technique we can construct the exact distribution of the least squares estimate of \tilde{B}_1 and \tilde{B}_2 . Also with this background information we can perform useful simulation studies, as a test of the estimation scheme, and obtain least squares associated error cone estimates for simulation or real cases.

The ultimate goal of our least squares error analysis is not to obtain best estimates of \tilde{B}_1 and \tilde{B}_2 but to obtain the best possible estimate of the true shock normal \tilde{n} . This is functionally related to \tilde{B}_1 and \tilde{B}_2 by

$$\tilde{n} = \bar{F}(\tilde{B}_1, \tilde{B}_2) , \quad (B - 22)$$

where, from Equation (A - 6),

$$\bar{n} = \frac{\Delta \bar{B} \times (\bar{B}_1 \times \bar{B}_2)}{|\Delta \bar{B} \times (\bar{B}_1 \times \bar{B}_2)|} = \bar{F}(\bar{B}_1, \bar{B}_2) \quad (B - 23)$$

with

$$\overline{\Delta B} = \overline{B}_2 - \overline{B}_1 .$$

But since we do not possess the true values \tilde{B}_1 and \tilde{B}_2 (except in the cases of simulation studies), we must be satisfied with our least squares best estimates \hat{B}_1 and \hat{B}_2 and obtain an estimate \hat{n} of \tilde{n} as

$$\hat{n} = \overline{F}(\hat{B}_1, \hat{B}_2) = \overline{F}(\hat{Z}') . \quad (\text{B} - 24)$$

Of major interest to us then is the statistical distribution of the error made in estimating \tilde{n} by \hat{n} . A natural measure of this error is the angle between \tilde{n} and \hat{n} . Thus, we define the function $\phi(\hat{n})$ as

$$\phi(\hat{n}) = \cos^{-1}(\tilde{n} \cdot \hat{n}) , \quad (\text{B} - 25)$$

where the principal value is understood. Obviously $\phi(\hat{n})$ is the angular error introduced by using \hat{n} as an estimate of the true normal. Now we introduce another function $\psi(\hat{Z}')$ as

$$\psi(\hat{Z}') = \phi[\overline{F}(\hat{Z}')] . \quad (\text{B} - 26)$$

$\psi(\hat{Z}')$ can be interpreted as the angular error in the normal estimate caused by using the least squares estimates of \tilde{B}_1 and \tilde{B}_2 rather than their inaccessible true values. In carrying out the least squares procedure for estimating normals, it is the statistical distribution of $\psi(\hat{Z}')$ rather than that of \hat{Z}' which is of interest. Since the function ψ is highly nonlinear the only reliable procedure for estimating the distribution of $\psi(\hat{Z}')$ is a Monte Carlo one. As constructed, the distribution of $\psi(\hat{Z}')$ lies between zero and 180° , and our goal is to estimate a cone angle α such that 95% of the distribution lies between zero and α . [The error cone geometrical interpretation is given in Section IV-A.] In other words, the probability is 0.95 that our estimate of the shock normal obtained by our least squares procedure will lie in this cone. This 95% error cone clearly has intuitive appeal as a measure of our ability to estimate shock normals with the least squares procedure. It has the disadvantage, however, of being a single parameter measure of a cone that more precisely should not be described as being right circular. That is, strictly speaking the covariance matrix resulting from the least squares scheme contains enough information to be used to obtain a cone with an elliptical cross-section rather than a circular one. There is no reason to expect an "isotropic noise" situation to exist in general, and, in fact, there is good reason to expect otherwise for an average interplanetary type shock. But within the capability of the overall scheme, considering its limiting assumptions, the single parameter measure of an error cone should certainly be adequate.

With the covariance matrix of \hat{Z}' in our possession we can implement the Monte Carlo process for estimating α by the following steps [Note: These same steps are used for obtaining the mean value error cone using its covariance matrix as discussed in Section IV-A]:

1. Sample K times randomly from the distribution for \hat{Z}' as defined by its covariance matrix.
2. Evaluate the function $\psi(\hat{Z}')$ at each of these K points and thereby obtain K functional values of ψ .
3. Choose the functional value which is the smallest value that is larger than 95% of the K functional values obtained from step 2. This value is an unbiased estimate of α .

The variance of the estimate of α obtained from steps 1, 2, and 3 above is inversely proportional to the Monte Carlo sample size K. From elementary probability theory it can be easily shown that, to a 95% certainty, the true percentage of the distribution of \hat{n} contained in the 95% critical error cone centered at \tilde{n} is not less than 94% if $K \geq 2,420$. For greater reliability we choose $K = 3,000$ for each cone angle calculation.

APPENDIX C

COMPUTER PROGRAMS USED IN SCHEME

The programs listed here, and used in this work, were written for the IBM 360-75 J computer.

C.1 Program to Obtain Best-Estimates; Main and Subroutines

On the eight pages following this preface there appears the shock program listing for real and simulated shocks. Table 5 shows the input format for the relevant input quantities.

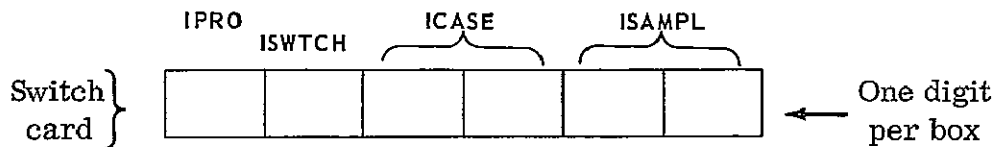
Table 5
Input Format

	Quantity	Format Designation	Descriptive Notes
Switches	{	I PRO	I 1 Integer with MFW* of 1
		I SWTCH	I 1 Integer with MFW of 1
		I CASE	I 2 Integer with MFW of 2, right adjusted
		I SAMPL	I 2 Integer with MFW of 2, right adjusted
	XSTART	8 F 6.2	FPN** with MFW of 6
	SIG	11 F 6.2	FPN with MFW of 6
	NN	11 I 6	Integer with MFW of 6, right adjusted
	Y	11 F 6.2	FPN with MFW of 6

*MFW means maximum field width.

**FPN means floating point number.

Recall that input XSTART, which is the starting vector for real shock studies, is \bar{Z}_{true} (See Section IV-B) for simulated shock studies. [A sample of the printed output is given in Appendix D.1 and described in Section IV-B.] The four switches comprise four numbers on a single input card as shown below:



The switch card is the first data card. The second data card is the XSTART card carrying eight numbers. The third card is SIG with eleven numbers. The fourth is NN with eleven numbers. And the last set of cards comprises the Y data array, each card of eleven numbers until all $N (= \sum NN(i))$ data points are listed. For example, if N is 28, then the first Y card has eleven numbers, the second eleven also, and the third card has six numbers. Table 5 shows this overall order for the cards. The Y array is used only for real shock cases; for simulated shocks no Y data is necessary, of course. In all other respects the above comments hold for both real and simulated shock cases. If in the case of a real shock a second or third, etc., XSTART is used, these are placed in order immediately after the Y array. And if another real shock is to be processed, the entire order of cards, from the 1st XSTART to the last XSTART, is repeated. And repeated again for a third shock, etc. But each separate real shock case must have the same number of XSTART's. In the simulated cases of more than

one shock the set of XSTART, SIG, NN is simply repeated for each case. For any given computer run, for a real or simulated study, only one switch card is used and it is always the 1st card after the control cards. Table 6 schematically represents the card order for real and simulated cases. Below we describe the switches and how they are used. IPRO is used to control whether a real or simulated shock is to be processed. ISWTCH can switch from XSTART unaltered to XSTART changed to XMEAN (from Y array) as the starting vector of the

Table 6

Input Data Card Order (One card for each line)

Real Study		Simulated Study		
<u>Switch Card</u>		<u>Switch Card</u>		
XSTART(1)	}	XSTART	}	
SIG		SIG		1st shock
NN		NN		case
Y	}		}	
...				2nd shock
...	}	(repeat	}	
		order)		case
XSTART(2)	}			
XSTART(3)				
etc.				
(repeat order		}		}
with same no.	2nd shock			
of XSTART's)		case		

iteration process. ICASE is just the number of different shocks (or cases) to be studied. ISAMPL is the number of samples of a given shock case (from the random number generator) to be considered for a simulated case, but it is the number of starting vectors for any given real case. [Note: Program is arranged to require the same number of "samples" for each shock case, for both real and simulated studies]. Table 7 shows what values the switches must have to perform the duties described above. Section IV-B gives an example of their use for a simulation study.

