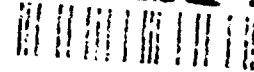


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Algorithms for Interpolating and Approximating Radiance Profiles

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# ALGORITHMS FOR INTERPOLATING AND APPROXIMATING RADIANCE PROFILES

Steven J. Leon

## 1 Introduction

In recent years there has been a considerable amount of work by J. I. F. King and others developing methods for remote temperature sensing based on applying transform theory to the radiative transfer equation. King, Hohlfeld, and Kilian, [9] have shown that using differential inversion it is possible to successfully determine temperature profiles based on measurements of the upwelling intensities in the atmosphere. A second transform method proposed by Jean I. F. King is based on optical measure theory. This technique has been studied by King and Leon, [11,12]. The optical measure theory method has the advantage that it does not require any computations of numerical derivatives. Instead the radiance profile is approximated by a rational function. The Planck intensity is then determined as the inverse transform of the rational function. In this paper we present techniques for approximating the radiance profile based on rational interpolation and nonlinear least squares data fitting.

In the final section of the paper we discuss general matrix methods for solving integral equations of the first kind. In particular, using regularization techniques, the inversion problem can be solved as a linear system with quadratic constraints. Numerical algorithms have been developed for solving these constrained problems. However, these algorithms proved unsuccessful when applied to data sets obtained from the NOAA TIROS Operational Vertical Sounder (TOVS). A singular value analysis is given which shows why the matrix techniques fail.

## 2 Rational Approximation of Radiance Profiles

Using radiative transfer theory one can relate the Planck intensity to the upwelling intensity of the atmosphere. This relationship can be expressed in terms of an integral equation of the first kind. Specifically the relationship is given by

$$R(\bar{p}) = \int_0^{\infty} B(p)W(p/\bar{p})dp/p \quad (1)$$

where  $W(p/\bar{p})$  is a kernel weight function that peaks at  $p = \bar{p}$  and  $R(\bar{p})$  denotes the radiance of the wavelength channel whose weight function peaks at  $p = \bar{p}$ .

If we set

$$W(z) = ze^{-z} \quad \text{and} \quad s = \frac{1}{\bar{p}}$$

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then the integral equation (2) can be expressed as a Laplace transform and consequently we can solve for the Planck function

$$B(p) = \mathcal{L}^{-1} \left( \frac{R(\frac{1}{s})}{s} \right)$$

We can think of  $B(p)$  and  $R(\hat{p})$  as transform pairs. Once a representation for  $R$  has been decided upon, then  $B$  can be determined analytically as an inverse Laplace transform. In Section 4 we will consider other choices for the weight function  $\mathcal{W}(z)$ . Optical measure theory permits the inversion of non-Laplacian exponential kernels.

The  $H$ -function inversion theory of Chandrasekhar [2] suggests that  $R$  should be represented as a rational function. If we set

$$R(\hat{p}) = d_1 + d_2\hat{p} + \dots + d_{j+1}\hat{p}^j + \sum_{i=1}^l \frac{w_i}{1 + c_i\hat{p}} \quad (2)$$

then

$$\frac{R(\frac{1}{s})}{s} = \frac{d_1}{s} + \frac{d_2}{s^2} + \dots + \frac{d_{j+1}}{s^{j+1}} + \sum_{i=1}^l \frac{w_i}{s + c_i}$$

and

$$B(p) = d_1 + d_2p + \dots + \frac{d_{j+1}}{j!} p^j + \sum_{i=1}^l w_i e^{-c_i p} \quad (3)$$

