AN EVALUATION OF LEAST SQUARES ALGORITHMS USED IN ATMOSPHERIC RETRIEVALS

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1. INTRODUCTION

The retrieval of atmospheric temperature and moisture profiles from satellite radiance observations involves many different steps including calibration, geolocation, transmittance calculation and radiative transfer computation. Various numerical methods are employed in these computational tasks. This paper examines one particular numerical method, the solution of the least squares problem, which is encountered in the computation of atmospheric retrievals. In order to produce atmospheric retrievals of known accuracy, it is desirable to use a least squares algorithm which has consistent and reliable performance. This is particularly the case for high spectral resolution data where it is desired to maximise the information retrieved from radiance measurements. It is also desirable to distinguish between "bad" retrievals which are caused by a lack of information in the input data, and those which are "bad" because the least squares algorithm failed.

Two least squares algorithms are examined; the Normal Equation method and the QR decomposition method. Examples of the computational accuracy of these two methods in the solution of an ill-conditioned Hilbert matrix system are presented. The accuracy of the two methods is then examined in the computation of retrievals of atmospheric temperature from synthetic radiance observations using the International TOVS Processing Package Version 3 (ITPP3) (Smith et. al., 1985).

2. THE PHYSICAL RETRIEVAL SCHEME

In the physical retrieval scheme the perturbation form of the radiative transfer equation is replaced by a system of linear equations (Smith et. al., 1989), and expressed in the form

$$Ax = b\,, \tag{1}$$

where A is an m row by n column matrix of basis functions, b is a column vector of m radiance observations, and x is the solution column vector of n coefficients. Since the retrieval problem involves the use of spectrally interdependent radiance observations, it is required that there be more observations in the vector b than coefficients in the solution vector x. For the ITPP3 retrieval algorithm, there are 22 elements in b and 10 coefficients in the solution vector x.

It is well known that the inversion of equation (1) to return the vector x is an ill-conditioned problem. The instability in the solution is evident in that small variations in b cause large variations in x. In the case of physical retrievals, this instability may arise from several sources including measurement errors, numerical roundoff errors, approximations to atmospheric transmittances, and approximations to the Planck function. This instability is exhibited in a measurable sense by the condition number of A.

A preferred approach is to not solve the ill-conditioned problem but to solve a related system in a least squares sense, while imposing some constraints to avoid poor solutions. The aim is to use a robust method; one which has the ability to obtain good answers or at least indicate when the answer might be poor. The method should also be relatively insensitive to error in the input data, or if this is not known, then the method should be able to estimate the error in the result. This paper compares the performance of

(i) the normal equation method, and
(ii) the QR decomposition method.

3. THE NORMAL EQUATION METHOD

In the normal equation method, the quantity

$$\| b - Ax \|_p \tag{2}$$

is minimized using a suitable choice of p. There are occasions where $p=1$ or $p=\infty$ are used, but usually $p=2$ is selected and (2) is then known as the 2-norm. Thus the problem reduces to minimizing the sum of the squares of the residuals, or the Euclidean norm i.e.

$$\min_x (b - Ax)^2 .$$

The solution is well known and is given by the normal equations as

$$x = (A^T A)^{-1} A^T b . \tag{3}$$

However for the inversion of the radiative transfer equation, $A^T A$ tends to have small eigenvalues and the problem is ill-conditioned. Consequently, atmospheric retrieval problems avoid using this form of the solution. The procedure used is known as the

minimum information method, or the constrained least squares method, where a smoothness criterion is used to control the shape of the solution.

If $x^T x$ is minimized subject to the constraint that

$$(Ax - b)^T B(Ax - b)$$

is a constant, where B depends on the measurement error, then the solution is given by

$$x = (A^T A + \gamma I)^{-1} A^T b$$

assuming measurement errors are random. The relation to the least squares solution in (3) is apparent with the addition of the Lagrangian multiplier γ. This serves to increase the size of the eigenvalues of $A^T A$ and hence stabilize the solution. Though γ can in theory be obtained precisely from the constraints this is not feasible computationally, and it is usual to guess an initial value for γ and iterate until the solution converges.

4. THE QR DECOMPOSITION METHOD

This method involves the conversion of the least squares problem into an equivalent easily solved problem by the use of orthogonal transforms.

The least squares problem

$$\min_x \| b - Ax \|_2$$

may be converted to an equivalent problem

$$\min_x \| Q^T b - Q^T Ax \|_2 \qquad (4)$$

where Q is an orthogonal matrix ($Q^T Q = I$ and $\|Q\| = 1$). This is the basis of robust methods such as the QR decomposition method and the Singular Value Decomposition (SVD) method (Golub et. al., 1983).

In the QR decomposition method, the matrix is factored as the product QR where Q is an orthogonal matrix and R is an upper triangular matrix. This is done in two stages. First A is transformed to a similar matrix which is tridiagonal if A is symmetric, or upper Hessenberg if it is not. This is usually achieved by Householder or Givens transformations. The final factorization into the form QR is via an iterative process involving the repetitive use of orthogonal transformations until convergence is achieved.