Table 7

Program Switches

$$\text{IPRO} = \begin{cases} 0, & \text{real shock(s) being processed} \\ 1, & \text{simulated shock(s) being processed.} \end{cases}$$

$$\text{ISWTCH} = \begin{cases} 0, & \text{unaltered XSTART} \\ 1, & \text{XSTART changed to XMEAN for iteration} \end{cases}$$

$$\text{ICASE} = \text{from 1 to 99 equal to number of shocks}$$

$$\text{ISAMPL} = \text{from 1 to 99 equal to number of samples for each shock.}$$

As an example of the use of the switches in a real shock study of two shocks using three starting vectors, the switches would be:

IPRO = 0	}	Switch card					
ISWTCH = 0		0	0	0	2	0	3
ICASE = 2							
ISAMPL = 3							

[Note: If ISAMPL is other than 1, ISWTCH should be 0 for a real case. If this is not adhered to, the program will successfully run but waste computer time through repeated operations].

For a real study of a single shock of $N = 90$ (number of components of \bar{Y}) with one starting vector the total program running time on the IBM 360-75-J is only about 0.3 minutes.

```

      IMPLICIT REAL*8 (A-H,M,O-Z)
      DIMENSION X(15),G(7),NN(11),Y(550),XXX(8), XX(26,15),
1B(8,8),A(550,8),Q(550),M(11),C(11,8),SIG(11),GK(11)
      DIMENSION XMEAN(15),ZZ(16),XSTART(15),XLOSS(16),QUAL(16)
      COMMON/XSQR/G4A,G5A,G6A,G4B,G5B,G6B,G4E,G5E,G6E,
1XNINE,TEN,ELEVEN,XLOSSM,QUAL,ZZ,QUALM,ISWTCH
      COMMON/AASUB/C
      CONV=57.29578D0

      IPRO TELLS THE PROGRAM WHETHER OR NOT WE WILL USE XMONTE TO
      GENERATE THE Y ARRAY (IPRO=1 USE XMONTE(SIMULATED SHOCK) IPRO=0
      USE XMONTE(REAL SHOCK))

      ISWTCH TELLS SUBROUTINE XSQ WHETHER OR NOT TO SET XSTART=XMEAN. IF
      ISWTCH=1 SET XSTART(I),FOR I=1,8,EQUAL TO XMEAN(I) IF ISWTCH=0 DO
      NOT SET THEM EQUAL.

      ICASE IS THE NUMBER OF DIFFERENT CASES TO BE PROCESSED

      ISAMPL FOR SIMULATED SHOCKS IS THE NUMBER OF SAMPLES PER CASE. FOR
      SHOCKS ISAMPL IS THE NUMBER OF XSTARTS PER CASE.

      READ(5,09)IPRO,ISWTCH,ICASE,ISAMPL
      ISSAME=0
      ITOTAL=1
      ITOTLE=ICASE*ISAMPL
      8 FORMAT(11I6)
      25 FORMAT(1H0,'INPUT XSTART WAS ',08(F9.3,1X))
      111 FORMAT(1H0,'XSTART REPLACED BY XMEAN')
      113 FORMAT(1H,'SIMULATED SHOCK BEING PROCESSED')
      112 FORMAT(1H,'REAL SHOCK BEING PROCESSED')
      31 FORMAT(1H1,'SHOCK PROGRAM OUTPUT')
      6 FORMAT(11F6.2)
      27 FORMAT(1H0,'THE TOTAL NUMBER OF DATA POINTS,N,IS ',I4)
      18 FORMAT(1H0,'THE INPUT Y ARRAY WAS ')
      32 FORMAT(1H,11(F9.3,1X))
      9 FORMAT(2I1,2I2)
      57 FORMAT(1H0,24X,3HB1X,7X,3HB1Y,7X,3HB1Z,7X,3HB2X,7X,3HB2Y,
      17X,3HB2Z,7X,3H WY,7X,3H WZ,7X,3H N1,7X,3H N2,7X,3H WX)
      26 FORMAT(1H,'THE INPUT SIG WAS ',11(F9.3,1X))
      28 FORMAT(1H,'THE INPUT NN WAS ',11(I9,1X))
      55 FORMAT(1H0,'THE CORRESPONDING G VALUES ARE')
      70 FORMAT(1H,7(F9.3,1X))
      56 FORMAT(1H,6X,2HN1,8X,2HN2,8X,2HWX,8X,2HNX,8X,2HNY,8X
      1,2HNZ,8X,2HDP)
      11 FORMAT(1H0,'THE NUMBER OF ITERATIONS,L,IS ',I5)
      12 FORMAT(1H0,'THE BEST ESTIMATE INDEPENDENT PARAMETER MATRIX IS')
      67 FORMAT(1H,5X,3HB1X,7X,3HB1Y,7X,3HB1Z,7X,3HB2X,7X,3HB2Y,7X,
      13HB2Z,7X,3H WY,7X,3H WZ,7X,3H N1,7X,3H N2,7X,3H WX)
      50 FORMAT(1H,84X,F16.5,'=LOSS M'//)
      114 FORMAT(1H,8(F9.3,1X),4X,F16.5,'=LOSS ',I2,' Z= ',F8.4)
      44 FORMAT(1H,8(F9.3,1X),4X,F16.5,'=LOSS ',I2)
      106 FORMAT(1H0,'THE BEST ESTIMATE DEPENDENT PARAMETER MATRIX IS ')
      107 FORMAT(1H,16X,2HN1,8X,2HN2,8X,2HWX,8X,2HNX,8X,2HNY,8X,2HNZ,
      18X,2HDP)
      109 FORMAT(1H,10X,7(F9.3,1X),04X,F16.5,'=QUALITY ',I2)
      105 FORMAT(1H,10HMEAN'S G'S,7(F9.3,1X),4X,F16.5,'=QUALITY M'//)
      16 FORMAT(1H0,'B, THE COVARIANCE MATRIX OF FINAL ESTIMATE, IS ')
      29 FORMAT(1H,11(F9.3,1X),'MEAN VALUES')
      40 FORMAT(1H0,'THE CONTRACTED FORM OF DERIVATIVE MATRIX,A, IS')
      23 FORMAT(1H,8(F9.3,1X),10X)
      21 FORMAT(1H,8(F9.5,1X))
      71 FORMAT(1H0,'AAVE=' ,F7.3,5X,'ABE=' ,F7.3,5X,'AVE,ABE=' ,F7.3)
      1114 FORMAT(8F6.2)
      1115 FORMAT(1H0,'THE NUMBER OF DIFFERENT CASES TO BE PROCESSED IS ',I3)
      3 READ(5,1114)(X(I),I=1,08)
      DO 115 I=1,8
      115 XXX(I)=X(I)
      READ(5,6)SIG
      READ(5,8)NN
      NTOT=NN(1)+NN(2)+NN(3)+NN(4)+NN(5)+NN(6)+NN(7)+NN(8)+NN(9)+NN(10)
      1+NN(11)
      230 WRITE(6,31)
      IF(ISWTCH.EQ.1)WRITE(6,111)
      IF(IPRO.EQ.0)WRITE(6,112)
      IF(IPRO.EQ.1)WRITE(6,113)
      WRITE(6,1115)ICASE
      WRITE(6,27)NTOT
      IF(IPRO.EQ.1)GO TO 24