The coefficients in equation (2) can be determined from the data by rational interpolation or by nonlinear least squares. If one sets

$$R_i = R(\hat{p}_i) \quad i = 1, \dots, m$$

and expresses  $R$  as a quotient

$$R(\hat{p}) = \frac{a_1\hat{p}^n + a_2\hat{p}^{n-1} + \dots + a_{n+1}}{\hat{p}^l - a_{n+2}\hat{p}^{l-1} - \dots - a_m} \quad (n + l = m + 1)$$

then  $R$  will interpolate  $(\hat{p}_i, R_i)$  if and only if

$$a_1\hat{p}_i^n + a_2\hat{p}_i^{n-1} + \dots + a_{n+1} + a_{n+2}\hat{p}_i^{l-1} R_i + \dots + a_m R_i = \hat{p}_i^l R_i \quad (4)$$

$i = 1, \dots, m$

The coefficients  $a_i$  are determined by solving the linear system (4). The residue form of  $R$  can be computed as an inverse convolution and from this one can determine the coefficients for equations (2) and (3). In practice these equations will only have a small number of components. Generally, it is possible to get a good fit with  $j = 1$  or  $2$  and  $l = 3 - j$ . If one takes  $j = 1$  and  $l = 2$ , it is possible that for some data sets the interpolating function will have a positive pole ( $c_i < 0$ ), even though this is impossible for an actual radiance profile. When this happens the weight  $w_i$  corresponding to the pole will be much smaller than the weight corresponding to the other rational component. Thus if one sets  $w_i = 0$ , then the resulting function will give a good approximation to the data points.

The rational interpolating function can be taken as starting approximation for an iteratively computed nonlinear least squares fit to the data of the form

$$R(\bar{p}) = x_1 \bar{p} + x_2 + \frac{x_3}{1 + x_5^2 \bar{p}} + \frac{x_4}{1 + x_6^2 \bar{p}} \quad (5)$$

Initially the  $x_i$  coefficients are determined by the coefficients of the rational interpolating function. If the interpolating function has no positive poles, then set

$$x_1 = a_1, \quad x_2 = a_2, \quad x_3 = w_1, \quad x_4 = w_2, \quad x_5 = \sqrt{c_1}, \quad x_6 = \sqrt{c_2}$$

If the first pole of the interpolating function is positive, set  $x_3 = 0$  and  $x_5 = 1$ . Similarly if the second pole is positive set  $x_4 = 0$  and  $x_6 = 1$ .

The choice of a rational function to represent the radiance data is motivated by the physics of the atmosphere. In practice the nonlinear least squares approximation gives a very good fit to the radiance data. The coefficients of the rational function can be used to determine a Planck function of the form (3).

### 3 Generalized Exponential Inversion

In the generalized exponential inversion proposed by Jean I. F. King it is assumed that

$$W(z) = W_k(z) = \gamma_k z \exp_k(z)$$

where

$$\gamma_k = \frac{1}{k^{1/k} \Gamma\left(\frac{k+1}{k}\right)}$$

and

$$\exp_k(z) = \exp(-z^k/k)$$

King has shown that if

$$R(\bar{p}) = \int_0^\infty B(p) W_k(p/\bar{p}) \frac{dp}{p}$$

and  $R(\bar{p})$  is of the form (2), then the Planck intensity  $B(p) = B_k(p)$  will be of the form

$$B_k(p) = d_1 + d_2 p + \dots + \frac{d_{j+1}}{j!} p^j + \sum_{i=1}^l w_i \exp_k(c_i p) \quad (6)$$

Note that equations (3) and (6) are the same in the case  $k = 1$ .

### 4 Test Results

The interpolation and nonlinear least squares algorithms have been tested extensively on simulated data and on the TOVS data. The algorithms are numerically stable. Figures 1 through 5 were generated from a typical data set of the TOVS data. In Figure 1 the radiance has been derived by a nonlinear least squares fit of the form given in equation (5). The radiance values are plotted as a function of the pressure in millibars. Figure 2 shows

a semilog plot of the temperature profile for the same data set. The pressures are given in millibars on the vertical axis. Figure 3 shows the temperature profile for that data set derived by generalized exponential inversion with  $k = 0.8$ . Figure 4 shows the temperature profile derived by generalized exponential inversion with  $k = 1.2$ . Figure 5 shows all three Planck plotted as functions of  $p$  on the same axis system.

