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A Method to Calculate the Temperature Error Amplitude in Temperature/Emissivity Retrieval

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Abstract: Thermal infrared (TIR) data are collected by orbital sensors in order to analyze targets on the Earth's surface in a local or global scale. The radiance captured by the sensors in the TIR is dependent on two physical quantities: temperature (T) and emissivity (ε) of the surface. In this case, Planck's law, which describes the relation between these variables, leads to an equation without a single solution. Many methods have been proposed in the last decades and each technique has a set of restrictions that must be observed in order to generate reliable results. In this paper, we present the Cauchy-Schwarz Inequality Temperature Based (CSI-TB) algorithm to T and ε retrieval. This new approach allows calculating both the range and the standard deviation of the errors related to temperature estimation. Initially, the problem of separating the T and ε from radiance data will be treated as a comparison between vectors. The Cauchy-Schwarz inequality (CSI) is applied to sort the spectral similarity between vectors. The vectors are formed by radiance data from the sensor and reference data. The reference data are formed by a database (DB) of a given target with spectral signatures of radiance measured at different temperatures. Thus, the first estimate for T will be the temperature corresponding to the most similar spectrum of the DB, with proportional error to the differences between the temperatures of the DB. In the second step of the algorithm, linear regression is applied in the parameters for a 2nd degree polynomial between the results from CSI (ordinate axis) and temperatures (abscissa axis). In this case, the final estimate for T will be the abscissa of the vertex of the 2nd degree polynomial generated by the regression. The inclusion of this step allows obtaining more accurate estimates for the T when comparing the estimates of the first stage. The algorithm was tested in simulated radiance, temperature and emissivity data in which the target of interest is the quartz mineral, since it has a known spectral signature, associated with the Si-O bond in the TIR region. The simulated sensor was the TIR/ASTER subsystem onboard the EOS-Terra satellite. The results of the simulations obtained performance within the theoretical limits predicted by the method.

Key words: thermal infrared, temperature and emissivity retrieval, algorithm development

1. Introduction

With the development of the urban economy, the pursuit of high economic benefits from the limited land has become the dominant impetus affecting urban spaces in many metropolises.

Radiation measurements by orbital sensors are valuable for the study of the terrestrial environment and its natural and anthropic changes. Most studies are carried out from the recording of electromagnetic energy between the region of the visible to the shortwave infrared, where information of reflectance of targets allows its physical and chemical characterization.

Less common, but not least important, the thermal infrared region is mainly used for studies of energy balance on the Earth's surface (temperature data), as well as an alternative for a spectral characterization and composition of targets (emissivity data).

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In these situations, terrestrial remote sensing works with a radiation emitted in the atmospheric windows between 8 and 14µm, corrected to the top of the atmosphere, in which the emitted radiation of the surface is function of its temperature (T) and emissivity (ε). However, there is a limitation in the separation of these terrestrial variables, since it is an indeterminate problem characterized by a nonlinear function [1].

For n spectral bands, there are n+1 unknowns (spectral emissivity + temperature).

Several methods were developed in the last decades in the attempt of recovering with reliability the temperature and emissivity of the terrestrial surface from orbital data sensors radiance [2-15].

Here we developed a method to retrieve T and ε from radiance data providing, previously, the error amplitude of T from a target database measured at different temperatures. First, the Cauchy-Schwarz Inequality (CSI) is used, treating the problem as a comparison between radiance vectors from inner product operations. One of these vectors is formed by data collected by the sensor. The others are composed of elements of a data base obtained by controlled experiments. In the second part, linear regression is applied in the parameters for a second degree polynomial between inner products and temperatures. This is a new method of separating temperature and emissivity that allows calculating the minimum and maximum errors of the temperature estimate.

In order to test the method, pixels were simulated from laboratory-collected data of a quartz mineral (SiO_2) free of impurities and with a known spectral signature, associated with the Si-O bond in the thermal infrared region (8-14 µm) [16, 17]. These data are free of noise and do not have interference from the atmosphere. The simulated sensor was the Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER), onboard the EOS Terra satellite, which has a thermal infrared (TIR) subsystem that records data in 5 spectral bands centered at the following wavelengths (8.3, 8.6, 9.1, 10.6 and 11.2 µm) [18].