If A is factored as QR and the least squares is rewritten in the form of equation (4), then the solution is achieved by letting

$$d = Q^T b$$

and solving

$$Q^T Ax = Q^T QRx = Rx = d$$

by back substitution since R is upper triangular. The solution is unique if A is of full rank. If A is rank deficient (rank A < n) then the least squares solution is non-unique. In this situation, the SVD method must be applied.

In order to monitor the stability of the QR decomposition method, it is necessary to check that the machine precision of the computer system does not affect the derived solution. If the matrix A is rank deficient, this implies linear dependency among the columns of A so that there is a non-zero vector z such that

$$Az = 0$$

and the solution is not unique. When A is square, this is the same as having A singular. One method of determining whether this situation applies is to compute a condition estimate for A, and check that this is not less than the machine precision of the computer system. If it is less, then A is numerically indistinguishable from a rank deficient matrix, and results from the QR decomposition method are unreliable (Dongarra et. al., 1978). One condition estimate which may be used is the 1-norm condition number, which is a computed estimate of

$$\| A \|_1 \| A^{-1} \|_1 . \qquad (5)$$

The test for rank deficiency then becomes

$$1 / (\| A \|_1 \| A^{-1} \|_1) < \text{epsilon} ,$$

where epsilon is the machine precision. If this test is true, then the matrix A is effectively rank deficient.

5. ERROR PROPAGATION IN COMPUTATIONAL IMPLEMENTATIONS

If the least squares problem

$$\min_x \| b - Ax \|_2$$

is solved by reducing to the normal equations

$$A^T Ax = A^T b$$

and solving this linear system by Choleski decomposition, then it may be shown (Golub et. al., 1983) that the accuracy of the computed solution depends on the square of the condition number of the matrix A. This implies that the method is highly unstable. The QR decomposition method using Householder transformations produces an orthogonal matrix Q such that

$$Q^T A = R$$

or

$$A = QR$$

where R is upper triangular. The resultant solution by backward substitution can be shown to be considerably more stable. Stewart (1977) states that the perturbations in Q and R caused by errors in A are bounded by the condition number of A times the relative change in A. This implies a considerable reduction in the growth of errors using the QR decomposition method.

6. NUMERICAL SOLUTIONS OF AN ILL-CONDITIONED LEAST SQUARES SYSTEM

In order to evaluate the relative accuracy of the normal equation and QR decomposition methods, results from computer implementations of the two algorithms in FORTRAN-77 are presented. The QR decomposition is performed by the LINPACK subroutine package (Dongarra et. al., 1978). This version of the QR decomposition method computes the machine precision (epsilon) and utilizes the reciprocal of the 1-norm condition number to test for rank deficiency. Both single and double precision versions are tested. The normal equation method is the double precision version with Lagrangian multiplier that is used in the physical retrieval code of the ITPP3. This version does not test the matrix A in equation (1) for rank deficiency.

Computer system: 80386 PC with 80387 coprocessor, Microsoft MS-DOS Version 4.01 operating system, Microsoft FORTRAN Version 5.00 compiler with no optimization.

A is a 5 row by 5 column Hilbert matrix that is known to be ill-conditioned and defined by

$$A(i,j) = 1 / (i + j - 1)$$

which gives the values of A as

```
1.0000E+00  5.0000E-01  3.3333E-01  2.5000E-01  2.0000E-01
5.0000E-01  3.3333E-01  2.5000E-01  2.0000E-01  1.6667E-01
3.3333E-01  2.5000E-01  2.0000E-01  1.6667E-01  1.4286E-01
2.5000E-01  2.0000E-01  1.6667E-01  1.4286E-01  1.2500E-01
2.0000E-01  1.6667E-01  1.4286E-01  1.2500E-01  1.1111E-01 ,
```

x is a 5 element column vector

```
x = ( -1.0, 1.0 , -1.0, 1.0, -1.0 ),
```

b is the computed product of A and x, i.e.

b = Ax.

The least squares algorithms are given A and b and are used to compute the solution vector x′. The Euclidean norm of the residual vector (Ax′ - Ax) is used as an indicator of the goodness of fit of the derived solution vector.

Example 1 : Single precision LINPACK QR decomposition

Reciprocal of 1-norm condition number = 1.5647E-06
Epsilon (machine precision) = 1.1921E-07

Solution vector x′ is

```
-1.0000E+00  1.0001E+00 -1.0006E+00  1.0009E+00 -1.0004E+00
```

Residual vector (Ax′ - Ax) is

```
 1.1921E-07  0.0000E+00  0.0000E+00  0.0000E+00  1.4901E-08
```

Euclidean norm is 1.2014E-07

Example 2 : Double precision LINPACK QR decomposition

Reciprocal of 1-norm condition number = 1.5616E-06
Epsilon (machine precision) = 2.2204E-16

Solution vector x′ is

```
-9.9998E-01  9.9956E-01 -9.9815E-01  9.9722E-01 -9.9865E-01
```

Residual vector (Ax' - Ax) is

```
 0.0000E+00  2.9802E-08  0.0000E+00  1.4901E-08  0.0000E+00
```

