COMPARISON OF SEVERAL OPTIMIZATION METHODS TO EXTRACT CANOPY BIOPHYSICAL PARAMETERS - APPLICATION TO CAESAR DATA

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ABSTRACT

An improved version of the SAIL model which includes the hot spot effect and the spectral variation of vegetation reflectance is used to retrieve canopy biophysical parameters from visible and near infrared radiometric data. The leaf mesophyll structure, the chlorophyll a+b concentration, the leaf area index, the mean leaf inclination angle and the hot spot size parameter are determined by inversion of the coupled PROSPECT+SAIL model. Four different optimization methods (Quasi-Newton, Marquardt, Simplex, Genetic Algorithms+Quasi-Newton) are tested with several kinds of data (synthetic data and airborne data acquired with the CAESAR sensor) and compared in terms of accuracy and computation time.

KEY WORDS: canopy reflectance, models, inversion

INTRODUCTION

The interpretation of optical remote sensing data for agricultural and ecological applications is still problematic. A classical approach involves vegetation indices built from reflectance values acquired in the red and near infrared by spaceborne sensors. The development of a new generation of instruments capable of measuring the spectral radiance at several viewing angles may be accompanied by new methods of interpretation. Among these, the inversion of physically-based reflectance models appears very promising because it allows to separate the influence of surface variables on the measured radiometric signal (Flasse, 1993). Estimating properly canopy biophysical variables from reflectance measurements implies first an appropriate model and second an appropriate inversion procedure!

In an inversion perspective, the choice of the model is governed by a certain number of rules. Remote sensing, as many scientific disciplines, uses modelling which consists in creating an abstract and reduced version of reality. If we use a sufficiently high number of parameters, it is clear that we can always construct a mathematical model describing any situation. But obviously that is not the real problem: the challenge consists in constructing a model which does not rely too heavily on mathematical hypotheses. Thus there is a conflict between a strict adherence to empirical data, commonly called a fit, and the quantity of parameters used in a model: a lot of parameters may provide a good fit but also imply a complicated model. When inverting them, best models are those which make a compromise between a few parameters and a good fit (Thom, 1983). However this condition is not sufficient since the description of canopy reflectance with mathematical model leaves aside the physical principles governing the reflectance. The model parameters must correspond to quantities measurable in the field and interpretable in terms of physical and biological properties. Finally, due to the great variability of plant canopies (homogeneous, row, sparse or mixed crops), it is perhaps futile to try to build a universal model applicable to complex media (Pinty and Verstraete, 1992). Different models have been inverted to extract information on vegetation from bidirectional (Goel and Thompson, 1984; Otterman, 1990; Pinty et al., 1990; Kuusk, 1991a; Deering et al., 1992), spectral (Schmuck et al., 1993; Baret and Jacquemoud, 1994), or both bidirectional and spectral (Kuusk, 1994) reflectance measurements.

According to the method of least squares, inverting a canopy reflectance model consists in determining simultaneously the values of the parameters of the model which minimize the distance between the measured and the simulated data. For this purpose, one defines a merit function $\Delta^2=\Sigma[R_{mes}-R_{mod}(P)]^2$ where R_{mes} is the measured reflectance and $R_{mod}(P)$ the reflectance modeled with the set of parameters P influencing

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the propagation of light in the canopy. The inversion problem reduces to minimizing Δ^2. In most cases, the complexity of models prevents an analytical inversion so that numerical methods are required. There are a number of ways of achieving it. Search strategies refer to a variety of algorithms whose performances depend on many factors closely linked to the method of search but also to the model to be inverted. A typical recommendation should be to try several of them; this may result in excessive computation time and is bluntly unrealistic when thousands of inversions have to be performed, for example on pixels of a remote sensing image. According to the literature, it appears in practice that the choice of the optimization method is above all determined by the availability of an inversion routine in a mathematical library (IMSL, NAG, SAS,...) and rarely guided by criteria of convergence, reliability, accuracy or computation time. These criteria have been used in Renders et al. (1992) to compare different optimization methods to invert a canopy bidirectional reflectance model with synthetic data.

In this paper, we make an attempt to apply these methods to real conditions. We first analyze the performance of optimization methods with "noisy" synthetic data. Secondly, we use these methods with real data from the CAESAR (CCD Airborne Experimental Scanner for Applications in Remote Sensing) multispectral sensor for which radiometric data and some of the associated ground data were available.

