ESTIMATING THE CORRECT DEGREE OF SMOOTHING IN THE SIMULTANEOUS RETRIEVAL METHOD

Jan Svensson
The Swedish Meteorological and Hydrological Institute (SMHI)
Norrköping, Sweden

1. INTRODUCTION

The International TOVS Processing Package, version 3 (ITPP3), developed by the Cooperative Institute for Meteorological Satellite Studies (CIMSS), Madison, Wisconsin,has been implemented on the VAX 8600 computer system at SMHI. Test data were taken from the Meso-scale Analysis Area for PROMIS 600 at SMHI (appr. 54-61°N, 6-28°E), see Gustafsson and Törnevik (1984), during the period May 3-26, 1983. Fifteen satellite passages were processed. The same data have been used in the test of ITPP2, see Svensson (1984, 1985 a). The test results for the temperature profiles are compared in Figure 1. This figure shows a significant improvement in ITPP3, especially for cloudy retrievals. The filtering programs, in ITPP2 and ITPP3 respectively, were used before comparison with radiosonde data. In ITPP2 24.8% of all soundings were rejected, while in ITPP3 only 8.2% were rejected. Another advantage is that ITPP3 seems to be faster. ITPP2 was implemented on a SPERRY 1122, which means that an exact comparison of execution times is difficult to do. The estimated CPU-time for one satellite passage is 9.5 minutes and estimated elapsed time is 19 minutes for ITPP3 on VAX 8600. One simple, but effective, modification of the program TOVRET in ITPP3 was done. The coefficients for HIRS radiative-transfer computations were stored in the virtual memory once and for all. In the original version the coefficients were reread every sounding. The I/O count in TOVRET was reduced with nearly 45% with our modification.

We will later implement the inversion method THAP, described by Svensson (1985 a, 1985 b) in ITPP3. The intention is to use the generalized cross-validation (GCV) in order to automatically select the regularization parameter. The GCV is more difficult to use in THAP than in the ordinary inversion method. Thus it seems reasonable to try to use the GCV in the ordinary inversion method first. In Section 2 we describe briefly the inversion method in ITPP3 and in Section 3 we describe the GCV. In section 4 we show some test results.

2. THE INVERSION METHOD IN ITPP3

The inversion method in ITPP3, also known as 'the simultaneous retrieval method', is described by Smith et al (1985). We shall here make a very short description of the method.

We start with an initial guess of the temperature and moisture profiles. We will then estimate a perturbation from the initial profiles. We have to solve the least-squares problem

$$\min_{\underset{\sim}{x}} \; || \underset{\approx}{A} \cdot \underset{\sim}{x} - \underset{\sim}{B} ||_2^2$$

where $\underset{\sim}{B}$ is a radiance vector, $\underset{\approx}{A}$ is a matrix calculated from the radiative transfer equation and $\underset{\sim}{x}$ is the perturbation vector to be found (more details are found in Smith et al (1985) or Svensson (1985 a, 1985 b). This least squares problem is ill-conditioned, that is taken the least-squares solution

$$\underset{\sim}{x} = (\underset{\approx}{A}^T \cdot \underset{\approx}{A})^{-1} \cdot \underset{\approx}{A}^T \cdot \underset{\sim}{B}$$

will give a physically unacceptable solution. If we add a regularization term

$$\underset{\sim}{x} = (\underset{\approx}{A}^T \cdot \underset{\approx}{A} + \lambda \cdot \underset{\approx}{I})^{-1} \cdot \underset{\approx}{A}^T \cdot \underset{\sim}{B} \qquad (1)$$

where λ is the regularization parameter and $\underset{\approx}{I}$ is the unit matrix, then we have a more well-conditioned problem with a physically acceptable solution. The parameter λ gives the degree of smoothing. If $\lambda \to 0$, then we will have the least-squares solution and if $\lambda \to \infty$, then we will have the initial profile as the solution.

