

# Regularization of Atmospheric Temperature Retrieval Problems\*

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## 1 Introduction

Passive remote sensing of the atmosphere is used to determine the atmospheric state. A radiometer measures microwave emissions from earth's atmosphere and surface. The radiance measured by the radiometer is proportional to the brightness temperature. This brightness temperature can be used to estimate atmospheric parameters such as temperature and water vapor content. These quantities are of primary importance for different applications in meteorology, oceanography, and geophysical sciences. Depending on the range in the electromagnetic spectrum being measured by the radiometer and the atmospheric quantities to be estimated, the retrieval or inverse problem of determining atmospheric parameters from brightness temperature might be linear or nonlinear. In most applications, the retrieval problem requires the inversion of a Fredholm integral equation of the first kind making this an ill-posed problem. The numerical solution of the retrieval problem requires the transformation of the continuous problem into a discrete problem. The ill-posedness of the continuous problem translates into ill-conditioning or ill-posedness of the discrete problem. Regularization methods are used to convert the ill-posed problem into a well-posed one.

In this paper, we present some results of our work in applying different regularization techniques to atmospheric temperature retrievals using brightness temperatures measured with the SSM/T-1 sensor. Simulation results are presented which show the potential of these techniques to improve temperature retrievals. In particular, no statistical assumptions are needed and the algorithms were capable of correctly estimating the temperature profile corner at the tropopause independent of the initial guess.

## 2 Radiative Transfer Theory in the Microwave Region

Radiative transfer theory describes the intensity of radiation propagating in a general class of media that absorbs, emit, and scatter the radiation [5]. The radiative transfer equation for a plane-parallel atmosphere is given by

$$\cos \theta \frac{dI_\nu}{dz} = -\sigma(z)I_\nu + J_\nu(z) \quad (1)$$

where  $I_\nu(z)$  is the instantaneous radiant intensity that flows at each point in the medium per unit area, per unit of solid angle, at a given frequency  $\nu$ ;  $\sigma(z)$  is the extinction coefficient; and  $J$  is a source term. These last two quantities describe the loss/gain into the given direction. The angle  $\theta$  is the direction angle with respect to the vertical axis  $z$  with  $\theta = 0$  when pointing upwards.

In the general case, scattering into and from other directions can lead to both gains and losses to the intensity and are taken care by the terms  $\sigma$  and  $J$ . For the microwave region, the scattering term is usually neglected [3]. If scattering is neglected, the only source term to consider is that due to local emission and the extinction coefficient reduces to the absorption coefficient  $\sigma_a$ . Assuming local thermodynamic equilibrium, each point can be characterized by a temperature  $T$  and from Kirchoff's law we get

$$J_\nu(z) = \sigma_a(z)B_\nu(T(z)) \quad (2)$$

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where  $B_\nu(T)$  is the Planck function:

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp h\nu/kT - 1} \quad (3)$$

where  $h = 6.625 \times 10^{-34}$  Js is Planck's constant,  $c = 2.988 \times 10^8$  m/s is the speed of light, and  $k = 1.381 \times 10^{-23}$  J/K. Equation (1) is a linear non-homogeneous first-order differential equation with solution

$$I_\nu(z) = I_\nu(z_o) e^{-\sec\theta \int_{z_o}^z \sigma_a(z) dz} + \sec\theta \int_{z_o}^z \sigma_a(z) e^{-\sec\theta \int_\gamma^z \sigma_a(\xi) d\xi} B_\nu(T(\gamma)) d\gamma \quad (4)$$

where  $I_\nu(z_o)$  is the boundary condition, In the microwave region of the spectrum

$$h\nu \ll kT$$

which results in (3) taking the form

$$B_\nu(T) = \frac{2\nu^2 kT}{c^2} = \frac{2kT}{\lambda^2} \quad (5)$$

where  $\lambda$  is the wavelength. This is known as the Raleigh-Jeans approximation. From this expression, it is clear that in the microwave region the energy emitted is proportional to the physical temperature T. Another commonly used result from this relation is to define a scaling of the intensity  $I_\nu$  as follows

$$T_b = \frac{\lambda^2}{2k} I_\nu \quad (6)$$

The quantity  $T_b(\nu)$  is called the *brightness temperature* which is commonly used in the microwave retrieval literature instead of  $I_\nu$ . In terms of brightness temperature and using (5), (4) takes the form

$$T_b(z) = T_b(z_o) e^{-(\delta(z_o) - \delta(z)) \sec\theta} + \sec\theta \int_{z_o}^z \sigma_a(\gamma) e^{-(\delta(\gamma) - \delta(z)) \sec\theta} T(\gamma) d\gamma \quad (7)$$

where

$$\delta(z) = \int_z^\infty \sigma_a(\xi) d\xi \quad (8)$$

is the optical thickness and  $z_o$  represents the top of the atmosphere (TOA). Here the dependency of all these quantities in frequency  $\nu$  is not shown for convenience