## 5 Matrix Methods

Equation (1) can be regarded as a Fredholm integral equation of the first kind. By this we mean an equation of the form

$$\int_a^b f(y)K(x, y)dy = g(x) \quad (7)$$

where the functions  $g(x)$  and  $K(x, y)$  are known and the solution  $f(y)$  must be determined. The difficulty with this type of equation is that the solution does not depend continuously on the data. It is possible to have function  $H(y)$  that oscillates wildly on  $[a, b]$  such that

$$\int_a^b H(y)K(x, y)dy = \epsilon(x) \approx 0$$

Thus if  $F$  is a solution to (7), then  $F_1 = F + H$  is a solution to

$$\int_a^b f(y)K(x, y)dy = g_1(x)$$

where  $g_1(x) = g(x) + \epsilon(x)$ . The functions  $F$  and  $F_1$  will differ greatly even though  $g$  and  $g_1$  are close. In practice the known function  $g(x)$  is represented by a discrete data set which involves some experimental error. In general because the problem is ill-posed, the numerically computed solution is not likely to be close to the true solution. This is particularly true when the function  $g(x)$  is sampled at only a small number of data points.

In this section we will discuss general matrix methods involving regularization conditions which can be used for solving integral equations of the first kind. We will examine how well these methods can be applied to the transfer equation.

Equation (7) can be discretized using an appropriate quadrature formula to give an equation of the form

$$\sum_{j=1}^n w_j K(x_i, y_j) f(y_j) = g(x_i)$$

Setting

$$a_{ij} = w_j K(x_i, y_j) \quad z_j = f(y_j) \quad b_i = g(x_i) \quad i = 1, \dots, m \quad j = 1, \dots, n$$

the discretized equation can then be represented as a linear system

$$Az = b$$

If  $A$  has singular value decomposition  $U\Sigma V^T$ , then the solution is given by

$$\mathbf{z} = A^+ \mathbf{b} = V\Sigma^+ U^T \mathbf{b}$$

Because the problem is ill-posed, the computed solution  $\mathbf{z}$  may vary greatly from the true solution. A standard technique is to require that the solution  $f(y)$  satisfy a smoothness constraint in order to eliminate wildly oscillating components. The regularization condition one usually imposes is that the norm of one or more of the derivatives of  $f$  be bounded. When this constraint is discretized one ends with a constrained least squares problem of the form

Minimize

$$\|A\mathbf{z} - \mathbf{b}\|_2$$

subject to

$$\|C\mathbf{z}\|_2 \leq d \quad (C \in \mathbb{R}^{p \times n})$$

This constrained problem can be solved using the method of W. Gander [5]. First we note that if  $A^+ \mathbf{b}$  is not feasible, then the solution  $\mathbf{z}$  must satisfy the constraint  $\|C\mathbf{z}\|_2 = d$ . We are then left with the equality constrained problem which can be solved using Lagrange multipliers. This leads to the generalized normal equations

$$(A^T A + \lambda C^T C)\mathbf{z} = A^T \mathbf{b}$$

These equations can be solved using the generalized singular value decomposition,

$$U^T A X = \text{diag}(\alpha_1, \dots, \alpha_n) = D_1$$

$$V^T C X = \text{diag}(\beta_1, \dots, \beta_q) = D_2$$

where

$$q = \min(p, n) \quad U^T U = I_m \quad V^T V = I_p$$

and  $X$  is a nonsingular  $n \times n$  matrix. If we set  $\mathbf{w} = X^{-1} \mathbf{z}$  and  $\mathbf{c} = U^T \mathbf{b}$ , then

$$\|A\mathbf{z} - \mathbf{b}\|_2 = \|D_1 \mathbf{w} - \mathbf{c}\|_2$$

and the generalized normal equations reduce to

$$(D_1^T D_1 + \lambda D_2^T D_2)\mathbf{w} = D_1^T \mathbf{c}$$

We can solve for  $\mathbf{w}$  as a function of  $\lambda$ .

