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RETRIEVAL OF VERTICAL TEMPERATURE PROFILES IN THE ATMOSPHERE

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ABSTRACT

In this paper a new regularization technique is introduced and applied to the problem of retrieval of vertical temperature profiles in the atmosphere from remote sensing data. This is a key issue in Meteorology since it provides an important input for weather forecasting models, mainly in the Southern Hemisphere, where there are large areas uncovered by data collecting ground stations. The new regularization technique is derived from the well known Maximum Entropy method, and is based on the maximization of the entropy of the vector of *second-differences* of the unknown parameters. Simulations using real satellite data achieved a good agreement with radiosonde measurements. Numerical simulations have also shown that the temperature profiles retrieved with the new technique are relatively independent on the choice of the initial guess.

INTRODUCTION

Basic to most regularization techniques is the idea of restoring the well-posedness of the original problem by restricting the class of admissible solutions with the help of suitable *a priori* information. Prior knowledge is normally exploited under the form of a stabilizing functional that impose constraints on the variations of the model parameters, bounding them to such a degree that the final solution looks physically reasonable. Generally, this rather vague notion of reasonable means in fact smoothness.

First proposed as a general inference procedure by Jaynes (1957), on the basis of Shannon's axiomatic characterization of the amount of information (Shannon and Weaver, 1949), the maximum entropy (MaxEnt) principle emerged at the end of the 60's as a highly successful regularization technique, mainly due to the pioneering contributions of Burg (1967), Frieden (1972), Wernecke and D'Addario (1977), and Gull and Daniel (1978). Since then, the MaxEnt principle has successfully been applied to a variety of fields, from computerized tomography (Smith *et al.*, 1991) or non-destructive testing (Ramos and Giovannini, 1995), to pattern recognition (Fleisher *et al.*, 1990) or crystallography (de Boissieu *et al.*, 1991).

As with others standard regularization techniques, such as Occam's razor (Constable, 1987) or Tikhonov's regularization (Tikhonov and Arsenin, 1977), MaxEnt searches for solutions that display *global* regularity. Thus, for a suitable choice of the penalty or regularization parameter, MaxEnt regularization yields the smoothest reconstructions which are consistent with the available data. However, in spite of being very effective in preventing the solutions to be contaminated by artifacts, many times explicit penalizing roughness during the inversion procedure may not be the best approach to be followed. If, for instance, it is realistic to expect spikiness in the reconstruction of an image, or if there is prior evidence on the smoothness of the, say, second-derivatives of the true model, imposing an isotropic smoothing directly on the entire solution may lead to an unnecessary loss of resolution or to an unacceptable bias. In other words, the solution so obtained may no longer reflect the physical reality.

In this work, we describe a generalization of the standard MaxEnt regularization method which allows for a greater flexibility when introducing prior information about the expected structure of the true physical model, or of its derivatives, into

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the inversion procedure. Also, we discuss a particular implementation of this generalization, called "second-order maximum entropy (MaxEnt-2) regularization", and applied it to problem of retrieval of vertical temperature profiles in the atmosphere from remote sensing data.

ENTROPIC REGULARIZATION OF HIGHER ORDER

We assumed that the inverse problem to be solved is defined as follows (Ramos and Campos Velho, 1996; Campos Velho and Ramos, 1997):

$$\text{find } \mathbf{x} \text{ such that } \mathbf{y} = A(\mathbf{x}) \ , \tag{1}$$

where $\mathbf{x} \in R^n$ denotes the unknown parameters, $\mathbf{y} \in R^m$ the data-vector and $A : R^n \to R^m$ is an operator, linear or not, modeling the relation between $\mathbf{x}$ and $\mathbf{y}$.

A traditional approach for solving (1) is to determine $\mathbf{x}$ in the least square sense. Unfortunately, minimization of the distance between computed and experimental data alone does not provide a safe inversion technique, due to the presence of noise in $\mathbf{y}$. A better approach, is to formulate the inverse problem as:

$$\min_{\mathbf{x} \in R^n} \ \{\rho(\mathbf{y}, A(\mathbf{x})) + \gamma r(\mathbf{x})\} \tag{2}$$

where ρ is a suitable norm, usually the Euclidean square norm $\rho(\mathbf{y}, A(\mathbf{x})) = \|\mathbf{y} - A(\mathbf{x})\|^2$, r is a regularization function and γ is the regularization parameter. The function $r(\mathbf{x})$ generally expresses our prior beliefs about the unknown physical model. For instance, the zero-th order Tikhonov regularization corresponds to the case $r(\mathbf{x}) = \|\mathbf{x}\|^2$, with $\gamma > 0$. In the case of MaxEnt regularization, $r(\mathbf{x})$ takes the form of Shannon's missing information measure:

$$r(\mathbf{x}) = S(\mathbf{x}) = -\sum_{i=1}^{n} q_i \log q_i \quad \text{with} \quad q_i = \frac{x_i}{\sum_{i=1}^{n} x_i} \tag{3}$$

and $\gamma < 0$. $S(\mathbf{x})$ attain its global maximum when all q_i are the same, which corresponds to a uniform distribution with a value of $S_{max} = \log n$. On the other hand, the lowest entropy level, $S_{min} = 0$, is attained when all elements q_i but one are set to zero. MaxEnt regularization selects the simplest possible solution, containing the minimum of structure required to fit the data.

