Canopy biophysical parameter retrieval by inversion of the PROSPECT-SAIL radiative transfer models using three different techniques: an iterative minimisation algorithm, a look-up table approach and a neural network

Master thesis
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Abstract

The goal of this work is to invert a radiative transfer model (RTM) combination upon hand-held spectroradiometer ground measurements of reflectances of the jute variety corchorus capsularis, a fiber crop which is of great socio-economic importance in the state of West Bengal, Eastern India.

A RT model simulates spectral reflectance of vegetation as a function of different biophysical and biochemical parameters. If the model simulates properly the plant or canopy under investigation, and if the model is invertible, then the parameters which describe biochemistry and plant structure can be retrieved by inversion of the function (model).

In a field sampling and measurement expedition in Kalyani, 40 km north of Kolkata, 4 different growth stages of corchorus capsularis were measured at canopy level, plus one stage (8 weeks) at leaf level. Different biochemical parameters (leaf chlorophyll a & b content, leaf water and dry matter content) were measured in BCKV Agricultural University in Mohanpur.

The simulation at leaf level is done with the PROSPECT model, a widely used leaf model; the canopy is simulated with SAIL. At both levels, there are problems with the simulation, i.e. the simulated reflectances based upon the field measured parameters show significant differences to the measured reflectances.

Three inversion methods are used, first with synthetic reflectances to test the invertibility of the model combination, then with the field measured reflectances. These are: an iterative minimisation algorithm (a Nelder-Mead Simplex), a look-up table approach (LUT) and a neural network with different training algorithms and network structures.

At the synthetic level, the minimisation algorithm performs best, while with the measured data it is unprecise and time and computer intensive, thus not operational over a satellite pixel image. Both other methods yield parameter values with errors under 20%; both are operational because the computer intensive part is done previously. A combination of both methods as a means of cross check can further reduce the uncertainty.

This study has not the pretention to have exhaustively investigated the three methods. At every stage of this work, from the field and laboratory work to the model inversion, there are matters that may be investigated deeper and more precisely. Following every path would have gone beyond the scope of this master thesis, which was to go through the different steps of a forward simulation and inversion.
Aknowledgements

This small section is meant to thank the different persons for the help and/or possibilities I have benefited from throughout the development of the work, from the first contacts between IBF and the University until the final office work to finish with these lines. I would like to proceed chronologically to put clarity into the accruement, and to avoid the task of deciding who helped most. Different people have helped in various manners at distinct moments in different situations. But certainly I would not have been part of the project if Michael Schaepman had not donated some of his time, experience, talent of organisation and understanding to haul me back in. Thank you, Michael. I would like to thank Mr. Till Grether for coming up with this project, thereby creating the opportunity for me to take part in an interesting project. We could take a glimpse of what it is like at the frontier between academia and private business; I value that as rich experience. Special thanks to Mathias Kneubühler who accompanied and chaperoned us scientifically, and who was a good field leader, always thoughtful of maintaining a positive disposition in a sometimes stressful situation; he was an agreeable partner to work with. My respect and gratitude to Prof. Dr. Klaus I. Itten, head of the Remote Sensing Laboratories, for making the collaboration possible. Thank you and good luck to Margarita Osses and Christian Gemperli, who were part of the field team, who took their share of work and °celsius, for gathering the material of our respective works. Back in Switzerland, I would like to thank Ben Kötz for his help, guidance and tips about what to pay attention to, and trouble-shooting while wrestling with the different Matlab codes. I know I owe many more people and not citing them is not at all a shame to give offense, but rather just the will not to extend the list to largely. In no way are they forgotten, by the exercise of writing this they were recalled to mind.

Gil Meienberger
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1. Introduction

■ The West Bengal Jute Project

At the origin of this work is the West Bengal Jute Project (WBJP) that is led by IBF AG and EMPA. IBF AG (Innovative Bio Fibre Corporation) is a firm that specializes on comprehensive supply management of sustainably developed plant fiber raw material for future oriented industrial partners. EMPA is the Swiss federal laboratories for materials testing and research.

The background of the project is the fact that the supply of raw fibres like kenaf or jute is hardly predictable. This represents a major drawback for the industrial application of renewable fibre products. This is more and more an issue as disposal of used goods gets problematic and economic growth without ecological sustainability as hidden agenda a mortgage for the future.

Fibre plants are cultivated in third-world countries by small farmers in rotation of crops; therefore the plots are continuously changing. Agricultural maps are not precise or widely lacking, while gathering local information on crop distribution is equally difficult. These constraints can be resolved by applying remote sensing techniques for the survey of fibre crop cultivation. Agricultural applications of remote sensing include crop type classification, crop condition assessment and crop yield estimation, for example. The goal of this project is to foster sustainable management of fiber crops in the state of West Bengal, eastern India. In order to manage crops for estimation or whatever purposes, one needs parameters that characterise them. These can be inferred with techniques from remote sensing data.

■ Canopy parameters and current status of canopy parameter retrieval

Remote sensing data are used to infer canopy biophysical variables like LAI (leaf area index), or Cab (chlorophyll a & b) among others, which are involved in the important physical and/or physiological processes governing crop growth (Combal, 2002).

LAI is the main vegetation structure variable and one of the main drivers of canopy primary production (Weiss, 1999). It is thus of prime interest for crop yield models and soil-vegetation-atmosphere-transfer (SVAT) models. It is functionally linked with the evolution of canopy spectral reflectance over the growth season (Broge, 2001). Cab is also involved in the production process; it is an important variable in photosynthesis, and it is closely linked to nitrogen status (Baret, 1997). What is more, both can be used for yield estimation (Baret, 2000), and maybe even for quality assessment of the plant’s raw fiber.

Plant water content is related to plant biomass and LAI (Champagne, 2003); it increases as LAI if the quantity of leaves increases. It is therefore an indicator of canopy structure (Champagne, 2003), which could give informations on changes in the biomass. If it is suitable for biomass characterization, it could also be linked to a pest risk management or stress (Baret, 2000). It seems important to be able to link leaf water (Cw) content with the plant water content. Cw has a large effect on the spectra in the shortwave infrared (SWIR) wavelengths (1250-2500nm) (Kneubuehler, 2002).

The leaf orientation, and thus the average leaf angle (ala), is critical as well, because it defines the area projected by the foliage element onto the horizontal plane; it therefore determines its absorption ability (Atzberger, 1998). Finally, the dry matter content Cm is important as it is an input parameter in numerous crop models.

As to point two, according to (SPREAD, 2002), LAI, Cab, Cm and Cw play the leading roles in impacting on the canopy. They should therefore be all retrievable.
If inferred accurately, these variables may then be fed to canopy primary production models (crop yield prediction models for example).

To do this, it is necessary to relate vegetation properties to reflectance measurements. In general, two different approaches may be considered (Jacquemoud, 1993):

- The semi-empirical approach, which consists in using statistical techniques to obtain a correlation between the target and its spectral signature. An example of these methods are the vegetation indices (VI), which combinations of spectral measurements in different wavelengths as recorded by a sensor. They have been related to canopy variables of interest like LAI for example (Weiss, 1999). (Baret, 1991) gives a list of commonly used VIs in remote sensing. They are often calibrated with experimental observations, and therefore not easily transferable to other sites at other moments. Thus, the major drawback of the VI is that they can be sampling and site-specific (Privette, 1996), and lack the physical basis that would make them widely applicable. Their advantages are that this technique is simple and easy to compute (Qi, 2000).

- The physical model approach, which consists, in a first step, in describing the interactions between the sunlight and the canopy through an analytical model. The functional dependance between the spectral signature of the target and the target parameters has to be established, if possible with physical laws; this is called the direct problem, or forward modelling. In the relation (1)

\[ R = M(V, C) + \varepsilon \]  

\[ R \] is the simulated reflectance, \( M \) the model with inputs \( V \) as canopy biophysical variables and \( C \) as the corresponding measurement configuration (the sun illumination direction, the observation angles). The uncertainty \( \varepsilon \) accounts for both measurement and model uncertainties. It represents the adequacy between the simulated and measured canopy reflectance. The measurement uncertainties result from the noise associated with the sensor and the data processing, the model uncertainties are related to the assumptions on canopy architecture, which may not be consistent with that of the actual canopy (Combal, 2003).

Physically-based models range in complexity from simple nonlinear models to complex numerical radiative transfer models for realistic three-dimensional vegetation canopies (Kimes, 2000). In (Goel, 2000) there is a review of canopy reflectance models published in the literature with their strengths and shortcomings: geometrical models, turbid medium models, hybrid models, computer simulation models and some other types. These models, also known as radiative transfer models, have been used since the 1960s to model scattering from canopies at optical wavelengths (Ross, 1981). They attempt to relate radiation leaving a vegetation canopy in a given direction to the characteristics of the incident radiation and those of the canopy (Goel, 2000). While modelling canopy scattering, one wishes to state the scattered quantity as an intrinsic property of the canopy, rather than stating a scattered intensity as a function of incident intensity. This allows for the comparison, for instance, of measurements made under differing illumination...
intensities. The fundamental intrinsic scattering quantity at optical wavelengths is known as the Bidirectional Reflectance Distribution Function (BRDF) (Tomiyasu, 1988). BRDF models usually consist of a set of equations that relate surface physical properties to the observed signals as a function of wavelength (Qi, 2000).

The model used in this study belongs to the group of turbid medium models, and is best suited for dense canopies with small vegetation elements (Goel, 2000). Once a certain model has been calibrated (like the leaf model PROSPECT) and validated on experimental data sets, i.e. has proven its ability to successfully model certain kinds of canopies, the inversion procedure, i.e. the estimation of the biophysical variables from reflectance measurements, is possible by the inversion of the functional relationship mentioned in equation (1); the procedure consists in finding an estimate of the variables $V$ from the measured radiation $R$. This is the analytical, conceptual inversion of a radiative transfer model (Combal, 2002); however, not every model is invertible analytically because of its complexity so many different inversion methods were developed and are presently available. (Kimes, 2000) identifies three major categories of inversion algorithms:

a) Traditional inversion methods (Bacour, 2001): they include four main components: (i) measured reflectance data, (ii) a vegetation reflectance model that simulates vegetation reflectance, (iii) an iterative standard optimization algorithm, and (iv) a figure-of-merit function that must be minimised. This technique consists of updating the values of the unknown input canopy RT model variables until the reflectance simulations closely match the corresponding measurements (Baret, 2000). The merit function provides a numerical "resemblance" between measured and simulated reflectance values. When dealing with large sets of satellite imagery, traditional inversion methods cannot be used operationally on a per pixel basis because they are iterative and therefore time and computer-demanding. Most used optimization algorithms are the downhill simplex method, the conjugate direction set method and the quasi Newton method (Gastellu-Etchegorry, 2003). Another problem is the difficulty of getting optimal solutions (multiple solutions at local minima) (Fang, 2003).

b) Look-up table (LUT) approaches (Estève, 1998, Knyazikhin, 1998): they consist in the search of a pre-computed look-up table of reflectance spectra in order to find out the reflectance that most resembles the measured reflectance; input to these spectra are either synthetically generated parameter values or field values. The LUT may be constituted of synthetic or measured spectra; it should be mentioned that a LUT made of purely measured reflectances would require huge field measurement efforts. Once the most resembling spectra of the LUT are determined, it is easy to find the constituting parameters since these spectra have precisely been built with known variable values. The parameter retrieval can be fast because the most computationally expensive part of the inversion procedure is completed before the inversion itself. Thus, LUTs are well suited to computationally expensive complex reflectance models. In order to obtain accurate inversion products, reflectance values of the look-up table must be simulated for a wide range of the model-input parameters that most affect the reflectance.

c) Neural network methods (Abuelgasim, 1998, Kimes, 2000): neural networks enable to relate a given set of input variables to a set of output variables, irrespective to any known functional relationship between input and output, provided an implicit relationship exists between these sets. This approach is fundamentally different from LUT and the minimisation algorithm that require the model M to compute some cost function $C_f$ (Combal, 2003). With the help of a learning set of reflectance measurements/simulations, they are able to determine the optimal underlying relationship that maps input parameters (i.e., canopy optical and structural parameters) of the reflectance model.
to outputs (i.e., simulated/measured reflectances). Multi-layer feed-forward neural networks can approximate any continuous input-output relation of interest to any degree of accuracy, provided sufficiently many hidden units are used (Cybenko, 1989, Hornik, 1989). Nevertheless, the neural networks have not been generalized to handle any arbitrary subset of directional data (Kimes, 2000).

- **Goal of this work**

The main objective of this work is to evaluate the possibility of inferring canopy biophysical variables by inversion of a radiative transfer model using canopy reflectance spectra acquired in the field with a high spectral resolution radiometer. This work contains a theoretical as well as an experimental part and shall be an evaluation of how RTM inversion could be used in an operational way.

Three of the most widely applied methods of inversion are tested, namely an iterative minimization algorithm, a look-up table approach and a neural network. Two conditions are to be fulfilled. First, the combination of the two models used has to simulate accurately the jute variety JRO 524 (*corchorus capsularis*) under investigation. Second, the selected model must be invertible. This means that the inversion process, were the model fully invertible, should produce an unique solution. But as some models are complex and the retrieval algorithms not perfectly adapted to the task (the algorithms are more mathematical than physical), partly invertible models are also useful, just that the results shall be considered with the necessary caution.

If the two conditions are fulfilled, then one could tackle the next problems if one were to invert satellite image data for retrieval of biophysical parameters: the atmosphere and the different satellite sensor configurations. But this extends the scope of this thesis, and will most probably be subject of following works.

Concerning the first condition, a comparison and a descriptive analysis are made between the field and forward simulated reflectances (see Fig.1), and the results are presented and discussed in chapter 4.

![Fig.1: Forward modelling (Kimes, 2000)](image)

Concerning the second condition, a synthetic data set with reflectances and the corresponding parameters is created with the coupled PROSPECT-SAIL model. Since we have the reflectances and the corresponding parameters, if an inversion method can not retrieve the parameters from the reflectance, then the model is not fully invertible and the inversion method must be adapted until it supplies reasonable results. The three inversion methods are applied, and the results discussed.

The work is structured as follows: in chapter 2, the measured data is presented; there is a description of how it was collected and what it is. Chapter 3 handles the methods of the two directions of modelling: forward and backward. In the first part, the models, the parameters and their measurement or calculation necessary for the reflectance simulation
are presented. The analysis of the measured spectra is also in this part. In the second part, the inversion methods are presented. Chapter 4 lays out the results and the path that led to them. A summary and a discussion of all findings of chapter 4 is made in the following chapter. Chapter 6 presents the concluding remarks; chapter 7 lists the tables, program codes and chapter 8 the cited references.

2. Description of the data

2.1. Data from the fieldwork

The field campaign was conducted in fields curtly outside the town of Kalyani, approximately 50 km north of Central Kolkata, capital of the state of West Bengal, in the lowlands of the Ganga basin (Fig.2). This region of West Bengal is situated along the deep moist Eastern end of the monsoon trough. For a climatic overview of the region, see Fig.3. From 23th May to 6th June 2003, different kind of data was gathered. Jute cultivation plots were characterized by spectral, physical and chemical parameters. Some determinations were conducted in the fields and others in the laboratories of BCKV (Bhidan Chandra Krishi Viswavidyalaya) Agricultural University in Mohanpur, West Bengal.
Fig. 2: Schematic map of Kolkata and surroundings, with its location within the MODIS image (image courtesy: NASA Visible Earth on [http://www.gesource.ac.uk](http://www.gesource.ac.uk)) of the Ganges and Brahmaputra rivers through Eastern India and Bangladesh. The red circle symbolises the town of Kalyani, the site of the field work (map not to scale, edited from map on [http://www.mapsofindia.com](http://www.mapsofindia.com)).