1 - DESCRIPTION OF THE MODEL AND THE MINIMIZATION METHODS

1.1. The PROSPECT+SAIL Model

PROSPECT (Jacquemoud and Baret, 1990) is a radiative transfer model which simulates the leaf reflectance and transmittance from 400 to 2500 nm as a function of the leaf mesophyll structure parameter N, the chlorophyll a+b concentration C_{ab} (μg cm^{-2}), and the water depth C_w (cm). For given solar θ_s and viewing θ_o zenith angles, and a given relative azimuth φ_o angle, SAIL (Verhoef, 1984, 1985) calculates the canopy bidirectional reflectance using leaf optical properties, soil reflectance, and canopy architecture; the latter is represented by the leaf area index LAI, the mean leaf inclination angle θ_l, and the hot spot size-parameter S_l defined as S_l=L/H where L is the horizontal correlation length which depends on the mean size of the leaves and on the shape of the leaves, and H is the canopy height (Kuusk, 1991b). The association of the two models permits the simulation of canopy spectral reflectance for any configuration of measurement. By combining these spectra to the three CAESAR (Looyen and Dekker, 1991) gaussian filter functions centred on 550 nm ($\delta\lambda$ =30 nm), 670 nm ($\delta\lambda$=30 nm), and 870 nm ($\delta\lambda$=50 nm), we can reproduce the equivalent reflectance measured by this sensor (Figure 1). As these bands are outside the water absorption wavelengths, N, C_{ab}, LAI, θ_l, and S_l are the five independent variables of the PROSPECT+SAIL model that characterize the physical and biological properties of the plant canopy. The soil reflectance is assumed to be known: Figure 1 shows the spectral reflectance of the clayey soil we selected in this paper.

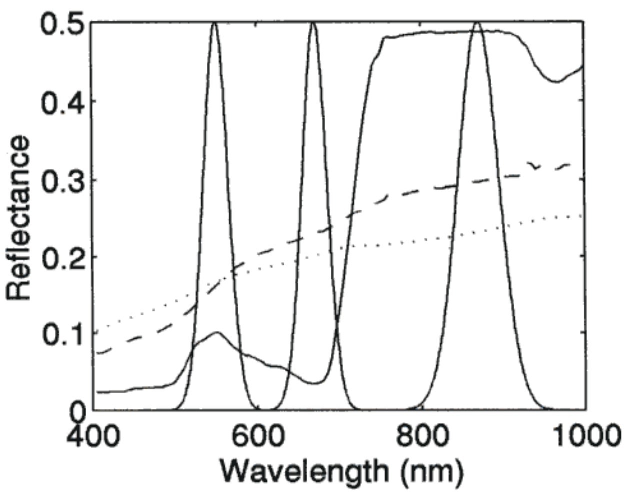


Figure 1. CAESAR spectral bands superposed on the reflectance spectra of the clayey soil used for the simulation study (---) and the bare soil selected in the Flevoland site for the application study (…). The typical reflectance spectrum of a plant canopy is also provided (—).

1.2. The Minimization Methods

There are various kinds of optimization methods, often classified following their strategies of search:

1. The search space is explored using a single point. The method exploits the local information (gradient) to find a better next point (e.g., Quasi-Newton and Marquardt methods).

2. The search space is explored using a family of points. The method exploits the relative order between the candidate points to drive the search in a better direction (e.g., Simplex method).

3. The search space is explored using a population of points. The method identifies the subdomain in which the global minimum is located (e.g., Genetic Algorithms method).

Four minimization methods have been tested in this study: Quasi-Newton (QN) and Marquardt (MQ) often used in least squares minimization, Simplex (SP), and a coupled method Genetic Algorithms + QN (GQ). Very briefly, the QN method (Gill and Murray, 1972) minimizes, at each iteration, a quadratic approximation of the merit function Δ^2. We used here the routine E04JAF of the NAG library. The MQ method (Marquardt, 1963) combines the best features of the gradient search (steepest descent) with a linearization of the fitting function (Taylor's expansion). The HAUS59 routine (Roux and Tomassone, 1973) was used. Instead of starting from a single point in the p-dimensional search space, the SP method (Nelder and Mead, 1965) considers a geometrical figure consisting of p+1 points, the simplex. Through a sequence of elementary geometric transformations (reflection, contraction, and extension), the initial simplex progresses in parameter space until it surrounds the minimum. We used the routine E04CCF of the NAG library. Finally, the GQ method (Renders et al., 1992) combines the explorative qualities of Genetics Algorithms with those of exploitation of the QN method; Genetic Algorithms (Goldberg, 1989) is a global search method based on an analogy with the process of natural selection and evolutionary genetics; in the coupled method, Genetic Algorithms create generations of points while QN drives the selection of individuals. The GQ method used in this paper is the Lamarck-inspired of Renders et al. (1992).

