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TO: Distribution

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SUBJECT: Partial Prereduction of the Normal Equations

For some types of research carried out with PEP there has been a history of increasing model complexity and an increasing number of parameters adjusted at one time. For the study of solar system dynamics and tests of gravity theory, economic limits and the physical limitations of available computers have encumbered the use of large parameter sets. However, there is ample evidence that it would be useful to be able to make much larger solutions (i.e., solutions of the normal equations with much larger numbers of parameters). Planetary topography, now represented by a 123 term 2-dimensional Fourier series, is the limiting factor for the Mars radar data. Expansion of the model to at least 203 terms is indicated.

Even the 123-term model has been considered to be too large to be used for all three inner planets (Mercury, Venus, Mars) if the data are to be analyzed simultaneously. The inclusion of the optical data in the solution requires 200 to 350 extra bias parameters as well as outer planet initial conditions to be included in the parameter set. The resulting combined normal equations, including all parameters which it now appears would be useful (800 to 1000 of them!) would require 2.5-4. megabytes of core and from 50 to 100 minutes of inversion time, using an in-core inverter on an IBM 360/75. The core/system limitations on the Draper Lab. 360/75 put a bound of about 700 on the size of the largest set of normal equations that PEP can solve (by special arrangement); the inversion time would be 35 minutes. (The Lincoln Lab 370/168 is about 3.5 times faster than the Draper Lab 360 and should be able to invert a matrix for nearly 2000 parameters.)

While the cost of forming a single solution (at $6.00 per minute) is by no means prohibitive, upwards of a hundred solutions would require unusually strong funding. However, that is a realistic number to wish to be able to make in a given study. Thus there is a need to find a less costly way of working.

Among the large number of solutions that go into a study there are groups within which the only difference is in the choice of parameter set. Generally, within these groups the intersection of the individual parameter sets contains nearly as many parameters as the individual sets. This fact is the main motivation for the work that follows.

## The Partial Prereduction Technique

The normal equations are of the form

$$U = BX \tag{1}$$

where X is an adjustment vector of length n, B is the n by n coefficient matrix, and the right hand side (RHS) vector, U, of length n is formed using the prefit residuals. We partition these using the parameter subsets $\{\alpha\}$ and $\{\beta\}$ such that $\{\beta\}$ contains as many of the parameters common to all solutions as is convenient, and $\{\alpha\}$ contains all of the remaining parameters.

$$U = \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} C & F \\ F^{\dagger} & D \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} \tag{2}$$

where v is the "$\alpha$ part" of U and w is the "$\beta$ part", etc. Then

$$v = Cy + Fz$$

$$w = F^{\dagger} y + Dz$$

$$z = D^{-1}(w - F^{\dagger}_{y}) \tag{3}$$

$$y = \bar{C}^{-1} \bar{v} \tag{4}$$

where

$$\bar{C} = C - FD^{-1}F^{\dagger}$$

$$\bar{v} = v - FD^{-1}w \tag{5}$$

It is not hard to see that a sub-set $\{\alpha'\}$ of the $\{\alpha\}$ of parameters represented in Equation (4) could be extracted and solved in the same way as PEP usually treats saved normal equations (SNE).

If by suitable choice of $\{\beta\}$ all of the "parameters of interest" are in $\{\alpha\}$, then no further work is needed. If, however, this condition fails or if predicted

residuals are to be calculated then we proceed:

$$z = \bar{z} - \bar{F}^{\dagger} y \tag{6}$$

$$\bar{z} = D^{-1} w$$

$$\bar{F}^{\dagger} = D^{-1} F^{\dagger} \tag{7}$$

If the predicted residuals are not needed, but the RMS of the weighted predicted residuals is needed we may use the method of the memorandum Distribution/RDR dated 24 Jan 1974. The change in the RMS weighted residual is related to the square of the norm of the adjustment, $N^2$, and

$$N^2 = X^{\dagger} U = y^{\dagger} v + z^{\dagger} w$$

$$= y^{\dagger} \bar{v} + N_0^2$$

$$N_0^2 = w^{\dagger} D^{-1} w \tag{8}$$

The equations for including a priori information in a solution are given in the memorandum Distribution/RDR dated 28 July 1975. Applying these to Equation (2) yields

$$\begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} C+C_0 & F+F_0 \\ F^{\dagger}+F_0^{\dagger} & D+D_0 \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} - \begin{pmatrix} C_0 & F_0 \\ F_0^{\dagger} & D_0 \end{pmatrix} \begin{pmatrix} y_0 \\ z_0 \end{pmatrix} \tag{9}$$

