Atmospheric temperature retrieval from satellite data using the maximum non-extensive entropy principle

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The regularization theory appeared in the 60's as a general method for solving inverse problems [9]. In this approach, the non-linear least square problem is associated with a regularization term, in order to obtain a well-posed problem. A regularization technique was proposed by Tikhonov [9], where smoothness of the unknown function is searched. Similarly to Tikhonov's regularization, the maximum entropy formalism searchs for *global* regularity and yields the smoothest reconstructions which are consistent with the available data. In the middles of 90's, higher order procedures for entropic regularization have been introduced [5, 2] (see also [6] and references inside).

A non-extensive formulation for the entropy has been proposed by Tsallis [10, 11]. Recently, the non-extensive entropic form (S_q) was used as a new regularization operator [7], using only $q = 0.5$. For the $q = 1$ the Boltzmann-Gibbs-Shannon's entropy is recovered. The non-extensive entropy includes as a particular case the extensive entropy ($q = 1$): in which the maximum entropy principle can be used as a regularization method. However, another important particular case of the non-extensive entropy occurs when $q = 2$ [3].

Initial conditions for numerical weather prediction are obtained from the Earth observation system. Radiances measured by meteorological satellites is a component of this observation system. From these radiances, atmospheric temperature and humididy profiles can be determined. Several methodologies and models have been developed to compute this estimation. A method using the second order entropy approach [6] was proposed as a solution for this inverse problem. Here, the higher order non-extensive entropy will be used to improve the previous inverse solution.

Non-extensive Entropy as a New Regularization Operator

Typically, inverse problems are ill-posed – existence, uniqueness and stability of their solutions cannot be ensured. An inverse solution can be formulated to obtain existence and uniqueness, but this solution can still be unstable under the presence of noise in the experimental data. Hence, it requires some regularization technique, i.e., the incorporation in the inversion procedure of some available information about the true solution. Following the Tikhonov's approach [9], a regularized solution is obtained by choosing the function p^* that minimizes the following functional

$$J_\alpha[\tilde{\Phi}, p] = \left\| \tilde{\Phi} - \Phi(p) \right\|_2^2 + \alpha\, \Omega[p] \qquad (1)$$

where $\tilde{\Phi}$ is the experimental data, $\Phi(p)$ is the answer computed from the forward model, $\Omega[p]$ denotes the regularization operator, α is the regularization parameter, and $\|\cdot\|_2$ is the L_2 norm. The regularization parameter α is chosen using several mehods: Morozov's discrepancy principle, L-curve, and others [1]. The regularization term $\Omega[p]$ will be expressed by the non-extensive form of entropy [10]:

$$S_q(\mathbf{p}) = \frac{k}{q-1}\left[1 - \sum_{i=1}^{N_p} p_i^q\right] \quad (2)$$

where p_i is a probability, and q is a free parameter. In thermodynamics the parameter k is known as the Boltzmann's constant. Similarly as in the mathematical theory of information, $k = 1$ is considered in the regularization theory. Tsallis' entropy reduces to the the usual Boltzmann-Gibbs-Shanon formula

$$S_q(\mathbf{p}) = -k\sum_{i=1}^{N_p} p_i \ln p_i \quad (3)$$

in the limit $q \to 1$. The parameter q is called the *non-extensivity parameter.*

As for extensive form of entropy, the equiprobability condition produces the maximum for the non-extensive entropy function. This condition leads the regularization function defined by the operator $S_q(\mathbf{p})$, given by Eq. (2), to search the smoothest solution for the of the unknown vector $\mathbf{p}$. The next theorem shows that the extensive entropy and Thikhonov's regularizations are particular cases of the non-extensive entropy.

Theorem *For particular values for non-extensive entropy $q = 1$ and $q = 2$ are equivalents to the extensive entropy and Tikhonov regularizations, respectively.*

Proof: (i) $q = 1$: Taking the limit,

$$\begin{aligned} \lim_{q\to 1} S_q(\mathbf{p}) &= \lim_{q\to 1} \frac{1 - \sum_{i=1}^{N_p} p_i^q}{q-1} \\ &= -\sum_{i=1}^{N_p} p_i \log p_i \end{aligned} \quad (4)$$

(ii) $q = 2$: $\max S_2$ is equivalent to $\min(-S_2)$:

$$\begin{aligned} \max S_2(\mathbf{p}) &= \max\left(1 - \sum_{i=1}^{N_p} p_i^2\right) \\ &= \min\left(\sum_{i=1}^{N_p} p_i^2 - 1\right) \end{aligned} \quad (5)$$

now, for the maximum (minimum) value holds $\nabla_{\mathbf{p}} S_2 = 0$, therefore

$$\begin{aligned} \nabla_p S_2(\mathbf{p}) &= \nabla_p\left(\sum_{i=1}^{N_p} p_i^2 - 1\right) \\ &= \nabla_p \|\mathbf{p}\|_2^2 . \end{aligned} \quad (6)$$

In conclusion: $\max S_2(\mathbf{p}) = \min \|\mathbf{p}\|_2^2$, the zeroth-order Tikhonov regularization!

Retrieval of Atmospheric Temperature

The retrieval of temperature and humidity profiles from satellite radiance data is important for applications such as weather analyses and data assimilation in numerical weather predictions models.