2. Recovery of the Temperature and Emissivity of the Terrestrial Surface

Recovering T and ε from radiance data from orbital sensors is a challenging task, as it is an undetermined problem characterized by a non-linear function of these two variables [1]. The spectral radiance can be defined using the Planck equation (Eq. 1).

$$B(\lambda,T)=\frac{C_1}{\lambda^5\left(e^{\frac{C_2}{\lambda T}}-1\right)} \tag{1}$$

where B(λ, T) is the spectral radiance reemitted by the blackbody ($Wm^{-2}sr^{-1}\mu m^{-1}$), T is the surface temperature in Kelvin (K), λ is the wavelength (µm), C1 is the first radiation constant (3.74151×10^{-16} Wm^2) and C2 is the second radiation constant (1.43879×10^{-2} mK).

The emissivity (ε) is defined by the ratio between the radiance of a given material R(λ, T) and the radiance of a blackbody B(λ, T) under the same wavelength λ and the same temperature (T) (Eq. 2).

$$\varepsilon(\lambda,T)=\frac{R(\lambda,t)}{B(\lambda,T)} \tag{2}$$

Since the radiance of a material cannot be greater than the radiance of a blackbody, then emissivity is a dimensionless parameter between zero and one.

In this case, to find a relation between T and ε, we use the Planck equation (Eq. (1)) and the definition of emissivity (Eq. (2)).

By combining the Eq. (1) and Eq. (2), we have the following equation:

$$R(\lambda,T)=\varepsilon(\lambda,T)\frac{C_1}{\lambda^5\left(e^{\frac{C_2}{\lambda T}}-1\right)} \tag{3}$$

The Eq. (3) is a relation between the variables: radiance, temperature and emissivity, which results in an indeterminate equation, since R(λ, T) is the radiance measured by the sensor, two variables must be determined (T and ε). Thus, the temperature of a target and its emissivity define the infrared energy emitted by the object. In the case of terrestrial targets, these two parameters can be measured in the TIR range where the dominant radiation is approximately between 3-14 μm [19].

3. Methodology

Before applying the method, a spectral library of the target of interest must be generated in a controlled environment to measure the radiance at different temperatures. Let us give preference to equal spacings between the target temperatures to compose the DB and define this spacing by Δ. In addition, the effect of the atmosphere on the radiance data recorded by the sensor must be corrected. That is, this procedure must precede the application of the algorithm.

The first part of the method compares sensor data with a spectral library using the Cauchy-Schwarz inequality[1] to identify the DB spectrum closest to the sensor data. Consequently, this spectral signature, which was measured at a certain temperature, will be the first estimate of T for the analyzed pixel.

Since the DB temperature set is finite, a second step is added which uses the first temperature estimate to generate a linear regression on the parameters for a second degree function between the inner product with temperature. The vertex of this function is used for the final temperature estimation. With the sensor radiance and the estimated temperature, the emissivity (ε) can be calculated.

If the spectral signatures that compose the DB are at equally spaced temperatures, then one can calculate error amplitudes of the estimated T variable. It should be noted that this method is only valid for pixels that represent the same target of the spectral library.

4. Cauchy-Schwarz Inequality Temperature Based (CSI-TB)

Let $X = [x_1, \dots, x_n]^T$ be the vector with radiance data recorded by the sensor with *n* bands. In this case, X is a pixel of dimension $n \times 1$. And the matrix $A = [a_{l,c}]$ represents the m spectral signatures of DB resampled to a given sensor with n bands. Each line of A refers to the spectral signature at a specific temperature, where $L_l = [a_{l1,}a_{l2,\dots,}a_{ln}]$ refers to l-th line of the array A. Thus, the matrix A has dimensions m × n. The (Algorithm 1) describes the method in more detail.

Algorithm 1 Temperature and emissivity retrieval

Input: X e A

Output: T e ε

1: The $\boldsymbol{X}$ vector will be multiplied by the $\boldsymbol{A}$ to generate

$$AX = \begin{bmatrix} \langle L_1, X \rangle \\ \vdots \\ \langle L_m, X \rangle \end{bmatrix} \tag{4}$$

Where $\langle\ ,\ \rangle$ represents the inner product operation.