The solution is received in two steps in ITPP3. In step 1 only the microwave channels and HIRS channels 1-3 and 11-12 are used. These channels are less affected by clouds, which means that they can be used for cloud correction of the other HIRS channels. In step 2 as many as nineteen different radiances are used. In step 1 the regularization parameter $\lambda = 1.0$ and in step 2, $\lambda = 0.1$ for clear retrievals and $\lambda = 1.0$ for cloudy retrievals. An automatic selection of λ would be preferable. Such an automatic selection would distinguish between good or bad initial guesses and between good or bad cloud corrections. The GCV is such an automatic method.

3. GENERALIZED CROSS-VALIDATION

The method of generalized cross-validation, described by Craven and Wahba (1979) and Golub et al (1979), determines the regularization parameter from the data, that is in our case from the radiances. The parameter λ in (1) is determined as the minimizer of

$$V(\lambda) = \| (\underset{\approx}{I} - \underset{\approx}{K}(\lambda)) \cdot \underset{\sim}{B} \|_2^2 / (\text{trace } (\underset{\approx}{I} - \underset{\approx}{K}(\lambda)))^2$$

where

$$\underset{\approx}{K}(\lambda) = \underset{\approx}{A} (\underset{\approx}{A}^T \cdot \underset{\approx}{A} + \lambda \cdot \underset{\approx}{I})^{-1} \cdot \underset{\approx}{A}^T$$

We may calculate $V(\lambda)$ and $V'(\lambda)$ from the singular value decomposition of $\underset{\approx}{A}$, see Golub et al (1979) or from the bidiagonal decomposition, see Eldén (1984). We use the method of Eldén in the calculation of $V(\lambda)$ and use a golden section search, see Gill et al (1981), for the minima search. We prefer to make the minimization in a $\log(\lambda)$ scale as proposed by O'Sullivan and Wahba (1985).

The GCV gives a good estimation of the optimum λ when the errors in $\underset{\sim}{B}$ are uncorrelated with no bias. A Monte Carlo experiment with this assumption, using data from TOVS, is described by O'Sullivan and Wahba (1985).

4. TEST RESULTS

We have implemented the GCV algorithm in step 2 in the simultaneous retrieval method. In step 1 the regularization parameter is still fixed. The first attempt with GCV was rather discouraging. The values of λ were for some cases much less than 0.1 and for other cases much greater than 1.0. The RMS differences to the radiosonde data were more than 5°C. We then limited the range of λ from 0.1 to 1.0. The RMS differences between satellite soundings and radiosondes are shown in Figure 2. This figure shows almost the same result for the soundings with fixed λ and those with λ decided by the GCV. The standard deviations between satellite soundings and radiosondes are shown in Figure 3. A small improvement when using the GCV is indicated for the cloudy retrievals.

One explanation of why we did not receive a more significant improvement of the satellite soundings, is that the assumption of uncorrelated errors with no bias is not fulfilled. We may suppose that there might be a bias, e g if the cloud algorithm fails to detect clouds for some situations, then we will have a negative bias. The cloud correction algorithm also makes the radiance errors correlated, because errors in the radiances used in step 1 will introduce errors in the cloud corrected radiances. A better understanding of the error statistics of the cloud corrected radiances would be valuable. The use of AVHRR for cloud correction might give a better agreement to the assumption of uncorrelated radiance errors with no bias.

It should be pointed out that the GCV is very inexpensive for such small least-squares problems like this one. The CPU time for the inversion method does not increase, when we added the GCV subroutines. The use of GCV seems encouraging, but more work must be done before it can be used in operational systems.