It is not the intention of this paper to describe in detail the mechanism of these optimization methods; the reader is referred to the above references for more information. However, several points are worthy of note: these algorithms only require function evaluations (no analytical derivative) which makes them easy to use. In order to avoid function evaluations at infeasible points, they were bounded according to the domain of applicability of the model parameters: $1<N<2.5$, $1<C_{ab}<100$ µg cm^{-2}, $0.1<LAI<10$, $5°<\theta_l<85°$, and $0<S_l<1$. When required, the initial guesses have been fixed to $N=1.75$, $C_{ab}=50.5$ µg cm^{-2}, $LAI=5.05$, $\theta_l=45°$, and $S_l=0.5$. Note that one of the difficulties which may arise when inverting the model is that there may be more than one local minimum for the merit function within a reasonable range of values for the parameters; while the first three strategies (QN, MQ, SP) are likely to provide local minima, GQ is assumed to identify the global minimum of the merit function.

2 - EXPERIMENTATION

2.1. Synthetic Data

In order to compare the different methods, a number of inversion procedures were performed using reflectances generated with the PROSPECT+SAIL model. Five surfaces representing five different vegetation canopies have been defined by varying the model parameters (Table 1).

Surface	N	C_{ab}	LAI	θ_l	S_l
A	1.28	36.6	3.46	27.7	0.77
B	2.14	5.7	2.00	54.9	0.48
C	1.65	62.2	0.54	79.9	0.24
D	1.41	25.5	5.62	10.3	0.36
E	1.07	16.6	1.10	64.3	0.16

Table 1. Canopy parameters used to simulate the synthetic reflectances.

For each surface, three types of data set were built with n=6, 9, and 27 reflectance values. These data sets respectively correspond to 2 (0°/+52°), 3 (0°/±52°), and 9 (0°/±25.8°/±45.6°/±60°/±72.5°) viewing angles distributed in the principal plane ($\varphi_o=0°$) for a constant solar zenith ($\theta_s=40°$) and the three CAESAR wavebands. The first two situations refer to the nominal looking angles of CAESAR, the third one to the nominal looking angles of the MISR (Multiangle Imaging SpectroRadiometer) instrument (Diner et al., 1991).

In the view of being close to a real context where measurements are contaminated by noise due to the instrument and to external conditions, a random noise component (gaussian distribution of zero mean and variance σ=0.01) was added to the reflectance values and this operation was repeated 50 times. In total we analysed the results of 5 surfaces × 3 data sets × 50 noise × 4 optimization procedures: that is to say 3000 inversions! The inversion of the PROSPECT+SAIL model consists in determining by iterations the set of parameters P=(N, C_{ab}, LAI, θ_l, S_l) which minimizes Δ^2 defined as:

$$\Delta^2 = \sum_{i=1}^{3}\sum_{j=1}^{n}\left[R_{\text{mes}} - R_{\text{mod}}(\lambda_i, \theta_j, P)\right]^2 \tag{1}$$

where R_{mes} is the measured and R_{mod} the modeled canopy reflectance. The summation is over the 3 CAESAR channels (λ_i) and the n viewing angles (θ_j). The criterion used to stop the inversion is to assume convergence if the relative change occuring between two successive iterations is less than some prescribed quantity. The optimization methods have been compared in terms of accuracy and computation time: the accuracy, distance from the solution to the global minimum, is assessed by the Error defined as:

$$Error = \sqrt{\sum_{k=1}^{5}(p_i - p_i^*)^2} \tag{2}$$

where p_i and p_i^* are respectively the normalized values of the real and fitted parameters. The computation time (Cntr) can be defined as the mean number of calls to the function to be minimized.