Fig. 3: Climate diagram of Kolkata at Kolkata NSCB International Airport: average monthly temperature (plus minimum and maximum in dotted lines), air average humidity, and monthly rainfall (source: [www.worldclimate.com](http://www.worldclimate.com))
Brief description of jute

Corchorus capsularis, alias white jute, is a strong, coarse fiber used for making burlap, gunny, cordage, etc. This annual plant is sown before or in the early rainy season (February-April) by direct seeding, depending on the species; the harvest is 3-5 months after sowing. The whole stem is harvested for retting. After harvesting, plants are bundled together with required number of plants, and kept standing for 5-7 days in the field for shading off the leaves. Then the bundles are put under water. Clear slow flowing water is the best thing possible for good retting. After 12-15 days, when proper retting is completed, the fibre is separated from the stick by hand and then washed and dried in sunlight. After drying, farmers sell the fibre in the local market. Jute grows well where the annual rainfall is 1500 mm or more, with at least 250 mm during each of the months of March, April and May. The optimum range of temperature required is 18˚-33˚C. Cultivation largely depends upon pre-monsoon showers and moisture conditions. C. capsularis is more water tolerant than other species and thus generally can be grown in low lands, and even under water logging conditions.

Jute is basically self-pollinated and has fourteen diploid chromosomes. It needs long day light for growth. The fibre is obtained from the bast or phloem layer of the stem. Jute cultivation is labour intensive and is mostly grown by marginal, poor, and small landowners. For successful cultivation, land preparation is very important. It needs 3-5 times cross ploughing and laddering for uniform smooth soil, which must have more than 20% organic content. Cow dung is generally used, along with NPK in appropriate proportion, according to the soil type. The preferred soil of this crop is river silt alluvium, with a pH of 5.4 - 6.4.

With a spacing of 25 cm x 7 cm, there are 570 000 plants/ha. During cultivation weeding is usually done in addition to thinning (Ratikanta, 1997).
Spectroradiometric characterization of jute

For the radiometric characterization of the jute leaves and canopy, a field spectroradiometer (FieldSpec Pro FR, Analytical Spectral Devices Inc.), consecutively called ASD, was used; the device takes reflectance measurements in the range 350-2500nm (interval 1nm). The field of view (FOV) used was 25°. Measurements were taken from the nadir, at a height of 0.5 to 1m above the canopy. For the leaves’ reflectances, special attention was given to avoid that the recorded area was not outside the leaf area. The measurings were taken a few centimeters above the leaf.

A white Spectralon panel was used for calibration of the sensor. Spectralon reflectance standards and materials are highly lambertian over their effective spectral range, and therefore can put into relation a reflectance that is almost complete to a reflectance of a material that does absorb as well.

If atmospheric conditions were stable (i.e. incident radiation on plants is more or less constant), one white reference measurement was made at the beginning of each transect, otherwise more.

Measurements were taken in 10 fields, all of which were rectangular. The plot sizes varied from approximately 20*15m to 10*7.5m. Two diagonal transects were taken per jute field, on each transect one spectroradiometric measurement every 2m, otherwise only one transect. For each point measured on the transect, five spectra were measured, taking care to rotate the fibre optic during recording, in order to integrate vegetation, soil, shadow effects, etc.

Of these 10 measured fields, 6 had the jute variety JRO 524 at 4 different growing stages: 4, 5, 6 (twice) and 8 (twice) weeks old crops (see Fig.6 & 7). The 4 other fields were bare soil with different partial covering or structure. F4 had been plowed two days ago, the three others had born rice; these last three fields were partly covered with weeds and parts of the cut rice stems (Tab.1). The soil under the different canopies was smooth, and almost weed-free. Under the dense canopies, the soil contained a slight humidity in comparison with the very dry soils of the more open canopies. For every field, there are at least one hundred reflectance spectra (Tab.1). The variability within the fields is demonstrated in Fig.8. This is the field with the largest variability; all other fields are more homogeneous.
Fig. 6: Two phenological stages of jute: in the front, a four weeks old canopy (field 2), in the back, a six weeks old canopy (field 1). Canopy heights are 20-30cm respectively 75-100cm.
Fig. 7: Canopy detail of field 1 (six weeks old).

The sensor has been perturbed by atmospheric water absorption in the regions that range between 1348 and 1426nm, and between 1795 and 1955nm, leading to large fluctuations in the readings, producing very unstable spectra. Thus the two regions mentioned have been removed. So for every spectrum, there are 1765 reflectance values (bands).

Every measurement of five spectra is accompanied by a GPS reading (instrument Garmin GPS 12 XL), and a rough description of the recorded area regarding vegetation density, soil fraction, dryness of soil, wind moving the plants in the canopy, sky conditions and time of measurement.
Fig. 8: Measured reflectances of field 1. There are 190 spectra in total; spectra displayed in beige indicate a rather high proportion of soil; the variance of the spectra is an indication of a relatively inhomogeneous canopy. The two vertically dotted lines indicate that wavelengths were excluded for sensor instability due to atmospheric water vapor.

<table>
<thead>
<tr>
<th>field, transect</th>
<th>remarks</th>
<th>field age (weeks)</th>
<th>number of spectra</th>
</tr>
</thead>
<tbody>
<tr>
<td>f1, 1</td>
<td>interrupted</td>
<td>6</td>
<td>50</td>
</tr>
<tr>
<td>f1, 1</td>
<td>second time</td>
<td>6</td>
<td>75</td>
</tr>
<tr>
<td>f1, 1</td>
<td>same way back as previous</td>
<td>6</td>
<td>65</td>
</tr>
<tr>
<td>f1, 2</td>
<td>second transect</td>
<td>6</td>
<td>165</td>
</tr>
<tr>
<td>f2, 1</td>
<td></td>
<td>4</td>
<td>65</td>
</tr>
<tr>
<td>f2, 2</td>
<td></td>
<td>4</td>
<td>65</td>
</tr>
<tr>
<td>f3, 1</td>
<td></td>
<td>6</td>
<td>70</td>
</tr>
<tr>
<td>f3, 2</td>
<td></td>
<td>6</td>
<td>65</td>
</tr>
<tr>
<td>f4, 1</td>
<td>freshly plowed field</td>
<td></td>
<td>50</td>
</tr>
<tr>
<td>f4, 2</td>
<td></td>
<td></td>
<td>40</td>
</tr>
<tr>
<td>f5, 1</td>
<td>leaves</td>
<td>8</td>
<td>145</td>
</tr>
<tr>
<td>f5, 2</td>
<td>canopy</td>
<td>8</td>
<td>158</td>
</tr>
<tr>
<td>f6, 1</td>
<td></td>
<td>5</td>
<td>56</td>
</tr>
<tr>
<td>f6, 2</td>
<td></td>
<td>5</td>
<td>55</td>
</tr>
<tr>
<td>f7, 1</td>
<td></td>
<td>8</td>
<td>55</td>
</tr>
<tr>
<td>f7, 2</td>
<td></td>
<td>8</td>
<td>45</td>
</tr>
<tr>
<td>f14, 1</td>
<td>harvested rice field, little weed</td>
<td></td>
<td>80</td>
</tr>
<tr>
<td>f15, 1</td>
<td>harvested rice field, rests of rice stems</td>
<td></td>
<td>92</td>
</tr>
<tr>
<td>f16, 1</td>
<td>harvested rice field, rests of rice stems</td>
<td></td>
<td>40</td>
</tr>
</tbody>
</table>

Tab. 1: Overview of the fields resp. their transects, with the field age and the number of spectra.
Canopy structure characterisation (hemispherical photography)

In the 6 fields with jute, hemispherical photographs were taken. Hemispherical photography is an optical, indirect, non-contact method for LAI measurement. These methods are more commonly implemented than direct methods, for the latter are extremely time-consuming and as a consequence making large-scale implementation only marginally feasible. These indirect methods are based on the measurement of light transmission through canopies (Jonckheere, 2004). Hemispherical photography is markedly cheaper than alternatives, rapid, and has already proven to be a powerful method for measuring various components of canopy structure and under story light regime. Analysis of hemispherical photographs has been successfully used in a diverse range of studies to characterise plant canopy structure (Jonckheere, 2004).

The digital camera (Nikon Coolpix 4500) with a fish eye lens was put on the ground, looking upwards. For each field, there are between 10 and 12 photos along a transect, and one transect for the field (examples Fig.9 & 10).

Fig.9: Hemispherical photography of field 2, the field with the lowest density.
Fig. 10: Hemispherical photography of field 5, the field with one of the highest densities.

- Biochemistry of the canopy

For each field, 10 samples of vegetation were taken. Each sample consisted of the first 5 fully grown leaves of the plant beginning from the top. They were put into plastic bags, placed in a cooling box with ice and driven to the lab for fresh and dry weight determination. For the fresh weight, the balance had an accuracy of 0.01g, for the dry weight 0.001g. The 5 leaves of each sample were additionally photocopied on millimeter paper for leaf area determination back home.

For the leaf chlorophyll content, 10 samples were taken for each field, each of which contained 5 leaves. The leaves were then brought to the lab in cooling boxes for chlorophyll extraction with spectrophotometry (Arnon’s method, (Arnon, 1949)). The operator who performed the spectrophotometry determination had never done the procedure before, and has warned about possible inaccuracy in the readings.

2.2. Transformation of the data

The ASD stores the reflectances in binary format. The binary format is converted to ASCII format, using the Portspec application in the DOS mode. This is done to import the spectra into ENVI, a remote sensing software, which allows for hyperspectral image analysis. Describing statistical analysis of the data is done calculating mean value and standard deviation of the spectra for each plot. Some spectra of some fields have been taken with a great fraction of soil; nevertheless, no spectrum has been deleted to avoid biases.
3. Methodology of parameter retrieval

3.1. Introduction to PROSPECT and SAIL

- **Leaf level: the PROSPECT model**

The radiative transfer model PROSPECT (PROpriétés SPECTrales) (Jacquemoud, 1990) idealizes a leaf as a pile of N identical elementary plates composed of absorbing and diffusing constituents. It considers that the interaction of electromagnetic radiation with plant leaves (reflection, transmission and absorption) depends on the chemical and physical characteristics of the leaves. The absorption of electromagnetic radiation by leaf constituents, for example, is essentially a function of changes in the spin and angular momentum of electrons, transition between orbital states of electrons in particular atoms (chlorophylls a & b, carotenoids, brown pigments and other accessory pigments) and vibrational-rotational modes within the polyatomic molecules (water). These processes are strongly dependent on wavelength (Atzberger, 1998). The latest version of this model (Jacquemoud et al., 2000), as used in this study, is a function of the chlorophyll a & b concentration (Cab), the leaf water content EWT (Equivalent water thickness) (Cw), the dry matter content (Cm), and the internal structure parameter (N). In abstract, N relates to the cellular arrangement within the leaf (Atzberger, 1998). Cab and Cw model the absorption with the corresponding specific spectral absorption coefficients Kab and Kw. These have been fitted using experimental data from a wide range of plant types and status, and do not depend on leaf type (Jacquemoud, 1996). With the exception of N, all parameters can be physically measured at leaf level. In short, PROSPECT computes spectra of the reflectance and transmittance of single leaves for the spectral range 400-2400nm; the spectral resolution is 1nm.

- **Canopy level: the SAIL model**

A vegetation canopy is not a large leaf, but a mosaic of leaves, soil background and shadow; it is a system where the various elements (leaves, stalkes, branches, etc.) are oriented in a complex manner. When entering the canopy, the directional and spectral composition of the incident radiation is altered, because the solar radiation is scattered and reflected between the leaves and the underlying soil (Atzberger, 1998). Nevertheless, one would like to relate part of this altered and reflected radiation intercepted by a remote sensing device to vegetation properties. All these difficulties have obliged the research scientist to simplify the real nature, which has led to a variety of canopy reflectance models (Goel, 1988).

The model used in this study, SAIL (Scattering of Arbitrarily Inclined Leaves) (Verhoef, 1984), belongs to the turbid medium models.

In this model, the canopy is considered as an horizontal, homogeneous, and infinitively extended layer made up of Lambertian scatterers (leaves), which are small and randomly distributed. The leaf optical properties are identical for the bottom and the top surfaces (Jacquemoud, 1993). The azimuth angle of the scatterers is assumed to be randomly distributed, while their zenith angle follows an ellipsoidal distribution characterized by a mean leaf inclination angle. Although it uses a simple description of the canopy structure, the SAIL model has already been validated on mature agricultural crops, like soybean, maize (Jacquemoud, 1995), orchards and sugar beet (Weiss, 2000), just to cite a few. This model is best suited for dense canopies with small vegetation elements (Goel, 2000).
3.2. Forward simulation

In (Ceccato, 2002a), the relative influence of variation in model input parameters in explaining variance in reflectance data at leaf level has been quantified with a sensitivity analysis using EFAST; it consists in studying how variation in the output of a model can be apportioned, qualitatively or quantitatively, to different sources of variation (Saltelli, 2000). In the visible region (400-700nm) for example, the total order sensitivity, (i. e. the variance of 1 parameter plus the variances of the interactions of this one parameter with all other parameters), showed Cab to explain between 60 and 80% of variance of model output. N is responsible for 15 to 35%. Both explain 95 % of the variance.

3.2.1. Determination of the PROSPECT parameters

The laboratory in Mohanpour provided three parameters: the water mass per leaf (fresh weight - dry weight), the dry matter mass per leaf and the chlorophyll a & b content. This last one was retrieved with the Arnon method. (Porra, 2002) describes the method as imprecise because faultily calibrated; the proposed following transformation is therefore applied to the chlorophyll values: new Cab values = (Arnon-Cab values)*0.895 (Porra, 2001).

To calculate the model parameters Cw and Cm, the leaf area of the leaves is necessary, according to the two following equations:

\[
C_w = \frac{\text{water mass}}{\text{unit leaf area}} \quad (\text{g/cm}^2) \quad (\text{Ceccato, 2001})
\]

\[
C_m = \frac{\text{dry mass}}{\text{unit leaf area}} \quad (\text{g/cm}^2) \quad (\text{Fourty, 1997})
\]

■ Method for the retrieval of leaf area

The leaf samples were photocopied in India on millimeter paper. Back in Switzerland the photocopies are scanned and imported in Photoshop 6.0. One square centimeter is selected with the selection tool, and the option statistics provides the pixel statistics of the selected area. This is the reference. With the magic wand tool, the leaves as a whole are selected and the statistics option provides again the number of pixels representing the leaf. Finally the leaf area pixels are divided by the reference number of pixels to get an area in square centimeters.

■ Method for determining the N structure parameter

Basically two different approaches are addressed. The first method consists of calculating N with two empirical relationships proposed in the literature. The other method is to set the laboratory values as fix and make an inversion of the PROSPECT model over N.

First, N is calculated with the relationship proposed by (Jacquemoud, 1990). Table A-1 in the annex shows the results of the calculations.

\[
N = \frac{0.95 \times \text{SLA} + 0.025}{\text{SLA} - 0.1}
\]  \hspace{1cm} (2)

where SLA is the leaf area/unit dry leaf weight.

The second equation (Ceccato et al., 2001):

\[
N = 4 \sqrt{\frac{1}{\text{SLA} - 0.1}}
\]  \hspace{1cm} (3)

These relationships between SLA and N are based on empirical rather than physical methods. They produce unrealistic results, because corchorus capsularis is a dicotyledon (http://plants.usda.gov/(November 2003)) and therefore should have an N value varying between 1.5 and 2.5 (Jacquemoud, 1996).
So the second method is used, i.e. the inversion of PROSPECT with fixed values for $C_w$, $C_m$, $C_{ab}$.