For our purpose, it is of interest to solve this equation to obtain the brightness temperature that a satellite will measure at the top of the atmosphere when looking to the surface at an angle  $\theta$  off nadir. This will correspond to  $z_o = 0$  surface (sfc) and  $z = \infty$  in (7). The boundary term  $T_b(0)$  is given by

$$T_b(0) = \epsilon T_s + (1 - \epsilon) T_d$$

where  $T_s$  is the surface temperature,  $T_d$  is the downwelling radiation reflected by the surface back towards the satellite, and  $\epsilon$  is the surface emissivity. For the reflected component, it is assumed that the surface is a smooth, homogeneous, and isothermal so only the radiation in the specular direction  $\theta$  is accounted for. In our reference coordinates, the propagation angle for the downwelling radiation is  $\pi - \theta$ . The downwelling radiation is obtained by solving the radiative transfer equation where integration is from the TOA to the surface with propagation angle  $\pi - \theta$ . This is taken care in (7) by setting  $z_o = \infty$  and  $z = 0$ . The boundary term in this case is given by the cosmic microwave background emission with  $T_c = 2.7$  K. The resulting expression for the brightness temperature at the TOA at an angle  $\theta$  off nadir

$$T_b = \left[ \epsilon T_s + (1 - \epsilon) T_c e^{-\delta(0) \sec\theta} \right] e^{-\delta(0) \sec\theta} + \int_0^\infty T(z) \left[ 1 - (1 - \epsilon) e^{-2(\delta(0) - \delta(z)) \sec\theta} \right] e^{-\delta(z) \sec\theta} dz \quad (9)$$

Simulation of this expression if all quantities were known is a simple matter. However, the computation of the optical thickness and the absorption parameter requires the use of databases containing information about the spectral characteristics of atmospheric constituents such as HITRAN. In our work, all optical depth computations were carried out using the FASE Radiative Transfer Code.

### 3 Atmospheric Remote Sensing

The satellite instrument measures radiance that arrives into its field of view. The radiance that arrives is the sum of the radiance emitted and reflected by the surface, emitted and reflected by the atmosphere, and that scattered by the atmosphere into the field of view of the instrument. The relative contribution of each component depends on the region of the spectra seen by the instrument. Remote sensing of the surface takes advantage of those regions of the spectrum where the atmosphere is transparent or nearly so. In the case of atmospheric remote sensing, the satellite sensor is looking at regions in the spectra where the atmosphere blocks the radiance emitted or reflected by the surface and therefore it receives that radiation that is emitted or reflected by the atmosphere. The interaction of electromagnetic waves with the atmosphere depends on the characteristics of the propagating wave (primarily its wavelength), the physical characteristics of the atmosphere and its constituents (pressure, temperature, density, absorbing gases, suspended particles). The mechanisms for interactions are: scattering, absorption, emission, and refraction. In regions where the atmospheric constituents characteristics are known or understood as in the 60 GHz oxygen and 183 GHz water vapor absorption lines, measurements of brightness temperature can be used to infer atmospheric properties of interest. The relation between atmospheric properties with brightness temperature is given by the radiative transfer equation (7). Therefore the problem of interest is to infer the atmospheric quantities of interest from measured brightness temperature by inversion of the radiative transfer equation.

### 4 Temperature Retrieval Problem

If the atmosphere strongly absorbs, most of the contribution to the measured brightness temperature will come from the atmosphere itself. In the case of the microwave region of the spectrum, scattering is negligible and the energy into the field of view of the sensor will come from atmospheric emission. Assuming that the satellite is looking at nadir (i.e.  $\theta = 0$ ), and that the surface temperature  $T_s$  and emissivity  $\epsilon$  are known, (9) can be rewritten as

$$\tilde{T}_b = \int_0^\infty T(z) K(\nu, z) dz \quad (10)$$

where

$$K(\nu, z) = \left[ 1 + (1 - \epsilon) e^{-2(\delta(0) - \delta(z))} \right] e^{-\delta(z)}$$