Interpretation of satellite radiances in terms of meteorological fields requires the inversion of the Radiative Transfer Equation (RTE) where measurements of radiation performed in different frequencies are related to the energy from different atmospheric regions. This solution is very unstable regarding the noises in the measuring process. Also, several methodologies have been developed to improve the satellite data processing. The direct problem may be expressed by [4]

$$I_\lambda(0) = B_\lambda(T_s)\Im_\lambda(p_s) + \int_{p_s}^{0} B_\lambda[T(p)]\frac{\partial \Im_\lambda(p)}{\partial p}dp, \quad (7)$$

where I_λ is the spectral radiance, λ is the channel frequency; $\Im$ is the layer to space atmospheric transmittance function, the subscript s denotes surface; and B is the Planck function which is a function of the temperature T (or pressure p):

$$B_\lambda(T) = \frac{2hc^2/\lambda^5}{[e^{hc/k_B\lambda T} - 1]} \quad (8)$$

being h the Planck constant, c the light speed, and k_B the Boltzmann constant. For practical purposes, equation (8) is discretized using central finite differences, for N_p atmospheric layers considered.

Some previous results have employed a generalization of the standard maximum entropy principle (MaxEnt-0) for solving this inverse problem [6]: the higher order entropy approach. The same strategy can be applied here.

Therefore, the non-extensive entropy of order-γ is defined as

$$S_q^\gamma \equiv \frac{k}{q-1}\left[1-\sum_{i=1}^{N_p} r_i^q\right] \quad ; \quad r_i = \frac{p_i}{\sum_{i=1}^{N_p}} \qquad (9)$$

and

$$\mathbf{r} = \Delta^\gamma \mathbf{p} \qquad (10)$$

where $\gamma = 0,\ 1,\ 2, \ldots$, and Δ is a discrete difference operator.The standard MaxEnt-0 can be derived from (9) and (10) imposing $\gamma = 0$ and $q = 1$. A small value should be added to the difference operator (say $\varsigma = 10^{-15}$) to assure a definite quantity for all values of q.

Figures 1 and 2 present the atmospheric temperature retrieval achieved using radiance data from the High Resolution Radiation Sounder (HIRS-2) of NOAA-14 satellite. HIRS-2 is one of the three sounding instruments of the TIROS Operational Vertical Sounder (TOVS). Results with NE-MaxEnt-1 and NE-MaxEnt-2 are compared to those obtained with MaxEnt-2 (such results have already been analysed against the profile computed by ITPP-5, a TOVS processing package [6] employed by weather service research centers throughout the world), and to *in situ* radiosonde measurements.

From figures 1 and 2 is hard to identify the better performance among the retrievals. Table 1 compares the RMS of NE-MaxEnt-2 and NE-MaxEnt-1 related to the MaxEnt-2. The layer defined by 500-250 hPa there is no significant diffences among the different regularization operators. But, for the layer 250-50 hPa, the best performance was obtained by the NE-MaxEnt-1, for the 700-500 hPa better result for the MaxEnt-0, and for the region 1000-750 hPa the NE-MaxEnt-2 ($q = 0.5$) has presented the better inversion.

Some improvement was obtained using the higher order of the non-extensive entropic approach. We note that the most important layer for numerical weather prediction lies into the levels 1000-700 hPa. The results suggest that we need to combine different techniques, considering different atmospheric layers, in order to have a better inverse solution.

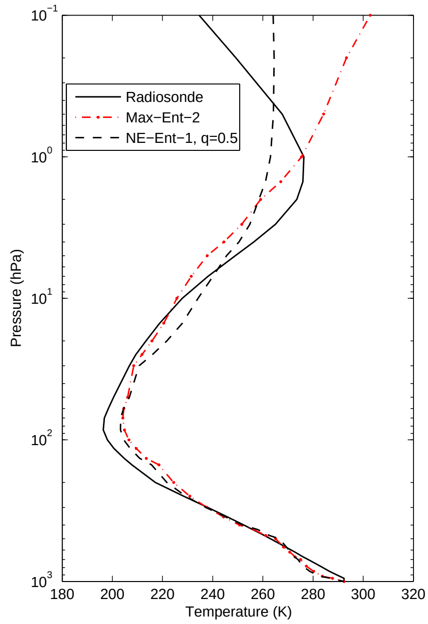

Figura 1: Reconstructions for temperature profile: $q = 1.0$.

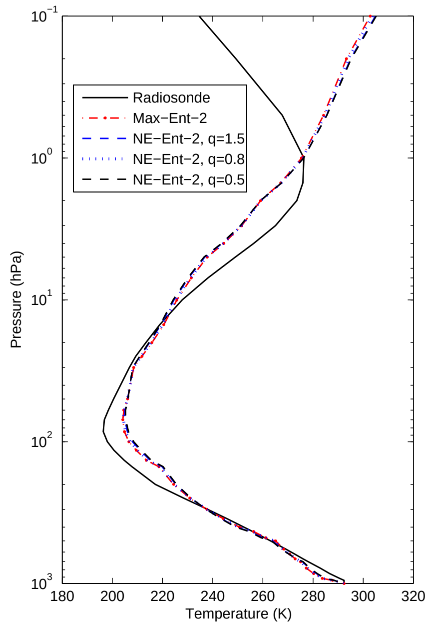

Figura 2: Reconstructions for temperature profile: $q = 2.0$.

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Tabela 1: Root-mean-square for MaxEnt-2 and Non-extensive MaxEnt of first and second orders (NE-MaxEnt-1 and NE-MaxEnt-2).

Pressure (hPa)	RMS Max-Ent-2	NE-MaxEnt-2 $q = 0.5$
50-0.1	13.248	13.646
250-50	7.442	8.723
500-250	5.216	5.508
700-500	**1.283**	1.817
1000-700	4.428	**3.475**
Pressure (hPa)	NE-MaxEnt-1 $q = 0.5$	NE-MaxEnt-0 $q = 0.5$
50-0.1	9.598	10.483
250-50	**5.818**	11.038
500-250	5.532	10.730
700-500	1.478	2.481
1000-700	5.334	17.518