For the inversion, a *Matlab* algorithm (*fminsearch*) is used, which minimises a merit function, i.e. the difference between the simulated and the measured reflectance. The result is $N=2.76$. The whole spectrum is considered because $N$ affects all wavelengths, even if it is maximal in the near infrared (NIR). (Jacquemoud, 1993) remarks that $N$ values over 2.5 represent senescent leaves with a disorganized internal structure. For that reason, another inversion is performed over the range [700,1350nm]; the result is $N=2.66$. In neither case are the results found in accordance with the cited author. It is decided to keep $N=2.76$. (Clevers, 1991) notices that the influence of a varying $N$ is not very important, so a slightly wrong value should not induce dramatic biases.

For the rest of the fields, as there are no reflectances for their specific leaves, it is assumed that $N$, as a structural parameter, does not vary greatly over the different vegetation stages.

### 3.2.2. Parameterisation of the SAIL model

**LAI, ala**

The LAI (leaf area index) and the ala (mean leaf angle to the nadir) are determined with the software *CAN_EYE* (Weiss, Baret: personal communication to B. Kötz) written in the *Matlab* code. Hemispherical photographs (camera on the ground, looking upwards) are the input. By selecting pixels, one classifies the hemisphere in sky, leaves, soil, bark, etc. In this study, it is solely distinguished between sky and vegetation.

Structures like branches, shoots, etc. dictate the spatial distribution of leaves; this distribution therefore cannot be assumed to be random, there is foliage clumping. The geometric distribution of gap sizes (physical dimension of an opening in the canopy) can be measured precisely. It contains information of canopy architecture and can so be used to quantify the effect of foliage clumping on indirect (i.e., non-destructive) measurements of LAI, like with the hemispherical camera.

**hot spot**

(Jacquemoud, 2000) presents an easy formula (from Kuusk, as a personal communication) to calculate the hot spot: average length of a single leaf/canopy height. This did not seem practical for all vegetation stages. At 2 weeks of age, the plants are quite short in height while the leaves are already broad and long. Therefore, a default value of 0.1 is used if the formula value looks too different from the others (0.43 for field 2). For a detailed overview of the parameter values used in this forward simulation of the SAIL model, see Tab.A-2 in the annex.

**soil reflectance**

Field F4 is not suitable to represent the soil under the canopies because it was ploughed, and ploughed fields reflect less than a flat ground (increased shading due to clods of earth). The weed fractions of field 15 and 16 (stubbles of harvested rice and weeds) were higher than the one beneath the canopies of interest. Therefore, field 14 is chosen to represent the underlying soil.

**viewing geometry parameters**

Because the sensor was at nadir, the view zenith angle and the azimuthal angle were set to zero. The solar zenith angle was calculated with an *IDL* program called *sunangles.pro*; inputs are time, latitude and longitude of a measurement.
diffuse fraction

Although the fraction of diffuse radiation depends on the wavelength and atmospheric conditions, it is assumed as constant at 0.2 (this corresponds to 50km visibility (Jacquemoud, 1993)), because no measurement were made to distinguish between the direct and the diffuse flux component. However, (Clevers, 1991) shows that the diffuse fraction has only a minor influence on simulated reflectance, so it should not affect the simulation results.

3.3. Inversion of the PROSPECT-SAIL model combination

Once a certain model has been calibrated and validated on experimental data sets, the inversion procedure, i.e. the estimation of the biophysical variables from reflectance measurements, is possible by the inversion of the functional relationship mentioned in the introduction.

By testing three methods of inversion, one wants to test the "integrity" of the methods. For this, a synthetic reflectance is simulated with PROSPECT-SAIL with parameters similar to those of field 5; this is to be the reference reflectance. Then, an inversion is done on this simulated reflectance and the retrieved parameters are compared with those that created it; in that way, the method of inversion can be judged. If the inversion instrument is deemed satisfactory, the inversions are done over the measured reflectances. Retrieved parameters which deviate by up to 5% from their reference are considered as good, those with 10% difference as satisfying results; a deviation of up to 20% is still sufficient, whereas higher deviations will be considered as too poor.

3.3.1. Traditional inversion method, the minimisation algorithm

This algorithm adjusts the free parameters in the model so as to simulate a reflectance whose difference with the measured reflectance is minimal (Kimes, 2000). The algorithm used is called a "climber", because it considers only its local information to find a better solution. There is a danger of converging towards a local minimum (Renders, 1995), but the risk can be reduced by starting the minimisation process from different locations in the parameter space.

The first method is a multidimensional unconstrained nonlinear minimisation algorithm, implemented in Matlab and called fminsearch; it uses the Nelder-Mead simplex (direct search) method. It is described as a robust technique that requires less a priori information, weaker assumptions, and finds the optimum solution more reliably than other traditional techniques (Renders, 1992).

Methods

The important and interesting parameters to be retrieved are listed in the introduction: LAI, Cab, Cw, ala and Cm.

The next task is to settle the constraints of their ranges. The algorithm is defined as unconstrained, but then the free parameters can assume any value. Because physically-based model parameters have a predictable nature (exempli gratia LAI>0), a priori information should be used to constrain the parameter space. Otherwise, the inversion solution is normally based strictly on the minimisation of the merit function- this may lead to mathematical singularities-, the physical sensibility is not assessed during the
The minimisation algorithm implemented in Matlab asks for an initial parameter set from where to start in the parameter space. In order to avoid biases, a Matlab program is designed to produce 200 starting sets. The retrieval process is launched and the results are compared to the references. If the results are satisfying, then the validation with field spectra can be done.

<table>
<thead>
<tr>
<th>free parameters</th>
<th>field range</th>
<th>range width</th>
<th>constrained range</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAI</td>
<td>1.4-2.8</td>
<td>1.4</td>
<td>0.8-3.4</td>
</tr>
<tr>
<td>ala</td>
<td>30-62</td>
<td>30</td>
<td>10-80°</td>
</tr>
<tr>
<td>Cab</td>
<td>56.2-86.2</td>
<td>30</td>
<td>30-90 μg/cm²</td>
</tr>
<tr>
<td>Cm</td>
<td>0.004-0.007</td>
<td>0.003</td>
<td>0.001-0.01 g/cm²</td>
</tr>
<tr>
<td>Cw</td>
<td>0.017-0.026</td>
<td>0.009</td>
<td>0.01-0.04 g/cm²</td>
</tr>
</tbody>
</table>

Tab.2: Inversion method with the minimisation algorithm: the free parameters and their ranges.

3.3.2. The look-up table inversion method

This inversion method is intuitively the simplest method to grasp: one simulates a great number of reflectances by varying all relevant parameters within a certain range. By choosing the amount of simulations, one can decide how precisely the range must be covered; for a range of 3 (0.5-3.5) for example, shall there be 10, 50 or 100 intervals? For a start, 50'000 simulations are taken, just to test the performance of the method. (Weiss, 2000) suggests a 100'000 cases table, which provides a good compromise between the computer resources requirements and the accuracy of canopy variable estimates, whereas in this study, 130'000 entries are taken. The parameter values are quantified by a Matlab random numbers generator (uniform distribution) within the following ranges (Tab.3). In the choice of the ranges, care is taken to englobe with a comfortable security all values measured in the field, as for the method with the minimisation algorithm.

<table>
<thead>
<tr>
<th>free parameters</th>
<th>range</th>
<th>fix parameters</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAI</td>
<td>0.5-4.5</td>
<td>sun zenith angle</td>
<td>4</td>
</tr>
<tr>
<td>ala</td>
<td>10-80°</td>
<td>view zenith angle</td>
<td>0</td>
</tr>
<tr>
<td>Cab</td>
<td>25-100 μg/cm²</td>
<td>azimuthal angle</td>
<td>0</td>
</tr>
<tr>
<td>Cm</td>
<td>0.001-0.01 g/cm²</td>
<td>diffuse fraction</td>
<td>0.2</td>
</tr>
<tr>
<td>Cw</td>
<td>0.01-0.04 g/cm²</td>
<td>hot spot</td>
<td>0.07</td>
</tr>
<tr>
<td>N</td>
<td>2-2.9</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Tab.3: Inversion method with the LUT approach: the free parameters and their ranges, the fix ones and their values. The ranges for LAI, and Cab are slightly larger than those of the iterative algorithm in the previous section to be sure to englobe every possible value occuring in the field.

The different parameters are not of the same sensitivity for the simulated reflectance: the impact of the variations of Cm on the reflectance is not as critical as those of LAI might be. Neither are they necessarily distributed following the law of Poisson. In the literature, several different distribution are used depending on the parameter (Weiss, 2000). Nevertheless, for simplification, each parameter is given the same distribution.
The reference reflectance, i.e. the field reflectance for which the parameters are sought, is again first a synthetic reflectance with characteristics similar to field 5. This is done in order to have an idea on how well the method works "mathematically". This means that the LUT and the reference are generated by the same function, and the considerations about how well the PROSPECT-SAIL models can model the field fall away. The concentration can thus be oriented on the number of entries in the LUT, and on the thematic of the ill-posed problem. This issue, inherent to the inverse problem, consists of two separate aspects: First, the solution of the inverse problem is not necessarily unique, but a set of solutions could lead to similar matches between the measured and the simulated reflectance values. Second, the measurement and model uncertainties may induce large variation in the solution of the inverse problem (Combal, 2003).

As soon as an operational LUT method stands, it is applied to measured field data. The synthetic reference reflectance has the following constituting parameters (Tab.4)

<table>
<thead>
<tr>
<th>Synthetic reference reflectance</th>
<th>Cab</th>
<th>Cw</th>
<th>Cm</th>
<th>N</th>
<th>LAI</th>
<th>ala</th>
<th>h.s.</th>
<th>vza</th>
<th>sza</th>
<th>skyl</th>
<th>d.f.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Synth estic reference reflectance</td>
<td>85</td>
<td>0.025</td>
<td>0.006</td>
<td>2.6</td>
<td>2.9</td>
<td>50</td>
<td>0.07</td>
<td>0</td>
<td>4</td>
<td>0</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Tab.4: The constituting parameters of the synthetic reference reflectance. Abbreviation h.s. means hot spot, vza and sza view and solar zenith angle respectively, skyl is the view azimuth angle and d.f. the diffuse fraction.

By building the LUTs for the synthetic analysis part, some parameters are set free while the others are fixed to the value of the synthetic reference reflectance (Tab.3).

With the cost function (4), the sums of the differences between the reference reflectance \( (\text{mes}) \) and the simulated reflectances \( (\text{sim}) \) of the LUT are calculated over all wavelengths, for all cases, and then sorted.

\[
\sum_{i=1}^{1765} (\pi_i, \text{mes} - (\pi_i, \text{sim}))^2
\]

(4)

The best 50 fits (Weiss, 2000) with their corresponding parameters are taken out and compared with the reference.

Then the same exercise is done with a table of 130'000 entries.

The computational cost of building a LUT is as follows: on a Sun Sparc computer (900MHz, 17Gb RAM), it takes roughly 10 hours to build a table of 130000 spectra. To search it for the best solutions only takes a couple of seconds. For storage, the reflectance table requires 1.74 Gb, the parameter table 2.6Mb. The storage place can be reduced by half by multiplying the reflectance table by 10’000 and saving it as single precision values instead of double.

3.3.3. The neural network

3.3.3.1. Introduction

Neural networks are broadly used in remote sensing, from classification applications to inverse problem resolution (Baret, 1995).

They are composed of single neurones connected to each other and characterized by a transfer function, and associated weight and bias (Weiss, 1999). These structures can map the inputs (in our case spectral reflectances) to the desired outputs (biophysical parameters) by learning the mathematical function or relationship underlying the system.
by means of a supervised training. Training does not mean that the network will memorize the training data, but rather that the network will model the underlying generator of the data (Bishop, 1995). We do not need any knowledge or make assumptions about the mathematical representation to relate these inputs and outputs. The neural network algorithm can be understood as building the relation that transforms the measured reflectance for several wavelengths into the canopy variable values. This approach is fundamentally different from the LUT or the traditional iterative minimisation algorithm that require a model M (a functional relationship between variables and reflectance) to compute a cost function $C_f$ (Combal, 2003). The network may be composed of any number of layers, each layer having any number of neurons. Multilayer feedforward networks, as (Cybenko, 1989) and others have shown, can approximate any continuous input-output relation of interest to any degree of accuracy, provided sufficiently many hidden units are used (Kimes, 2002).

3.3.3.2. Neural network training and testing

- Neuron model and network architecture

As the basic element, the neuron model is described (Fig.11).

![Neural network concept](https://example.com/fig11)

Fig.11: The neural network concept. Left side: neuron model with vector input ($p_i$). On the right side: a layer with 3 neurons, generating three outputs $a$, which can be inputs to new neurons (inspired from the Matlab help facility).

The scalar input $p_i$ is transmitted through a connection that multiplies it by the weight $w_i$ (Fig.11 left). The transfer function has the following elements as argument (4),

$$ t = f\left( \sum_{i=1}^{n} w_i \cdot p_i + b \right) $$

and can be linear, logistic, hard-limit or else; the transfer function will determine the neuron output $a$. The hard-limit transfer function relates any input to either 0 or 1 (binary coding); the linear function processes the input linearly, as the name suggests, and can adopt any value. The tan-sigmoid and log-sigmoid are logistic functions; logsig compresses the input between 0 and 1, while the tansig function does it into the range [-1,1].

The parameters $w$ and $b$ are both adjustable scalars. The central idea of neural networks is that these parameters can be adjusted so that the network exhibits some desired behaviour, i.e. that inputs can be transformed by the different mathematical operations that are enabled to some desired outputs. The sketch in Fig.12 is a general network...
architecture. The number of layers, the number of neurons within them, and the transfer function determine the complexity and the range of tasks the network can handle. The two-layer sigmoid/linear network with biases can represent any functional relationship between inputs and outputs if the sigmoid layer has enough neurons (Hagan, 1996).

![Diagram of a three-layer network](image)

Fig. 12: Three-layer network, abbreviated notation. P is an R-length vector, aj and bj are S-length vectors. (inspired from the Matlab help program.)

The number of neurons of the output layer is determined by the desired output of the network. So the remaining unknown is the number of neurons in the "hidden" layer. The higher the number of neurons is, the complexer the function that can be imitated by the network.

For the nomenclature, a [50,5] designation means a network with 2 layers: a hidden one with 50 nodes or neurons, and the output layer with 5 neurons.

- Training

The first step in training a feed-forward neural network is to create its architecture (Matlab function: for a detailed explanation of the code, see code 4 in annex). Once the network stands, it is ready for training. This training process requires a set of examples of proper network behaviour—network inputs p and target outputs t. These training patterns act as the "real world", or at least as a reference. For a conceptual overview of canopy reflectance model inversion using a neural network, see Fig. 13.

During training, the weights and biases of the network are iteratively adjusted to minimise the network performance function, which as by default is the mean square error mse—the average squared error between the network outputs a and the target outputs t for all training patterns.

Several training algorithms implemented in Matlab use the gradient of the performance function to determine how to adjust the weights and biases to minimise the error. This gradient is determined using a technique called backpropagation, which involves performing computations backwards through the network (Hagan, 1996). These algorithms are called backpropagation algorithms and are popular to solve the problem of analysis of spectral data (Bishop, 1995).

Once the training is done, the network can be applied with great speed. As with more traditional regression techniques, neural networks can produce models which underfit or overfit the data. If the training error is high, the algorithm is unable to converge; that is characteristic of underfitting. On the other hand, high testing error is characteristic of overfitting. One would like a close correspondence between the two error types (Kimes, 2000).