		QN		MQ		SP		GQ	
data set	surface	Error	Cntr	Error	Cntr	Error	Cntr	Error	Cntr
n=6	A	0.1899	920	0.3524	**132**	**0.1166**	327	0.6066	2354
	B	0.1770	300	0.1950	**104**	**0.1235**	363	0.1874	1319
	C	0.2464	786	0.2175	239	0.1326	**226**	**0.0810**	2433
	D	0.2571	1131	0.3476	635	**0.1767**	**275**	×	×
	E	**0.0949**	321	0.3965	**163**	0.2200	378	×	×
n=9	A	0.0804	302	**0.0467**	**82**	0.1302	327	0.2756	1239
	B	**0.0135**	244	0.2231	**65**	0.0276	381	**0.0135**	1082
	C	0.0049	233	0.0049	**61**	0.0049	237	**0.0046**	968
	D	**0.1539**	550	0.3281	**325**	0.1925	356	×	×
	E	**0.0014**	188	0.0324	**67**	0.0247	477	×	×
n=27	A	0.0215	192	**0.0214**	**62**	0.0218	378	0.0215	977
	B	**0.0022**	193	0.1458	**64**	0.0129	351	**0.0022**	979
	C	0.0015	244	0.0015	**54**	0.0015	275	**0.0012**	917
	D	**0.0281**	244	**0.0281**	**59**	0.0540	420	×	×
	E	**0.0004**	173	**0.0004**	**59**	0.0007	407	×	×

Table 2. Accuracy (Error) and computation time (Cntr) as determined for the different study cases (values are the average outputs of 50 noise-disturbed inversions). For each data set and each surface, the best performances in terms of Error and Cntr have been printed in bold.

From a general point of view, it emerges from Table 2 that, whatever the method, the more data values available the higher the accuracy. The computation time follows the opposite trend for QN, MQ, and GQ but it seems to be rather constant for SP. These two criteria are also dependent on the type of surface: for instance, inversions performed on surfaces A and D which correspond to dense and planophile canopies (high LAI and low θ_l values) are the less efficient; this is not surprising because both visible and near infrared reflectances aim at saturation in such conditions. One can also notice great Error's for QG with surface A: a detailed analysis of the fitted parameters shows that N, θ_l, and S_l are rather far from their actual values even if canopy reflectances are well reconstructed by the model. As already observed by Jacquemoud (1993) on reflectance spectra, it means that different sets of parameters can account for almost similar surfaces. Let us compare now the different optimization methods for the same data set: no real trend can be observed for the accuracy; on the other hand, there are great disparities in the computation time. MQ is on average the fastest method, at least 3 times faster than QN, twice faster than SP, while GQ takes far more computation time. These results are consistent with simulations of Renders et al. (1992) mainly performed on "clean" synthetic data.

In conclusion, the choice of an optimization method may depend on the priority given to the solution (accuracy or computation time). Concerning the accuracy, QN and GQ are the most outstanding when the number of data is much greater than the number of parameters, SP when only few measurements are available. Concerning the computation time, MQ emerges as the winner of this comparison for almost all the cases.

2.2. Airborne Data

In order to test the applicability of such optimization methods on real remote sensing data, measurements acquired in Flevoland (The Netherlands) during the 1991 Mac Europe Campaign have been investigated. Several CAESAR images were recorded on three dates during the growing season (July 4th, 23rd, and August 29th 1991) for several crops but, due to the perfect atmospheric conditions observed on July 4th, only data acquired at that time have been analysed. We selected fives differents crops (peas, sugar beet, wheat, onions, and potato) for which radiometric and ground measurements were available (Büker et al., 1992a, 1992b). To create angular variability on the reflectance, two images of the same target were obtained in down-looking mode (θ_o=0) and in forward-looking mode (θ_o=52°). In fact, this latter angle is a nominal value only valid for the near infrared band; the viewing angles in the green and red are respectively 45° and 59° but, due to the low reflectance levels in these two bands and to the non-significant variation of the reflectance induced by a 7° variation of θ_o outside the hot spot region, we used the nominal value. At flight time, the solar zenith angle θ_s was 36.1° and the relative azimuth angle φ_o (angle between solar plane and forward-looking plane) estimated at 7.4°. The calibration of CAESAR was performed by using reference targets in the field (Büker et al., 1992b). Since plots were not too distant, we assigned to them the same soil spectral reflectance (Figure 1) measured in the field during the experiment. Although soil roughness may induce great variations of reflectance from one measurement configuration to another, we assumed that soil reflectance was lambertian.