Proceeding as above, we get

$$y = \tilde{C}^{-1} \tilde{v} \tag{10}$$

where

$$\tilde{C} = C + C_0 - (F+F_0)(D+D_0)^{-1}(F^{\dagger}-F_0^{\dagger})$$

$$\tilde{v} = v - (F+F_0)(D+D_0)^{-1}(w+F_0^{\dagger}y_0 + D_0 z_0) + C_0 y_0 + F_0 z_0 \tag{11}$$

Since the principal reason for the use of Equation (4) is to avoid having to invert a matrix the size of D for each solution, it follows from Equation (11) that if a priori information is to be added then either 1) it will be added just before Equation (5) is used or 2) $D_0$ (and thus $F_0$ and $z_0$) will be zero and Equation (11) will take the form

$$\tilde{C} = \bar{C} + C_0$$

$$\tilde{v} = \bar{v} + C_0 y \qquad (12)$$

It will be seen later that for studies of solar system dynamics, the matrix D may be too large to invert conveniently. (See Appendix A.) Fortunately there are a number of possible ways to handle the inversion. With a little effort in the choice of $\{\alpha\}$, D can be made block diagonal, and thus easy to invert. If this is not reasonable, D can be put in the form

$$D = \begin{matrix} G & H_1 & N_2 \\ H_1^\dagger & M_1 & O \\ H_2^\dagger & O & M_2 \end{matrix}$$

Such matrices can be inverted in small parts. There may also be packaged matrix inverters that operate on a matrix stored on a direct access device. Finally, it may be possible to use the partial prereduction technique recursively. (This has not been investigated.)

Realization of the Partial Prereduction Technique in PEP

The equations given above show that it is possible to work with a very large set of normal equations and perform numerous inexpensive numerical experiments (i.e., make solutions with different parameter sets) as long as there is a large set of parameters which is common to all solutions. (This is the usual case.) The PEP implementation should be easy to use and should maintain the potential of the method for high efficiency.

Using the partial prereduction technique, solutions are made from SNE in two steps. In the first, an investment is made in generating a set of reduced total saved normal equations (RTSNE). In the second, the RTSNE are used and a solution of the normal equations is found. Much of the savings comes from the ability to repeat this second step. This suggests that the control scheme be designed to permit multiple-solution runs.

In both of the above-mentioned two steps it is necessary to identify a main set, $\{\pi\} = \{\alpha\} \cup \{\beta\}$, of

parameters and a subset. The usual PEP "L vectors" can be used to identify $\{\pi\}$. The various subsets, such as $\{\alpha\}$, can be identified using parameter-name lists. Since we are considering multisolution runs, it should be possible to generate a list by modifying a previously generated list. A set of two-word commands, as listed in Table I, provides the needed flexibility.

After a parameter set, $\{\alpha'\} \subseteq \{\alpha\}$, has been selected, the program functions necessary to use the RTSNE are defined by Equation (4) -- or (10) and (12) -- and (7). Each use will include the inversion of the matrix C', a sub-matrix of C, and the calculation of the solutions for the $\{\alpha'\}$ parameters. The prediction of the postfit RMS weighted residual will also be performed. The calculation of the solutions for the $\{\beta\}$ parameters should be programmed as an option.

Before the RTSNE can be used they must be generated. This will be done according to Equations (5), (8), and (7) starting with SNE, either "total", TSNE, or "series-by-series", SSNE. (See Appendix B for the format.) Since the B matrix may be very large, the sub-matrices C, D, and F will be formed separately. Further, if the D matrix is to be treated as a block diagonal, each block of D and each corresponding block of F will be formed separately. Thus the SNE data set must be read a minimum of three times.

The following is a suggested order of operations, assuming all pointers have already been set up and the IDENTIFICATION and POINTER GROUPS of records have been written on the RTSNE data set.

1. Read SNE to form U, C. Save C on the first temporary data set (TDS 1).

2. Read SNE to form F; save on TDS 2.

3. Read SNE to form D. Invert D and save $D^{-1}$ on TDS 3. Form $D^{-1}$ W.

4. Read TDS 2 and TDS 3. Form $FD^{-1}$ and save on TDS 4. Form $FD^{-1}W$.

5. Form $W^{+}D^{-1}W$ and write the pointer group on the RTSNE data set.

6. Add V to $FD^{-1}W$ and write $\overline{V}$ on the RTSNE data set.

7. Read TDS 2 and TDS 4. Form $-FD^{-1}F$. Read TDS 1 and form $\overline{C}$. Write $\overline{C}$ on RTSNE data set.

Table I

| | Verb | Noun | Notes |
|---|---|---|---|
| * | NAME | solname | used to identify the list |
| | DEFINE | MASTER | used to define a basic list |
| * | | solname | which can be modified |
| * | | ABOVE | "solname" refers to any |
| | | LIST | previously used name |
| | ADD | LIST | these are used to modify |
| | DELETE | LIST | a defined list |