$$\tilde{T}_b = T_b - \epsilon T_s + (1 - \epsilon) T_e e^{-\delta(0)}$$

If the absorber is uniformly mixed with a known concentration, as  $O_2$ , the quantity  $K(\nu, z)$  is known and the temperature profile  $T(z)$  could be retrieved by inverting (10). The function  $K(\nu, z)$  is called in the literature [3] the *weighting function*. From this point on, in our discussion we would not distinguish between  $T_b$  and  $\tilde{T}_b$  in (10).  $O_2$  has several absorption lines around between 50 and 60 GHz. The Special Sensor Microwave Temperature-1 (SSM/T-1) sensor of the sensor suite of the DMSP satellite has 7 channels located in the 50 to 60 GHz range used for temperature retrievals. A summary of the SSM/T-1 sensor characteristics is given in [6]. In the  $O_2$  band, the shape of the weighting function is independent of the temperature making the inversion of (10) a linear inversion problem.

#### 4.1 Problem Discretization

To numerically solve the temperature retrieval problem, first we discretize (10) by approximating the integral with a numerical integration formula. This results in the algebraic linear system of equation

$$T_b = KT + e \quad (U)$$

where  $T_b \in \mathcal{R}^m$  and  $T \in \mathcal{R}^n$  are the brightness and atmospheric temperature vector;  $K \in \mathcal{R}^{m \times n}$  is the matrix of weighting functions; and  $e$  is an error term associated with measurement noise and the truncation error arising from the discretization of the integral equation. The number of measured brightness temperatures  $m$  is usually smaller than the vertical resolution or number of temperature levels  $n$  to estimate. In the case of the SSM/T-1 sensor, there are  $m = 7$  channels and normally  $n \geq 20$  temperature levels. Therefore the resulting algebraic linear system of equations (11) is under constrained (i.e. there are more unknowns than equations).

## 4.2 Regularization of the Discrete Problem

The temperature retrieval problem is related to the solution of the linear system of equations (11). This problem has two major difficulties associated with it: (i) ill-conditioning due to the ill-posedness of the associated integral equation, and (ii) multiple solutions because of trying to estimate more temperature levels than measurements available. To overcome these difficulties, we will use the so called regularization methods. Regularization theory [1] transforms an ill-posed problem to a well-posed one, using a *priori* knowledge on the nature of the solution. Depending on the prior information, regularization techniques can be classified into two major groups: statistical and deterministic.

### 4.2.1 Statistical Regularization

In statistical regularization, prior statistical information is used to regularize the temperature retrieval problem. Our prior information in this case is the prior distribution of the temperature profiles  $p_T(T)$  and the conditional distribution  $p_{T_b/T}(T_b)$ . According to Bayesian estimation theory [4], the best estimator  $T$  based on the brightness temperature observation  $T_b$  of the temperature profile  $T$  in a mean square sense is the conditional mean

$$T = E(T/T_b) \quad (12)$$

We will refer to this estimator as the minimum mean square estimator (MMSE). The analytical determination of this function might be a very difficult task. In many instances, the estimator is constrained to be linear which results in the Linear Minimum Mean Squares Estimator (LMMSE) [4]

$$\mathbf{T} = \mathbf{T} + \mathbf{\Lambda}_{T,T_b} \mathbf{\Lambda}_{T_b,T_b}^{-1} (\mathbf{T}_b - \bar{\mathbf{T}}_b) \quad (13)$$

where  $T$  is the a priori mean of  $T$ ,  $\bar{\mathbf{T}}_b$  is the mean of  $\mathbf{T}_b$  given  $T$ ,  $\mathbf{\Lambda}_{T,T_b}$  is the cross covariance between  $T$  and  $\mathbf{T}_b$ , and  $\mathbf{\Lambda}_{T_b,T_b}$  is the conditional covariance of the brightness temperature. The LMMSE is easy to construct, since only the first and second order statistics are needed rather than their complete probability densities. Also, if  $T$  and  $\mathbf{T}_b$  are jointly Gaussian, the LMMSE is the optimal Bayesian MMSE.

### 4.2.2 Deterministic Methods

In this section, we will look at two regularization methods for ill-posed linear algebraic systems of equations: Tikhonov regularization, and discrepancy principle regularization. Other methods are discussed in [2]. Computation of the regularized solution was done using the MATLAB Regularization Toolbox presented in [2].

#### Tikhonov's Regularization

One way to regularize (11) is computing  $T$  as the solution to the optimization problem

$$\hat{T}_\lambda = \arg \min_{T \in \mathcal{R}^n} \left[ \|\mathbf{K}T - \mathbf{T}_b\|^2 + \lambda^2 \|\mathbf{L}(T - T_o)\|^2 \right] \quad (14)$$

where  $T_o$  is a prior temperature profile estimate,  $\|\cdot\|$  is the 2-norm, and  $\lambda$  is the regularization parameter.