2: Each line l of the vector $\boldsymbol{AX}$ will be normalized

$$Z = \begin{bmatrix} cos\left(\frac{\langle L_1, X\rangle}{\|L_1\|\|X\|}\right) \\ \vdots \\ cos\left(\frac{\langle L_m, X\rangle}{\|L_m\|\|X\|}\right) \end{bmatrix} \tag{5}$$

where $0 \le \boldsymbol{Z_l} \le 1$, since the input data are all positive.

3: Select the line l_{max} of the $\boldsymbol{Z}$ vector that has the closest value of one.

4: Check which is the temperature ($t_{l_{max}}$) related to the l_{max} line. This value will be the first estimate for T in a given pixel of the image.

5: Select the following set of points: ($t_{l_{max-1}}, Z_{l_{max-1}}$), ($t_{l_{max}}, Z_{l_{max}}$), ($t_{l_{max+1}}, Z_{l_{max+1}}$). With these three points, regression is applied to a polynomial of the second degree to find the parameters a_0, a_1 e a_2 related to the function $y = a_0 + a_1x + a_2x^2$.

6: Calculate the vertex abscissa (x_v): $x_v = -\frac{a_1}{2a_2}$.

7: If $x_v \in [t_{l_{inf}}, t_{l_{sup}}]$, where $t_{l_{inf}}$ and $t_{l_{sup}}$ are the lowest and the highest temperature of the DB respectively, then $T = x_v$. Otherwise, $T = t_{l_{max}}$.

8: return T.

9: Calculate the emissivity:

$$\varepsilon(\lambda, T) = R(\lambda, T)\frac{\lambda^5\pi\left(e^{\frac{c_2}{\lambda T}}-1\right)}{c_1} \tag{6}$$

with the estimated value of the temperature (T) and the radiance (R) provided by the sensor for a given band, the emissivity (ε) is calculated for this band centered at its respective wavelength (λ).

10: return ε.

4.1 Temperature Estimation Error

The method allows to know the amplitude of the errors of the first estimate of T referring to the Algorithm 1 — steps 1 to 4. This work will not mathematically demonstrate the limits of errors

[1] Appendix A

referring to the final estimate of T — steps 5 to 10 of the proposed method. However, the simulations indicate that the maximum and minimum errors of the final estimate are smaller when compared to the first estimate (see Table 2).

The error amplitude of the first estimate of T can be represented as a quantization error, since the true temperature, T_R, should be classified into one of the possible temperature values of the DB (T_{DB}).

The quantizer ($Q_{DB}(.)$) is a function that aims to transform the n-th entry $T_R[n]$ into a single value of a finite set of possibilities [20]. This operation is represented as follows:

$$\hat{T}_R[n] = Q_{DB}(T_R[n]) \tag{7}$$

and refers to $\hat{T}_R[n]$) as the n-th quantized sample that is equal to some temperature value (T_{DB}) of the DB.

For this analysis, we will consider a uniform quantizer that covers a temperature interval [T_{min}, T_{max}] of a random variable T with m intervals. Thus, the step size of the quantizer is described as follows:

$$\Delta = \frac{T_{max} - T_{min}}{m} \tag{8}$$

The possibility of values for $\hat{T}_R[n]$ is called quantized levels and in practice will depend on the experiment performed to construct the reference DB. In other words, what are the temperature values that compose the DB.

Generally, the quantized sample $\hat{T}_R[n]$ will be different from the sample of true values $T_R[n]$. The difference between them is the quantization error, defined by

$$e[n] = T_R[n] - \hat{T}_R[n] \tag{9}$$

Samples are rounded to the nearest quantization level, in other words, to the most similar spectrum of DB, which results in

$$-\Delta/2 \le e[n] \le \Delta/2 \tag{10}$$

The statistical representation of quantization errors is based on the following assumptions:

(1) The sequence of errors e[n] is a sample of a stationary stochastic process;

(2) The sequence of errors e[n] is not correlated with the sequence $T_R[n]$;

(3) The random variables of this stochastic process are not correlated.