$$w_i(\lambda) = \frac{\alpha_i c_i}{\alpha_i^2 + \lambda \beta_i^2} \quad i = 1, \dots, n$$

The secular equation

$$\phi(\lambda) \equiv \|D_2 \mathbf{w}(\lambda)\|_2^2 = d^2$$

will have only one positive real solution  $\lambda^*$  and this is the solution which minimizes  $\|D_1 \mathbf{w}(\lambda) - \mathbf{c}\|_2$ . (See Gander [5]). The solution to the constrained least squares problem is then given by

$$\mathbf{z} = X \mathbf{w}(\lambda^*)$$

In the case that the system  $Az = b$  is underdetermined ( $m < n$ ) one may consider reversing the conditions. This leads to the second regularization problem:

Minimize

$$\|Cz\|_2$$

subject to the condition

$$\|Az - b\|_2 = \min$$

This second problem is a much easier problem to solve. If  $A$  has singular value decomposition  $U\Sigma V^T$  and

$$\Sigma = \begin{pmatrix} \Sigma_1 & O \\ O & O \end{pmatrix}$$

where  $\Sigma_1$  is nonsingular, then set

$$y = V^T z = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \quad c = U^T b = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

We can minimize  $\|Az - b\|_2$  by setting

$$y_1 = \Sigma_1^{-1} c_1$$

The vector  $y_2$  must then be chosen so as to minimize  $\|Cz\|_2$ . To do this set

$$E = CV = (E_1 \ E_2) \quad \text{and} \quad e = -E_1 y_1$$

It follows that

$$\begin{aligned} \|Cz\|_2 &= \|Ey\|_2 \\ &= \|E_2 y_2 - e\|_2 \end{aligned}$$

Thus  $\|Cz\|_2$  can be minimized by setting  $y_2 = E_2^+ e$ . The solution to the second regularization problem is then given by

$$z = Vy$$

These regularization methods can be applied to the transfer equation. Generally, because the only useful measurements are those taken at wavelengths near  $15 \mu\text{m}$ , one is usually limited to approximately 6 data points. Thus if equation (1) is discretized using 16 point Gauss-Laguerre quadrature, then the resulting coefficient matrix  $A$  will have dimensions  $6 \times 16$ . In practice, most of the singular values of  $A$  will be quite small. For a typical matrix determined by a sample of data from the NOAA TIROS Operational Vertical Sounder the computed singular values (rounded to 2 digits) were:  $0.28 \times 10^0$ ,  $0.45 \times 10^{-1}$ ,  $0.60 \times 10^{-3}$ ,  $0.22 \times 10^{-5}$ ,  $0.30 \times 10^{-8}$ ,  $0.78 \times 10^{-12}$ . Because the numerical rank of  $A$  is so low relative to the precision of the data, the matrix methods discussed earlier do not work. If the first matrix method is used then, for any reasonable constraints, the computed residuals turn out to be unacceptably large. On the other hand, if the second method is used, it is not possible to obtain a reasonable constraint at all. There just simply is not enough information for the regularization methods to work.

## 6 Conclusions

Although transfer theory can be used to relate the Planck Intensity to the upwelling intensity in the atmosphere, the relation is expressed in the form of an integral equation of the first kind. Such equations are ill-posed and consequently do not have unique numerical solutions. Adding regularization conditions does not solve the problem. For data sets like those obtained from the TOVS data, there is not enough information to determine the Planck function using matrix methods with appropriate smoothness constraints. More assumptions relative to the physics of the atmosphere must be added. In this regard the transform methods based on optical measure theory seem to work well. The key step is the representation of the radiance profile by a rational function. This can be accomplished in a numerically stable manner using nonlinear least squares fitting algorithms.