Euclidean norm is `3.3320E-08`

Example 3 : Double precision normal equation solution, Lagrangian multiplier γ = 1.0

Solution vector is

```
-3.3917E-01 -1.8460E-01 -1.2882E-01 -9.9453E-02 -8.1181E-02
```

Residual vector (Ax' - Ax) is

```
 2.6783E-01  8.6590E-02  4.6381E-02  3.1272E-02  2.3847E-02
```

Euclidean norm is `2.8797E-01`

Example 4 : Double precision normal equation solution, Lagrangian multiplier γ = 0.1

Solution vector x' is

```
-5.2833E-01 -2.1689E-01 -1.2500E-01 -8.3617E-02 -6.0937E-02
```

Residual vector (Ax' - Ax) is

```
 7.1795E-02 -1.1261E-02 -1.8452E-02 -1.7048E-02 -1.4594E-02
```

Euclidean norm is `7.8265E-02`

Example 5 : Double precision normal equation solution, Lagrangian multiplier γ = 0.0

Solution vector x' is

```
-9.8592E-01  7.3803E-01  1.2574E-01 -6.9540E-01 -1.7240E-01
```

Residual vector (Ax' - Ax) is

```
 9.6546E-05  7.2083E-05  5.9816E-05  5.1684E-05  4.5683E-05
```

Euclidean norm is `1.5117E-04`

The sizes of the Euclidean norms indicate that the LINPACK method achieves considerably better results than the ITPP3 normal equation method for this ill-conditioned system. The single precision LINPACK routine shows a reciprocal 1-norm condition number of comparable size to epsilon, indicating that the matrix is partially rank deficient. However the x′ result is still indicated to be reliable, with a relatively small error indicated by the Euclidean norm. The double precision LINPACK routine is able to solve for x′ without difficulty as the epsilon for double precision arithmetic is far smaller, and a slightly smaller Euclidean norm than the single precision result is achieved. The normal equation routine with Lagrangian multiplier $\gamma = 1.0$ yields a relatively large Euclidean norm, which implies the vector x′ is inaccurate. Setting $\gamma = 0.1$ only marginally improves the accuracy of x′. Even with $\gamma = 0.0$ the error in the solution is still larger than the LINPACK results, with no other indication as to whether the solution is reliable.

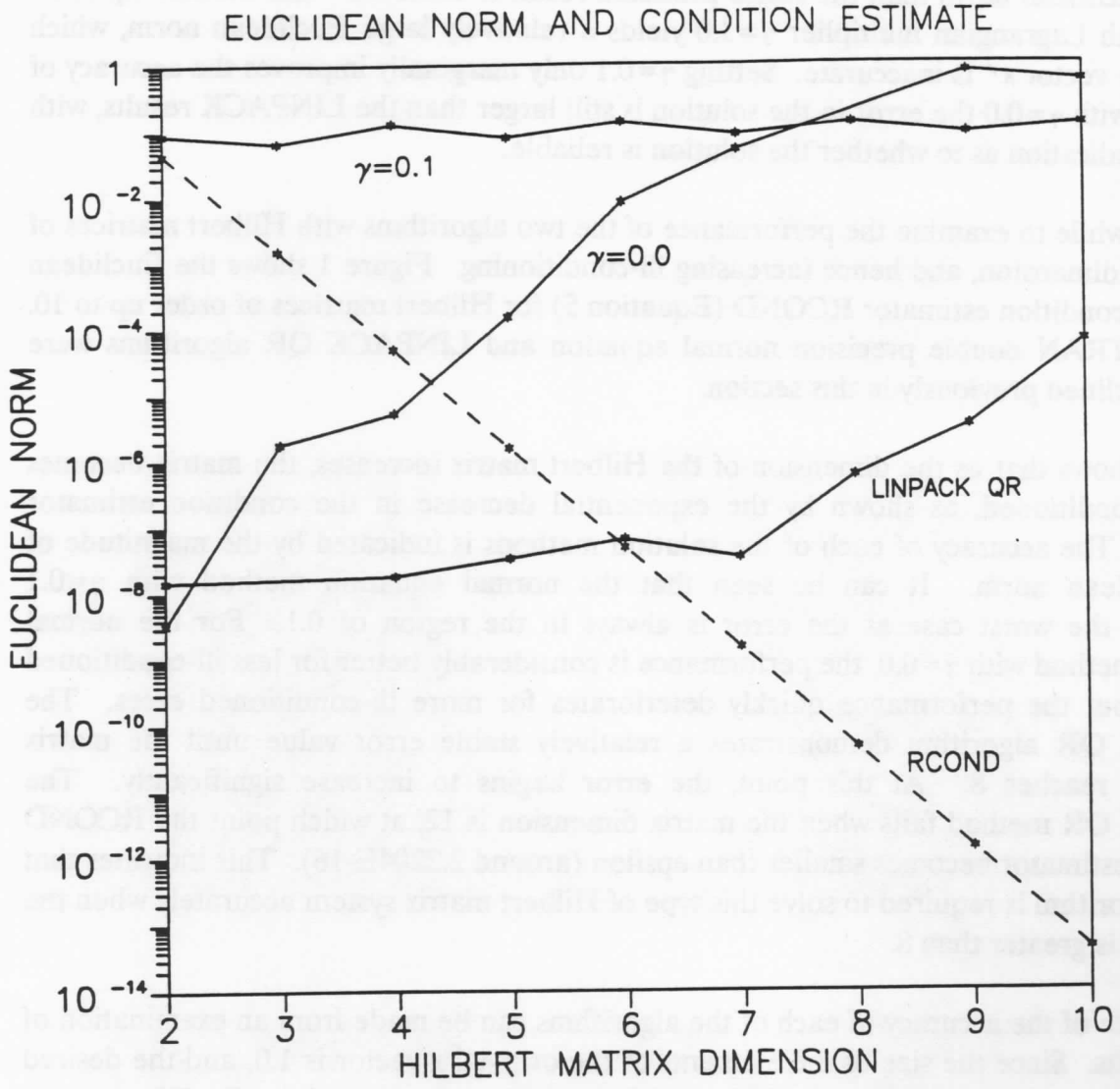
It is worthwhile to examine the performance of the two algorithms with Hilbert matrices of increasing dimension, and hence increasing ill-conditioning. Figure 1 shows the Euclidean norm and condition estimator RCOND (Equation 5) for Hilbert matrices of order up to 10. The FORTRAN double precision normal equation and LINPACK QR algorithms were used as outlined previously in this section.

