Improved Estimates of Vegetation Biophysical Variables from Satellite Observations using Spatial and Temporal Constraints

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Abstract: A new method for estimating canopy biophysical variables from the satellite observations is developed based on a variational assimilation technique. This allows accounting for the spatial and temporal constraints in the estimation process of crop characteristics. Inversion will be achieved concurrently over an ensemble of pixels belonging to a spatial and temporal window. This ensures the problem to be better posed than when solved over single pixels and dates. Atmospheric characteristics are assumed steady within the spatial window, but vary from date to date. Conversely, surface characteristics are assumed to be steady within the limited temporal window, but spatially variable. This paper explains the variational assimilation theory used here, the surface and atmosphere radiative transfer models considered, and the ensemble assimilation scheme applied to account for the spatial and temporal constraints.

1. Introduction

Estimates of canopy biophysical variables from the satellite observations is one of the key issues in remote sensing. In the last few years, a number of studies have reported encouraging results using radiative transfer model inversion techniques.

Recent reviews of biophysical properties retrieval methods (Combal, *et al.*, 2002 ; Baret *et al.,* 2003) showed that most of radiative transfer inversion techniques were based on iterative optimization (Jacquemoud *et al.,* 2000) or neural networks methods (Weiss *et al.*, 2002; Beal *et al.*, 2005). However, the inversion of radiative transfer models is a severely ill-posed problem that may lead to significant uncertainties in the biophysical variables estimates when limited information is used. The improvement of the performances of the inversion process requires more information to be exploited including better radiative transfer models, exploitation of proper prior information on the distribution of the canopy and atmosphere variables, knowledge of uncertainties in satellite measurements, as well as possible spatial and temporal constraints. In this study we focus on the use of coupled surface-atmosphere radiative transfer models (SMAC and SAIL+PROSPECT) and on the exploitation of the possible spatial and temporal constraints to estimate more accurate LAI values from the satellite observations. For this purpose, an ensemble of pixels belonging to a spatial and temporal window will be considered simultaneously, representing a very large inversion problem as compared to inversion applied to the single pixels. The coupled model is inverted with a variational method particularly efficient for very large inverse problems. Its implementation is based on the computation of the adjoint model and a Bayesian cost function allowing accounting also for prior information on the distribution of the variables.

This paper explains the variational assimilation theory used here, the surface and atmosphere radiative transfer models considered, and the ensemble assimilation scheme applied to account for the spatial and temporal constraints.

2. Variationnal Data Assimilation Method

2.1 Principles of the method

For sake of simplicity, the method is explained in its most synthetic form, inspired from Le Dimet and Talagrand (1985).

Let consider a system (D) that expresses the temporal evolution of a state variable X, as a function of the direct model F and some control variables K and of its initial conditions U at time 0:

$$\left\{\begin{array}{lcl} \dfrac{dX}{dt} & = & F(X,K) \\ X(0) & = & U \end{array}\right. \qquad \text{(D)}$$

The system (D) has a unique solution if U and K are known. Considering that observations X_{obs} of the state variable X are acquired, the method consists in estimating the control variables K for which the simulated time course of the state variable best matches the observations. This is performed by minimizing the cost function measuring the discrepancy between 1) the solution X of the model and the observations X_{obs}, 2) the initial condition U and corresponding prior information U_0, and 3) the control variable K and some *a priori* information K_0 on it.

$$J(K) = \frac{1}{2}\int_0^T \|X - X_{obs}\|^2 + \frac{1}{2}\|U - U_0\|^2 + \frac{1}{2}\|K - K_0\|^2$$

The optimal values for the parameters are determined in such a way that they minimize the cost function J. They are characterized by the Euler-Lagrange Condition of Optimality:

$$\left\{\begin{array}{lcl} \nabla_U J(U,K) & = & 0 \\ \nabla_K J(U,K) & = & 0 \end{array}\right.$$

where $\nabla_U J(.)$ and $\nabla_K J(.)$ are the gradients of J with respect to U and K. Their calculation will be performed analytically by introducing an adjoint variable P of the state variable X ; P is solution of the Adjoint Model (D*):

$$\begin{cases} \frac{dp}{dt} + \left[\frac{\partial F}{\partial X}\right]^T p = X - X_{obs} \\ p(T) = 0 \end{cases} \qquad \text{(D*)}$$

Thanks to mathematical properties of the adjoint variable P, the backward integration of the adjoint model (D*) permits to express the gradients as:

$$\begin{cases} \nabla_U J(U,K) = -p(0) + U - U_0 \\ \nabla_K J(U,K) = -\int_0^T \left[\frac{\partial F}{\partial K}\right]^T dt + K - K_0 \end{cases} \qquad \text{(GradJ)}$$

2.2 Minimization Algorithm

From a computational point of view, the estimation of the optimal parameter set is performed by plugging the value of the gradient (GradJ) in a descent type method of optimization (conjugate gradient, Quasi-Newton, Truncated-Newton, for instance). At each iteration, an evaluation of the model and of the gradient is achieved by the adjoint model. The minimisation algorithm used in this work is N1QN3, which consists in a Quasi-Newton optimization technique with BFGS update (Gilbert and Lemarechal, 1989).