There are several training algorithms and each has a different computation and storage requirement. None is suited for all purposes, some are not suited for a given task. For a start, an algorithm that the Matlab toolbox help describes as "very good general purpose algorithm" is chosen; it is called trainscg.
There are some advantages to the neural networks. First, this method can be applied to the most complex model without reducing the number of parameters or simplifying the physical processes. The models that have many parameters and include most physical processes tend to be the most accurate and robust models. Thus, the methods applied to full models may, potentially, find more relationships between the desired input and output variables (Kimes, 2000). The method does not require any initial guesses for the parameters, as do the traditional minimisation algorithms, and it can be applied to new data very quickly (Goel, 2000). Consequently, it can be applied on a per pixel basis.

A main disadvantage is the fact that some experimentation is required to find the optimum network structure. Also, the neural nets have not been generalised to handle any arbitrary subset of directional/spectral data (Goel, 2000). What is more, the neural networks suffer from the same problems as all other methods. They are dependant upon the fidelity/accuracy of the physically-based model (if trained with generated spectra) (Kimes, 2000).

**Methods**

A number of elements precondition the architecture to build: 1765 input bands should produce 5 parameters (LAI, ala, Cm, Cab, Cw). For that, the output layer is to have 5 neurons. (Udelhoven, 2000) uses 15 neurons in the hidden layer, for 46 input bands to
relate to 5 parameters. So a two-layer network is used, the respective transfer functions are sigmoid and linear, and the number of neurons in the hidden layer arbitrarily set to 150. The thought is to start with a small network and progressively expand it if necessary. (Bishop, 1995) writes that empirically, it is often found that "tanh" functions give rise to faster convergence of training algorithms than logistic functions. For this reason, the \textit{tansig} function is preferred to the \textit{logsig} one in the hidden layer.

The strategy is as follows: first, the net is to be calibrated over a training set of synthetic data. As soon as the network produces satisfying estimations, the measured data is applied to see how fine the network infers those parameters.

The goal is to get 19 approximations of parameters within 5\% of their reference out of 20 synthetic reflectances.

From the LUT with 50000 entries described in 3.2.2., every 16th spectrum for the training set (approx. 4000 spectra and corresponding parameters) and every 43th spectrum for the validation or control set (approx. 1000 spectra and corresponding parameters) are selected for calibration and control. If the training results are not satisfying, either the number of iterations during training or the number of nodes is increased until the expected accuracy is achieved.

4. Results

In a first part, the results of the comparisons between the simulated leaf reflectances and measured field leaf reflectances are presented and discussed.

In a second part, the inversions are presented, as explained earlier, first with data on a purely synthetic basis, then with the data collected in the fields.

4.1. Modelling

- Comparison \textit{measured leaf reflectance vs. simulated reflectance}, and discussion

As a reference, the mean and standard deviation of the 145 leaf reflectance measurements of field 5 are taken. There were no leaf measurements for the other fields. This reference is compared to the simulated reflectance of leaves of each field, computed with the parameter values measured in the lab.

Except for most of the visible region (VIS, 400-700nm) where the simulated reflectance is overestimated, the simulated leaf spectra of the different fields are within one standard deviation of the measured mean (Fig.14). As the photosynthetic pigments absorb strongly in this region (Ceccato, 2002), this could indicate a low Cab value as model input parameter; this is however not very plausible, as the value of 86.2\mu g/cm^2 of field 5 is \textit{per se} quite high. Besides that, tests with higher values have not bettered the curve fitting, as saturation occurs beyond a certain value. A hypothesis that could explain the difference is that \textit{corchorus capsularis}, a tropical breed, was not considered when PROSPECT was calibrated; it may lack certain pigments that are in the calibration leaves. (Haboudane, 2004) writes that living leaves can have similar structural characteristics but various pigment contents. Albeit plausible, it does not seem the most realistic possibility. Another factor which would lower the reflectance is a smaller N; but in the same time, it lowers also the reflectance in the near infra-red (NIR, 700-1300nm), and the short wave IR (SWIR, 1300-2500nm), regions that are relatively precisely modelled.
(Le Maire, 2004) remarks that PROSPECT cannot simulate the correct reflectances at both the 550nm peak and the near-infrared shoulder around 750 nm, whatever the value of N is. Off course, the inconsistencies could also simply be attributed to bad measurements. Whatever the reason, it seems that PROSPECT has difficulties in modelling jute in the VIS.

![Simulated leaf spectra of the 6 fields](image)

**Comparison simulated canopy vs. measured canopy reflectance, and discussion**

The output from the SAIL simulation are reflectance values for every wavelength of the input. Fig.15 shows the comparison of the measured with the simulated values. For field 1, there are 3 different transects recorded at different times (a,b,c), which means there are three varying sun-zenith angles. Field 2 and 3 have each two illumination geometries, the rest of the fields one. Every spectral region in which the simulated reflectance is within one standard deviation of the transect’s or the field’s measured mean spectrum is considered appropriately modeled.

According to (Jacquemoud, 1993, Asner, 1998), the different parameters influence different spectral regions. Cab shapes the VIS, LAI and ala are the dominant parameters controlling the canopy reflectance. Cw has a great influence from 1000nm to 2400nm. Cm has influence in the NIR.

A few transects show a great overestimation of their reflectance in the VIS: d), g), i) and j) in (Fig.15). This can indicate too low Cab input values, although this answer is not quite satisfying as the Cab values are quite high. As the reflectance at leaf level in the VIS is
already overestimated by PROSPECT, it seems logical that SAIL does the same; the reason why it does not do it for all the fields and transects is not clear. Both transects of field 2 show a high NIR reflectance, but the range beyond is once over-, then undersimulated. So this seems to indicate that ala is only minorly responsible in this faulty deviation. Cab might be slightly underestimated, but if so, it is only for transect 1. Tendentially, the opinion is that LAI is overestimated for field 2. Tests with lower LAIs show less reflection in the NIR and less absorption around 660nm. (Pinty, 1990) notes that a sparse vegetation with a low LAI (which is the case of field 2) is not well accounted for by the model SAIL. So this is also a factor to take into account.

For i, the overshot in the NIR is possibly due to the low ala value of 30°. This value is the lowest of all fields and does not fit into the rule of thumb that the denser the canopies, the higher the LAI and thus the lower the ala. Field 6 was 5 weeks old, very developed compared to field 2 but much less dense than the 8 weeks old fields. Simulation with higher ala values show a decrease of the reflection in the NIR.

Field 7 is overestimated in the VIS; the Cab input value is low compared to fields of the same age; what is more, the rest of the spectrum is fairly well modelled. The guess is a low Cab value. Again, tests can show a stronger absorption if the Cab values are higher.

Of course there are no proofs of flawed measurements. The operator in India who measured Cab admitted never having used the method before, thereby warning of possible errors. Therefore it does not seem farfetched if the assumptions are partly inexact Cab values. The second source of errors is the LAI and the ala, which are both derived with the same method. The program used had just been freshly written by the time the calculations were done. Newly developed software does need some adjustments when applied to real problems, and the author of this study has used it without being told if there are specials to observe. It has been mentioned earlier that the way the classification is done may influence the results.

To explain the erroneous parts of the modelled spectra with measurement errors is a solution which permits to qualify the PROSPECT-SAIL model for this purpose. It is by far not perfect, but if we leave away field 2 for it has sparse vegetational cover, and therefore is not well accounted for by SAIL, the results, at least for wavelengths above 700nm, become acceptable: in a majority of cases, the simulated reflectance is within one standard deviation of the mean of the measured spectra. For the wavelengths below 700nm, it is PROSPECT that overestimates the reflectance; little surprisingly, SAIL tendentially does the same. Therefore, it can be said that corchorus capsularis can be fairly well simulated by PROSPECT-SAIL, taking into account the simplifications that SAIL makes about the canopy.
Fig. 15: Simulated and measured jute spectra. In red, the simulated spectrum of the different transects and fields; in black, the standard deviations (dashes) and the mean of the measured transects and fields. a,b,c: 3 transects of field 1; d,e: field 2; f,g: field 3; h,i,j: fields 5,6,7 respectively. On the x-axis, spectral bands [1349-1425nm] and [1796-1954nm] are cut out because of instability of the reflectance values due to atmospheric water vapor absorption.
Results from the hemispheric camera and the *Can_Eye* software (Weiss & Baret)

The average leaf angle (ala) is related with LAI. When the density of the vegetation is not very high, the leaves are disposed in a more horizontal position, because there is space. The LAI is low (relatively few leaves), but the ala (angle to the nadir) is high. The denser it gets, the more vertical the leaves tend to be (Jacquemoud, 1993). For that reason, the ala value for field 6 (age: 5w, ala=30°) is too low compared to the other fields. There is a little variance in the results, depending on how one classifies. It is difficult to say what it depends on, for the matter has not been investigated any further than the use of the software required.

4.2. The inversion techniques

4.2.1. Traditional minimisation algorithm

As mentioned before, the minimisation algorithm requires a starting set of parameters; with this initial set it will model a spectrum and compare it to the reference spectrum. Then it will search for a set of parameters for which the difference between its modelled spectrum with the reference spectrum will be smaller, and so on. In order to exclude biases and omissions regarding spots in the parameter space, 200 randomly generated parameter sets are taken, and the retrieval algorithm is launched 200 times. As a consequence, in about 83 cases out of a hundred, one finds an inverted Cab value within 10 % of the reference, or 8 of ten retrievals would only deviate by 5% maximum (Tab.5). For the other parameters (Cw, Cm, LAI, ala), only 50 % of the starting parameter sets produce a satisfying inversion.

<table>
<thead>
<tr>
<th></th>
<th>Cab</th>
<th>Cw</th>
<th>Cm</th>
<th>LAI</th>
<th>ala</th>
</tr>
</thead>
<tbody>
<tr>
<td>dev. from ref: &lt;5%</td>
<td>79%</td>
<td>43%</td>
<td>45.5%</td>
<td>41%</td>
<td>43%</td>
</tr>
<tr>
<td>dev. from ref: &lt;10%</td>
<td>83.5%</td>
<td>55.5%</td>
<td>47%</td>
<td>46.5%</td>
<td>50.5%</td>
</tr>
</tbody>
</table>

Tab.5: Retrieval results of the minimisation algorithm after 200 iterations (see 3.2.1, Methods): for each parameter, percentage of retrievals that deviate by 5% resp. 10% from their respective references are given.

Numerically, this method does not produce the expected results. A more qualitative analysis is considered: the histograms and the distribution of the retrieval results are taken into account. For every parameter, except for Cab, the value most often retrieved relatively to the others is exactly the reference values (Fig.16).

![Fig.16: Analysis of the histograms of the retrieved values: on the x-axis are the parameter values, on the y-axis, the number of times the value is retrieved.](image)
In this way, the algorithm has, while delivering values over a quite large spectrum, in each case a pronounced preference for the desired value.

■ Validation with field measurements

After the functional efficiency of an inversion of a synthetic reflectance is proven, the method is applied to the measured spectra of the different fields. Starting with 200 iterations from different places in the parameter space does not produce the same results as with the synthetic spectrum. Some isolated values are under 5% deviation from the reference, but they are the minority. Even a deviation of 10% is rare. It gives the impression that there is no system; the satisfying respectively poor retrievals are seemingly randomly distributed, so that one cannot derive usable findings (see Tab.6).

<table>
<thead>
<tr>
<th>Field, transect</th>
<th>f1,1</th>
<th>f1,2</th>
<th>f1,3</th>
<th>f2,1</th>
<th>f2,2</th>
<th>f3,1</th>
<th>f3,2</th>
<th>f5</th>
<th>f6</th>
<th>f7</th>
<th>f1</th>
<th>f2</th>
<th>f3</th>
</tr>
</thead>
<tbody>
<tr>
<td>[%] deviation from ref. Cab</td>
<td>12.5</td>
<td>0.5</td>
<td>2.5</td>
<td>38</td>
<td>43</td>
<td>8.5</td>
<td>24</td>
<td>19.5</td>
<td>1</td>
<td>13.5</td>
<td>0</td>
<td>38.5</td>
<td>16.5</td>
</tr>
<tr>
<td>[%] deviation from ref. Cw</td>
<td>4</td>
<td>0</td>
<td>2.5</td>
<td>n.r.</td>
<td>n.r.</td>
<td>2</td>
<td>15</td>
<td>23</td>
<td>36</td>
<td>15</td>
<td>0</td>
<td>41</td>
<td>8</td>
</tr>
<tr>
<td>[%] deviation from ref. Cm</td>
<td>33</td>
<td>53</td>
<td>35</td>
<td>10</td>
<td>57</td>
<td>66</td>
<td>65</td>
<td>71</td>
<td>36</td>
<td>35</td>
<td>44.5</td>
<td>40</td>
<td>68</td>
</tr>
<tr>
<td>[%] deviation from ref. LAI</td>
<td>24</td>
<td>5.5</td>
<td>10</td>
<td>67</td>
<td>39</td>
<td>11.5</td>
<td>33</td>
<td>8</td>
<td>32</td>
<td>3.5</td>
<td>0</td>
<td>38</td>
<td>8</td>
</tr>
<tr>
<td>[%] deviation from ref. ala</td>
<td>29</td>
<td>0</td>
<td>4.5</td>
<td>n.r.</td>
<td>27.5</td>
<td>5</td>
<td>43</td>
<td>4</td>
<td>90</td>
<td>24</td>
<td>1</td>
<td>27</td>
<td>27.5</td>
</tr>
</tbody>
</table>

Tab.6: 200 different starting points in the parameter space with the field transect resp. whole field spectra as reference: the deviation of the most often retrieved value in the histogram from the respective field parameter, for each parameter. Grey-filled cells highlight a deviation within 10%. The abbreviation n.r. means not retrievable, because the retrieved parameters are clustered at one or both parameter range boundaries.

Fields 1, 2 and 3 are taken by transect; between these transects, there are significant differences. The values of the last 3 columns of Tab.6 show that value differences between transects tend to be averaged when the field is considered as a whole; the results are better because the badness of the worst transect value is attenuated by the relative better values of the other(s). Field 2 as a whole is the only field for which it has not been possible to retrieve the parameters by considering the histogram: the values were strongly scattered. For that reason, the median of the retrieved values is used to calculate the deviation.

4.2.2. The look-up table approach

In a first stage, the method of inversion of a spectrum to parameters by means of a look-up table is to be tested with synthetic data only; it is to be evaluated which size and which parameters are to be set free or constrained. Then, as the method proves successful, the field spectra shall be inverted. 5 different LUTs are evaluated, the first has 50'000, the following 130’000 entries. The first two LUTs have no constraints on the 6 parameters whose ranges are defined in Tab.3. The following have constraints on one or two of these parameters in order to determine if and to which extent the other parameters are inferable.

■ LUT 50’000 entries, all 6 parameters free (within their ranges)

The sum of the differences between the wavelengths of every reflectance spectrum of the LUT and the reference is made, and the fifty smallest differences are selected: they represent the best spectral fits. The corresponding parameters do not show an unitary value for each parameter over the fifty values. Here again the difficulty of modelling with
PROSPECT-SAIL is visible, i.e. different sets of parameter produce similar spectra. To elude the problem, the median of the 50 retrievals is taken. Tab.7 shows the medians of the best 50 fits of the first LUT with the deviation to the corresponding reference parameters.

<table>
<thead>
<tr>
<th></th>
<th>LAI</th>
<th>ala</th>
<th>Cm</th>
<th>Cab</th>
<th>Cw</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>LUT_best, median</td>
<td>2.32</td>
<td>49</td>
<td>0.0054</td>
<td>82.6</td>
<td>0.029</td>
<td>2.34</td>
</tr>
<tr>
<td>stdev</td>
<td>0.6</td>
<td>10</td>
<td>0.0026</td>
<td>10</td>
<td>0.005</td>
<td>0.24</td>
</tr>
<tr>
<td>reference</td>
<td>2.9</td>
<td>50</td>
<td>0.006</td>
<td>85</td>
<td>0.025</td>
<td>2.6</td>
</tr>
<tr>
<td>deviation: med./ref. (%)</td>
<td>20</td>
<td>2</td>
<td>10</td>
<td>2.8</td>
<td>14</td>
<td>10</td>
</tr>
</tbody>
</table>

Tab.7: LUT with 50’000 entries: retrieval results are within 5% deviation from reference for Cab and ala (last row of column).