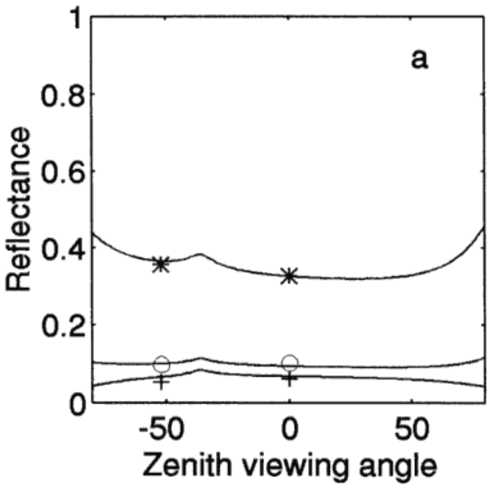
As for the theoretical study, inversions were performed on each surface using QN, MQ, SP, and QG. Let us introduce the root mean square error of the fit (RMSE) defined as $(\Delta^2/n)^{½}$ where n is the number of data points (n=6): RMSE gives an information on how well the calculated canopy reflectances (using the model and the estimated parameters values) compare with the corresponding measured values. The fitted parameters, the computation time (Cntr), and RMSE's are presented in Table 3.

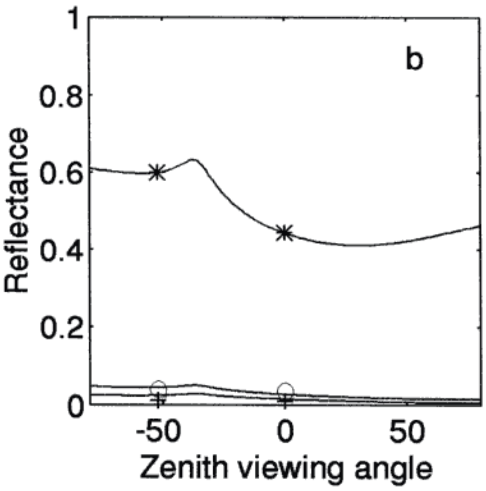
surface	method	N	C_{ab}	LAI	θ_l	S_l	Cntr	RMSE
peas LAI≈1	QN	1.00	51.7	1.03	43.5	0.05	135	0.0081
	MQ	1.41	36.4	0.80	39.3	0.05	177	0.0184
	SP	1.00	51.7	1.03	43.6	0.05	350	0.0081
	GQ	1.00	51.7	1.03	43.5	0.05	948	0.0081
sugar beet LAI≈2	QN	1.00	59.5	2.84	42.8	0.05	174	0.0116
	MQ	2.50	35.1	1.59	20.7	0.05	243	0.0253
	SP	1.02	59.1	2.81	42.5	0.05	489	0.0116
	GQ	1.00	59.5	2.84	42.9	0.05	951	0.0116
wheat LAI≈2-5	QN	2.50	79.2	4.93	61.3	0.05	446	0.0069
	MQ	2.50	74.3	6.06	62.6	0.05	116	0.0114
	SP	2.48	79.5	4.80	61.0	0.05	260	0.0070
	GQ	2.50	79.2	4.93	61.3	0.05	1041	0.0069
onions LAI?	QN	1.00	58.8	2.64	45.7	0.05	156	0.0126
	MQ	1.90	38.8	2.16	46.9	0.05	122	0.0188
	SP	1.00	58.8	2.64	45.7	0.05	441	0.0126
	GQ	1.00	58.8	2.64	45.7	0.05	938	0.0126
potato LAI>5	QN	1.77	73.5	10.0	39.6	0.07	302	0.0129
	MQ	1.86	62.8	9.94	30.9	0.05	97	0.0148
	SP	1.60	74.6	8.45	41.7	0.09	452	0.0130
	GQ	1.77	73.5	10.0	39.6	0.07	1108	0.0126

Table 3. Inversion of the PROSPECT+SAIL model on CAESAR data.

One can immediately notice that QN, SP, and GQ provide similar results in terms of retrieved parameters and the lowest RMSE's indicate the best reconstruction of the measured reflectances; MQ systematically finds other solutions and seems to be less efficient. QN and GQ have the best RMSE but QG requires much more computation time. In the absence of precise information on the measured biophysical characteristics of these canopies, it is somewhat difficult to interpret this difference we did not note when running inversions with synthetic data.