```

```

      IF((IPRO.EQ.0).AND.(ISSAME.NE.0))GO TO 120
      DO 17 I=1,NTOT,11
      IKK=I+10
17  READ(5,6)(Y(JXC),JXC=I,IKK)
120  WRITE(6,18)
      DO 19 I=1,NTOT,11
      IKK=I+10
      WRITE(6,32)(Y(JXC),JXC=I,IKK)
19  CONTINUE
24  WRITE(6,57)
      WRITE(6,26)SIG
      WRITE(6,28)NN
      CALL CON(X,G)
      WRITE(6,25)(X(I),I=1,08)
      WRITE(6,55)
      WRITE(6,56)
      WRITE(6,70)G
      IF(IPRO.EQ.1)CALL XMONTE(SIG,NN,Y,X)
      CALL XSQ(SIG,NN,Y,X,XX,L,B,XLOSS,XMEAN)
      WRITE(6,11)L
      WRITE(6,12)
      WRITE(6,67)
      JTOP=L+1
      DO 13 I=1,JTOP
      IF(I.EQ.1)WRITE(6,29)(XMEAN(LM),LM=1,8),XNINE,TEN,ELEVEN
      IF(I.EQ.1)WRITE(6,50)XLOSSM
      NCOUNT=I-1
      JJTOP=16
      IF(I.EQ.JJTOP)WRITE(6,44)(XX(I,LM),LM=1,8),XLOSS(I),NCOUNT
      IF(I.NE.JJTOP)WRITE(6,114)(XX(I,LM),LM=1,8),XLOSS(I),NCOUNT,ZZ(I)
      IF(I.EQ.JTOP)GO TO 100
      GO TO 13
100  DO 101 II=1,8
      GK(II)=XX(I,II)
101  CONTINUE
13  CONTINUE
      WRITE(6,106)
      WRITE(6,107)
      DO 102 I=1,JTOP
      NCOUNT=I-1
      IF(I.EQ.1)WRITE(6,105)(XMEAN(LM),LM=9,15),QUALM
      WRITE(6,109)(XX(I,LM),LM=9,15),QUAL(I),NCOUNT
102  CONTINUE
      CALL AA(GK,NN,A)
      WRITE(6,16)
      DO 41 I=1,8
      WRITE(6,21)(B(I,LM),LM=1,8)
41  CONTINUE
      WRITE(6,40)
      DO 20 I=1,11
      WRITE(6,23)(C(I,LM),LM=1,8)
20  CONTINUE
      CEA=((G4E*G4A)+(G5E*G5A)+(G6E*G6A))
      CEB=((G4E*G4B)+(G5E*G5B)+(G6E*G6B))
      CAB=((G4A*G4B)+(G5A*G5B)+(G6A*G6B))
      CC=DARCOS(CEA)
      BB=DARCOS(CEB)
      DD=DARCOS(CAB)
      AAVE=CC*CONV
      ABE=BB*CONV
      AVEABE=DD*CONV
      WRITE(6,71)AAVE,ABE,AVEABE
      IF(ITOTAL.EQ.ITOTLE)GO TO 99
      ITOTAL=ITOTAL+1
      ISSAME=ISSAME+1
      IF(ISSAME.EQ.ISAMPL)ISSAME=0
      IF(IPRO.EQ.0)GO TO 118
      DO 116 I=1,8
116  X(I)=XXX(I)
      GO TO 119
118  IF((IPRO.EQ.0).AND.(ISSAME.NE.0))READ(5,1114)(X(I),I=1,08)
119  IF(ISSAME.EQ.0)GO TO 3
      GO TO 230
99  STOP
      END
      SUBROUTINE CON(X,G)
      IMPLICIT REAL*8 (A-H,M,O-Z)
      REAL*8 N1,N2
      DIMENSION X(15),G(7)

```

```

B1X=X(1)
B1Y=X(2)
B1Z=X(3)
B2X=X(4)
B2Y=X(5)
B2Z=X(6)
WY=X(7)
WZ=X(8)
XX=B2X-B1X
Y=B2Y-B1Y
Z=B2Z-B1Z
PIE=3.1415927
F=(XX**2+Y**2+Z**2)/(4.0D0*PIE)
A=B2X**2+B2Y**2+B2Z**2-B1X**2-B1Y**2-B1Z**2
QX=(B1Y*B2Z)-(B1Z*B2Y)
QY=(B1Z*B2X)-(B1X*B2Z)
QZ=(B1X*B2Y)-(B1Y*B2X)
MX=(QZ*Y)-(QY*Z)
MY=(QX*Z)-(QZ*XX)
MZ=(QY*XX)-(QX*Y)
E=-((WY*QY)+(WZ*QZ))/QX
T=E*XX+WY*Y+WZ*Z
D=E*MX+WY*MY+WZ*MZ
GG=B1X*MX+B1Y*MY+B1Z*MZ
M=DSQRT(MX**2+MY**2+MZ**2)
SX=WY*QZ-WZ*QY
SY=WZ*QX-E*QZ
SZ=E*QY-WY*QX
R=(B2X*SX+B2Y*SY+B2Z*SZ)/(B1X*SX+B1Y*SY+B1Z*SZ)
RR=-((F*GG)/(T*D))
WX=E
N1=((R-1.0D0)/R)*(5979.14D0*RR)
N2=(R-1.0D0)*(5979.14D0*RR)
G(1)=N1
G(2)=N2
G(3)=WX
G(4)=MX/M
G(5)=MY/M
G(6)=MZ/M
G(7)=(((RR*D**2)/(M**2))-(A/(8.*PIE)))
RETURN
END

```

```

SUBROUTINE FI(X,NN,F)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION X(15),NN(11),F(550),M(11),G(7)
C FI CALCULATES EXPECTED VALUE OF OBSERVATIONS AND STORES THEM IN F
C NN(I) IS NUMBER OF OBSERVATIONS OF ITH VARIABLE
C X ARRAY CONTAINS SHOCK PARAMETERS
CALL CON(X,G)
X(9)=G(1)
X(10)=G(2)
X(11)=G(3)
N=0
DO 1 J=1,11
N=N+NN(J)
1 M(J)=N
J=1
DO 2 I=1,N
IF(I.LE.M(J))GO TO 2
J=J+1
2 F(I)=X(J)
RETURN
END

```

```

FUNCTION XL(X,SIG,Y,NN)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION X(15),SIG(11),Y(550),Q(550),NN(11),B(11),F(550),M(11)
1,G(7)
C XL IS THE LOSS FUNCTION
C X IS THE ESTIMATE OF SHOCK PARAMETERS
C SIG(I) IS THE SIGMA VALUE ON ITH VARIABLE
C Y(I) IS THE ITH OBSERVATION
C NN(I) IS NUMBER OF OBSERVATIONS ON ITH VARIABLE
J=1
N=0
DO 1 I=1,11
B(I)=1.0D0/(SIG(I)*SIG(I))
N=N+NN(I)
1 M(I)=N
DO 2 I=1,N