The results are good for ala and Cab (<5% deviation from the reference), satisfying for N and Cm (<10%), sufficient for Cw and unsatisfying for LAI.

- LUT 130’000, all parameters free

According to the citations in 3.2.2., another table with 130000 entries is generated, all previously free parameters are still free.

<table>
<thead>
<tr>
<th></th>
<th>LAI</th>
<th>ala</th>
<th>Cm</th>
<th>Cab</th>
<th>Cw</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>best 50, median</td>
<td>2.34</td>
<td>52.6</td>
<td>0.0061</td>
<td>84</td>
<td>0.029</td>
<td>2.35</td>
</tr>
<tr>
<td>standard dev.</td>
<td>0.06</td>
<td>21</td>
<td>0.003</td>
<td>6.8</td>
<td>0.002</td>
<td>0.22</td>
</tr>
<tr>
<td>reference</td>
<td>2.9</td>
<td>50</td>
<td>0.006</td>
<td>85</td>
<td>0.025</td>
<td>2.6</td>
</tr>
<tr>
<td>deviation: med./ref. (%)</td>
<td>19</td>
<td>5</td>
<td>1.5</td>
<td>1</td>
<td>16</td>
<td>10</td>
</tr>
</tbody>
</table>

Tab.8: LUT with 130’000 entries: Cm, Cab and ala are within 5% deviation. Results are similar to Tab.7.

Like for the previous LUT, Cab, ala and newcomer Cm are well retrieved (Tab.8); the results’ quality varies very little. Only the standard deviation is smaller, except for ala. LAI has a particularly little dispersion, which is an indicator of stability of the inversion process. The question is how to improve the LAI and Cw retrievals. Fig.17 shows how well the fifty best spectra fit the reference. That means that spectrally, it is very difficult to
retrieve optimal results with the LUT, as several sets of parameter produce the same spectrum (cf. ill-posed problem).

![Graph](image)

Fig.17: The black line is the synthetic reference, the grey thick line represents the 50 spectra with smallest differences to reference spectrum. The two vertical dotted lines are the places where data is excluded because of atmospheric vapor absorption. The statistical distribution of the retrieved parameters can be viewed in Tab.8.

(Bacour, 2002) states that LAI and Cab have interactions, as well as LAI and ala. As LAI and Cab are prime parameters, they should remain unconstrained. As a consequence, if ala is fixed to 50°, this might let converge LAI to more desirable values.

■ LUT 130'000, ala fix

In the following LUT (130'000 entries) the mean leaf angle ala is fixed to 50°. Again the best fifty fits are selected and the median computed out of the corresponding parameters. Tab.9 lists the results.

<table>
<thead>
<tr>
<th></th>
<th>LAI</th>
<th>Cm</th>
<th>Cab</th>
<th>Cw</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>LUT, median</td>
<td>2.34</td>
<td>0.0061</td>
<td>84</td>
<td>0.029</td>
<td>2.35</td>
</tr>
<tr>
<td>stdev</td>
<td>0.06</td>
<td>0.0025</td>
<td>7.85</td>
<td>0.0017</td>
<td>0.196</td>
</tr>
<tr>
<td>reference</td>
<td>2.9</td>
<td>0.006</td>
<td>85</td>
<td>0.025</td>
<td>2.6</td>
</tr>
<tr>
<td>deviation</td>
<td>20</td>
<td>1.5</td>
<td>1</td>
<td>16</td>
<td>10</td>
</tr>
</tbody>
</table>

Tab.9: LUT with 130'000 entries and a fix ala=50°. Results are nearly the same as in Tab.8.

The results are good for Cab and Cm, sufficient for Cw, but unsatisfying for LAI again. Because there is no improvement in fixing ala, as a next step, N is considered. It is not a parameter for retrieval; it has been fixed by inversion of a leaf spectrum earlier in this work. Besides that, there is a relatively strong correlation between N and LAI for the best 50 fits (see Fig.18). The higher the N, the lower the LAI; and typically, LAI is underestimated in this case (Tab.9). This may be the hampering element hindering the retrieval of a more precise LAI value. To check this out, another LUT is generated with 130'000 entries, this time with a fixed N=2.6. As the results between the LUT with fixed
ala and the one with free ala are minimal (Tab.8 and Tab.9), ala is set free again for this investigation.

Fig.18: Correlation between N and LAI for the best 50 spectra retrieved with the cost function.

- **LUT 130’000, N fixed**

Regretfully, the LAI retrieval value is not improved, but worsened, if only by a little. To fix N to a high value constrains LAI to a lower value. The rest of the parameters are retrieved as with the other LUTs (see Tab.10). This was somehow predictable with Fig.18.

<table>
<thead>
<tr>
<th>LUT</th>
<th>LAI</th>
<th>ala</th>
<th>Cm</th>
<th>Cab</th>
<th>Cw</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.29</td>
<td>50.5</td>
<td>0.0061</td>
<td>87.6</td>
<td>0.031</td>
<td></td>
</tr>
<tr>
<td>0.49</td>
<td>6.8</td>
<td>0.0027</td>
<td>10.7</td>
<td>0.0043</td>
<td></td>
</tr>
<tr>
<td>2.9</td>
<td>50</td>
<td>0.006</td>
<td>85</td>
<td>0.025</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>1</td>
<td>1.5</td>
<td>3</td>
<td>24</td>
<td></td>
</tr>
</tbody>
</table>

Tab.10: LUT 130’000, with a fixed N: retrieval of Cw and LAI is worse than in Tab.4.2.3.

- **LUT 130’000, N and ala fixed**

One last experiment is performed to see if there is a solution to improve the retrieval of LAI: the structure parameter N is set to 2.6, and ala to 50°. The results are not very different from the preceding tables (Tab.11).

<table>
<thead>
<tr>
<th>LAI</th>
<th>ala</th>
<th>Cm</th>
<th>Cab</th>
<th>Cw</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.27</td>
<td>0.0065</td>
<td>89</td>
<td>0.031</td>
<td></td>
</tr>
<tr>
<td>0.027</td>
<td>0.0027</td>
<td>4.5</td>
<td>0.0006</td>
<td></td>
</tr>
<tr>
<td>2.9</td>
<td>0.006</td>
<td>85</td>
<td>0.025</td>
<td></td>
</tr>
<tr>
<td>22.5</td>
<td>8</td>
<td>5</td>
<td>24</td>
<td></td>
</tr>
</tbody>
</table>

Tab.11: LUT 130’000, with fixed N and ala: LAI and Cw still remain unsatisfyingly retrieved.

- **Validation with field spectra**

The previous LUTs show that the best results can be expected with a LUT with 130’000 entries with all parameters free. The field measured spectra of different vegetation stages and different illumination geometries are to be applied to one LUT, thus some variables specific to each field have to be averaged: the hot spot takes the value 0.1, the average sun zenith angle over all fields is 5°.
A LUT with 130'000 entries is built. The results do not correspond to the results of the synthetic data retrieval. Especially the promising 5% of ala, Cm and Cab are not met. They are met for a 10% deviation for the transects of field 1. For the other fields, this mark is met only sporadically. Tab.12 summarizes the findings.

<table>
<thead>
<tr>
<th>deviation [%] from ref. LAI</th>
<th>f1,1</th>
<th>f1,2</th>
<th>f1,3</th>
<th>f2,1</th>
<th>f2,2</th>
<th>f3,1</th>
<th>f3,2</th>
<th>f1</th>
<th>f2</th>
<th>f3</th>
<th>f5</th>
<th>f6</th>
<th>f7</th>
</tr>
</thead>
<tbody>
<tr>
<td>deviation [%] from ref. ala</td>
<td>11.5</td>
<td>7.5</td>
<td>27</td>
<td>11.5</td>
<td>18</td>
<td>12.5</td>
<td>8.5</td>
<td>19</td>
<td>5.5</td>
<td>18</td>
<td>3</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>deviation [%] from ref. Cm</td>
<td>0</td>
<td>0</td>
<td>5</td>
<td>32</td>
<td>37.5</td>
<td>26.5</td>
<td>10</td>
<td>27.5</td>
<td>13</td>
<td>31.5</td>
<td>0</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td>deviation [%] from ref. Cab</td>
<td>2.5</td>
<td>9</td>
<td>1</td>
<td>23.5</td>
<td>14.5</td>
<td>15.5</td>
<td>21.5</td>
<td>9</td>
<td>14</td>
<td>16.5</td>
<td>25.5</td>
<td>9</td>
<td>3.5</td>
</tr>
</tbody>
</table>

Tab.12: LUT 130’000 with all parameters free: deviations of the median (best 50 spectral fits) from the reference values (measured field and laboratory values). The cells in grey highlight the deviations within 10%.

4.2.3. Neural network

In a first step, the networks are created and trained with a certain number of spectra from the LUT 130'000, all parameters are set free; then, a validation set of spectra, different from the first but from the same LUT, is used to check how well the network can generalize to new spectra. This has proven to be an error, since no method such as the neural networks needs the link to reality more if it is to make sense. To try a validation with spectra of the same origin (and same noise) as the training set is not robust as soon as different data are used upon the network. Nevertheless, as in a second step, field data is used to validate the network. This first section (captioned "Training and validation with the LUT") is left in the text to pay tribute to the whole development of the knowledge about these networks.

■ Training and validation with the LUT

At first, an architecture is randomly chosen. After each training and control phase, the network architecture or the number of iterations are altered in order to improve the performance. If it is not specified explicitly, then every reference to a training means the network is trained with the training algorithm trainscg (see 3.2.3.2. Neural network training and testing). Unfortunately, it turns out that if Cab and ala are easily inferred within reasonable limits, the network produces negative values for Cw and Cm; LAI is difficult to find also (Tab.13).

<table>
<thead>
<tr>
<th>LAI</th>
<th>ala</th>
<th>Cm</th>
<th>Cab</th>
<th>Cw</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;20%</td>
<td>95.8%</td>
<td>99%</td>
<td>0%</td>
<td>100%</td>
</tr>
<tr>
<td>&lt;10%</td>
<td>84.6%</td>
<td>97%</td>
<td>0%</td>
<td>99.5%</td>
</tr>
<tr>
<td>&lt;5%</td>
<td>63%</td>
<td>92%</td>
<td>0%</td>
<td>96.6%</td>
</tr>
</tbody>
</table>

Tab.13: Percent of inferred parameters (e.g. LAI) which are within 5,10 or 20% deviation of the target parameters. Results for a [150,5] network, 6000 iterations (see code 5 in annex for more details).

(Bacour, 2002) warns of interactions between parameters: LAI-Cab for example, or LAI-ala. Thus there is danger of compensation between parameters. Besides that, as there is a linear relationship in the last layer, it may be difficult for an algorithm to accurately map values in the fifties and above (ala and Cab), and in the same time, with the same weights and biases, values below 0.1 (Cm and Cw); the range to map becomes too wide. LAI, which by order of magnitude is somewhere in between (although
closer to the "big ones" (Cab, ala)), is mapped accordingly: not quite as good as the big ones, but scores better than the small ones (Cm, Cw).

Taking this as a guideline, instead of creating gigantic networks which would take ages to train and might only produce partially satisfying results, the problem is split: in place of 1 network for retrieval of 5 parameters, 5 networks in parallel are combined which focus each on a single parameter only. These networks are called expert networks (Bishop, 1995).

■ Expert networks

Every expert network is trained and tested so as to achieve a retrieval rate of 95% within 5% deviation of the reference. The training and testing sets, although different, are from the same LUT 130000 which is used at the synthetic level in th LUT section 4.2.

Cab

The network architecture is [55,1], the number of iterations is 7000. For a summary of the networks’ structures, see Tab.14; for the retrieval results, see Tab.15.

LAI

Its range is [0.5,4.5]. Training the net with this range produces good training results but bad testing results. There is suspicion of overfitting. A too small target range seems to hinder the network from accurate mapping. (Kimes, 1998) proposes to manipulate numerically the inputs if the training leads to overfitting. The training targets and validation targets are multiplied by 50; the range is thus extended to [25,225]. The same net improves the retrieval within 10% of deviation by more than 50% after the numerical manipulation. By trial and error the net is improved until it reaches a maximum (93.3% within 5%). Further augmenting the number of iterations and/or the number of nodes seems to lead to overtraining, and the testing results get accordingly bad. At this point, the net tends to fit more the noise of the data then the general "idea" of the relation, because the larger the network, the more complex the "functions" the net can approximate. In that case, the net will not be able to generalize well to new data, which noise structure might be different.

There seems to be an optimum for a variable to be retrieved; it must be in relation with the concrete impact it has on the canopy. The net’s architecture is: [45,1], 7000 iterations.

Cw

Cw is taken to train a net on its own as well. Its range is [0.01,0.04]. As for LAI, the targets of the training and the targets of the validation set are multiplied by 2000 to a range of [20,80]. That makes it easier for the net to find distinguishable weights and biases to map the relationship in "sharper tones". The net is a [60,1] structure, 6000 iterations.

Cm

The same strategy is applied to Cm, which is multiplied by 10’000 (range [10,100]). Unfortunately, this parameter is not retrievable with this method. The training results are bad, even if the iteration number or the hidden layer nodes are augmented. As the training results are very bad, the testing results are not good either. For a drastically downsized network, the algorithm converges quite fast, but the testing results encourage the investigator to cast away that option.

<table>
<thead>
<tr>
<th>hidden, output layer</th>
<th>Cab</th>
<th>ala</th>
<th>LAI</th>
<th>Cw</th>
<th>Cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>55,1</td>
<td>65,1</td>
<td>45,1</td>
<td>60,1</td>
<td>60,1</td>
<td></td>
</tr>
</tbody>
</table>
Tab.14: The structures of the expert networks

<table>
<thead>
<tr>
<th></th>
<th>number of iterations</th>
<th>Cab</th>
<th>ala</th>
<th>LAI</th>
<th>Cw</th>
<th>Cm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>7000</td>
<td>0.1</td>
<td>99.9%</td>
<td>99.9%</td>
<td>99.9%</td>
<td>48.2%</td>
</tr>
<tr>
<td></td>
<td>8000</td>
<td>0.1</td>
<td>99.7%</td>
<td>99.9%</td>
<td>99.6%</td>
<td>23.7%</td>
</tr>
<tr>
<td></td>
<td>7000</td>
<td>0.1</td>
<td>98%</td>
<td>99.2%</td>
<td>99.6%</td>
<td>12.2%</td>
</tr>
<tr>
<td></td>
<td>6000</td>
<td>0.1</td>
<td>96.9%</td>
<td>93%</td>
<td>93.3%</td>
<td>12.2%</td>
</tr>
<tr>
<td></td>
<td>6000</td>
<td>0.1</td>
<td>96.9%</td>
<td>93%</td>
<td>96.9%</td>
<td>12.2%</td>
</tr>
</tbody>
</table>

Tab.15: Retrieval performance with the training and testing sets taken from the LUT 130'000, all parameters free.

These results seem very promising for the validation through field spectra.

■ Validation with field data

All fields are taken by transect, except field 1 where the second and the third of four transects are taken together because it is almost the same route forth and backwards and done without brake, thus featuring the same illumination geometry. Tab.16. shows the deviation of the estimated values from the measured field parameters.