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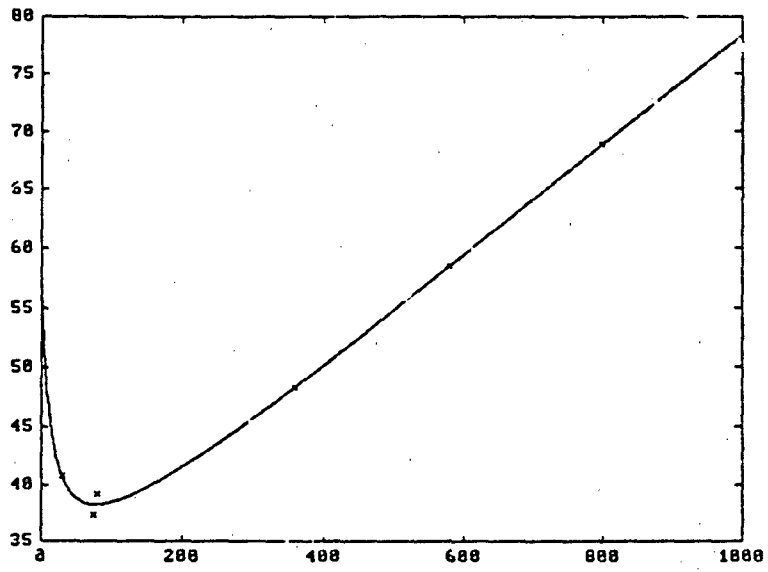