```

```

IF(I.LE.M(J))GO TO 2
J=J+1
2 Q(I)=B(J)
CALL FI(X,NN,F)
DO 3 I=1,N
3 F(I)=F(I)-Y(I)
XL=0.0D0
DO 4 I=1,N
4 XL=XL+(Q(I)*F(I)*F(I))
RETURN
END
SUBROUTINE AA(X,NN,A)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION X(15),NN(11),A(550,8),B(6),ID(8,8),XK(3,6)
1,C(11,8),YM(3,6),D1(6),G1(6),T1(6),F1(6),XJ(6),SS(3,6),XETA(6),
2XXI(6),W(3),Q(3),XM(3),S(3),H(6),WS(3,3),WE(3),WW(3),V(3),TW(3),
3DW(3),U(3),M(11)
COMMON/AASUB/C
DO 1 I=1,6
1 B(I)=X(I)
W(2)=X(7)
W(3)=X(8)
XX=B(4)-B(1)
Y=B(5)-B(2)
Z=B(6)-B(3)
PIE=3.1415927D0
F=(XX**2+Y**2+Z**2)/(4.0D0*PIE)
Q(1)=(B(2)*B(6))-(B(3)*B(5))
Q(2)=(B(3)*B(4))-(B(1)*B(6))
Q(3)=(B(1)*B(5))-(B(2)*B(4))
XM(1)=(Q(3)*Y)-(Q(2)*Z)
XM(2)=(Q(1)*Z)-(Q(3)*XX)
XM(3)=(Q(2)*XX)-(Q(1)*Y)
E=-((W(2)*Q(2))+(W(3)*Q(3)))/Q(1)
T=E*XX+W(2)*Y+W(3)*Z
D=E*XM(1)+W(2)*XM(2)+W(3)*XM(3)
G=B(1)*XM(1)+B(2)*XM(2)+B(3)*XM(3)
S(1)=W(2)*Q(3)-W(3)*Q(2)
S(2)=W(3)*Q(1)-E*Q(3)
S(3)=E*Q(2)-W(2)*Q(1)
ETA=B(4)*S(1)+B(5)*S(2)+B(6)*S(3)
XI=B(1)*S(1)+B(2)*S(2)+B(3)*S(3)
R=ETA/XI
RR=-((F*G)/(T*D))
DEN=(R-1.0D0)*(5979.14D0*RR)
DO 2 I=1,8
DO 2 J=1,8
ID(I,J)=0
IF(I.EQ.J)ID(I,J)=1
2 CONTINUE
DO 3 I=1,6
XK(1,I)=B(6)*ID(2,I)+B(2)*ID(6,I)-B(5)*ID(3,I)
1 -B(3)*ID(5,I)
XK(2,I)=B(3)*ID(4,I)+B(4)*ID(3,I)-B(1)*ID(6,I)
1-B(6)*ID(1,I)
XK(3,I)=B(1)*ID(5,I)+B(5)*ID(1,I)-B(2)*ID(4,I)
1-B(4)*ID(2,I)
3 CONTINUE
DO 4 I=1,6
C(11,I)=-((E*XK(1,I)+W(2)*XK(2,I)+W(3)*XK(3,I))/(Q(1)))
4 CONTINUE
DO 5 I=2,3
5 C(11,I+5)=-((Q(2)*ID(2,I)+Q(3)*ID(3,I))/(Q(1)))
DO 6 I=1,6
YM(1,I)=XK(3,I)*Y-XK(2,I)*Z+Q(3)*(ID(5,I)-ID(2,I))
1-Q(2)*(ID(6,I)-ID(3,I))
YM(2,I)=XK(1,I)*Z-XK(3,I)*XX+Q(1)*(ID(6,I)-ID(3,I))
1-Q(3)*(ID(4,I)-ID(1,I))
YM(3,I)=XK(2,I)*XX-XK(1,I)*Y+Q(2)*(ID(4,I)-ID(1,I))
1-O(1)*(ID(5,I)-ID(2,I))
D1(I)=E*YM(1,I)+W(2)*YM(2,I)+W(3)*YM(3,I)+XM(1)*C(11,I)
G1(I)=0.0D0
DO 7 J=1,3
7 G1(I)=G1(I)+ID(J,I)*XM(J)+B(J)*YM(J,I)
T1(I)=E*(ID(4,I)-ID(1,I))+W(2)*(ID(5,I)-ID(2,I))+W(3)
1*(ID(6,I)-ID(3,I))+XX*C(11,I)
F1(I)=(XX*(ID(4,I)-ID(1,I))+Y*(ID(5,I)-ID(2,I))+Z
1*(ID(6,I)-ID(3,I)))/(2.0D0*PIE)
XJ(I)=RR*(F1(I)/F+G1(I)/G-T1(I)/T-D1(I)/D)

```

```

SS(1,I)=W(2)*XK(3,I)-W(3)*XK(2,I)
SS(2,I)=W(3)*XK(1,I)-E*XK(3,I)-Q(3)*C(11,I)
SS(3,I)=E*XK(2,I)-W(2)*XK(1,I)+Q(2)*C(11,I)
XETA(I)=0.0D0
XXI(I)=0.0D0
DO 8 J=1,3
XXI(I)=XXI(I)+ID(J,I)*S(J)+B(J)*SS(J,I)
8 XETA(I)=XETA(I)+ID(J+3,I)*S(J)+B(J+3)*SS(J,I)
H(I)=(XI*XETA(I)-ETA*XXI(I))/(XI**2)
C(10,I)=DEN*(H(I)/(R-1.0D0)+XJ(I)/RR)
C(9,I)=(R*C(10,I)-DEN*H(I))/(R**2)
6 CONTINUE
DO 9 I=2,3
WS(1,I)=Q(3)*ID(2,I)-Q(2)*ID(3,I)
WS(2,I)=Q(1)*ID(3,I)-Q(3)*C(11,I+5)
WS(3,I)=Q(2)*C(11,I+5)-Q(1)*ID(2,I)
WW(I)=0.0D0
WE(I)=0.0D0
DO 10 J=1,3
WE(I)=WE(I)+B(J+3)*WS(J,I)
10 WW(I)=WW(I)+B(J)*WS(J,I)
V(I)=(XI*WE(I)-ETA*WW(I))/(XI**2)
TW(I)=XX*C(11,I+5)+Y*ID(2,I)+Z*ID(3,I)
DW(I)=XM(1)*C(11,I+5)+XM(2)*ID(2,I)+XM(3)*ID(3,I)
U(I)=-RR*(TW(I)/T+DW(I)/D)
C(10,I+5)=DEN*(U(I)/RR+V(I))/(R-1.0D0)
C(9,I+5)=(R*C(10,I+5)-DEN*V(I))/(R**2)
9 CONTINUE
DO 11 I=1,8
DO 12 J=1,8
C(J,I)=ID(J,I)
12 CONTINUE
11 CONTINUE
N=0
DO 13 L=1,11
N=N+NN(L)
13 M(L)=N
DO 15 K=1,8
J=1
DO 14 I=1,N
IF(I.LE.M(J))GO TO 14
J=J+1
14 A(I,K)=C(J,K)
15 CONTINUE
RETURN
END

```

```

SUBROUTINE XSQ(SIG,NN,Y,XSTART,XX,L,B,XLOSS,XMEAN)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION SIG(11),NN(11),Y(550),XSTART(15),XX(26,15),ZZ(16),
1B(8,8),XLOSS(16),XMEAN(15),Q(550),G(7),G1(7),C(8),M(11),QUAL(16)
COMMON/XSQR/G4A,G5A,G6A,G4B,G5B,G6B,G4E,G5E,G6E,
1XNINE,TEN,ELEVEN,XLOSSM,QUAL,ZZ,QUALM,ISWTC
C SIG(I) IS SIGMA VALUE ON ITH PARAMETER
C NN(I) IS NUMBER OF OBSERVATIONS OF ITH PARAMETER
C Y(I) IS ITH OBSERVATION,OR ITH COMPONENT OF DATA ARRAY
C XSTART IS STARTING VECTOR FOR NUMERICAL SOLUTION
C XX(I,J) IS ITH ESTIMATE OF JTH PARAMETER
C L IS NUMBER OF ITERATIONS USED
C B IS FINAL PROPAGATED COVARIANCE MATRIX OF BEST ESTIMATE
C XLOSS(I) IS VALUE OF LOSS FUNCTION FOR ITH STEP OF ITERATION
C XMEAN IS DATA AVERAGE VALUE PARAMETER ARRAY
MTT=0
N=0
CNORM=0.0D0
J=1
XNORM=0.0D0
DO 1 I=1,11
XMEAN(I)=0.0D0
N=N+NN(I)
1 M(I)=N
DO 2 I=1,N
IF(I.LE.M(J))GO TO 3
J=J+1
3 Q(I)=1.0D0/(SIG(J)*SIG(J))
2 XMEAN(J)=XMEAN(J)+(Y(I)/NN(J))
XNINE=XMEAN(9)
TEN=XMEAN(10)
ELEVEN=XMEAN(11)
XLOSSM=XL(XMEAN,SIG,Y,NN)