<table>
<thead>
<tr>
<th></th>
<th>f1,1</th>
<th>f1,2</th>
<th>f1,3</th>
<th>f2,1</th>
<th>f2,2</th>
<th>f3,1</th>
<th>f3,2</th>
<th>f5</th>
<th>f6</th>
<th>f7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cab</td>
<td>50%</td>
<td>60%</td>
<td>37%</td>
<td>64%</td>
<td>51%</td>
<td>60%</td>
<td>99%</td>
<td>99%</td>
<td>40%</td>
<td>80%</td>
</tr>
<tr>
<td>Cw</td>
<td>23.5%</td>
<td>0.5%</td>
<td>21%</td>
<td>50%</td>
<td>40%</td>
<td>25%</td>
<td>11%</td>
<td>19%</td>
<td>15%</td>
<td>25%</td>
</tr>
<tr>
<td>LAI</td>
<td>27%</td>
<td>2%</td>
<td>27%</td>
<td>5%</td>
<td>3.5%</td>
<td>31%</td>
<td>41%</td>
<td>7%</td>
<td>9%</td>
<td>6%</td>
</tr>
<tr>
<td>ala</td>
<td>93%</td>
<td>2%</td>
<td>8%</td>
<td>24%</td>
<td>37%</td>
<td>34%</td>
<td>59%</td>
<td>1%</td>
<td>75%</td>
<td>22%</td>
</tr>
</tbody>
</table>

Tab.16: Retrieval values per parameter for every transect; the percentage expresses the deviation of the retrieved value to the reference value. Cells highlighted in grey indicate a deviation under 10%.

The very disappointing character of the quality of these results tends to indicate a poor generalization to new data, although the testing set is quite large (~1000) and in its range certainly seems to encompass the field spectra. The results, although comparable to those of the previous two methods, is in quality worse.

Unability to handle new spectra can mean the network is overtrained; apparently, the network has memorized the training examples and cannot adapt to new data.

During neural network training, the true error, which is the error of a virtual validation set, will usually decrease initially. However, as training continues, the true error can start to increase, while the training error still decreases. This is because as training continues, weights become more tuned to particular features of the training data, which may be vagaries of the particular training set or noise, and as such specific to a data set. Different sets may have different noise features.

The Matlab help facility about network generalisation writes as a rule of thumb: if the number of parameters (weights and biases) is much smaller than the number of training patterns of the training set, then there is little chance of overfitting. This is evidently not the case here: the number of parameters is \((1765*50)+50+(50*1)+1=87'701\) parameters for a \([50,1]\) network, while the training patterns amount to 4000! One legitimate question with this method is certainly the one that asks about the sense of using hyperspectral data: Price (1994) indicates that for natural materials, 15-25 spectral bands are sufficient, suggesting redundancy in the numerous bands. Two possibilities arise to improve the efficiency of the method in case what is written above holds. Either the relevant bands for each parameter are selected, and the networks trained with them, or all wavelengths are kept. In this case, four techniques can be applied.
Improvements of the networks

From here on the training and testing is done with synthetic data and the validation with measured field spectra; the field data is incorporated much earlier in the process to prevent the building of networks like the expert networks. Several techniques can improve network generalization or at least prevent from overfitting:

a) Use of a minimal network architecture size: the goal is to use a network that is just large enough to provide an adequate fit. The larger a network being used, the more complex the functions the network can create. If a small enough network is chosen, it will not have enough power to overfit the training data and thus be able to generalize to new data.

b) Increase of the training data: if more data can be collected without too much effort and the size of the training set is easily increased, then there is no need to worry about the following techniques to prevent overfitting. As the training data set to calibrate the network in this study is generated with a RT model, the training data is not scarce; the validation with field data sets is more of an availability problem, especially if the fields are taken as one averaged reflectance of all the measurements over the two transects. The following two methods apply to those situations in which there is a limited supply of data.

c) Early stopping (implemented in Matlab): during training, the error on the validation set is monitored, and training is stopped when the validation set error starts to increase. Early stopping is very widely used and can allow the use of networks with architectures with more weights than the rule of thumb above would allow.

d) Regularization: this involves modifying the performance function, which is normally chosen to be the sum of squares of the network errors (mse) on the training set. It is possible to improve generalization by adding a term that consists of the mean of the sum of squares of the network weights and biases (msw). A performance ratio parameter (range: [0,1]) is used as a factor of both mse and msw. A value of 0.5 gives equal weight to mse and msw. Using this performance function will cause the network to have smaller weights and biases, and this will force the network response to be smoother and less likely to overfit. The problem with regularization is that it is difficult to determine the optimum value for the performance ratio parameter. If the ratio is too high, the chances are that the network overfits training data; a too low ratio will not permit adequate training. The trainbr algorithm, implemented in Matlab, is a routine that automatically sets the optimal performance parameters to achieve the best generalization. It generally works best when the network inputs and targets are scaled so that they fall approximately in the range [-1,1].

In the following lines, the four techniques for improvement of the generalization of the network are tested. The use of the first technique to reduce the architecture’s complexity does not yield better results. As for the network meant to retrieve Cab, originally built as a [55,1] network, the stepwise reduction of either the hidden layer or the number of iterations by one at a time has no benefit over the resulting retrieval; the finding one may extract from this is that the networks in their previous architecture are much too complex, and that single parameters may be difficult to retrieve alone. The rule of thumb seems to apply in this case, i.e., the number of input parameters is too high for the little number of training spectra. The next step is to augment the training spectra set; this is done by taking 25’000 spectra in the validation LUT with the different ranges characteristic to each parameter (SPREAD,
A network of 10 nodes in the hidden layer, trained over 100 epochs with \textit{trainscg}, is used. The network is trained in less than a quarter of an hour. See Tab.17 for an overview.

<table>
<thead>
<tr>
<th>range [nm]</th>
<th>f1</th>
<th>f2</th>
<th>f3</th>
<th>f5</th>
<th>f6</th>
<th>f7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cab</td>
<td>400-700</td>
<td>4</td>
<td>5.5</td>
<td>19.5</td>
<td>30</td>
<td>1.5</td>
</tr>
<tr>
<td>LAI</td>
<td>1400-2400</td>
<td>12</td>
<td>15.5</td>
<td>30.5</td>
<td>4.5</td>
<td>21.5</td>
</tr>
<tr>
<td>Cw</td>
<td>1100-1370</td>
<td>47</td>
<td>47</td>
<td>25</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

Tab.17: Enlargement of the training set, while in the same time reducing the network architecture produces these results (deviation from the reference parameter) for the individual parameters of the different fields. The values within 20% deviation are highlighted in grey.

The relatively short training time coupled with the partly good results encourages further investigation. According to (Broge, 2001), several parameters impact in the VIS-NIR; maybe the separation of the parameters into expert networks, as introduced at the beginning of this section, is not the best solution to this problem, as many parameters interact. The canopy reflectance is thus only explainable by their interaction. It is decided to consider again all parameters together for retrieval.

The idea of small architectures is kept, whereas that of large training sets is discarded because the melioration of the results is not spectacular.

The process is started with a [25,5] network with 4000 training spectra over 200 iterations. A reduction to a [20,5] network trained with \textit{trainscg} with 4000 training spectra yields promising but unsecure results (Tab.18): two networks (same spectra, same architecture), produce different results at validation. The reason for this is that every time a network is created, the weights and biases are initialized randomly. This random choice of initial weights and biases affects the performance of the algorithm and produces a different mean square error every time a new training is done.

<table>
<thead>
<tr>
<th>deviation from ref. LAI [%]</th>
<th>11.5</th>
<th>46</th>
<th>4</th>
<th>8.6</th>
<th>14.8</th>
<th>2</th>
<th>15</th>
<th>13.4</th>
<th>16.7</th>
<th>18.7</th>
<th>5</th>
<th>13.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>deviation from ref. ala [%]</td>
<td>3.35</td>
<td>4.8</td>
<td>0</td>
<td>19.7</td>
<td>27.9</td>
<td>9.5</td>
<td>6.5</td>
<td>5.6</td>
<td>16.8</td>
<td>1</td>
<td>63.8</td>
<td>12.1</td>
</tr>
<tr>
<td>deviation from ref. Cm [%]</td>
<td>8.8</td>
<td>32</td>
<td>17.6</td>
<td>27.5</td>
<td>12.7</td>
<td>15.4</td>
<td>9.3</td>
<td>70.9</td>
<td>7.5</td>
<td>5.5</td>
<td>2.3</td>
<td>7.7</td>
</tr>
<tr>
<td>deviation from ref. Cab [%]</td>
<td>17.2</td>
<td>2</td>
<td>8</td>
<td>11.5</td>
<td>5</td>
<td>22.3</td>
<td>9.5</td>
<td>10.1</td>
<td>9</td>
<td>15.7</td>
<td>4.2</td>
<td>12.5</td>
</tr>
<tr>
<td>deviation from ref. Cw [%]</td>
<td>29</td>
<td>17.6</td>
<td>20.2</td>
<td>8.7</td>
<td>12.5</td>
<td>26.9</td>
<td>32.1</td>
<td>35.8</td>
<td>20.7</td>
<td>6.2</td>
<td>23.4</td>
<td>37.2</td>
</tr>
</tbody>
</table>

Tab.18: Same network and method ([20,5], 4000 spectra, 100 iterations), similar but nevertheless different results: left and right of the thick line through the table. Grey-shaded cells show deviations of less than 20% of the reference parameters. With a few exceptions, LAI, ala and Cab (but not Cw) can be retrieved within 20% deviation of its reference. The results on the right are slightly better for LAI, ala and Cab than on the left.

The results from Tab.18 ask for a quantification of the probability that a network produces a tendentially better or worse retrieval result. For this reason, fifty equal networks are trained and validated; after each validation, the net is reinitialized. Tab.19 summarizes the findings.

<table>
<thead>
<tr>
<th>probability of LAI within 20%</th>
<th>61</th>
<th>44</th>
<th>74</th>
<th>72</th>
<th>40</th>
<th>66</th>
</tr>
</thead>
<tbody>
<tr>
<td>probability of ala within 20%</td>
<td>82</td>
<td>68</td>
<td>76</td>
<td>78</td>
<td>2</td>
<td>82</td>
</tr>
<tr>
<td>probability of Cm within 20%</td>
<td>88</td>
<td>24</td>
<td>82</td>
<td>52</td>
<td>86</td>
<td>84</td>
</tr>
<tr>
<td>probability of Cab within 20%</td>
<td>76</td>
<td>76</td>
<td>74</td>
<td>48</td>
<td>84</td>
<td>78</td>
</tr>
<tr>
<td>probability of Cw within 20%</td>
<td>1</td>
<td>12</td>
<td>10</td>
<td>72</td>
<td>74</td>
<td>0</td>
</tr>
</tbody>
</table>

Tab.19: With 50 networks of [20,5], 4000 training spectra and 100 iterations, the probability for each parameter to be retrieved within 20% deviation of its reference. The cells in grey highlight probabilities over 0.75.
The technique *early stopping* described earlier is implemented in *Matlab*; 500 spectra are taken from the LUT as the training set. For the validation set, which acts as the data set with which the algorithm decides when the training is enough, 50 measured spectra from each field (300 in total) are chosen randomly and given the corresponding field parameter values. The network has an architecture of [15,5]; the early stopping algorithm stops after 30 iterations (depending on the initial values of the weights and biases; done several times, it could yield slightly different iteration numbers). Then the network is tested with the mean spectra of each field. The results are summarized in Tab.20.

<table>
<thead>
<tr>
<th>field number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>deviation of LAI from ref. [%]</td>
<td>0</td>
<td>10.6</td>
<td>9.2</td>
<td>17.7</td>
<td>26.8</td>
<td>10.9</td>
</tr>
<tr>
<td>deviation of ala from ref. [%]</td>
<td>26.9</td>
<td>8.4</td>
<td>11.7</td>
<td>11.7</td>
<td>50.2</td>
<td>1.1</td>
</tr>
<tr>
<td>deviation of Cm from ref. [%]</td>
<td>0</td>
<td>2.4</td>
<td>12.4</td>
<td>12.4</td>
<td>4.8</td>
<td>2.2</td>
</tr>
<tr>
<td>deviation of Cab from ref. [%]</td>
<td>13.3</td>
<td>30.7</td>
<td>33.4</td>
<td>33.4</td>
<td>27.2</td>
<td>13.5</td>
</tr>
<tr>
<td>deviation of Cw from ref. [%]</td>
<td>50.2</td>
<td>25.7</td>
<td>2.8</td>
<td>2.8</td>
<td>7</td>
<td>48</td>
</tr>
</tbody>
</table>

Tab.20: Network training stopped after 30 iterations by the algorithm: for each field, the deviation of retrieved value from the reference (in grey, values within 20%).

The *regularization* technique asks for small input data sets: this condition concerns the number of spectral bands as a minimum number of spectra, guaranteeing a certain diversity, should be given. So the point earlier discussed is met again: the redundancy of the numerous spectral bands. 62 wavelengths that replicate most faithfully the dominant features of a vegetation reflectance are chosen (Fig.19). The spectrum is divided into its most marked features: the VIS, the NIR, and the following two reflectance humps. If the structure is complex, there are many wavelengths selected (like in the VIS); if it is rather a simple form like the region 1500-1700nm, there are fewer points.
Fig.19: The reduction of all wavelengths to a few (62) that "summarize" the general features of a typical vegetation reflectance spectrum. The red circles are the chosen wavelengths, the two dotted vertical lines indicate where unstable spectrum portions have been let aside due to water absorption features.

As the input vector (62 wavelengths) is significantly smaller than for the other networks used in this study, the present network gets a downsized architecture of [8,5]. The training algorithm is \textit{trainbfg} (a quasi-Newton algorithm); the performance ratio parameter, a coefficient that modifies the performance function, is set to 0.4. The maximum number of training epochs is set to 60, because previous tests have shown that the additional decrease of the mean square error (target-retrieved) gets smaller with more iterations, thus increasing the probability of overtraining. In order to guarantee a stable result, the regularization algorithm is launched 50 times, and after each training the network is reinitialized (results Tab.21).

<table>
<thead>
<tr>
<th>field number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>% of LAI within 20%</td>
<td>98%</td>
<td>81%</td>
<td>100%</td>
<td>98%</td>
<td>2%</td>
<td>100%</td>
</tr>
<tr>
<td>% of ala within 20%</td>
<td>81%</td>
<td>100%</td>
<td>98%</td>
<td>98%</td>
<td>0%</td>
<td>100%</td>
</tr>
<tr>
<td>% of Cm within 20%</td>
<td>100%</td>
<td>2%</td>
<td>100%</td>
<td>72%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>% of Cab within 20%</td>
<td>100%</td>
<td>98%</td>
<td>0%</td>
<td>0%</td>
<td>36%</td>
<td>100%</td>
</tr>
<tr>
<td>% of Cw within 20%</td>
<td>0%</td>
<td>1%</td>
<td>10%</td>
<td>100%</td>
<td>100%</td>
<td>0%</td>
</tr>
</tbody>
</table>

Tab.21: Results for the 50 trainings with the \textit{trainbfg} algorithm; the performance ratio parameter is 0.4. For 50 trainings, the percentage of retrievals which are within 20% of reference value are given. Highlighted cells in grey call attention to retrieval rates with little probability (under 80%).

5. Discussion

■ Field data

As has been mentioned earlier in this work, little attention was given to how data was collected and measured. For each field, there are at least a hundred spectra measured around roughly 20 points. A few among them are biased by shadowing, error by handling the sensor, or else, but the amount of measurements seems to permit a good approximation of the reflectance of the field as a whole.

Within the fields, there is a variance regarding the sensor height over the canopy, as the canopy was not homogeneous and no ruler was used to determine the height. The sensor is handheld and slightly rotated: two more arguable points which do not permit perfectly equal measurements over the field.

The field measurements were performed by four different people, at different times of the day. Three of these four persons were doing it for the first time, and were thus lacking the practice and a sure hand.