Figure 1 shows that as the dimension of the Hilbert matrix increases, the matrix becomes more ill-conditioned, as shown by the exponential decrease in the condition estimator RCOND. The accuracy of each of the solution methods is indicated by the magnitude of the Euclidean norm. It can be seen that the normal equation method with $\gamma = 0.1$ represents the worst case as the error is always in the region of 0.1. For the normal equation method with $\gamma = 0.0$, the performance is considerably better for less ill-conditioned matrices, but the performance quickly deteriorates for more ill-conditioned cases. The LINPACK QR algorithm demonstrates a relatively stable error value until the matrix dimension reaches 8. At this point, the error begins to increase significantly. The LINPACK QR method fails when the matrix dimension is 12, at which point the RCOND condition estimator becomes smaller than epsilon (around 2.2204E-16). This indicates that a SVD algorithm is required to solve this type of Hilbert matrix system accurately when the dimension is greater than 8.

An estimate of the accuracy of each of the algorithms can be made from an examination of these results. Since the size of the elements of the original x vector is 1.0, and the desired solution vector x′ should have size also equal to 1.0, then the size of the Euclidean norm indicates the accuracy of the solution method, in terms of the number of accurate decimal places in the solution vector. For example, when the Hilbert matrix is of dimension 6, the LINPACK QR decomposition method returns a Euclidean norm of order 10^{-7}. This implies that the method is accurate to 7 decimal places in this case. Similarly, the normal equation method with $\gamma = 0.0$ returns a Euclidean norm of order 10^{-2} and is therefore accurate to 2 decimal places, while the normal equation method with $\gamma = 0.1$ is accurate to 1 decimal place.

FIGURE 1

Euclidean norm and condition estimate $1/(\|A\|_1 \|A^{-1}\|_1)$, for Normal Equation method with $\gamma=0.1$, $\gamma=0.0$, and double precision LINPACK QR decomposition method.



It should be noted that this is a demanding test of the least squares algorithms. If a real world least squares problem was encountered where the RCOND condition estimator was less than 10^{-16} then it would be advisable to re-examine the formulation of the problem. These results emphasise the need to examine the condition of a given least squares problem before a solution method is applied. It is vital to ensure that the least squares algorithm will be able to solve a given set of problems consistently and reliably with known accuracy. This is especially true if the software is to be ported to other computer systems while maintaining the desired level of accuracy.

7. COMPARISON OF LEAST SQUARES METHODS IN ATMOSPHERIC RETRIEVALS

Following the testing of the least squares algorithms in solving a Hilbert matrix system, it was decided to examine the impact of the different algorithms on the performance of an atmospheric retrieval scheme. While it should be noted that this is not the best to way to test the performance of a least squares algorithm, it does provide an insight into how the selection of a particular algorithm can affect "real world" results.

An ITPP3 synthetic retrieval package was developed as an aid in assessing retrieval performance (Gumley et. al., 1989). This package allows a synthetic atmospheric profile to be entered, computes TOVS sensor brightness temperatures for the profile, and then uses the ITPP3 physical retrieval algorithm to invert the radiative transfer equation and return a computed atmospheric profile for comparison.

The ITPP3 retrieval program TOVRET was modified to include

- user defined HIRS/2 and MSU radiance data,
- user defined surface data,
- selection of transmittance gammas and deltas,
- optional cloud checking,
- user defined first guess profile,
- user defined surface skin temperature estimation,
- selection of normal equation or QR decomposition least squares algorithm.