5. REFERENCES

Craven, P. and G. Wahba, 1979: **Smoothing Noisy Data with Spline Functions: Estimating the Correct Degree of Smoothing by the Method of Generalized Cross-Validation. Numerische Mathematik, 31, 377-403.**

Eldén, L., 1984: **A note on the computation of the generalized cross-validation function for ill-conditioned least squares problems, BIT, 24, 467-472.**

Gill, P.E., W. Murray and M.H. Wright, 1981: **Practical Optimization, Academic Press, London.**

Golub, G.H., M. Heath and G. Wahba, 1979: **Generalized Cross-Validation as a Method for Choosing a Good Ridge Parameter. Technometrics, 21, 215-223.**

Gustafsson, N. and H. Törnevik, 1984: **Development of an Operational System for Very-Short-Range Forecasting (VSRF) at SMHI. Proceedings of the Second International Symposium on Nowcasting, Norrköping, Sweden, 3-7 September, 1984, 473-477.**

O'Sullivan, F. and G. Wahba, 1985: **A Cross Validated Bayesian Retrieval Algorithm for Nonlinear Remote Sensing Experiments. Journal of Computational Physics, 59, 441-455.**

Smith, W.L., H.M. Woolf, C.M. Hayden and A.J. Schreiner, 1985: **The simultaneous retrieval export package. Technical Proceedings of The Second International TOVS Study Conference, Igls, Austria, 18-22 February, 1985, 224-253.**

Svensson, J., 1984: **Temperature profile retrievals from TIROS Operational Vertical Sounder during the ONSAM-experiment. R & D notes 33, SMHI, Norrköping, Sweden, 13 pp.**

Svensson, J., 1985a: **Remote sensing of atmospheric temperature profiles by TIROS Operational Vertical Sounder, RMK 45, SMHI, Norrköping, Sweden, 61 pp.**

Svensson, J, 1985b: **Numerical treatment of an ill-posed problem in remote sensing of atmospheric temperature profiles, Report LiU-TEK-LIC-1985:23, Dept of Mathematics, Linköping University, 69 pp.**