It is reasonable to assume that e[n] is a random variable with mean equals to zero and uniform distribution between $-\Delta/2$ e $\Delta/2$. Therefore, the probability density function for the quantized error is $1/\Delta$, and the variance is

$$\sigma_e^2 = \int_{-\Delta/2}^{\Delta/2} e^2 \frac{1}{\Delta} de = \frac{\Delta^2}{12} \tag{11}$$

Therefore, the standard deviation is

$$\sigma_e = \frac{\Delta}{2\sqrt{3}} \tag{12}$$

5. Simulation

The article deals with an approach of how to recover the T from a target. The error in the estimation of T is given by the expression (10) and the standard deviation of the error by (12). These results are theoretical and dependent on certain hypotheses. Thus, the method allows to calculate (10) and (12) before applying the algorithm to estimate the temperature, since they depend solely on the difference between temperatures (Δ) of a database of spectral signatures of a target. In this way, it is clear that the simulations are not limited. In fact, they are not necessary, but they serve to show that the simulations are in agreement with the theoretical results.

In order to show that the simulations are in agreement with the theoretical results proposed in Section 4, we used raw data acquired in the laboratory to create synthetic data in order to construct a DB and to simulate the data recorded by a sensor. The target was the quartz mineral, because it has a well-defined spectral signature, associated with the Si-O bond in the TIR region. The simulated sensor was the TIR/ASTER subsystem onboard the EOS-Terra satellite.

The experiment was developed mainly to determine if the error amplitudes of the algorithms are within the theoretical limits developed in the Section (4). The simulated sensor data did not suffer interference from the atmosphere.

5.1 Temperature Estimation Error

To simulate the quartz radiance intercepted by the TIR/ASTER sensor, a data set was created for temperatures between 16°C and 36°C. To simulate an approximately continuous spectrum of the target of interest, a linear regression was applied generating 2001 values of radiance as a function of temperature. In this case, the difference between the temperatures is 0.01°C. The spectral signatures of the radiance were resampled to the five bands of the TIR/ASTER subsystem.

As it is written in the Section (3) the atmospheric correction must be performed before applying the method proposed in this paper.

5.2 Temperature Estimation Error

Five databases were constructed. They were simulated similarly to the ASTER data, the difference lies in the spacing between the temperature values. Here, DBs with fixed spacings of 1°C, 2°C, 4°C, 5°C and 10°C were simulated.

According to the description of the Subsection (5.1), radiances were simulated for temperatures between 16°C and 36°C. Thus, the DBs have, respectively, the following amounts of elements: 21, 11, 6, 5, and 3 spectra to compare with the sensor data.

6. Results

The analysis of the errors (real value minus the estimated value) of the estimates were performed in two parts: the first where the Cauchy-Schwarz inequality (steps 1 to 4) and the second part in which linear regression is applied (steps 5 to 10).

The Table 1 shows that the errors of the estimates of the simulations are in agreement with the theoretical results. For, the error amplitude is within the theoretical limits for each Δ spacing of the DB. There was no difference between the standard deviation of the theoretical error (σ_e) calculated by Eq. (12) and the standard deviation of the error from the application of the algorithm. In addition, the negative means indicate that the method tends to overestimate the temperature values.

Unlike the first part of the (Algorithm 1) (steps 1 to 4), a function to calculate the error amplitude for the second part of the algorithm (steps 5 to 10) has not yet been developed. But the simulation results show that the error limits are smaller when compared to the first part results. It can be seen that for Δ = 1 the amplitude of the error was 0.06 and for Δ = 10 was 4.59, that is, they correspond respectively to 6% and 45.9% of the theoretical error. The same analysis can be performed when we compare the results of the standard deviation, which also does not have an established function. For Δ = 1 the value of σ_e = 0.01 and for Δ = 10 the value of σ_e = 1.34, which represents 3.4% and 46% of the theoretical error respectively. Similarly to the first part of the algorithm, the negative means indicate that the method tends to overestimate the temperature values.

Table 1 Descriptive statistics of Algorithm errors 1 (steps 1 to 4)

	Error (°C) (Real temperature minus estimated temperature)				
Δ	Minimum	Maximum	Range	Average	σ_e
1	-0.50	0.49	0.99	-0.01	0.29
2	-1.02	0.98	2.00	-0.02	0.58
4	-2.08	1.92	4.00	-0.08	1.15
5	-2.62	2.38	5.00	-0.12	1.44
10	-5.50	4.51	10.01	-0.50	2.89

Table 2 Descriptive statistics of Algorithm errors 1 (steps 5 to 10).