The ITPP3 forward radiance computation programs RAOBHIRS and RAOBMSU were used to compute HIRS/2 and MSU radiances for a set of atmospheric profiles obtained from a TOVS sonde/satellite matched set provided by L. McMillin (private communication, 1988). The retrieved temperature and moisture profiles were selected as these provided continuous data up to 0.1mb, whereas the sonde profiles had intermittent data at high altitudes. A total of 351 atmospheric profiles between latitudes 45N and 45S were used in the study. The least squares algorithms were compared by processing all profiles with the same options, except for the selection of the least squares solution algorithm. The options used in processing were

- nadir viewing radiances computed
- transmittance gammas and deltas set to 1.0 and 0.0 respectively in both forward radiance calculation and ITPP3 retrieval
- surface emissivity set to 1.0 in forward calculation
- use surface data defined for input profile in retrieval
- use input profile as first guess in retrieval
- disable cloud checking in retrieval
- user defined surface skin temperature estimation in retrieval
- set RMS error limits for HIRS channels at 0.25K in retrieval.

The ITPP3 retrieval algorithm involves the use of a "two-pass" approach, where the first guess profile is adjusted to match the observed radiances. On the first pass, only four of the HIRS channels are used to adjust the guess profile. On the second pass, the full complement of HIRS temperature sounding channels is used. The normal equation method is used in ITPP3 on both the first and second pass. On the first pass, $\gamma = 1.0$, and on the second pass, $\gamma = 0.1$.

The test results presented here used both the normal equation method and the LINPACK QR decomposition method. The first set of results were generated using the default ITPP3 method ($\gamma = 1.0$ on first pass, $\gamma = 0.1$ on second pass). The second set of results were generated using the default ITPP3 method, except that γ was set to 0.0 on the second pass.

The third set of results were generated using the LINPACK QR decomposition method. Before processing retrievals, it was necessary to check the condition of the basis function matrix A on the first and second passes. On the first pass, the condition estimator RCOND is typically of order 10^{-9}. The epsilon for FORTRAN single precision values is of order 10^{-7}, so single precision LINPACK QR decomposition could not be used on the first pass. The epsilon for FORTRAN double precision values is 10^{-16}, indicating that double precision LINPACK QR decomposition could be used on the first pass. However, problems were experienced with the limited memory space available in an MSDOS environment, and the double precision version could not be incorporated into the code easily. Thus the normal equation method with $\gamma = 1.0$ was used on the first pass. Since the condition estimator RCOND is typically of order 10^{-4} on the second pass, the single precision LINPACK QR decomposition method was used on the second pass. The second pass is the more important of the two passes since this is where the full complement of HIRS channels is used in the retrieval.

Mean and root-mean-square (RMS) statistics were computed for each set of retrievals using the 3 different least squares algorithms as shown:

$$\Delta T_i = T_{(r,i)} - T_{(0,i)} \qquad (i = 1000mb, 950mb, 920mb, ..., 300mb)$$

$$Mean = (\Sigma (\Delta T_i)) / n \qquad (n = 351)$$

$$RMS = ((\Sigma (\Delta T_i)^2) / n)^{1/2}$$

where $T_{(r,i)}$ is the retrieved temperature at each atmospheric level, and $T_{(0,i)}$ is the original input temperature at each level. The results are plotted in Figure 2, 3 and 4. Cubic splines were fitted to the data at the TOVS retrieval levels to produce smooth curves.

Figure 2 shows the temperature profile retrieval error for the normal equation method with $\gamma = 1.0$ on the first pass, and $\gamma = 0.1$ on the second pass of the retrieval. Figure 3 shows the temperature profile retrieval error for the normal equation method with $\gamma = 1.0$ on the first pass, and $\gamma = 0.0$ on the second pass of the retrieval. Figure 4 shows the temperature profile retrieval error for the LINPACK QR decomposition method on the second pass of the retrieval.

FIGURE 2

Temperature profile retrieval error for Normal Equation method with $\gamma = 1.0$ on retrieval first pass, $\gamma = 0.1$ on retrieval second pass.