```

```

QUALM =DSQRT(N/XLOSSM)
CALL CON(XMEAN,G)
G4A=G(4)
G5A=G(5)
G6A=G(6)
CALL CON(XSTART,G1)
G4E=G1(4)
G5E=G1(5)
G6E=G1(6)
DO 4 I=1,7
J=I+8
XMEAN(J)=G(I)
4 XSTART(J)=G1(I)
IF(ISWTCH.EQ.1)GO TO 10
GO TO 11
10 DO 12 I=1,15
12 XSTART(I)=XMEAN(I)
11 DO 5 I=1,15
5 XX(1,I)=XSTART(I)
XLOSS(1)=XL(XSTART,SIG,Y,NN)
QUAL(1)=DSQRT(N/XLOSS(1))
CALL P(XSTART,Q,NN,Y,B,C)
DO 20 L=2,16
DO 6 I=1,8
CNORM=CNORM+(C(I)*C(I))
6 XNORM=XNORM+(XSTART(I)*XSTART(I))
XNORM=DSQRT(XNORM)
CNORM=DSQRT(CNORM)
Z=CNORM/XNORM
IF(L.EQ.2)ZZ(1)=Z
IF(Z.LE..010D0)GO TO 25
MTT=L-1
ZZ(MTT)=Z
DO 7 I=1,8
7 XSTART(I)=XSTART(I)-C(I)
XLOSS(L)=XL(XSTART,SIG,Y,NN)
QUAL(L)=DSQRT(N/XLOSS(L))
CALL CON(XSTART,G)
DO 8 I=1,7
J=I+8
8 XSTART(J)=G(I)
DO 9 I=1,15
9 XX(L,I)=XSTART(I)
CALL P(XSTART,Q,NN,Y,B,C)
20 CONTINUE
25 KMT=MTT+1
ZZ(KMT)=Z
L=MTT
CALL CON(XSTART,G)
G4B=G(4)
G5B=G(5)
G6B=G(6)
RETURN
END

```

```

SUBROUTINE P(X,Q,NN,Y,P,C)
IMPLICIT REAL*8 (A-H,O-Z)
REAL*4 EPS
DIMENSION U(8,8),AFLAG(8),ATEMP(8),Q(550),X(15),NN(11),Y(550),
1 D(8,550),F(550),A(550,8),B(8,8),C(8),G(7)
NC=8
MR=8
NR=8
EPS=3.0
N=0
CALL AA(X,NN,A)
DO 1 I=1,8
C(I)=0.0D0
DO 2 J=1,8
2 B(I,J)=0.0D0
1 CONTINUE
DO 3 I=1,11
3 N=N+NN(I)
DO 4 I=1,8
DO 5 J=1,8
DO 6 L=1,N
6 B(I,J)=B(I,J)+(A(L,I)*Q(L)*A(L,J))
5 CONTINUE
4 CONTINUE
CALL GINV2(B,U,AFLAG,ATEMP,MR,NR,NC,NRANK,EPS)

```

```

DO 7 I=1,8
DO 8 J=1,8
8 B(I,J)=B(J,I)
7 CONTINUE
CALL FI(X,NN,F)
DO 9 I=1,N
9 F(I)=F(I)-Y(I)
DO 10 I=1,8
DO 11 J=1,N
11 D(I,J)=0.0D0
10 CONTINUE
DO 12 I=1,8
DO 13 J=1,N
DO 14 L=1,8
14 D(I,J)=D(I,J)+(B(I,L)*A(J,L))
13 CONTINUE
12 CONTINUE
DO 15 I=1,8
DO 16 J=1,N
16 C(I)=C(I)+(D(I,J)*Q(J)*F(J))
15 CONTINUE
RETURN
END

```

```

SUBROUTINE XMONTE(SIG,NN,Y,X)
IMPLICIT REAL *8 (A-H,O-Z)
DIMENSION SIG(11),NN(11),Y(550),X(15),M(11),G(7)
C SIG ARE SIGMA VALUES
C NN GIVES NUMBER OF EACH TYPE OF MEASUREMENT
C X IS TRUE SHOCK PARAMETERS
C Y IS MONTE CARLO SAMPLE OF MEASUREMENT
N=0
J=1
DO 1 I=1,11
N=N+NN(I)
1 M(I)=N
CALL CON(X,G)
X(9)=G(1)
X(10)=G(2)
X(11)=G(3)
DO 2 I=1,N
IF(I.LE.M(J))GO TO 3
J=J+1
3 Y(I)=X(J)+BARN1(-1,1,12787,SIG(J))
2 CONTINUE
RETURN
END

```

```

SUBROUTINE GAUSS(/IX/,S,AM,V,H)
IMPLICIT REAL*8 (A-H,O-Z)
K=H
A=0.0D0
DO 50 I=1,K
CALL RANDU(IX,IY,Y)
IX=IY
50 A=A+Y
HO=H/12.
H2=H/2.
V=(S*(A-H2))/DSQRT(HO)+AM
RETURN
END

```

```

SUBROUTINE RANDU(/IX/,IY,YFL)
IMPLICIT REAL*8 (A-H,O-Z)
DATA JJJ5/1027/
IY=IX*JJJ5
IF(IY)5,6,6
5 IY=IY+2147483647+1
6 YFL=IY
YFL=YFL*.4656613D-9
RETURN
END

```

```

FUNCTION BARN1(I,IKEY,IFRN,SD)
IMPLICIT REAL*8 (A-H,O-Z)
C SD-----THE DESIRED STANDARD DEVIATION
C AMEAN-----THE DESIRED MEAN
C H-----THE POPULATION SIZE
DATA AMEAN/0.0D0/
DATA IHERE/12787/
DATA H/36.0D0/
IF(IKEY)5,4,4

```



```

4 IHERE=IFRN
5 IF(I)6,7,7
6 CALL GAUSS(IHERE,SD,AMEAN,VAL,H)
  IFRN=IHERE
  GO TO 8
7 CALL RANDU(IHERE,IFRN,VAL)
  IHERE=IFRN
8 BARN1=VAL
  RETURN
  END

```

```

SUBROUTINE GINV2(A,U,AFLAG,ATEMP,MR,NR,NC,NR1,EPS)
DOUBLE PRECISION FAC,DOT,DOT1,DOT2,TOL,DSQRT
DOUBLE PRECISION A(MR,NC),U(NC,NC),AFLAG(NC),ATEMP(NC)
DO 10 I=1,NC
DO 5 J=1,NC
5 U(I,J)=0.
10 U(I,I)=1.
  FAC=DOT(MR,NR,A,1,1)
  FAC=1./DSQRT(FAC)
  DO 15 I=1,NR
15 A(I,1)=A(I,1)*FAC
  DO 20 I=1,NC
20 U(I,1)=U(I,1)*FAC
  AFLAG(1)=1.
  N=56
  NR1=NC
  TOL=(10.**EPS*.5**N)**2
  DO 100 J=2,NC
  DOT1=DOT(MR,NR,A,J,J)
  JM1=J-1
  DO 50 L=1,2
  DO 30 K=1,JM1
30 ATEMP(K)=DOT(MR,NR,A,J,K)
  DO 45 K=1,JM1
  DO 35 I=1,NR
35 A(I,J)=A(I,J)-ATEMP(K)*A(I,K)*AFLAG(K)
  DO 40 I=1,NC
40 U(I,J)=U(I,J)-ATEMP(K)*U(I,K)
45 CONTINUE
50 CONTINUE
  DOT2=DOT(MR,NR,A,J,J)
  IF((DOT2/DOT1)-TOL)55,55,70
55 DO 60 I=1,JM1
  ATEMP(I)=0.
  DO 60 K=1,I
60 ATEMP(I)=ATEMP(I)+U(K,I)*U(K,J)
  DO 65 I=1,NR
  A(I,J)=0.
  DO 65 K=1,JM1
65 A(I,J)=A(I,J)-A(I,K)*ATEMP(K)*AFLAG(K)
  AFLAG(J)=0.
  FAC=DOT(NC,NC,U,J,J)
  FAC=1./DSQRT(FAC)
  NR1=NR1-1
  GO TO 75
70 AFLAG(J)=1.
  FAC=1./DSQRT(DOT2)
75 DO 80 I=1,NR
80 A(I,J)=A(I,J)*FAC
  DO 85 I=1,NC
85 U(I,J)=U(I,J)*FAC
100 CONTINUE
  DO 130 J=1,NC
  DO 130 I=1,NR
  FAC=0.
  DO 120 K=J,NC
120 FAC=FAC+A(I,K)*U(J,K)
130 A(I,J)=FAC
  RETURN
  END