Figure 1: Radiance function of the form (5) for set of TOVS data

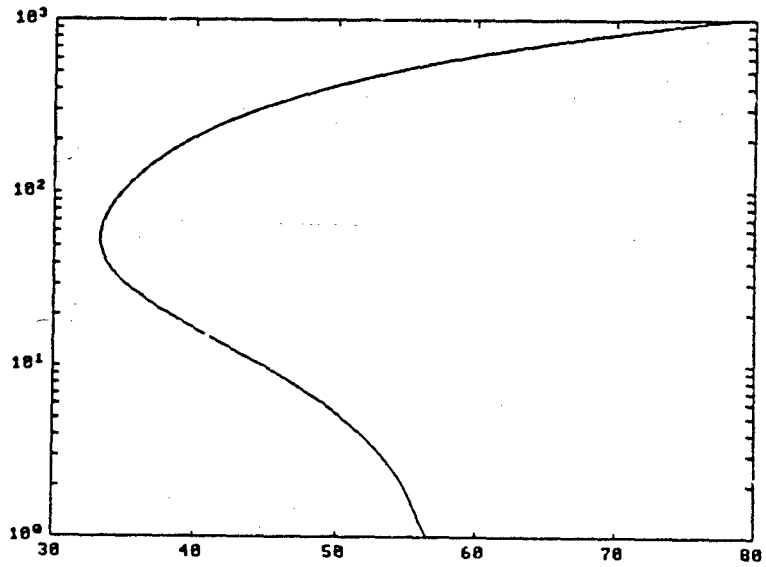


Figure 2: Temperature profile derived from set of TOVS data

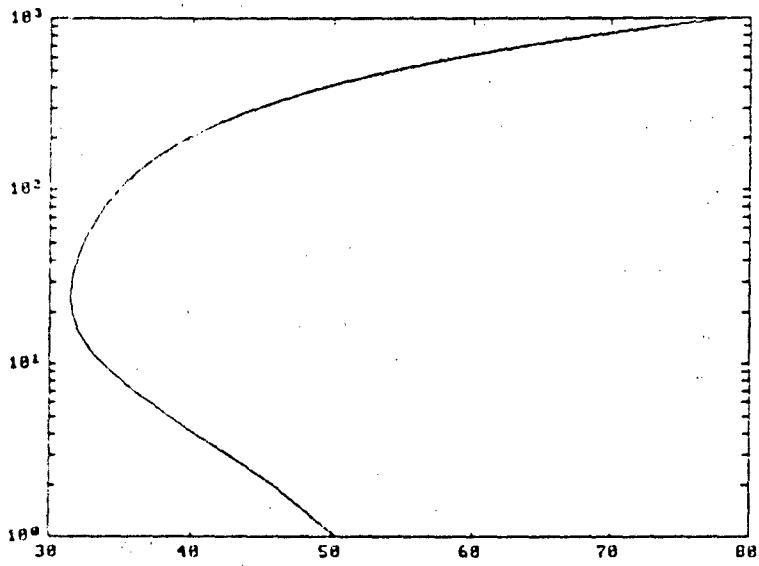


Figure 3 Generalized exponential inversion with  $k = 0.8$

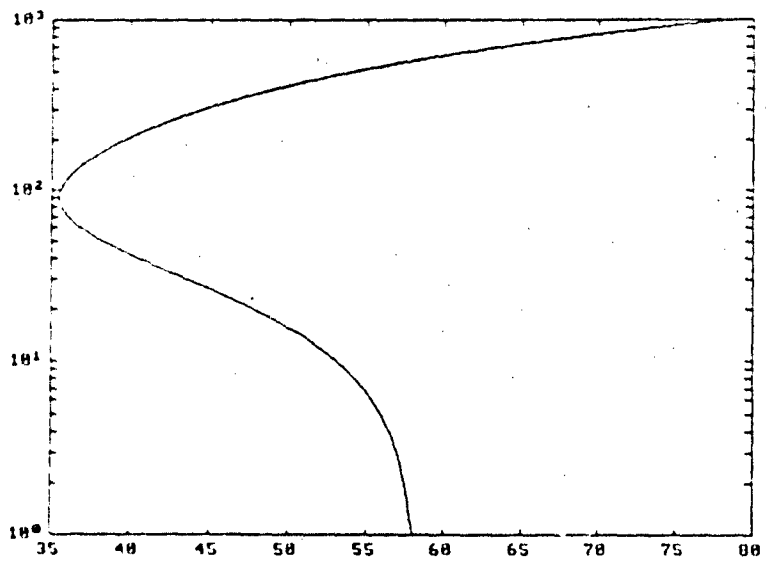


Figure 4. Generalized exponential inversion with  $k = 1.2$

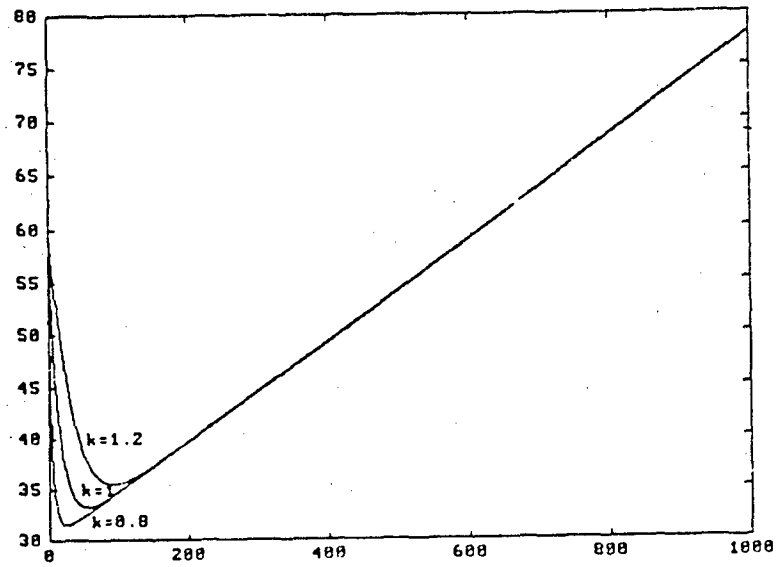


Figure 5:  $k = 0.8, 1, 1.2$  inverses plotted as functions of  $p$

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