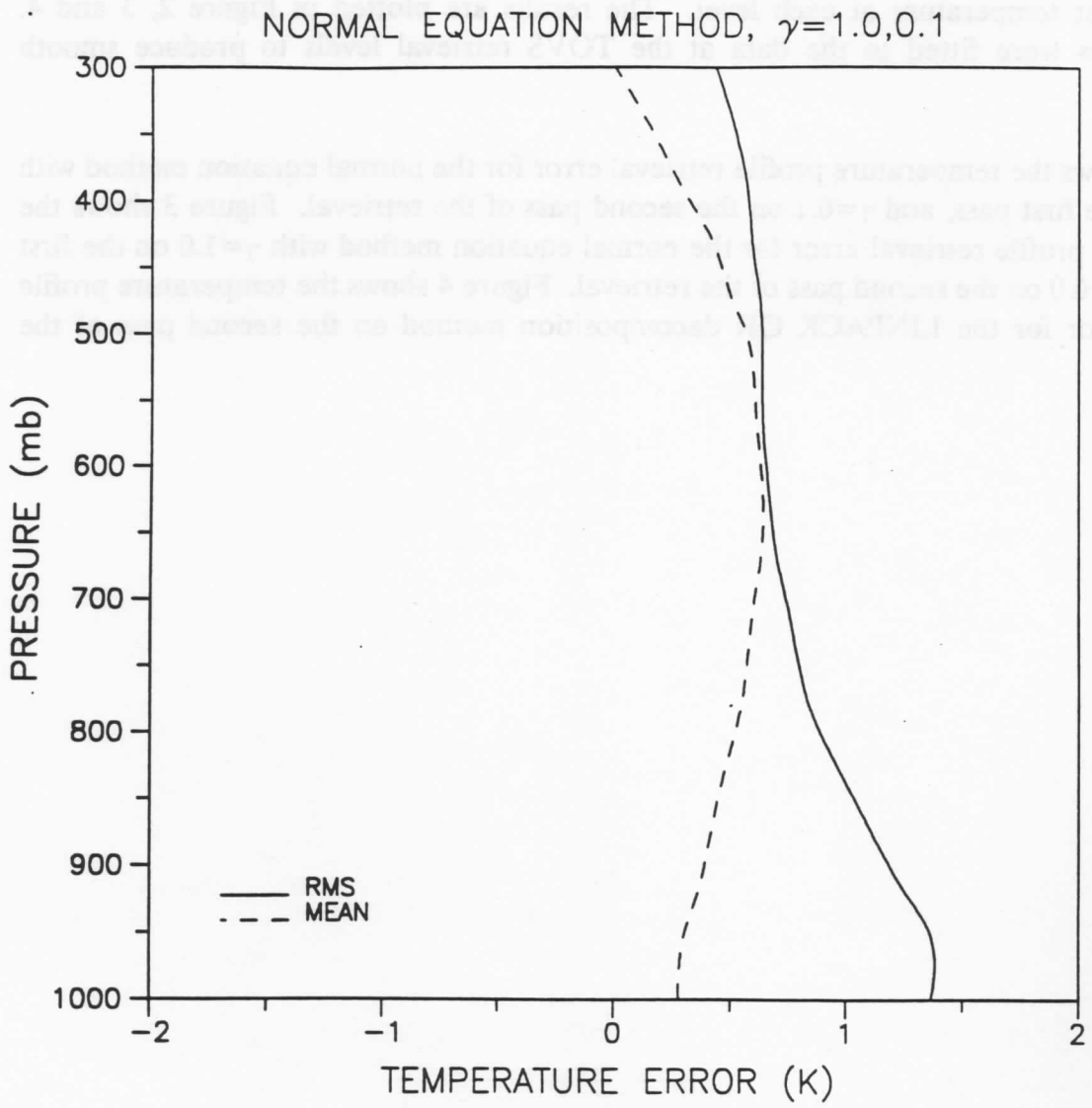


FIGURE 3

Temperature profile retrieval error
for Normal Equation method with $\gamma = 1.0$ on retrieval first pass,
$\gamma = 0.0$ on retrieval second pass.