```

```

FUNCTION DOT(MR,NR,A,J,K)
DOUBLE PRECISION A(MR,1),X,DOT
X=0.DO
DO 50 I=1,NR
X=X+A(I,J)*A(I,K)
50 CONTINUE
DOT=X
RETURN
END

```

C.2 Program to Generate Error Cone Angles; Main and Subroutines

On the five pages following this preface there appears the error cone program listing for real and simulated shocks. Table 8 shows the input format for the relevant input quantities. X refers to the first six components of \bar{Z}_{true} for a simulation study or of either \bar{Z}_{mean} or \bar{Z} (best estimate) for a real shock study (program must be run twice for real cases — See Section IV-A). SIG and NN refer to the first six components of the SIG's and NN's corresponding to the associated shock program, and N is the Monte Carlo sample size number (K in Appendix B.2) which is usually set equal to 3,000. B1 is the matrix $\underline{B}(\hat{Z})$ with the last two rows and columns deleted (See Appendix B.2 for explanation). The first four rows of Table 8 represent the first four data cards of the program in the order shown. The next six cards are the next six rows of the B1 matrix, respectively.

Table 8

Input Data Format

Quantity	Format Designation	Descriptive Notes
N	I 4	Integer with MFW* of 4, right adjusted
X	6 F 5.2	FPN** with MFW of 5
NN	6 I 3	Integer with MFW of 3, right adjusted
SIG	6 F 5.2	FPN with MFW of 5
B1	6 F 9.5 $\left(\begin{array}{l} \text{every} \\ \text{row of} \\ \text{matrix} \end{array} \right)$	FPN with MFW of 9

*MFW means maximum field width.

**FPN means floating point number.

The printed output of the program is given, in sample form, in Appendix D.2 and is described in Section IV-B. The total program running time for $N = 3,000$ and

$$\sum_{i=1}^6 NN(i) = 90$$

on the IBM 360-75 J computer is only about 3 minutes.

```

      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION B1(6,6),SIG(6),NN(6),X(6)
      READ(5,8)N
      READ(5,1)X
      READ(5,2)NN
      READ(5,1)SIG
      WRITE(6,3)X
      WRITE(6,6)SIG
      WRITE(6,4)N
      WRITE(6,5)NN
5    FORMAT(1H,'THE INPUT NN VALUES WERE ',6(I5,1X))
3    FORMAT(1H1,'THE INPUT X VALUES WERE ',6(F5.2,1X))
4    FORMAT(1H,'THE INPUT VALUE FOR N WAS ',I5)
6    FORMAT(1H,'THE INPUT SIG VALUES WERE ',6(F5.2,1X))
      WRITE(6,7)
7    FORMAT(1H0,'THE INPUT VALUES FOR B1 WERE ')
      DO 10 I=1,6
11   FORMAT(6F9.5)
      READ(5,11)(B1(I,J),J=1,6)
10   WRITE(6,12)(B1(I,J),J=1,6)
12   FORMAT(1H,'6(F9.5,1X))
1    FORMAT(6F5.2)
2    FORMAT(6I3)
8    FORMAT(I4)
      CALL CONE(B1,SIG,NN,X,N)
      RETURN
      END
-----
      SUBROUTINE FIND(MM,A)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(10000)
      XM=MM
      ISIG1=XM*(.05D0)+1.0D0
      ISIG2=XM*(.01D0)+1.0D0
      ISIG3=XM*(.005D0)+1.0D0
      WRITE(6,900)ISIG1,ISIG2,ISIG3
900  FORMAT(1H0,' ISIG1= ',I3,' ISIG2= ',I3,' ISIG3= ',I3)
      DO 15 I=1,ISIG1
      X=A(I)
      K=1
      DO 5 J=2,MM
      IF(X.GT.A(J))GO TO 5
      K=J
      X=A(J)
5    CONTINUE
      A(K)=--10.0D0
      IF(I.EQ.ISIG1.OR.I.EQ.ISIG2.OR.I.EQ.ISIG3)WRITE(6,1969)I,X
1969 FORMAT(1H0,'THE ',I3,' VALUE WAS ',D17.8)
15   CONTINUE
      RETURN
      END
-----
      SUBROUTINE CONE(B1,SIG,NN,X,N)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION B1(6,6),SIG(6),NN(6),X(6),XNN(6),A1(6),Z1(6)
1,  T2(6),E1(6),T1(6),FI1(10000),FI2(10000),XM1(6),XM2(6)
2,  XM(6),B2(6)
C    B1 IS COVARIANCE OF L.S. ESTIMATE
C    SIG IS DEVIATION ARRAY
C    NN ARRAY GIVES NUMBER OF READINGS IN EACH DATA CHANNEL
C    X ARRAY GIVES TRUE SHOCK PARAMETERS
C    N IS MONTECARLO SAMPLE SIZE
C    SUBSCRIPT 1 REFERS TO L.S. ESTIMATE
C    SUBSCRIPT 2 REFERS TO MEAN VALUE ESTIMATE
C    DATA ON L.S. CONE IS PRINTED FIRST
      CALL XNORM(X,XM)
      DO 1 I=1,6
      XNN(I)=NN(I)
1    B2(I)=SIG(I)/DSQRT(XNN(I))
      CALL EIGEN(B1,A1,6,1)
      DO 2 I=1,6
2    Z1(I)=DSQRT(A1(I))
      DO 100 I=1,N
      DO 10 L=1,6
10   T2(L)=BARN1(-1,1,12787,B2(L))
      E1(L)=BARN1(-1,1,12787,Z1(L))
      DO 89 LL=1,6
      F=0.0D0
      DO 85 LLL=1,6
85   F=F+(E1(LLL)*B1(LL,LLL))
89   T1(LL)=F

```

```

DO 15 L=1,6
T1(L)=T1(L)+X(L)
15 T2(L)=T2(L)+X(L)
CALL XNORM(T1,XM1)
CALL XNORM(T2,XM2)
DOT1=(XM(1)*XM1(1))+ (XM(2)*XM1(2))+ (XM(3)*XM1(3))
DOT2=(XM(1)*XM2(1))+ (XM(2)*XM2(2))+ (XM(3)*XM2(3))
FI1(I)=DARCOS(DOT1)
FI2(I)=DARCOS(DOT2)
FI1(I)=FI1(I)*57.29578D0
FI2(I)=FI2(I)*57.29578D0
100 CONTINUE
WRITE(6,70)
70 FORMAT(1H0,'WE WILL NOW PRINT FI1 RESULTS ')
CALL FIND(N,FI1)
WRITE(6,71)
71 FORMAT(1H0,'WE WILL NOW PRINT FI2 RESULTS ')
CALL FIND(N,FI2)
RETURN
END

```

```

SUBROUTINE XNORM(T1,M1)
IMPLICIT REAL*8 (A-H,M,O-Z)
DIMENSION T1(6),M1(3)
B1X=T1(1)
B1Y=T1(2)
B1Z=T1(3)
B2X=T1(4)
B2Y=T1(5)
B2Z=T1(6)
XX=B2X-B1X
Y=B2Y-B1Y
Z=B2Z-B1Z
QX=(B1Y*B2Z)-(B1Z*B2Y)
QY=(B1Z*B2X)-(B1X*B2Z)
QZ=(B1X*B2Y)-(B1Y*B2X)
MX=(QZ*Y)-(QY*Z)
MY=(QX*Z)-(QZ*XX)
MZ=(QY*XX)-(QX*Y)
M=DSQRT(MX**2+MY**2+MZ**2)
M1(1)=MX/M
M1(2)=MY/M
M1(3)=MZ/M
RETURN
END