At this point, we propose a generalization of the standard MaxEnt regularization method (hereafter, called MaxEnt-0) which allows for a greater flexibility when introducing prior information about the expected structure of the true physical model – or its derivatives –, into the inversion procedure. The entropic regularization function is defined as follows:

$$S_\alpha(\mathbf{x}) = -\sum_{i=1}^{n} q_i \log q_i \quad , \quad q_i = \frac{p_i}{\sum_{i=1}^{n} p_i} \tag{4}$$

and

$$\mathbf{p} = \mathbf{D}^\alpha \mathbf{x} \ , \tag{5}$$

where $\alpha = 0, 1, 2 \ldots$ and $\mathbf{D}$ is a discrete difference operator. The associated regularization parameter is denoted by γ_α. The standard MaxEnt-0 method can be derived from (4) and (5) imposing $\alpha = 0$ and $\gamma_0 < 0$. For $\alpha > 0$, equation (5) must be modified in order to assure that the logarithm in (4) will always have a definite value. Different formulations are possible and, whether $S_\alpha(\mathbf{x})$ must be maximized or minimized (i.e., whether $\gamma_\alpha < 0$ or $\gamma_\alpha > 0$), they give rise to different regularization approaches.

SECOND-ORDER MAXIMUM ENTROPY REGULARIZATION

We discuss now a particular implementation of equations (4) and (5), denoted MaxEnt-2 method, based on the maximization of the entropy of the vector of *second-differences* of $\mathbf{x}$. If we assume that $x_{min} < x_i < x_{max}$, $i = 1, \ldots, n$, and setting $\alpha = 2$, the elements of vector $\mathbf{p}$ are given by

$$p_i = x_{i+1} - 2x_i + x_{x-1} + 2(x_{max} - x_{min}) + \varsigma \ , \tag{6}$$

with $i = 2, \ldots, n-1$ and $\gamma_2 < 0$, ς being a small positive constant (say, $\varsigma = 10^{-15}$).

Since the quantity being extremized corresponds to the second-differences $\mathbf{x}$, a MaxEnt-2 solution tends to the second-order polynomial that better fits the data, when $\gamma_2 \to -\infty$. In comparison, under similar conditions, MaxEnt-0 will yield a uniform distribution and the second-order Tikhonov regularization will produce a straight line.

To illustrate the performance of the MaxEnt-2 method, we applied it to the problem of retrieval of vertical temperature profiles in the atmosphere from remote sensing data. This is a key issue in Meteorology since it provides an important input for weather forecasting models, mainly in the Southern Hemisphere, where there are large areas uncovered by data collecting ground stations; for full details on the solution of this inverse problem see Carvalho (1998).

The mathematical formulation of the problem of retrieving vertical temperature profiles from remote sensing data is given by the integral radiative transfer equation, and leads to the solution of a highly ill-conditioned Fredholm integral equation of the first kind. Moreover, this inverse problem turns out to be highly underconstrained since, due to technological limitations, the number of observations corresponds to a fraction of the number of temperatures to be estimated. For instance, in the example presented hereafter, 40 temperature values are estimated from 7 radiance measurements. In practice, operational inversion algorithms reduce the risk of being trapped in local minima by starting the iterative search process from an initial guess solution that is sufficiently close to the true profile. However, the dependence of the final solution on a good choice of the initial guess represents a fundamental weakness of such algorithms, particularly in regions where less *a priori* information is available (Chedin *et al.*, 1985).

Simulations using both synthetic and real satellite radiance data, from the High Resolution Radiation Sounder (HIRS-2) of NOAA-14 satellite, have been performed to evaluate the accuracy and the applicability of the MaxEnt-2 method. HIRS-2 is one of the three sounding instruments of the TIROS Operational Vertical Sounder (TOVS). The MaxEnt-2 results are compared to *in situ* radiosonde measurements and to temperature profiles computed by ITPP-5, a TOVS processing package employed by weather service research centers throughout the world. An initial guess generated by ITTP-5, based on climatological considerations, and a uniform profile have been used to start the computations.

Temperature versus atmospheric pressure plots, presented in figures 1 and 2, illustrate the agreement between computed results and the radiosonde measurements. In the range of 20-1000 hPa, the average error of MaxEnt-2 and ITTP-5 results is, respectively, 3.6 K and 2.0 K, when ITTP-5 initial guess is used to start both inversion algorithms, and 3.6 K and 25.2 K, when a uniform initial profile is employed. The salient feature of these results is the relative independence of MaxEnt-2 retrievals on the choice of the initial guess. This characteristic perfectly illustrates how the use of a suitable regularization technique can compensate the lack of information on the original data set. Moreover, it may be used whenever necessary to generate a good initial guess to processing packages like ITTP-5.