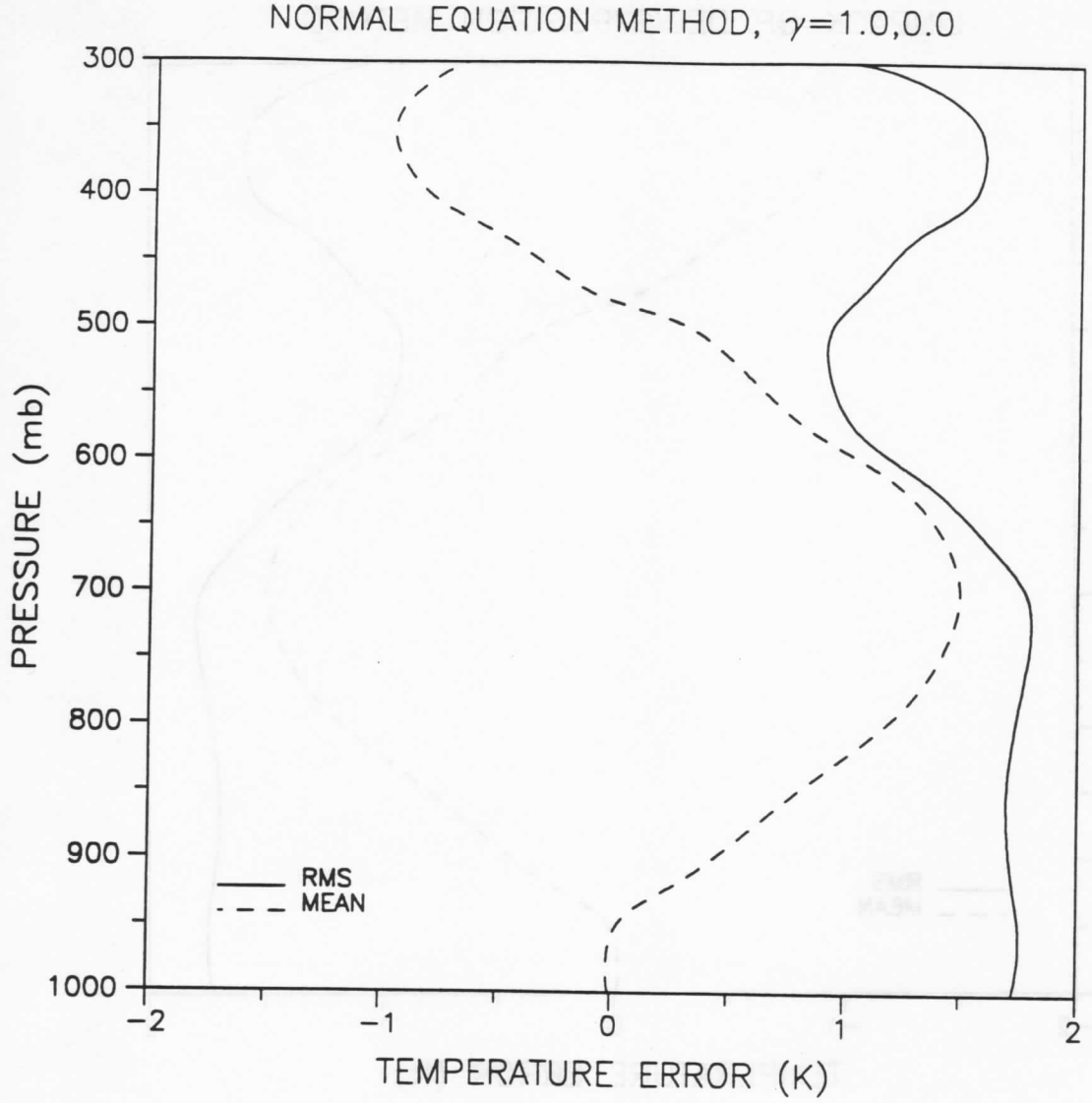
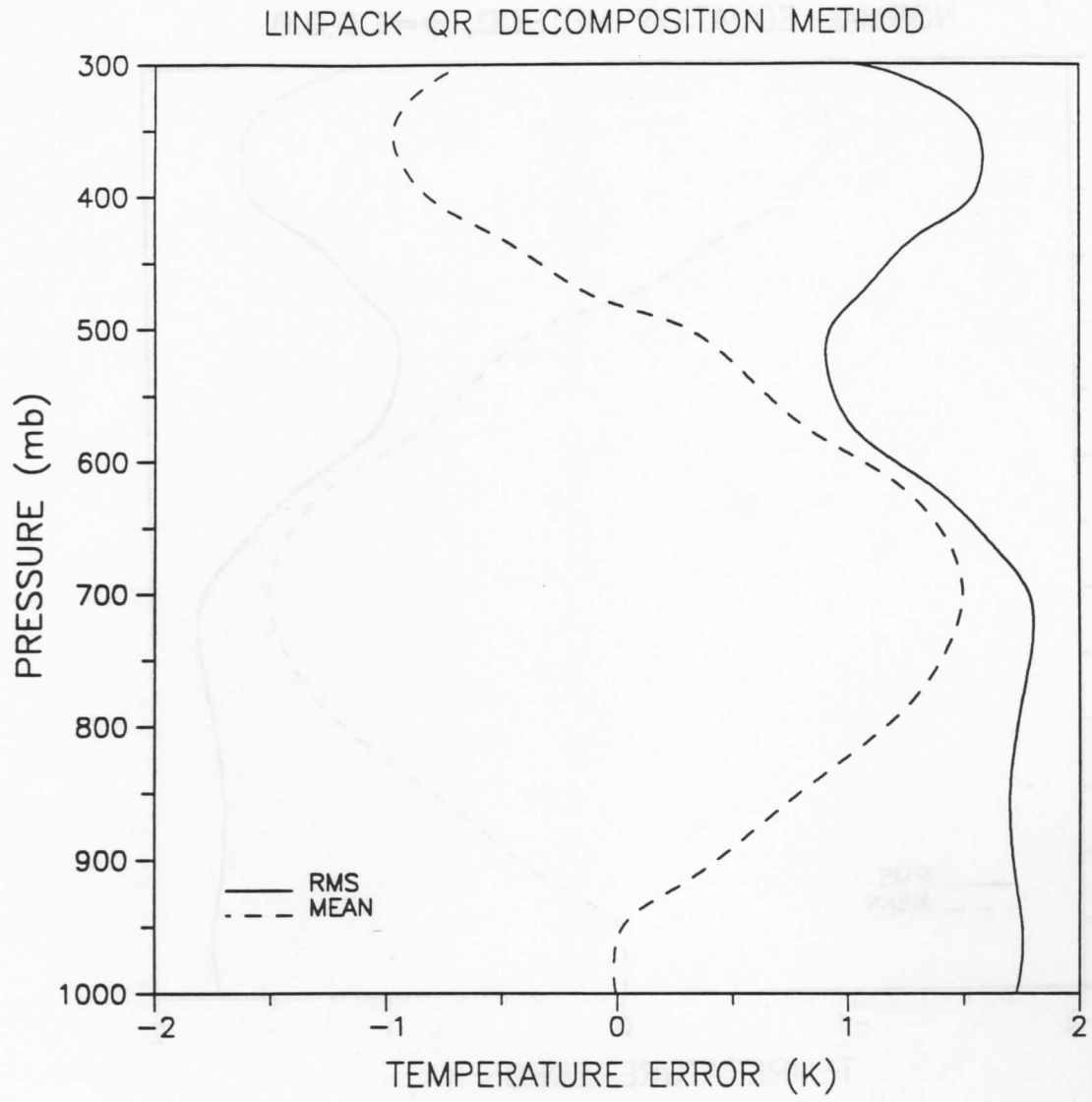