Notes:

- To generate a list there must be a DEFINE.
- The NAME is optional and of use only when a series of solutions is to be made
- The ADD and DELETE are optional. They follow the DEFINE and there may be any number of them in any order.
- LIST indicates that a list of parameter names follows. (It is like the IBM/JCL use of "*" or "DATA".)
- In generating the RTSNE only the DEFINE LIST command is used
- In using the RTSNE to form a solution, only the $\{\alpha'\}$ subset of $\{\alpha\}$ need be specified.
- In defining the $\{\alpha'\}$ the command word MASTER refers to $\{\alpha\}$.

*The implementation of these commands can be postponed.

8. Write $\overline{Z}$ on RTSNE data set.

9. Read TDS 4. Write $FD^{-1}$ on RTSNE data set.

Note that in the above procedures there are large matrix multiply operations which could take large amounts of storage. However, only one matrix needs to be in main storage. The other two can be read/written one line at a time. The actual multiply of the row of one matrix by the column of another should be done by an assembly routine such as DOT so as to keep the running sum in register. (This gains an extra eight bits precision.) To keep this operation efficient, care must be taken in setting up the one matrix stored in core. (A check of the code generated by IBM FORTRAN H/2 may show that the assembly routine is not needed.)

## APPENDIX A

### The Parameter Sets {α} and {β}

As an explicit example of the application of partial pre-reduction, the case of solar system dynamics is considered. Two possible divisions of the parameters are considered: (1) The set {α} is made small. (2) The matrix D is made block diagonal. In both cases there are ≈ 950 parameters and solutions would generally contain ≳ 900 of these.

#### Division 1

| NAME {α} | Number |
|---|---|
| Planet masses | 10 |
| Asteroid parameters | 7 |
| Lunar harmonics | 6 |
| Relativity | 15 |
| Principle of equivalence | 11 |
| Plasma and other solar system parameters | 12 |
| Earth IC | 6 |
| Radar station locations | 9 |
| Radar biases | 10 |
| Radii of planets | 5 |
| | 91 |

| {β} | |
|---|---|
| AT-UT | 50 |
| Planet IC | 54 |
| Mercury topography | 123 |
| Venus topography | 123 |
| Mars topography | 203 |
| Optical biases | 300 |
| Radar biases | 20 |
| | 873 |
| | 964 |

#### Division 2

Move Planet IC into {α}. There are then 145 elements in and 819 in {β}. The matrix D will be block diagonal with at least 4 blocks.

The example given does not represent an upper bound to the number of parameters that could be included in a single solution. A simple enlargement of the Mars topography model (from N = 20, M = 1 to N = 40, M = 4) would add 520 extra parameters. Although this would be an awkward way to model the topography (because of PEP internal limitations), it does indicate how fast topography models can add parameters to the estimation list.

A second, less dramatic example is the inclusion in the solar system model of the four largest moons of Jupiter. If we assume radar data from one of them and optical observations taken of all four, then this part of the model will add from 60 to 100 parameters to the estimation list.

APPENDIX B

Format of RTSNE Data Set

The data set consists of five separate groups. One of these, #4, will not be programmed initially.

1. IDENTIFICATION GROUP contains the title, general information, and "M-vector" records found in the usual SNE data set.

2. POINTER GROUP contains pointer vectors to identify the parameter subsets, nominal values, and a few indicative data:

   a. n total number of parameters

   b. m number in $\{\alpha\}$

   c. $N^2 = W\, D^{-1}\, W$

   d. NSER number of series-by-series right-hand-side vectors in group 4. NSER = 0 for first version.

   e. NAUX number of parameters included in group #5. If NAUX $\neq$ 0 and NAUX $\neq$ n-m, then an extra record of NAUX pointers must follow. NAUX = n-m for first version

3. PRIMARY RTSNE GROUP contains the vector $\overline{V}$ and matrix $\overline{C}$ in the usual SNE format.

4. SERIES-BY-SERIES GROUP contains the contributions to $\overline{V}$ from separate series. The equations for this are not explicitly included and the implementation of this feature should be delayed. For now, NSER = 0 in Group #2.

5. AUXILIARY RTSNE GROUP contains the vector $\overline{Z}$ and the matrix $\overline{F}$. The matrix is in the form of K-M records of M double precision words plus identification words.

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