THE PHYSICS OF SPECTRAL INVARIANTS

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ABSTRACT

To make full use of the increased possibilities of imaging spectroscopy (compared with the traditional multispectral instruments) for remote sensing of vegetation canopies, physically-based models should be used. The problem of retrieving the large number of model parameters from remotely sensed reflectance data is an ill-posed and underdetermined one. The physically-based spectral invariants approach may, in some cases, seem a lucrative alternative. However, the various formulations presented in literature are sometimes difficult to compare qualitatively or quantitatively. To develop a robust spectral-invariant based algorithm for vegetation remote sensing, empirical, mathematical and physical understanding of the problem has to be reached. We present connections between the photon recollision probability and the largest eigenvalue of the radiative transfer equation. Based on simple mathematical principles, the basic requirements set by the remote sensing process to a successful spectral invariant theory are presented.

Index Terms— photon recollision probability, canopy reflectance model, spectral invariants

1. INTRODUCTION

The advantage of imaging spectroscopy compared to other remote sensing techniques is its ability to directly provide information on the status and functioning of vegetation. This information can further be utilized in ecological or classification applications [1]. Despite this large potential, most studies dealing with forests (which exhibit a clear three-dimensional structure) have been statistical or limited case studies. Statistical (or empirical) algorithms utilize a few specifically selected wavebands to estimate the values of biophysical variables from hyperspectral remote sensing data. While this approach has proven successful in interpretation of multispectral remote sensing data (e.g., Landsat or SPOT satellite images), statistical studies can only indicate the true potential of imaging spectroscopy. To make full use of the spectroscopic nature of hyperspectral remote sensing data, physically-based canopy reflectance models provide a more reliable and robust tool.

Even relatively simple physically-based canopy reflectance models depend on at least a dozen input parameters [2]. For more comprehensive models that can be used to exactly predict the spectral and directional reflectance properties of boreal forests (e.g. FRT, 5scale; reviewed by [3]), the number of input parameters is several times larger. The inverse problem, or finding canopy structural and biochemical characteristics from the reflected signal measured by RS instruments, is therefore a complex task. It has been known for a long time that the inverse problem is ill-posed as very similar reflectance signatures can be produced by completely different canopies [2].

The variables determining the spectral reflectance properties of vegetation canopies (forests, grasslands, etc.) can be roughly divided into two categories: biochemical and structural variables. Biochemical variables, or the chemical composition of scattering elements, determine the optical properties of plant leaves or needles. Structural variables describe the spatial and directional distributions of these scattering elements and can thus be viewed as modulators of the biochemical reflectance signal. The separability of the influences of the two variable classes is not clear [4], at least using traditional IS techniques. However, such a separation would be desirable for a more reliable inversion.

Canopy spectral invariants, eigenvalues of the radiative transfer equation and photon recollision probability are some of the new theoretical tools that have been applied in this area of remote sensing (e.g. [5, 6, 7, 8]). These tools, although originating from the same background, differ slightly in their scope, computational algorithms, and interpretation. The spectral invariant theoretical approach, informally also referred to as '*p*-theory', owns its attractivity to several factors. Firstly, this approach provides a rapid and physically-based way of describing canopy scattering. Secondly, *p*-theory aims at parameterizing canopy structure in reflectance models using a simple and intuitive concept that can be applied at various structural levels, from the shoot to tree crown. The most comprehensive treatment of the eigenvalues of radiative transfer operator in vegetation canopies is given by [6], a more mathematical description is given by [9]. However, several ambiguities remain, for example in the limits of appli-

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cability of the p-theory and in the exact definition of photon recollision probability. The purpose of this article is to clarify the relations between the different approaches used in the theory of spectral invariants.

2. THE THEORETICAL BASIS

2.1. Photon recollision probability

Photon recollision probability theory is based on the assumption that the radiation scattered by a vegetation canopy can be written as the infinite sum

$$\frac{s}{i_0} = (1-p)\omega + p(1-p)\omega^2 + p^2(1-p)\omega^3 + \ldots + (1-p)\omega^i p^{i-1} + \ldots \quad (1)$$

where s is canopy scattering (the fraction of incident radiation not absorbed by the canopy), i_0 is canopy interceptance (the fraction of incident radiation not directly transmitted by the canopy), and p is the *photon recollision probability*. In the sum Eq. (1), $(1-p)\omega^i p^{i-1}$ equals the contribution of photons scattered i times inside the canopy to the total canopy scattering s. A closed form can be easily found for Eq. (1) [10]:

$$\frac{s}{i_0} = \frac{(1-p)\,\omega}{1-p\omega}. \quad (2)$$

Despite being an approximation, Eq. (2) describes well the spectral scattering properties of various natural and computer-simulated vegetation canopies [6, 7, 4, 11, 12, 13].