FIGURE 4

Temperature profile retrieval error
for Normal Equation method with $\gamma = 1.0$ on retrieval first pass,
LINPACK QR decomposition method on second pass.



8. DISCUSSION

Figure 2 shows that the mean and RMS temperature profile retrieval errors are well within acceptable error limits, compared to previous results (LeMarshall et. al., 1988). This gives confidence that the synthetic retrieval package is performing satisfactorily, as would be expected when the retrieval first guess is the original atmospheric profile. The retrieval error is greatest at the surface, and decreases for levels up to 300mb.

Figure 3, where $\gamma = 0.0$ on the second pass, shows markedly different mean and RMS error profiles. While the largest RMS error is still less than 2.0K, the error has increased at all levels from the surface up to 300mb. The reasons for the structure seen in the mean and RMS error profiles are not clear at this point, and were not investigated in this study.

Figure 4, where the LINPACK QR decomposition method was used, shows mean and RMS error profiles that are very similar to Figure 3. The error profiles for these plots are found to agree to three decimal places. This result bears some examination.

The first possibility is that the second pass of the retrieval algorithm has little bearing on the final result; that is, all the information necessary for profile retrieval is gleaned from the four HIRS channels used in the retrieval first pass. The retrieval profiles at the end of the first pass stage have not been examined in this study. However given the information content of just four channels, this possibility is thought to be unlikely.

The second possibility is that the second pass cases where $\gamma = 0.0$ and the QR method were used give results of a similar accuracy. The RCOND condition estimator on the second pass is always of order 10^{-4}. Referring back to Figure 1, it can be seen that for RCOND equal to 10^{-4}, the normal equation method with $\gamma = 0.0$ is accurate to around 5 decimal places, while the double precision LINPACK QR decomposition method is accurate to around 7 decimal places. The numerical results presented in Section 6 (Example 1) indicate that the single precision LINPACK QR decomposition method gives similar accuracy when RCOND $= 10^{-4}$. Thus, in this case where the basis function matrix is not too ill-conditioned, the normal equation method and the LINPACK QR decomposition method have accuracies which are not markedly different. However, as was seen with the Hilbert matrix example, this will not always be the case.

9. CONCLUSIONS

The solution of least squares systems is a standard problem which has received considerable attention in the literature (Golub et. al., 1983). Various algorithms have been formulated to solve such systems numerically. However, before any algorithm can be applied to a least squares problem, it is first necessary to be aware of the conditioning of the problem, and secondly to determine whether a given least squares algorithm can solve

the problem accurately and consistently, for different data sets and on different computer systems.

The solution of a least squares system with a Hilbert matrix as the basis is a severe test of least squares algorithms. The normal equation method is found to have problems solving such ill-conditioned systems, and no indication is available to the user as to whether the algorithm may have failed, or produced inaccurate results. The QR decomposition method however demonstrates consistent and accurate performance in solving this type of least squares system. For highly ill-conditioned systems, the LINPACK QR decomposition method will indicate whether machine precision limitations have made the solution unreliable. The need for a more specialised algorithm, such as SVD, is then indicated.

For retrievals processed with the ITPP3, it has been shown that there appears to be little benefit gained from changing to a LINPACK QR decomposition algorithm, in terms of retrieval accuracy. The normal equation method appears to work adequately when $\gamma=0.1$ on the retrieval second pass. However questions remain about the propagation of errors in the execution of the normal equation algorithm. It remains to be seen why the temperature profile retrieval errors are different when $\gamma=0.0$ rather than $\gamma=0.1$ is used on the second pass. The use of the LINPACK QR algorithm would however allow the user to be confident that the least squares algorithm did not "blow up" during computations, as the LINPACK QR algorithm has been demonstrated to work accurately and consistently for systems of condition comparable to that encountered in ITPP3 second pass retrievals.

For future retrieval algorithm development, it can be seen that if least squares algorithms are to be used, they must meet several requirements. A least squares algorithm must be able to solve a problem which has a certain level of ill-conditioning to a consistent accuracy. It should also indicate to the user when the results should not be trusted due to severe ill-conditioning. It should also provide the same consistency and accuracy when ported to different computer and compiler environments.

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TECHNICAL PROCEEDINGS OF THE SIXTH INTERNATIONAL TOVS STUDY CONFERENCE

AIRLIE, VIRGINIA

1-6 MAY 1991

Edited by

W. P. Menzel

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July 1991