A key issue in this method is the selection of the regularization parameter  $\lambda$ . The value used in the simulation results presented here was based on the L-curve method described in [2]. The optimal value of  $\lambda$  balances the prediction error  $\|\mathbf{K}T - \mathbf{T}_b\|$  with the regularization error  $\|\mathbf{L}(T - T_o)\|$ .

#### Discrepancy Method

Another possibility to regulate the temperature retrieval problem is by computing  $T$  as the solution to the quadratically constrained linear least squares problem

$$\hat{T}_\alpha = \arg \min_{T \in \mathcal{R}^n} \|\mathbf{L}(T - T_o)\|^2 \quad (15)$$

$$\text{subject to } \|\mathbf{K}T - \mathbf{T}_b\|^2 \leq \alpha^2$$

where  $\alpha$  plays the role of a regularization parameter. The solution to this problem can be made identical to  $\hat{T}_\lambda$  for a suitably chosen  $\alpha$  [2]. We prefer to select  $\alpha$  based on the measurement noise norm  $\|e\|$ .

## 5 Simulation Experiments

In this section, we present some simulation results that illustrate the use of deterministic methods to regularize the temperature retrieval problem. For the simulation experiments, a 98 layer atmosphere based on the US Standard Atmosphere model was used. The optical thickness for each layer was computed using the FASE code. The radiative transfer equation was numerically integrated using the trapezoidal rule. The implementation of Tikhonov's and the discrepancy algorithm available in the Matlab<sup>TM</sup> Regularization Toolbox were used to compute the temperature retrievals. All computations with the exception of the optical thickness were done under the MATLAB<sup>TM</sup> environment. In our simulations, the surface emissivity  $\epsilon$  was set to 0.9 and the surface temperature  $T_s$  set to 288.2 degrees Kelvin. Figures 1 and 2 show the results of applying Tikhonov's regularization to the temperature retrieval problem with perfect measurements (no noise). The regularization parameter  $\lambda$  was set 0.0044. The solid line is the retrieved temperature profile, the dashed line is the actual temperature profile, and the dash-dot line is the initial guess fed to the algorithm. We can see from this simulations that the algorithm was capable of estimating temperature up to 40 km. Beyond 40 km, the resulting estimate was identical to the initial guess. An important result is how the retrieval algorithm is capable of determining the height of tropopause corner when fed with initial guesses that have that corner at heights far from the actual height as shown in Figure 2. The importance of determining this peak comes from the fact that most important weather features are located at this region of the atmosphere. Also, the location of the tropopause peak serves as a figure of merit in evaluating the performance of temperature retrieval algorithms. We are not showing results for the algorithm based on the discrepancy principle regularization since they were similar to those of Tikhonov regularization.

Figures 3 and 4 show the performance of Tikhonov regularization under the presence of noisy data. The noise vector added to the measured brightness temperature has a normal distribution with zero mean and unit variance. The regularization parameter for this case was  $\lambda = 0.016$ . Notice that the noise causes the retrieved profile to be noisier with a maximum error in the first 20 km of 10 degrees Kelvin. Quite high compared to some retrieval methods that claim accuracies of 0.5 degrees Kelvin. However, the algorithm is still capable of determining the height of the tropopause.

Figures 5 and 6 show the results for the retrievals in the noisy case computed using discrepancy principle regularization. The regularization parameter for this case was set at  $\alpha = 3$ . That value corresponds to three standard deviations of the noise distribution. The resulting retrievals are smoother than those retrievals from Tikhonov regularization. The maximum error is in the neighborhood of 3 to 4 degrees Kelvin in the tropopause. The estimation of the location of the tropopause peak is also improved.

## 6 Conclusions and Final Comments

This paper presents some preliminary work in the application of regularization techniques to the linear problem of atmospheric temperature retrievals from microwave radiometry. The proposed techniques were evaluated using simulated data. We used algorithms implemented in the MATLAB Regularization Toolbox developed by [2]. The results obtained were quite encouraging. In particular, being able to estimate the location of the tropopause corner of the temperature profile even with bad initial guess and noisy data is a result not previously observed with other algorithms.