The hemispherical photos were not taken exactly on the spot where the spectra were recorded. Thus, the structure expressed by the LAI and ala after calculation with the program does not refer explicitly to one reflectance. For that reason, all photos were taken together and a mean LAI and ala were calculated.

The laboratory measurements are also difficult to judge: the leaf water and dry matter content do not pose problem, as the method is simple; for Cab retrieval, it is different. The method used (Arnon, 1949) is described as obsolete (Porra, 2002). The widely accepted method by (Lichtenthaler, 1987) was not used; besides that, the operator had never used the technique before.
Equally mentioned earlier, the calculation of LAI and ala was performed without knowing what is really relevant in the selection of the different classes. The difference between thorough selection compared to a superficial selection of the different categories (sky, leaves, etc.) for the final result were not investigated. As LAI is an expression of the vertical amount of leaves, the increase in LAI is expected to be linear or at least increasing with the age of the plant and its height. But in the results from the field photos, there are inconsistencies (field 6).

**Models**

(Kimes, 2000) writes that the use of physically-based models is potentially more effective (in generalisation and accuracy) than the application of more empirical models, including the vegetation indices. Especially, an advantage of the modelling approach is that it is physically based and is independent, to a certain extent, of the vegetation type (Qin, 2000); SAIL, for example, is not suited for modelling trees or forest canopies. Empirical relationships based on VIs are limited by the restricted amount of information used (generally red and infrared bands), when compared to the number of input variables that determine RT (Weiss, 1999). These relationships between a parameter and the VI are variable for different biomes. A prior knowledge about the particular biome is required in order to determine the empirical equation coefficients.

There are two major limitations in operational use of modelling with BRDF models. The first one is related to the inversion process of such a model. Some models have multiple solutions, and the inversion may not converge (Jacquemoud, 1993). This may result in unreliable estimates of the biophysical variables. The other limitation is the computational time involved in a number of inversion processes, which is a major barrier when using large satellite images (Qi, 2000); this can be circumvented by using techniques like the LUT or the neural network, because the computationally expensive part can be done in advance.

RT models based on plane-parallel geometry have been increasingly used in vegetation remote sensing due to their reasonable balance between accuracy of representing the reality and computational simplicity. To calculate canopy directional reflectance, the canopy radiative transfer equation has to be solved. This can be done numerically or analytically. Analytical solutions are fast and easy to implement, but may not be very accurate. Numerical solutions are accurate, but the iterative process is computationally expensive (Qin, 2000).

Analytical solutions can be obtained by either approximating the canopy RT equation and solving it with the Kubelka-Munk (KM) theory, or decomposing the canopy radiation field into unscattered, single scattering and multiple scattering components, then estimating multiple scattering.

SAIL is an RT model based on KM theory, which is used as a first approximation of the canopy RT equation (radiance fluxes within the canopy) to avoid solving that equation numerically. Thus, the KM theory deals with vertical fluxes rather than directional radiance. There are two major drawbacks to these simplifications. First, it is, strictly speaking, not suited for directional reflectance calculation. Second, it can only approximate multiple scattering (Qin, 2000).

The strategy of decomposing the canopy radiation field has allowed to greatly improve the accuracy of single scattering reflectance by capturing some important phenomena like the canopy hot spot, anisotropic reflectance from the soil, which are most pronounced in the first-order scattering (Qin, 2000).
Numerical solutions can be used to seek accurate solution for all orders of scattering. They are quite flexible, and can work on both one-dimensional and three-dimensional geometries. However, as said before, the cost of higher accuracy is usually associated with more expensive computation, which is an important factor in practical applications (Qin, 2000).

The choice of a right canopy model depends on the specific application case (such as the land cover type). There are many RT models available, and they have been validated with variable accuracy and detail over particular (local) vegetation canopies and soils available to the modelers. Thus, it is of prime interest, before using a specific model, to investigate the sensitivity of the modeled reflectance to the input canopy physical and structural parameters of interest. If the model is not sensitive to the parameter(s) of interest or if it produces the same solution for different combinations of input parameters, one will not expect to retrieve those parameters beyond a certain accuracy limit, no matter which information extraction methods are used (Qin, 2000). A concrete demonstration of this problem are the results of the spectral minimisation with the LUT where 50 very similar spectra are made of a rather wide range of parameters.

A second issue is to use optimal observations that are most likely to produce the best estimates for the parameters. The optimal sampling schemes can be obtained through a sensitivity analysis with multispectral and angular data (either from field/laboratory measurements or from highly accurate 3-D models) (Qin, 2000). The variability of the sun zenith angles and that of the view angles may increase the overall reflectance variability and thus the information content. The optimal angles probably depend on the canopy type and structure, as well as the atmosphere (Kimes, 2000).

The different assumptions of the SAIL model simplify the canopy, but do not take into account the reality: for example, properties like the leaf size and the spatial location of the leaf elements are ignored (Goel, 2000). The clump nature of vegetation canopies affects the reflectance considerably around nadir-viewing directions (Qin, 2000).

A further issue to be discussed are the fix parameters: although there are three respectively two different sun illumination geometries for field 1 resp. 2 and 3, the hot spot parameter value used is the same for all three sunangles. (Qin, 2000) writes that the hot spot effect influences canopy reflectance around the retro-illumination direction. As observation direction diverges from the illumination direction, more and more shadows are revealed and the reflected radiance decreases (Qin, 2000). Thus, it might be appropriate to use different values for the hot spot.

There are model uncertainties that are difficult to explain: the overestimation of the VIS with PROSPECT is the most important. Many other improvements of canopy RT models are discussed in the literature; this is not the place to do it, it is referred to a review of the evolution of canopy RT modeling (Qin, 2000).

The minimisation algorithm method

The analysis with the synthetic data qualifies the method: PROSPECT-SAIL is invertible with this method and for these parameters. The algorithm retrieves the correct or nearly correct values for a majority of launches within a desired accuracy. If there are enough trials, then the method can retrieve the correct value and be considered robust and stable. This is the proof that the model pair is numerically invertible.

The transition to field data is more delicate. At canopy level, according to the study of (Ceccato, 2002), Cab drives the reflectance in the VIS. The fields that are accurately modelled in the VIS should permit retrieval of Cab, like field 5. Unfortunately, this is not
the case. On the other hand, fields which are not modelled precisely in the VIS (field 6), exhibit a good retrieval value.

Another particularity is the fact that field 1 is the only field which features satisfying results for all important parameters except Cm (see Tab.6). All other fields have maximally two satisfying results and sometimes another which is sufficient in accuracy.

The hypothesis that the field best simulated by PROSPECT-SAIL allows the best retrievals does not hold. Field 5 is better modeled than field 1 in the VIS (at least the simulated spectral curves are nearer to the mean of the measured ones), but the Cab retrieval results are better in field 1. A hypothesis for this may be the fact that absorption in the VIS is not modelled linearly with increasing values of Cab; the higher the value, the smaller the additional absorption (expression of saturation). Considering that all fields have an overestimated reflectance in the VIS, it may be that the model is not suited perfectly for modelling jute in the VIS; it systematically exaggerates the reflectance. Thus a certain overestimation in the VIS would be normal, while a curve approaching the mean of the measured spectrum would indicate an exaggerated value of simulation input parameter Cab measured in the laboratory.

Another hypothesis is that fields whose sun zenith angle is greater show better results. This does not hold for transect1, field1, but in this case the changing illumination intensity due to unstable meteorological conditions during measurement might by the most contributing factor.

Errors are to be expected: noise in the sensor, shading, soil influence that is different from the standard soil chosen, errors in the reference parameter measurements and calculations, model shortcomings, among others. The data have been collected but little attention has been paid to a precise monitoring of how measurements (especially in the lab) have been done. As the model transforms the measured field parameters into spectra with the shortcomings to be seen in Fig.15, it seems obvious that an inversion against such spectra must produce errors, since an inversion introduces a higher level of complexity (e.g. large number of variables and physical processes, complex mathematical formulations), and/or a higher potential of ill-posed problems (Kimes, 2000).

Forward modelling and inversion with synthetic data rely on the mathematics of constitution of the data. With the field data and all the uncertainties about errors and quality mentioned above, the mathematical relationship is weakened and/or biased; this makes it difficult to assess which factor decisively induces errors and noise and hinders a correct retrieval.

There is a rather complete decoupling between the optimisation algorithm and a given BRDF application. The algorithm contains no built-in efficiencies for handling RT problems, despite the fact that the RT is well-understood and users can know a priori the general effects of a change in a given parameter value; it remains a research challenge to incorporate this RT knowledge into the algorithm (Kimes, 2000).

Aside from the quality of the results, the method does not seem to be operatively applicable for the purpose of this work; it would be very time-consuming. Each reflectance, i.e. a pixel in a satellite image, should be inverted with a least 30 different starting parameter sets to have a statistical security (unstability of the solution), which takes roughly 20 to 30 minutes. Over an image of 0.5 mio pixels (=reflectances), for example, this method would need more than 23 years to calculate it all!

- The look-up table approach

The first LUT with 130’000 entries and without any constraints except for the ranges produces the best results at the synthetic level. At this level, the retrieval possibilities are
as follows: LAI can be estimated within a 20% accuracy, Cw within 15%, the other parameters (ala, Cm and Cab) within 10%.

At the validation level with field reflectances, the results are different, except for LAI, which is still retrievable within 20%. The majority of the parameters (22 of 30 (5 parameters*6 fields=30)) for the different fields can be retrieved within 20% (Tab.12), more than half of which even within 10%. Some values which are not within the 20% threshold can be explained: ala of field 6, as already mentioned, invites to be handled with precaution, as the value of 30˚ seems nonsensical. For other ill-retrieved values, it is more difficult to find a clear answer. A factor that generally might have negatively influenced the retrieval quality is the use of averaged hot spot and sun zenith angle values for all fields for building the LUT from which the values are derived.

The mystery of field 5 being poorly retrieved, while precisely modelled, is still not solved. Again also, field 1 parameters are reasonably well retrieved, while those of field 2 are not. This is partly explainable by the fact that PROSPECT-SAIL does not simulate well fields with low vegetation cover and a high soil fraction (Jacquemoud, 1993); but field 1 is not perfectly simulated either, and certainly worse than field 5 for example. Also, the deviations of Cab from the respective references for fields 6 and 1 are much greater than for field 5; nevertheless, the retrieval success results inversely to what one might expect: fields 1 and 6 are within a 10% deviation for all parameters, field 5 clearly outside. There is no clear reason either why the Cw values of fields 6 and 7 are over 25% deviation, while the rest is hardly above 15%; performing a comparison between the spectra and their corresponding parameters does not show any apparent reason.

Minimising upon spectra with only spectral information taken from nadir with a LUT of this size cannot yield more accurate estimation of the parameters; indeed the 50 spectrally similar spectra (of the LUT retrieval) have a relatively large variation of the parameter values. Complementary directional data might contribute to improve retrieval of the parameters giving information about the structure of the canopy (LAI, ala).

The parameters that are input of the LUTs in this work are all generated according to a uniform distribution; this is not how they are actually distributed in "real nature"; there are mathematical distribution that should explain the different parameters in an more accurate way.

The LUT method can be applied to the most sophisticated model and still be applied on a per pixel basis, because the computationally intensive work can be done in advance. The LUT is inherently designed to handle any arbitrary set of sun-view angles, and finally, does not need an initial guess to the model variables as does the minimisation algorithm (Kimes, 2000).

- The neural network

The neural network is promising at a synthetic level, but more than another method does not make sense without validation data. To train a network without checking for over-fitting with validation or test data, as it is done at the beginning of the section concerning the neural network with the expert networks, does not make sense. (Udelhofen, 2000) uses 3000 training spectra, and after every 10th iteration a validation check with a test set is performed. This technique is in essence the earlier described early stopping method. Neural network training is a complex matter ruled by trial and error to a large extent. Several techniques are tried in this work; chronologically it runs as follows: first the attempt is made to train the network without testing its generalization ability on field data; it is only validated on data that has the same origin, i.e. the RT model. This cannot give useful information on its transferability to data with slightly other characteristics. It seems fine to
calibrate a network with synthetic data, but the control mechanism must intervene much earlier than done in this work. After this, the expert networks are trained again with a focus for reducing their sizes; the validation data this time is the field data. As the results are not convincing, the training sets are increased. Neither technique yields sufficiently good results. It is decided to get back to train the network for all parameters simultaneously, with small architectures. The results, presented in Tab.19, can be qualified as sufficient, while not being really satisfying: ala, Cab and Cm can be retrieved within 20% of their reference for probabilities over 3/4, except for a few exceptions (field 5, which has bad results for all techniques, and ala of field 6, which is for long deemed a doubtful value).

The next technique tested is early stopping. The results in Tab.20 are not really sufficient, because the method retrieves only LAI in an acceptable manner. The results found earlier (not published, while trying other networks) for training of such a network indicate tendentially too few training steps: indeed better results are found if the network is trained with more iterations.

The training algorithm is stopped after 30 iterations, because while the training data is quite homogeneous per se, the validation spectra measured with the ASD is not, especially if combined with the measured parameter values. The early stopping of the training tends to point out to an inhomogeneous validation data set; the algorithm leaves the network as general as possible, so that it might fit somehow the disparate data of the fields. If this hypothesis holds, then calibrating a network with spectra from a model that will produce homogeneous data is not best suited shall the network receive faulty and noisy field data to "invert". (Combal, 2003) proposes to add noise and/or biases to the generated data to account for these measurement and model uncertainties. In this technique, spectra have been used first to make the training stop, then to test the network, being part of the mean: they are so not perfectly independant. To be acceptable, the method should be tested with new field measurements.

Regularization is a promising method regarding some of the results: LAI is retrievable in at least 80% of the cases, but mostly with nearly 100% probability within a 20% deviation of its reference, except for field 6 (see Tab.21). The method seems sensitive to canopy geometry parameters; ala is retrieved with very similar succes. The retrieval of Cm within the 20% threshold is almost secure for four fields out of six; Cw on the contrary is only successfully retrieved for two fields, and Cab for three fields. Especially field 2 gets Cm and Cw values which are far from the reference. For Cm, it is partly explainable by the fact that the NIR is overestimated by PROSPECT-SAIL (see Fig.15) and the network is trained with those models’ synthetic data. This could be an indication of overfitting. As Cw and Cm are in a certain relation (leaf water is more or less 80% of leaf weight, and both Cm and Cm are related to the same leaf area), if the network produces a fair result for Cw and not for Cm or conversely, then one could gather from it the value of the other parameter and cross-check the results. Unfortunately, even if this method were secure, there would still be field 2 which is not in the range of any usable results. Cab is not retrievable in this way, which seems a bit surprising because it is a very "local" parameter (located in the VIS); what is more, the region with the most wavelengths in the selection (see Fig.19) is precisely the VIS.

Generally, it should be said that as the validation is done with only six spectra (means of the field reflectances), the results (especially the good) should be considered with some caution.

The neural network method can be applied to the most sophisticated models and still be applied on a per pixel basis, because the computationally intensive work can be done in advance. The neural networks have not been generalised, as of yet, to handle any
arbitrary set of angles, but they do not require any initial guesses for the parameters (Kimes, 2000).

6. Conclusions

Measurement and model uncertainties make it difficult to invert biophysical parameters with nadir-measured spectra from the jute plant below a 10 to 20% error, as seem to indicate the results of the three methods applied in this work. Indeed, (Asner, 2000) qualifies the behaviour of vegetation and soils as highly anisotropic; thus, at least for structural parameters, there may be more information in directional data, i.e. in spectral data measured from different angles.