```

```

SUBROUTINE GAUSS(/IX/,S,AM,V,H)
IMPLICIT REAL*8. (A-H,O-Z)
K=H
A=0.0D0
DO 50 I=1,K
CALL RANDU(IX,IY,Y)
IX=IY
50 A=A+Y
HO=H/12.
H2=H/2.
V=(S*(A-H2))/DSQRT(HO)+AM
RETURN
END

```

```

SUBROUTINE RANDU(/IX/,IY,YFL)
IMPLICIT REAL*8 (A-H,O-Z)
DATA JJJ5/1027/
IY=IX*JJJ5
IF(IY)5,6,6
5 IY=IY+2147483647+1
6 YFL=IY
YFL=YFL*.4656613D-9
RETURN
END

```

```

FUNCTION BARN1(I,IKEY,IFRN,SD)
IMPLICIT REAL*8 (A-H,O-Z)
C
C SD-----THE DESIRED STANDARD DEVIATION
C AMEAN-----THE DESIRED MEAN
C H-----THE POPULATION SIZE
DATA AMEAN/0.0D0/
DATA IHERE/12787/
DATA H/36.0D0/
IF(IKEY)5,4,4
4 IHERE=IFRN
5 IF(I)6,7,7

```

```

6 CALL GAUSS(IHERE,SD,AMEAN,VAL,H)
  IFRN=IHERE
  GO TO 8
7 CALL RANDU(IHERE,IFRN,VAL)
  IHERE=IFRN
8 BARN1=VAL
  RETURN
  END

```

```

SUBROUTINE EIGEN(AA,VALU,NR,M)
  IMPLICIT REAL*8(A-H,O-Z)
  REAL*8 IND
C----- EIGENVALUES AND EIGENVECTORS OF A REAL SYMMETRIC MATRIX
C----- CRITICAL NOTE EIGEN LIMITED . . . RANK MUST BE GE 2 OR LE 8
C----- NOT REALLY CAPABLE OF N X N MATRICES
C
C
C
  DIMENSION A(8,8),B(8,8),VALU(8),DIAG(8),SUPERD(7),Q(7),VALL(8)
  1,S(7),C(7),D(8),IND(8),U(8),DUMMY(94),AA(64)
  EQUIVALENCE (DIAG(1),DUMMY(1)), (SUPERD(1),DUMMY(9)),
  X (VALL(1),D(1),DUMMY(16)),(Q(1),S(1),DUMMY(24)),
  X (B(1,1),DUMMY(31)),(IND(1),U(1)),(II,MATCH),
  X (TAU,BETA),(P,PRODS),(T,SMALLD),(ANORM,ANORM2)
C
C
C
  CALCULATE NORM OF MATRIX
C
C
  N=NR
  ORMA = 0.00
  J = 1
  DO 1 I=1,N
    ORMA = ORMA+AA(J)
  1 J=J+N+1
  DO 2 I=1,N
    NI=N*(I-1)
    DO 2 J=1,N
      IJ=NI+J
  2 A(J,I) = AA(IJ)/ORMA
  3 ANORM2=0.000
  4 DO 6 I=1,N
    5 DO 6 J=1,N
      6 ANORM2=ANORM2+A(I,J)**2
  7 ANORM=DSQRT (ANORM2)
C
C
C
  GENERATE IDENTITY MATRIX
C
C
  9 IF (M) 10, 45, 10
  10 DO 40 I=1,N
  12 DO 40 J=1,N
  20 IF(I-J) 35, 25, 35
  25 B(I,J)=1.000
  30 GO TO 40
  35 B(I,J)=0.000
  40 CONTINUE
C
C
C
  PERFORM ROTATIONS TO REDUCE MATRIX TO JACOBI FORM
C
C
  45 IEXIT=1
  50 NN=N-2
  52 IF (NN) 890, 170, 55
  55 DO 160 I=1,NN
  60 II=I+2
  65 DO 160 J=II,N
  70 T1=A(I,I+1)
  75 T2=A(I,J)
  80 GO TO 900
  90 DO 105 K=I,N
  95 T2=CUS*A(K,I+1)+SUN*A(K,J)
  100 A(K,J)=CUS*A(K,J)-SUN*A(K,I+1)
  105 A(K,I+1)=T2
  110 DO 125 K=I,N
  115 T2=CUS*A(I+1,K)+SUN*A(J,K)
  120 A(J,K)=CUS*A(J,K)-SUN*A(I+1,K)
  125 A(I+1,K)=T2
  128 IF (M) 130, 160, 130
  130 DO 150 K=1,N
  135 T2=CUS*B(K,I+1)+SUN*B(K,J)
  140 B(K,J)=CUS*B(K,J)-SUN*B(K,I+1)
  150 B(K,I+1)=T2
  160 CONTINUE
C

```

```

C      MOVE JACOBI FORM ELEMENTS AND INITIALIZE EIGENVALUE BOUNDS
C
170 DO 200 I=1,N
180 DIAG(I)=A(I,I)
190 VALU(I)=ANORM
200 VALL(I)=-ANORM
210 DO 230 I=2,N
220 SUPERD(I-1)=A(I-1,I)
230 Q(I-1)=(SUPERD(I-1))**2
C
C      DETERMINE SIGNS OF PRINCIPAL MINORS
C
235 TAU=0.0D0
240 I=1
260 MATCH=0
270 T2=0.0D0
275 T1=1.0D0
277 DO 450 J=1,N
280 P=DIAG(J)-TAU
290 IF(T2) 300, 330, 300
300 IF(T1) 310, 370, 310
310 T=P*T1-Q(J-1)*T2
320 GO TO 410
330 IF(T1) 335, 350, 350
335 T1=-1.0D0
340 T=-P
345 GO TO 410
350 T1=1.0D0
355 T=P
360 GO TO 410
370 IF(Q(J-1)) 380, 350, 380
380 IF(T2) 400, 390, 390
390 T=-1.0D0
395 GO TO 410
400 T=1.0D0
C
C      COUNT AGREEMENTS IN SIGN
C
410 IF(T1) 425, 420, 420
420 IF(T) 440, 430, 430
425 IF(T) 430, 440, 440
430 MATCH=MATCH+1
440 T2=T1
450 T1=T
C
C      ESTABLISH TIGHTER BOUNDS ON EIGENVALUES
C
460 DO 530 K=1,N
465 IF (K-MATCH) 470, 470, 520
470 IF(TAU-VALL(K)) 530, 530, 480
480 VALL(K)=TAU
490 GO TO 530
520 IF(TAU-VALU(K)) 525, 530, 530
525 VALU(K)=TAU
530 CONTINUE
540 IF(VALU(I)-VALL(I)-5.0D-8) 570, 570, 550
550 IF(VALU(I)) 560, 580, 560
560 IF(DABS (VALL(I)/VALU(I)-1.0D0)-5.0D-8) 570, 570, 580
570 I=I+1
575 IF(I-N) 540, 540, 590
580 TAU=(VALL(I)+VALU(I))/2.0D0
585 GO TO 260
C
C      JACOBI EIGENVECTORS BY ROTATIONAL TRIANGULARIZATION
C
590 IF (M) 593, 890, 593
593 IEXIT=2
595 DO 610 I=1,N
600 DO 610 J=1,N
610 A(I,J)=0.0D0
615 DO 850 I=1,N
620 IF (I-1) 625, 625, 621
621 IF (VALU(I-1)-VALU(I)-5.0D-7) 730, 730, 622
622 IF (VALU(I-1)) 623, 625, 623
623 IF (DABS (VALU(I)/VALU(I-1)-1.0D0)-5.0D-7) 730, 730, 625
625 CUS=1.0D0
628 SUN=0.0D0
630 DO 700 J=1,N
635 IF(J-1) 680, 680, 640