Two parameters out of five (N and S_l) keep the value of the lower or upper bounds, whatever the method. This may mean that the measured reflectances do not incorporate enough variability due to these parameters. Jacquemoud (1993) already pointed out that the leaf mesophyll structure parameter N had little influence on canopy reflectance because the effect of a varying leaf reflectance was partly compensated by the varying leaf transmittance. As for the hot spot size parameter S_l, measured reflectances are too few and far from the hot spot region to permit its good estimation. To illustrate that point, we used the parameters estimated by the QN method to calculate the directional reflectance of three surfaces (peas, wheat, and potato) as a function of the viewing zenith angle θ_o (Figure 2).





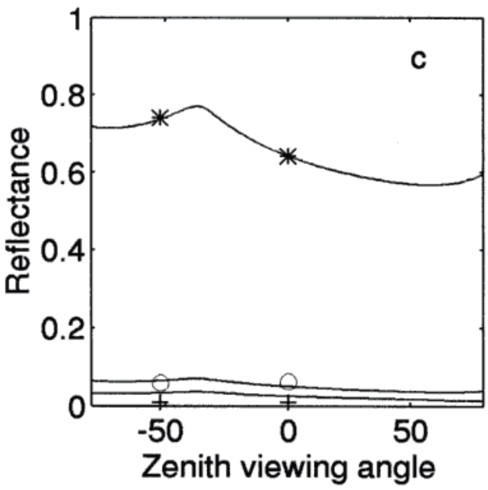


Figure 2. Comparison between the directional reflectances measured over three different patches (a → peas, b → wheat, c → potato) at the three CAESAR bands (green → circle, red → plus, near infrared → star) and those modeled with the PROSPECT+SAIL model using optimally fitted parameters. The measurement configurations are θ_s=36.1° and φ_o=7.4°.

Therefore, in future inversions in such experimental conditions it may be better to fix the value of these variables in order to avoid conflict with other variables and to save time in the inversion procedure. With regard to the other 3 parameters, retrieved values are generally consistent from one optimization method to another. Unfortunately, the ground truth was only available for the leaf area index and we had no available measured values of C_{ab} and θ_l with which to compare the inversion findings. One can see that fitted LAI's globally agree with measured values (first column of Table 3). Fitted chlorophyll a+b concentrations are those of plants in good health and seem quite reasonable for the studied crops. It is also significant to note that the leaf orientation estimated for the wheat crop indicates vertical leaves, and more horizontal leaves for the other crops which is the actual situation. Moreover, values retrieved for the sugar beet correspond to those cited in the literature for this particular crop (Baret and Jacquemoud, 1994). In the light of these results, little *a priori* guidance can be given as to the quality of the solution found by the nonlinear optimization alrorithms.

CONCLUSION

This study analysed different methods for the inversion of a canopy reflectance model, the PROSPECT+SAIL model, which simulates both the spectral and directional variation of vegetation reflectance. Comparisons were performed both on "noisy" synthetic data and airborne CAESAR data in terms of accuracy and computation time. It appeared that the experimental conditions had a great influence on the performances of the different methods and that the choice of the method depended on the priority given to the solution (accuracy or computation time). However, results obtained with synthetic data showed the pertinence of such an approach.

This first attempt to retrieve canopy biophysical characteristics by inversion of a radiative transfer model on real airborne remote sensing data was indeed very conclusive in the sense that the problem was very complex and that the reflectance measurements on which inversions have been performed did not represent an optimal sampling for this application. In this study, we allowed all five parameters to vary freely: due to the lack of measurements in the hot spot region and the low canopy reflectance sensitivity to the leaf mesophyll arrangement, it was not possible to provide a good estimate of the N and S_l parameters. It would be interesting in the future to fix these two parameters at their roughly measured values and to perform again new inversions. Be that as it may, since no guarantees can be given that a particular inversion method always work, it is necessary to check the computed solution even if the routine reports success.

Finally, this work is worthy to be continued with other field data sets and other experimental instruments. The development of airborne sensors such as ASAS (Advanced Solid-State Array) or POLDER (Polarization and Directionality of the Earth's Reflectance) which prefigure spaceborne instruments (respectively MISR and POLDER) capable of acquiring radiance measurements of the Earth surface both in several wavelengths and under several viewing angles, offers the possibilities to test these relatively new methods to extract surface properties from remote sensing data.

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