Studies in the literature (Baret, 1999, Pragnere, 1999) show that the LUT approach and the neural network approach generally perform best. (Kimes, 2000) finds that these two methods are efficient for regional and global applications. Both these methods can be applied on a per pixel basis for regional and global application. This is confirmed in this work. The traditional minimisation algorithm is not suitable for this kind of inversion; it is computationally to intensive. For some reason the algorithm seems to get trapped in local minima; besides that, there is the problem of the limitation of the modelling with PROSPECT-SAIL (non-uniqueness of the solutions).

Due to these limitations of the modelling, which concern all three methods, it might make sense to use a combination of methods (e.g. LUT and neural networks): first, use the strenghts of the respective methods in retrieving a certain parameter and second, diminish the uncertainty of the retrievals by cross-comparing them. The different results show that almost any parameter can be retrieved within 20% deviation of its reference with a reasonable security.

The LUT approach, while not being the ultimate method for inversion of nadir-view spectral data, certainly gives clues from where to start. LAI is to be retrieved within 20%, so as Cab (except for field 5). Cm and Cw, if considered as related, can allow a reciprocal improvement of their respective retrievals: each time one of them is badly retrieved for a field, the other is within the threshold and vice versa. Thus for Cm and Cw the probability to be retrieved properly within 20% is high. As retrieval accuracy with LUT depends directly on the model accuracy (Combal, 2003), it would be profitable to integrate much more prior information into the process to make up for the shortcomings of the model. The results of the spectral minimisation (Fig.17) seem to indicate that the ambiguities between variables are more intrinsic to the model structure than to the inversion.

The neural network approach, in the few applications illustrated in this study, shows that it is a relatively precise technique for certain parameters like LAI, ala or Cab. As the methods applied in this study show, it is relatively rapidly implemented; one can imagine that it could act as a security check upon retrieved values from a look-up table, for instance. An idea proposed earlier is to integrate noise and biases into the training set, thus lessening the gap between the homogeneous model data and the more inhomogeneous field data (Combal, 2003).

This study is not a comprehensive research work that compares three methods thoroughly to yield a definitive answer to the questions that were posed. There are definitively more issues to be looked into, for each of the three methods; simply, not every track could be followed and investigated in appropriate depth for a lack of time and scope of this master thesis. This work may be useful to recognise what has been done, and by that what is proven not to be operationable on a regional scale; there are many more uncertainties,
especially when the next step is taken, i.e. the coupling of an atmosphere model and the
calibration of the method(s) to specific or general sensor configurations.
There are also other possibilities. The method of the LUT or the neural networks could be
kept, but an more complex model as the PROSPECT-SAIL combination could be used.
Also, the investigated crop is spectrally known; if it can be discriminated from other major
crops grown in the region under scrutiny, it might make sense to determine several
optimal vegetation indices to relate to some parameters and use this empirical method, as
some of the drawbacks (extrapolation, vegetation heterogeneity) of these methods do not
or only partially apply in this case.

7. Annex

- Tables

Tab.A-1: Input parameters for the calculation of N with the 2 empirical formulas proposed by
(Ceccato, 2001)

<table>
<thead>
<tr>
<th>sample nb</th>
<th>mean leaf area [cm²]</th>
<th>dry leaf weight [g/cm²]</th>
<th>SLA ['']</th>
<th>N(Cecc.)</th>
<th>N(other)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>36.79</td>
<td>1.21 (5 leaves)</td>
<td>152.02</td>
<td>0.9</td>
<td>0.28</td>
</tr>
<tr>
<td>2</td>
<td>33.72</td>
<td>1.05 (5 leaves)</td>
<td>160.57</td>
<td>0.9</td>
<td>0.28</td>
</tr>
<tr>
<td>3</td>
<td>34.57</td>
<td>1.18 (5 leaves)</td>
<td>146.48</td>
<td>0.9</td>
<td>0.29</td>
</tr>
<tr>
<td>4</td>
<td>24.39</td>
<td>0.8 (5 leaves)</td>
<td>152.44</td>
<td>0.9</td>
<td>0.28</td>
</tr>
<tr>
<td>5</td>
<td>28.14</td>
<td>0.79 (5 leaves)</td>
<td>178.1</td>
<td>0.9</td>
<td>0.27</td>
</tr>
<tr>
<td>6</td>
<td>30.01</td>
<td>0.92 (5 leaves)</td>
<td>163.1</td>
<td>0.9</td>
<td>0.28</td>
</tr>
<tr>
<td>7</td>
<td>25.82</td>
<td>0.85 (5 leaves)</td>
<td>151.88</td>
<td>0.9</td>
<td>0.28</td>
</tr>
<tr>
<td>8</td>
<td>36.88</td>
<td>1.34 (5 leaves)</td>
<td>137.61</td>
<td>0.9</td>
<td>0.29</td>
</tr>
<tr>
<td>9</td>
<td>26.33</td>
<td>1.13 (5 leaves)</td>
<td>116.5</td>
<td>0.9</td>
<td>0.30</td>
</tr>
<tr>
<td>10</td>
<td>22.4</td>
<td>0.85 (5 leaves)</td>
<td>131.76</td>
<td>0.9</td>
<td>0.30</td>
</tr>
</tbody>
</table>

Tab.A-2: Parameter values of the measured fields, derived in the laboratory, with software or by
calculation. The fields are classified according to their age in weeks after day of sowing.

<table>
<thead>
<tr>
<th>fields</th>
<th>2</th>
<th>6</th>
<th>1</th>
<th>3</th>
<th>5</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cab [µg/cm²]</td>
<td>56.2</td>
<td>77.1</td>
<td>65.5</td>
<td>84.1</td>
<td>86.2</td>
<td>66.9</td>
</tr>
<tr>
<td>Cw [g/cm²]</td>
<td>0.017</td>
<td>0.026</td>
<td>0.017</td>
<td>0.02</td>
<td>0.026</td>
<td>0.017</td>
</tr>
<tr>
<td>Cm [g/cm²]</td>
<td>0.004</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.007</td>
<td>0.006</td>
</tr>
<tr>
<td>N</td>
<td>2.76</td>
<td>2.76</td>
<td>2.76</td>
<td>2.76</td>
<td>2.76</td>
<td>2.76</td>
</tr>
<tr>
<td>LAI</td>
<td>1.4</td>
<td>1.8</td>
<td>2.2</td>
<td>2.6</td>
<td>2.8</td>
<td>2.6</td>
</tr>
<tr>
<td>ala ['']</td>
<td>62</td>
<td>30</td>
<td>62</td>
<td>42</td>
<td>50</td>
<td>46</td>
</tr>
<tr>
<td>hot spot</td>
<td>0.1</td>
<td>0.09</td>
<td>0.12</td>
<td>0.12</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>sun zenith angle ['']</td>
<td>2, 6</td>
<td>2.12</td>
<td>28.9, 9.4, 6</td>
<td>10, 7.9</td>
<td>5.36</td>
<td>2.8</td>
</tr>
<tr>
<td>diffuse fraction</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>
Matlab codes

(Matlab commands are preceeded with >.)

These codes are shared by courtesy of F. Baret, S. Jacquemoud and B. Kötz.

---

**Code 1: minimisation algorithm**

Function name: it produces randomly start parameters for the minimization algorithm. Ref is the reference reflection upon which to minimise.

```
function params=machine(ref)
>v=rand(200,5);

Definition of parameter range: [min,max] => (max-min)*rdlutp+min
>v(:,1)=(100-1)*v(:,1)+1;   % Cab
>v(:,2)=(0.1-0.001)*v(:,2)+0.001;   % Cw
>v(:,3)=(0.09-0.0002)*v(:,3)+0.0002;   % Cm
>v(:,4)=(6-0.1)*v(:,4)+0.1;   % LAI
>v(:,5)=(85-5)*v(:,5)+5;   % ALA
>save v v
```

Call the function (invsail) that will minimize the merit function.

```
>for i=1:size(v,1)
>    x(i,:)=invsail(v(i,:),ref,50,0.07,4)
>end
```

---

Inversion function: start parameters, reference, leaf angle, hot spot, sun angle.

```
function var=invsail(v,refle,alaleaf,hs,sz)
    >coef_init=coefspe;
    >liste_wave=[400:1:2400]’;
    >for i=1:length(liste_wave);
        indice=find(coef_init(:,1)==round(liste_wave(i)));
        coef(i,:)=coef_init(indice,:);
    end
    >coef(1397:1555,:)=[];
    >coef(950:1026,:)=[];
    >load(’soil.dat’);
    >rs1=soil(:,2);
    >Refle=refle;
    >sz=sz*pi/180;
    >N=[2.6];
    >options=optimset(’MaxIter’,60000,’MaxFunEvals’,
            60000,’MaxFunEvals’,60000,’Display’,’iter’);
```

Matlab minimisation function: fminsearch

```
>var=fminsearch(’prosailgil’,v,options,Refle,N,alaleaf,hs,sz,
        coef,rs1);
```

Function ‘prosailgil’ called by fminsearch. This is the function we want to minimise.

```
v=[Cab Cw Cm LAI ala(canopy)]
```

Prospect code.

```
>k=v(1).*coef(:,4)+v(2).*coef(:,5)+v(3).*coef(:,3);
```
\[ \text{pe} = N; \]
\[ \text{lrt} = \text{noyau} (\text{coef}(:,2), \text{pe}, k./\text{pe}, \text{tav} (\text{alaleaf} \cdot \pi/180, \text{coef}(:,2))); \]
\[ \text{refl} = \text{lrt}( :, 1); \]
\[ \text{tran} = \text{lrt}( :, 2); \]

SAIL code.
\[ \text{rsail} = [\text{sail} \_ \text{marie}(v(4), v(5), \text{hs}, \text{refl}, \text{tran}, \text{rs1}, \text{rs1}, \text{rs1}, 0, \text{sz}, 0, 0.2)]; \]

Difference between reference and momentaneous simulated reflectance.
\[ \text{diff} = \text{norm} (\text{rsail} - \text{Refl}); \]
\[ \text{else} \]
\[ \text{diff} = 10000; \]
\[ \text{end} \]

**Code 2: generate parameters and create a look-up table**

Name of the function.
\[ \text{function f=gen_lutp}; \]

Create a matrix with 130000*6 values between 0 and 1.
\[ \text{rdlutp} = \text{rand}(130000,6); \]

Definition of parameter range: [min,max] = (max-min) * rdlutp+min.
\[ \text{rdlutp}( :, 1) = (4.5-0.5) \times \text{rdlutp}( :, 1) + 0.5; \quad \% \text{LAI} \]
\[ \text{rdlutp}( :, 2) = (80-10) \times \text{rdlutp}( :, 2) + 10; \quad \% \text{ALA} \]
\[ \text{rdlutp}( :, 3) = (0.01-0.001) \times \text{rdlutp}( :, 3) + 0.001; \quad \% \text{Cm} \]
\[ \text{rdlutp}( :, 4) = (100-25) \times \text{rdlutp}( :, 4) + 25; \quad \% \text{Cab} \]
\[ \text{rdlutp}( :, 5) = (0.04-0.01) \times \text{rdlutp}( :, 5) + 0.01; \quad \% \text{Cw} \]
\[ \text{rdlutp}( :, 6) = (2.9-2) \times \text{rdlutp}( :, 6) + 2; \quad \% \text{N} \]
\[ \text{lutp} = \text{rdlutp}; \]
\[ \text{save lutp lutp}; \]
\[ \text{clear lutp}; \]

Load soil reflectance.
\[ \text{load} (\text{soil.dat}); \]
\[ \text{rs1} = \text{soil}( :, 2); \]

Definition of sun angle and view angle.
\[ \text{angle} = \text{sz} \times \pi/180; \]
\[ \text{tobs} = 0 \times \pi/180; \]

Adapt coefficients for PROSPECT to wavelengths given by soil.
\[ \text{liste_wave} = [400:1:2400]'; \]
\[ \text{coef_init} = \text{coefspe}; \]
\[ \text{for i=1:length(liste_wave)} \]
\[ \quad \text{indice} = \text{find} (\text{coef_init}( :, 1) == \text{round} (\text{liste_wave}(i))); \]
\[ \quad \text{coef}(i, :) = \text{coef_init}(\text{indice}, :) ; \]
\[ \text{end} \]
\[ \text{for i=1:size(soil,1)} \]
\[ \quad x(i,:) = \text{coef}(\text{find}(\text{coef}(i,1)==\text{soil}(i,1))); \]
\[ \text{end} \]
\[ \text{coef} = x; \]
\[ \text{load} (\text{lutp}); \]
\[ \text{rdlutp} = \text{lutp}; \]

Calculation with PROSPECT (k,lrt) and SAIL (rdlutr)
\[ \text{for it=1:size(rdlutp,1)} \]
\[ k = 85.0 \times \text{coef}(i, 4) + \text{rdlutp}(it, 4) \times (\text{coef}(i, 5) + \text{coef}(i, 3) \times \text{rdlutp}(it, 2)) \]

\[ \text{lrt} = \text{noyau}(\text{coef}(i, 2), 2.6, k / 2.6, \text{tav}(50 \times \pi / 180, \text{coef}(i, 2))) \]

\[ \text{rdlutr}(it, :) = [\text{sail}_\text{marie}(\text{rdlutp}(it, 1), 50, \text{hs}, \text{lrt}(:, 1), \text{lrt}(:, 2), \text{rs}1, \text{rs}1, \text{rs}1, \text{tobs}, \text{angle}, 0, 0.20)]' \]

end

**Code 3: cost function of the look-up table**

Create a matrix the same size of rdlutr for substraction; rsail is reference.

\[ \text{ref} = \text{repmat}(\text{rsail}', \text{size}(\text{rdlutr}, 1), 1) \]

\[ \text{diff} = \text{sum}((\text{ref} - \text{rdlutr})^2, 2) \]

Select best 50 of sorted differences

\[ \text{diff}_{\text{sort}} = \text{sort}(	ext{diff}); \]

\[ \text{diff}_{\text{sort}, 50} = \text{diff}_{\text{sort}, (1:50,:)} \]

\[ \text{for } i = 1:50 \]

\[ \text{indice}(i, :) = \text{find}((\text{diff}_{\text{sort}, 50}(i, :) == \text{diff}) \]

end

Find corresponding parameters and corresponding reflectances.

\[ \text{par} \_\text{best} = \text{lutp}(\text{indice}, :) \]

\[ \text{ref} \_\text{best} = \text{rdlutr}(\text{indice}, :) \]

Median and standard deviation of best 50 parameters

\[ \text{median}50 = \text{median}((\text{par} \_\text{best}), 1) \]

\[ \text{stdev} = \text{std}((\text{par} \_\text{best}), 1) \]

**Code 4: create and train a network**

Create a new feed-forward network with 2 layers. First layer has 150 neurons, transfer function is tan-sigmoid; second layer has 2 nodes, transfer function is linear. For a vector input e.g., the desired output are 2 variables. Training algorithm is *trainscg*, options are: 5000 iterations maximum, performance function goal: 0.1; the rest of the options are left to the default. p is the training set of input vectors, minmax(p) indicates the range of "all possible occurrences". t is the training target set corresponding to p.

\[ \text{net} = \text{newff}((\text{minmax}(\text{p})), [150, 2], {'tansig', 'purelin'}, 'trainscg') \]

\[ \text{net} \_\text{trainParam}.\text{goal} = 0.1; \]

\[ \text{net} \_\text{trainParam}.\text{epochs} = 5000; \]

\[ \text{net} = \text{train}((\text{net}, \text{p}, \text{t}); \]

The training takes some time. p_val is the validation set of input vectors, t_val the corresponding targets. When it is done, test the net for efficacy:

\[ \text{simul} = \text{sim}((\text{net}, \text{p}_{\text{val}})) \]

Simul produces the parameters "guessed" from p_val. Compare with t_val for deviations.

**8. References**


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