2.3 Automatic Differentiation

Computation of the adjoint model is generally a tedious task. The adjoint model is better calculated with automatic differentiation tools when the model is complex enough. Automatic differentiation is a technique to evaluate the derivatives of a function defined by a computer program. The basic idea is to derive each statement of the direct code to obtain the directional derivatives (*tangent mode*) and transpose it to run backward in time and calculate the gradient (*reverse mode*) (Griewank, 1988).

Automatic differentiation was here performed by the TAPENADE software (Hascoët and Pascual, 2004). This tool takes the computer source program as an input and builds a new code that computes the gradient, which is called the adjoint model.

Even though automatic differentiation helped in the process of generating the adjoint model, it was difficult for some parts of the direct code that was not specifically written to be differentiated. Accurate adjoint model is mandatory because an error in the adjoint model will lead to a wrong gradient preventing from getting the right solution. The adjoint model has therefore to be carefully checked according to Taylor and scalar product tests.

2. The Radiative Transfer Models

Coupling the SAIL canopy reflectance model (Verhoef, 1984) with the PROSPECT leaf optical properties model (Jacquemoud and Baret, 1990) allows to simulate canopy reflectance from canopy structure, optical properties of vegetation elements, soil background reflectance, wavelength, view and illumination conditions. Background reflectance was assumed to be that of a typical soil with variation in its brightness using the brightness coefficient.

The SMAC model (Rahman and Dedieu, 1994) simulates the top of atmosphere reflectance as observed at the satellite level from top of canopy reflectance and atmospheric characteristics. SMAC was chosen because it is very computer efficient while keeping a good compromise in terms of accuracy compared to the physical and analytic 6S model from which it is derived (Vermote *et al,* 1997).

Coupling radiative transfer models SAIL+PROSPECT to an atmospheric correction allows relating the top of the atmosphere reflectance to the biophysical variables of interest such as Leaf Area Index (*LAI).*

The input variables of the models are the following:

- illumination and observation configuration that derives from satellite orbit characteristics and swath : the solar and view zenith angles, θs and θv and the relative azimuth φ.
- soil background reflectance spectrum and the brightness coefficient (Bs)
- leaf biophysical variables (N, Cab, Cw, Cm, and Cbp)
- canopy structure characteristics (LAI, ALA, Hotspot)
- atmosphere characteristics (τ_{550}, P_{atm}, C_{wv}, C_{03}).

3. Assimilation Scheme accounting for Temporal and Spatial Constraints

Implementation of several constraints requires creating a macro-model (MACRO-SPS) running simultaneously on several dates and pixels, where the spatial and temporal constraints are described by relations between the variables. Figure 1 shows how spatial and temporal constraints were here applied to atmosphere leaves, canopy, soil and geometry variables:

- atmosphere characteristics and geometry configuration, are fixed on a given temporal window:
  A = (τ_{550}, P_{atm}, C_{wv}, C_{03}, θv , θs , φ)
- Leaves and canopy properties are fixed on a given spatial window:
  C = (N, Cab, Cdm , Cs , LAI , ALA , Hotspot)
- The background brightness **Bs** can vary both temporally and spatially and is then unconstrained:

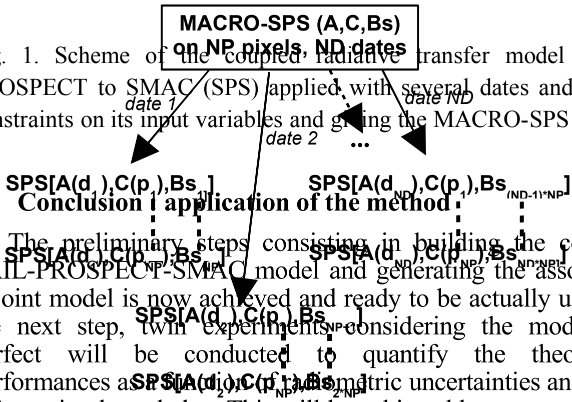

Fig. 1. Scheme of the coupled radiative transfer model SAIL-PROSPECT to SMAC (SPS) applied with several dates and pixels constraints on its input variables and giving the MACRO-SPS model.

4. Conclusion : application of the method

The preliminary steps consisting in building the coupled SAIL-PROSPECT-SMAC model and generating the associated adjoint model is now achieved and ready to be actually used. In the next step, twin experiments considering the models as perfect will be conducted to quantify the theoretical performances as a function of radiometric uncertainties and prior information knowledge. This will be achieved by comparison to more classical techniques applied over single individual pixels.

Then, the ensemble inversion will be applied to actual satellite observations to confront results to current biophysical products available. This innovative method could then be used to derive the best LAI values over a representative set of surface and atmosphere types. They could eventually constitute an ideal learning data base to train more operational algorithms such as neural networks to generate accurate products over large temporal and spatial coverage as required by the user community.

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