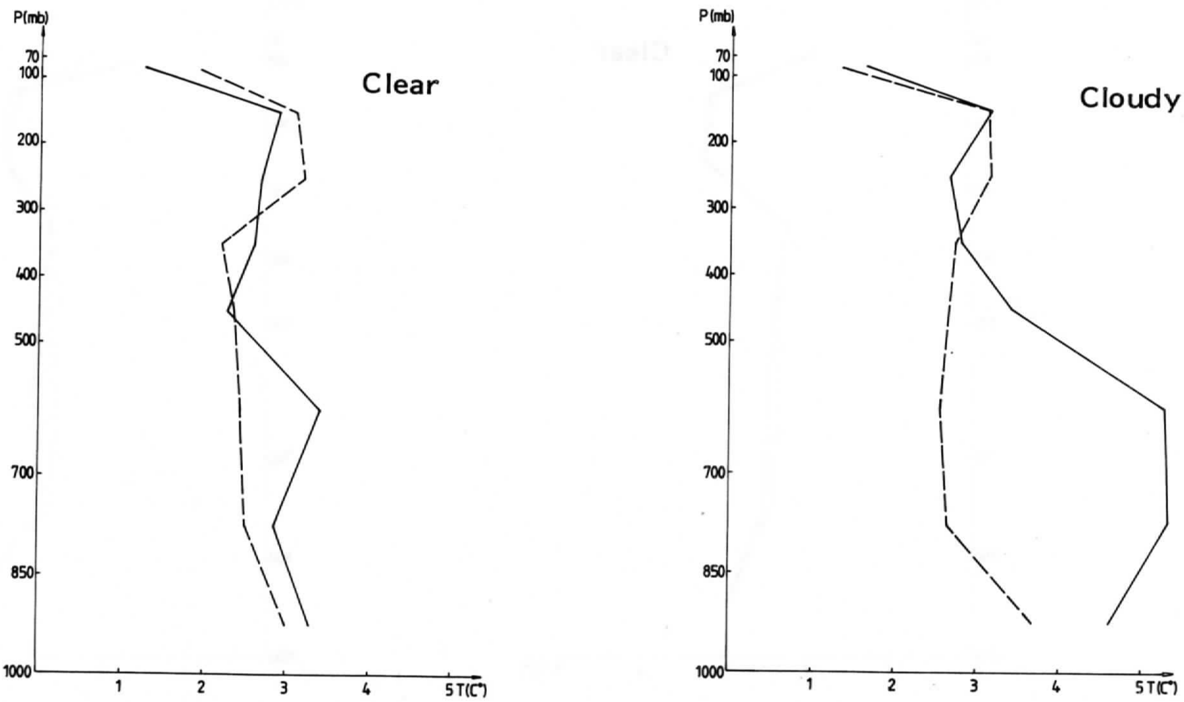

FIGURE 1. RMS differences in layer mean temperatures between satellite soundings and radiosondes launched in the Meso-scale Analysis Area.

—— = satellite soundings from ITPP2 (104 clear retrievals, 34 cloudy retrievals)

----- = satellite soundings from ITPP3 (71 clear retrievals, 93 cloudy retrievals)

First guess profile = climate.

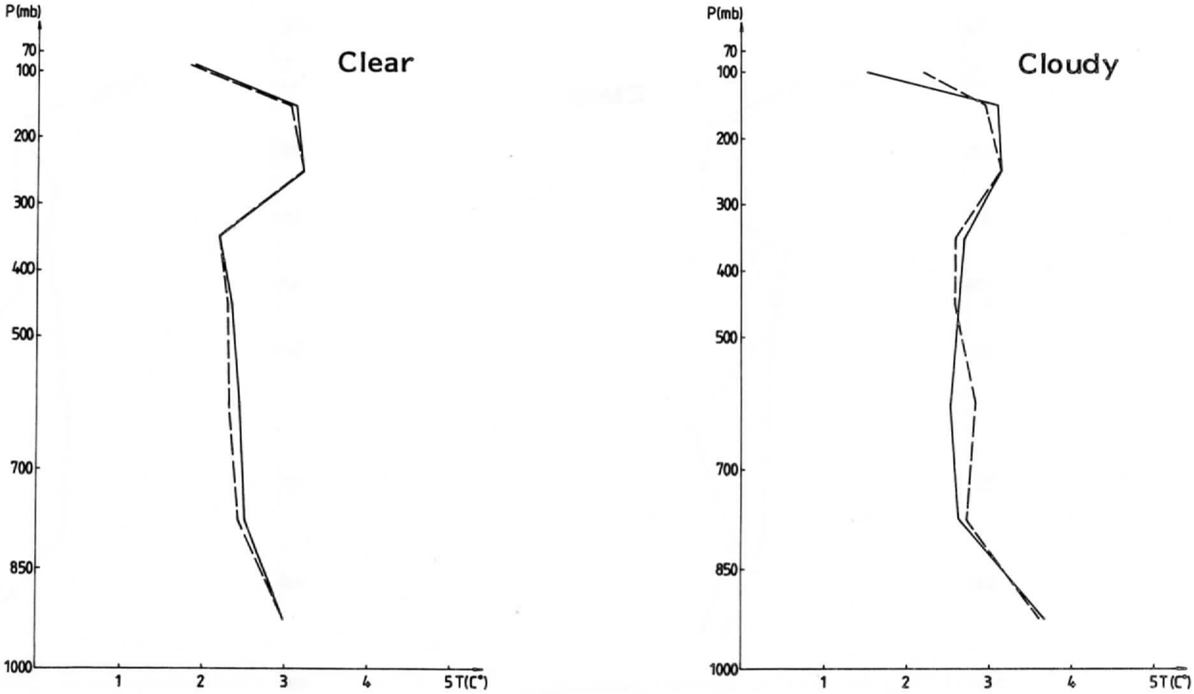

FIGURE 2. RMS differences in layer mean temperatures between satellite soundings and radiosondes launched in the Meso-scale Analysis Area.