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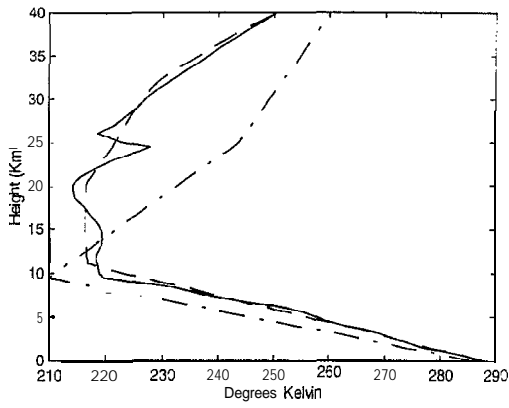


Figure 1: Tikhonov Regularization with 10 km Tropopause.

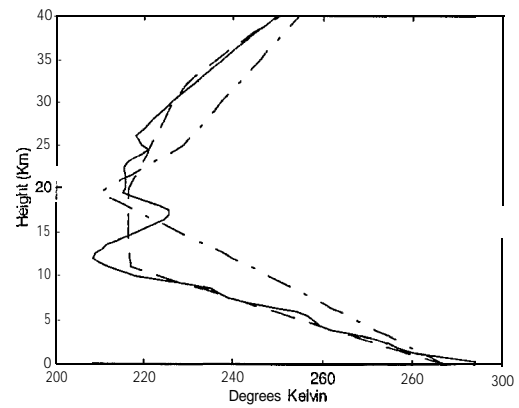


Figure 4: Tikhonov regularization with 20 km tropopause initial guess: noisy case.

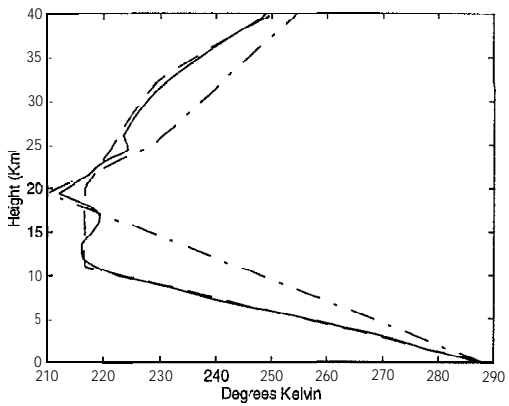


Figure 2: Tikhonov regularization with 20 km tropopause initial guess: noise free.

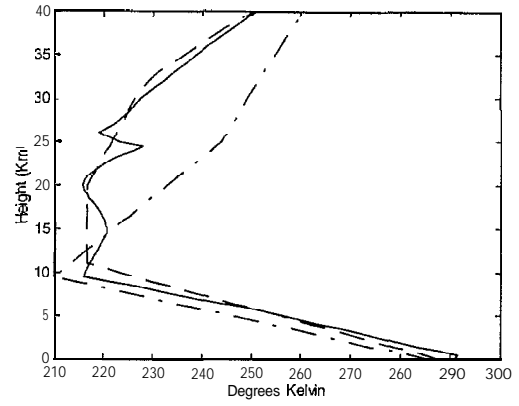


Figure 5: Discrepancy regularization with 10 km tropopause initial guess: noisy case.

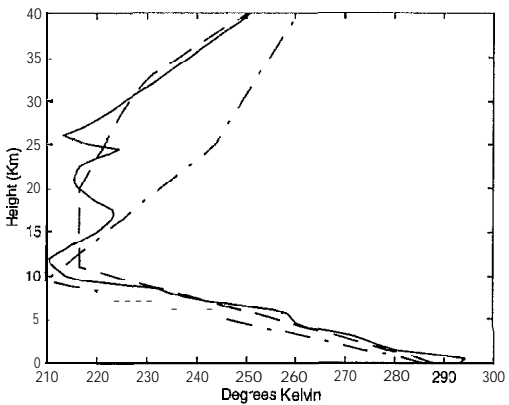


Figure 3: Tikhonov regularization with 10 km tropopause initial guess: noisy case.

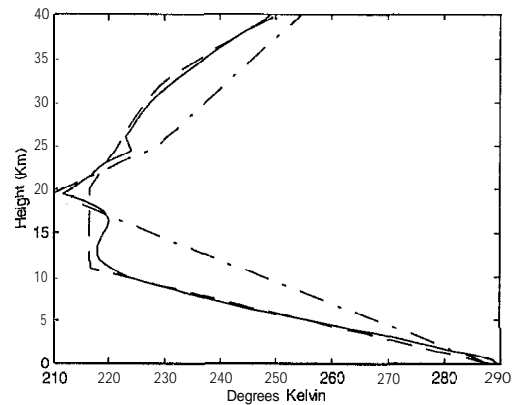


Figure 6: Discrepancy regularization with 20 km tropopause initial guess: noisy case.