	Error (°C) (Real temperature minus estimated temperature)				
Δ	Minimum	Maximum	Range	Average	σ_e
1	-0.02	0.03	0.06	-0.01	0.01
2	-0.08	0.14	0.22	-0.05	0.04
4	-0.33	0.51	0.84	-0.15	0.20
5	-0.51	0.77	1.28	-0.21	0.33
10	-1.99	2.60	4.59	-0.27	1.34

7. Discussion and Conclusion

The paper deals with an approach of how to recover the T and ε of a target, knowing previously the amplitude of the associated error from a radiance database. The estimate and standard deviation of the error are associated with the spectral contrast between the radiance curves of the specific target measured at different temperatures. In this sense, the CSI-DB proposed performed within the expected for simulated data without atmospheric interference. The accuracy/precisions of the estimates are related to the size (Δ) between the different temperatures at which the target was measured. These estimates have errors less than ±Δ/2. In average, the method tends to overestimate the temperature values. The algorithm CSI-DB does not restrict the number of sensor channels.

In this paper the quartz signature was used for different temperatures for geologic investigation purposes in mafic and ultramafic rocks. Meanwhile, new spectral libraries from various targets are being considered and will be tested in the near future.

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Appendix A. Cauchy-Schwarz Inequality

Theorem 1. If $\boldsymbol{V}$ is a vector space over $\mathbb{R}$ endowed with an inner product $\langle\ ,\ \rangle$, then for all $x,y \in \boldsymbol{V}$ we have

$$|\langle x, y\rangle| \leq \|x\|.\|y\| \quad \text{(A1)}$$

Therefore, by Theorem (1), results that

$$-1 \leq \frac{|\langle x,y\rangle|}{\|x\|.\|y\|} \leq 1 \text{ for all } x, y \in \mathrm{V} - \{0\} \quad \text{(A2)}$$

Thus, there exists a unique angle $\theta \in [0,\pi]$ satisfying

$$cos\theta = \frac{|\langle x,y\rangle|}{\|x\|.\|y\|} \quad \text{(A3)}$$

Where θ is the angle between the vectors x,y.
Since the elements of the vector are positive values, then $0 \leq cos\theta \leq 1$.

Appendix B. Regression to Second degree polynomial

According to (21) in the case where it is desired to use a second degree polynomial to fit the data (x_i, y_i) we have

$$y = a_0 + a_1 x + a_2 x^2 \quad \text{(B1)}$$

Thus, the residue is given by

$$R^2 = \sum_{i=1}^{n}[y_i - (a_0 + a_1 x_i + a_2 x_i^2)]^2 \quad \text{(B2)}$$

the partial derivatives are

$$\frac{\partial(R^2)}{\partial a_0} = -2\sum_{i=1}^{n}\left[y_i - \left(a_0 + a_1 x_i + a_2 x_i^2\right)\right] = 0 \quad \text{(B3)}$$

$$\frac{\partial(R^2)}{\partial a_1} = -2\sum_{i=1}^{n}\left[y_i - \left(a_0 + a_1 x_i + a_2 x_i^2\right)\right] x_i = 0 \quad \text{(B4)}$$

$$\frac{\partial(R^2)}{\partial a_2} = -2\sum_{i=1}^{n}\left[y_i - \left(a_0 + a_1 x_i + a_2 x_i^2\right)\right] x_i^2 = 0 \quad \text{(B5)}$$

these equations lead to

$$a_0 n + a_1 \sum_{i=1}^{n} x_i + a_2 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i \quad \text{(B6)}$$

$$a_0 \sum_{i=1}^{n} x_i + a_1 \sum_{i=1}^{n} x_i^2 + a_2 \sum_{i=1}^{n} x_i^3 = \sum_{i=1}^{n} x_i y_i \quad \text{(B7)}$$

$$a_0 \sum_{i=1}^{n} x_i^2 + a_1 \sum_{i=1}^{n} x_i^3 + a_2 \sum_{i=1}^{n} x_i^4 = \sum_{i=1}^{n} x_i^2 y_i \quad \text{(B8)}$$

or in matrix form

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix}\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{bmatrix} \quad \text{(B9)}$$

in matricial notation the Equation (B9), can be rewritten as follows

$$Xa = y \quad \text{(B10)}$$

This matrix equation can be solved numerically, or it can be inverted directly, if possible, to obtain the solution vector

$$a = (X^T X)^{-1} X^T y \quad \text{(B11)}$$