—— = satellite soundings from ITPP3, with fixed regularization parameter (71 clear retrievals, 93 cloudy retrievals)

----- = satellite soundings from ITPP3, with regularization parameter determined by the method of generalized cross-validation (72 clear retrievals, 92 cloudy retrivals)

First guess profile = climate.

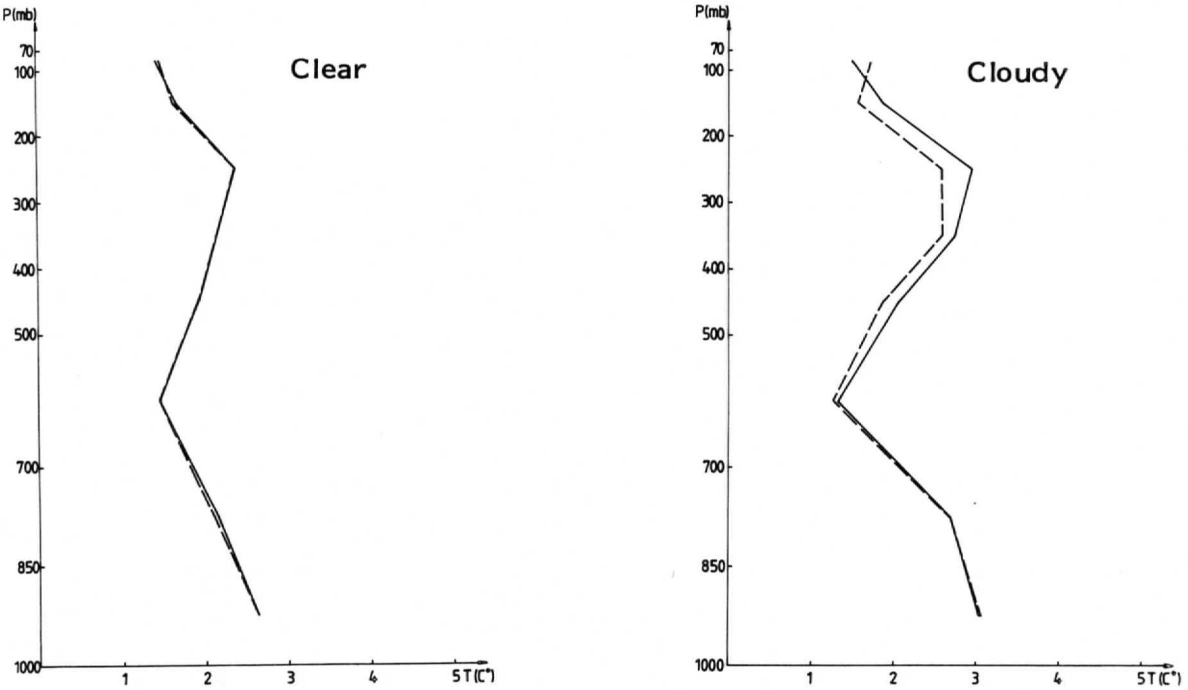

FIGURE 3. Standard deviation of differences in layer mean temperatures between satellite soundings and radiosondes launched in the Meso-scale Analysis Area.

—— = satellite soundings from ITPP3, with fixed regularization parameter (71 clear retrievals, 93 cloudy retrievals)

----- = satellite soundings from ITPP3, with regularization parameter determined by the method of generalized cross-validation (72 clear retrievals, 92 cloudy retrievals)

First guess profile = climate.

The Technical Proceedings of

The Third International TOVS Study Conference

Madison, Wisconsin

August 13 - 19, 1986

Edited by

W. P. Menzel

Cooperative Institute for Meteorological Satellite Studies
Space Science and Engineering Center
University of Wisconsin
1225 West Dayton Street
Madison, Wisconsin 53706
(608)262-0544

November 1986