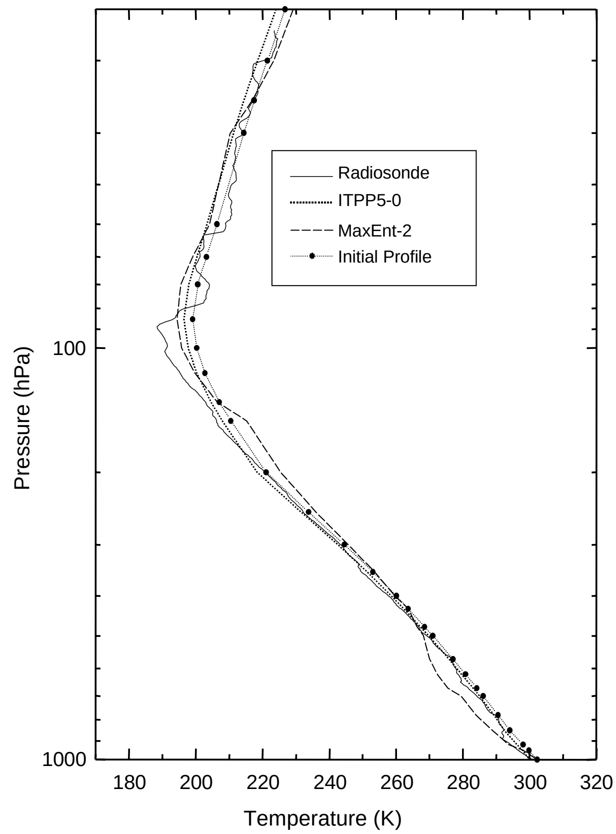

Figure 1. MaxEnt-2 and ITTP-5 atmospheric temperature retrievals achieved using radiance data from the High Resolution Radiation Sounder (HIRS-2) of NOAA-14 satellite; inversion procedure started with TOVS initial guess.

CONCLUSION

Many times, when solving an inverse problem, to impose an isotropic smoothing directly on the unknown parameters may lead to an unnecessary loss of resolution or to an unacceptable bias. To overcome these difficulties, we presented a generalization of the well-known Maximum Entropy regularization method. Also, we derived a particular implementation of this generalization, called “second-order maximum entropy (MaxEnt-2) regularization”, based on the maximization of the entropy of the vector of second-differences of the unknown parameters. For increasing values of the regularization parameter, MaxEnt-2 solutions tend to the second-order polynomial that better fits the data. Applied to the problem of retrieval of vertical temperature profiles in the atmosphere from remote sensing data, MaxEnt-2 results achieved a good agreement with radiosonde measurements. The numerical simulations also have shown that MaxEnt-2 retrievals are relatively independent on the choice of the initial guess.

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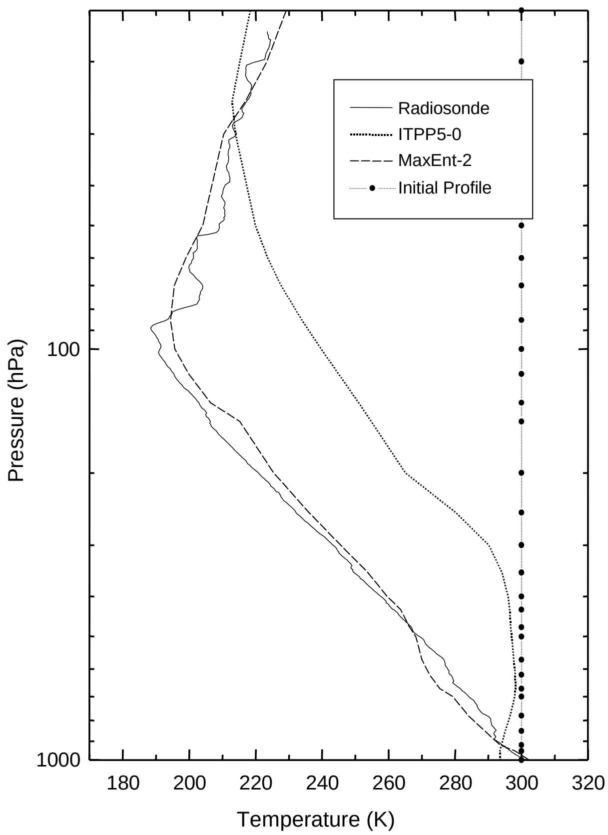

Figure 2. MaxEnt-2 and ITTP-5 atmospheric temperature retrievals achieved using radiance data from the High Resolution Radiation Sounder (HIRS-2) of NOAA-14 satellite; inversion procedure started with a uniform profile.

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