```

```

640 GO TO 900
650 S(J-1)=SUN
660 C(J-1)=CUS
670 D(J-1)=T1*CUS+T2*SUN
680 T1=(DIAG(J)-VALU(I))*CUS-BETA*SUN
690 T2=UPERD(J)
700 BETA=UPERD(J)*CUS
710 D(N)=T1
720 DO 725 J=1,N
725 IND(J)=0.0D0
730 SMALLD=ANORM
735 DO 780 J=1,N
740 IF (IDINT(IND(J))-1) 750,780,780
750 IF (DABS (SMALLD)-DABS (D(J)))780, 780, 760
760 SMALLD=D(J)
770 NN=J
780 CONTINUE
790 IND(NN)=1.0D0
800 PRODS=1.0D0
805 IF (NN-1) 810, 850, 810
810 DO 840 K=2,NN
820 II=NN+1-K
830 A(II+1,I)=C(II)*PRODS
840 PRODS=-PRODS*S(II)
850 A(1,I)=PRODS
C
C      FORM MATRIX PRODUCT OF ROTATION MATRIX WITH JACOBI VECTOR MATRIX
C
855 DO 885 J=1,N
860 DO 865 K=1,N
865 U(K)=A(K,J)
870 DO 8851 I=1,N
875 A(I,J)=0.0D0
880 DO 8852 K=1,N
      A(I,J)=B(I,K)*U(K)+A(I,J)
8852 CONTINUE
8851 CONTINUE
885 CONTINUE
      DO 886 I=1,N
      NI=N*(I-1)
      DO 886 J=1,N
      IJ=NI+J
886 AA(IJ)=A(J,I)
890 CONTINUE
      DO 891 I=1,N
891 VALU(I) = VALU(I)*ORMA
      RETURN
C
C      CALCULATE SINE AND COSINE OF ANGLE OF ROTATION
C
900 IF (T2) 910, 940, 910
910 T=DSQRT (T1**2+T2**2)
920 CUS=T1/T
925 SUN=T2/T
930 GO TO (90,650), IEXIT
940 GO TO (160,910), IEXIT
      RETURN
      END

```


APPENDIX D

SAMPLES OF OUTPUTS OF PROGRAMS

D.1 Shock Program Output

The output, as it appears in printed form (the upper portion on the next two pages; the lower portion appears on the two pages after that). The sample shown is for a simulated shock example and is fully described in Section IV-B of the report. A real shock sample output would be almost identical except that also printed out in the upper portion would be the \bar{Y} array, and XMEAN does not usually replace XSTART as in the simulated cases, but it can.

D.2 Cone Program Output

A sample of this output (appears on the single page following the Shock Program output sample). Section IV-B also fully describes this printed output for simulated shocks. It is identical in appearance for real shock cases.

B2Y	B2Z	WY	WZ	N1	N2	WX
1.100	1.300	10.000	10.000	0.700	1.000	10.000
10	10	10	10	10	10	10
9.000	-3.000	10.000	20.000			

~~DP~~
13.361

WY	WZ	N1	N2	WX	MEAN VALUES
4.255	17.983	6.890	13.486	71.404	8707.94392=LOSS M

4.255	17.983	8707.94392=LOSS	0 Z=	0.2197
6.930	22.003	270.71065=LOSS	1 Z=	0.1534
4.070	20.107	163.04689=LOSS	2 Z=	0.0931
3.515	21.027	137.36852=LOSS	3 Z=	0.0609
3.489	21.296	136.97695=LOSS	4 Z=	0.0487
3.503	21.323	136.97673=LOSS	5 Z=	0.0436
3.504	21.324	136.97673=LOSS	6 Z=	0.0413
3.504	21.324	136.97673=LOSS	7 Z=	0.0402
3.504	21.324	136.97673=LOSS	8 Z=	0.0397
3.504	21.324	136.97673=LOSS	9 Z=	0.0394
3.504	21.324	136.97673=LOSS	10 Z=	0.0393
3.504	21.324	136.97673=LOSS	11 Z=	0.0392
3.504	21.324	136.97673=LOSS	12 Z=	0.0392
3.504	21.324	136.97673=LOSS	13 Z=	0.0392
3.504	21.324	136.97673=LOSS	14 Z=	0.0392
3.504	21.324	136.97673=LOSS	15	

THE BEST ESTIMATE DEPENDENT PARAMETER MATRIX IS

	N1	N2	WX	NX	NY	NZ
MEAN'S G'S	18.943	36.918	36.737	0.903	0.254	0.347
	18.943	36.918	36.737	0.903	0.254	0.347
	7.232	14.048	107.708	0.977	0.115	0.180
	7.510	14.647	77.978	0.967	0.148	0.208
	7.000	13.600	71.850	0.959	0.170	0.225
	6.931	13.457	71.097	0.958	0.174	0.229
	6.932	13.458	71.072	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229
	6.932	13.458	71.071	0.958	0.174	0.229

THE COVARIANCE MATRIX OF FINAL ESTIMATE IS

0.00585	0.00016	0.00018	0.00173	0.00012	-0.00181	0.02443
0.00016	0.01068	0.00021	0.00071	0.00884	0.00284	0.03608
0.00018	-0.00021	0.00556	-0.00057	0.00104	0.00797	0.00433
0.00173	0.00071	0.00057	0.02461	0.00297	0.00291	0.18015
0.00012	0.00884	0.00104	-0.00297	0.07419	-0.01690	-0.29266
0.00181	0.00284	0.00797	0.00291	0.01690	0.05350	0.15013
0.02443	0.03608	0.00433	-0.18015	-0.29266	-0.15013	5.74353
0.02724	0.01494	0.02770	0.15660	0.00422	0.33189	2.01930

THE CONTRACTED FORM OF DERIVATIVE MATRIX, A, IS

1.000	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.000	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.000	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.000	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.000	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.000	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.000
-10.618	2.474	12.937	9.962	0.145	-5.866	0.445
20.614	2.226	25.539	19.340	1.608	11.606	0.939
33.718	-47.999	-104.491	-17.369	24.724	53.824	1.424

AAVE= 8.734 ABE= 3.088 AVE,ABE= 8.772

DP	
7.624	0.12680=QUALITY M
7.624	0.12680=QUALITY 0
27.292	0.70874=QUALITY 1
13.634	0.92663=QUALITY 2
10.354	1.00953=QUALITY 3
10.007	1.01097=QUALITY 4
10.003	1.01098=QUALITY 5
10.003	1.01098=QUALITY 6
10.003	1.01098=QUALITY 7
10.003	1.01098=QUALITY 8
10.003	1.01098=QUALITY 9
10.003	1.01098=QUALITY 10
10.003	1.01098=QUALITY 11
10.003	1.01098=QUALITY 12
10.003	1.01098=QUALITY 13
10.003	1.01098=QUALITY 14
10.003	1.01098=QUALITY 15
-0.02724	
0.01494	
0.02770	
0.15680	
0.00422	
-0.33189	
2.01930	
7.10262	
0.0	
0.0	
0.0	
0.0	
0.0	
0.0	
0.0	
1.000	
-0.723	
1.417	
3.099	

THE INPUT X VALUES WERE 4.00 5.00 1.00 3.50 9.00 3.00
THE INPUT SIG VALUES WERE 0.35 0.50 0.35 0.60 1.10 1.30
THE INPUT VALUE FOR N WAS 3000
THE INPUT NN VALUES WERE 20 20 20 10 10 10

THE INPUT VALUES FOR B1 WERE

0.00585	0.00016	0.00018	0.00173	0.00012	-0.00181
0.00016	0.01068	-0.00021	-0.00071	0.00884	0.00284
0.00018	-0.00021	0.00556	-0.00057	0.00104	0.00797
0.00173	-0.00071	-0.00057	0.02461	-0.00297	0.00291
0.00012	0.00884	0.00104	-0.00297	0.07419	-0.01690
-0.00181	0.00284	0.00797	0.00291	-0.01690	0.05350

WE WILL NOW PRINT F11 RESULTS

ISIG1= 150 ISIG2= 30 ISIG3= 15

THE 15 VALUE WAS 0.70037671D 01

THE 30 VALUE WAS 0.65018993D 01

THE 150 VALUE WAS 0.51747948D 01

WE WILL NOW PRINT F12 RESULTS

ISIG1= 150 ISIG2= 30 ISIG3= 15

THE 15 VALUE WAS 0.14611719D 02

THE 30 VALUE WAS 0.13564957D 02

THE 150 VALUE WAS 0.10634617D 02