2.2. Radiative transfer theory

We start by writing out the radiative transfer equation (RTE). Following the notation of [14] we write

$$(\Omega\cdot\nabla)I(\mathbf{r},\Omega) + \sigma(\mathbf{r},\Omega)I(\mathbf{r},\Omega) = \int_{4\pi} d\Omega' I(\mathbf{r},\Omega')\sigma_S(\mathbf{r},\Omega'\to\Omega) + Q_0(\mathbf{r},\Omega), \quad (3)$$

where $I(\mathbf{r},\Omega)$ is the scattered radiance in the direction Ω at the point $\mathbf{r}$ inside the canopy, σ is the volume extinction coefficient, σ_S is the volume scattering coefficient, and Q_0 is the source function due to incident radiation:

$$Q_0(\mathbf{r},\Omega) = \int_{4\pi} d\Omega' I_0(\mathbf{r},\Omega')\sigma_S(\mathbf{r},\Omega'\to\Omega), \quad (4)$$

where I_0 is the sum of the radiances of four radiation field components: incident direct solar radiation, diffuse sky radiation, ground-reflected unintercepted incident direct solar radiation, and ground-reflected unintercepted diffuse sky radiation. The volume extinction coefficient $\sigma(\mathbf{r},\Omega)$ is defined as the fraction of radiant energy traveling in the direction Ω intercepted by a unit volume of the vegetation canopy at the point $\mathbf{r}$. Similarly, the volume scattering coefficient $\sigma_S(\mathbf{r},\Omega'\to\Omega)$ gives the fraction of radiant energy traveling in the direction Ω' which is scattered by a unit canopy volume into a unit solid angle around Ω. Together with Eq. (3) we specify the boundary conditions

$$I(\mathbf{r},\Omega) = B(\mathbf{r},\Omega),\ \mathbf{r}\in\delta V,\ \mathbf{n}(\mathbf{r})\cdot\Omega < 0, \quad (5)$$

where δV is the canopy boundary, $\mathbf{n}(\mathbf{r})$ is the outward normal at the point $\mathbf{r}\in\delta V$, and $B(\mathbf{r},\Omega)$ is a wavelength-independent function defined on δV. The formulation of RTE as given by Eq. (3) assumes that $B(\mathbf{r},\Omega)$ at the canopy upper boundary δV_{top} is zero and incident radiation is described using the source term Q_0. At the bottom canopy surface δV_{bottom}, $B(\mathbf{r},\Omega)$ equals the ground-reflected diffuse flux,

$$\begin{cases} B(\mathbf{r},\Omega) = 0, & \mathbf{r}\in\delta V_{top},\ \mathbf{n}(\mathbf{r})\cdot\Omega<0 \\ B(\mathbf{r},\Omega) = \int\limits_{\mathbf{n}(\mathbf{r})\cdot\Omega>0} d\Omega' I(\mathbf{r},\Omega')\rho_{gnd}(\mathbf{r},\Omega'\to\Omega), & \\ & \mathbf{r}\in\delta V_{bottom},\ \mathbf{n}(\mathbf{r})\cdot\Omega<0. \end{cases} \quad (6)$$

When dealing with the eigenvalue problem, $\rho_{gnd}\equiv 0$.

2.3. The eigenvalue problem

The eigenvalue problem [7] in radiative transfer is finding the eigenvalues γ_i and eigenvectors ϕ_i of Eq. (3) satisfying

$$\gamma_i\left[(\Omega\cdot\nabla)\phi_i(\mathbf{r},\Omega) + \sigma(\mathbf{r},\Omega)\phi_i(\mathbf{r},\Omega)\right] = \int_{4\pi} d\Omega'\,\phi_i(\mathbf{r},\Omega')\sigma_S(\mathbf{r},\Omega'\to\Omega) \quad (7)$$

using vacuum boundary conditions: no radiation can enter the canopy from the outside. In practical terms, this means that the vegetation canopy is bounded from below by a black surface (soil) and no incident radiation exists, neither direct nor diffuse.

The eigenvalue problem (Eq. 7) is obtained from RTE (Eq. 3) by substituting the radiance I with ϕ_i, multiplying the left hand side Eq. 3 by γ_i and setting $Q_0\equiv 0$. According to [7], we should find the largest positive eigenvalue γ_1 corresponding to a unique positive eigenvector ϕ_1. The rest of the eigenvectors that are not positive throughout the vegetation canopy cannot be used alone (without the first eigenvector) to approximate the radiation field inside the canopy.

3. MERGING THE APPROACHES

3.1. Expansion into eigenvectors

One of the foundations of the spectral invariants theory is the expansion of the solution of the radiative transfer equation (Eq. (3)) into a series of eigenvectors. This technique is based on the completeness of the set of eigenvectors (i.e., any solution of RTE can be represented as a sum of eigenvectors) and the special properties of the radiative transfer problem allowing to derive the spectral dependence of the expansion coefficients [7, 9]. Thus, we can write

$$I(\mathbf{r},\Omega,\lambda) = \sum_{i=1}^{\infty} a_i(\lambda)\,\phi_i(\mathbf{r},\Omega). \tag{8}$$

The advantage of Eq. (8) is the separation of the functions of spectral and spatial variables. Further, giving a physical interpretation to Eq. (8) will let us use the the spectral dependence of $a_i(\lambda)$ to give us directly the p-theory. This approach has been used previously and we will not go into the details of the derivations. Thus, we can write that the spectral dependence of the expansion coefficients in Eq. (8) is given by Eq. (9):

$$a_i(\lambda) \sim \frac{p_i\omega(\lambda)}{1-p_i\omega(\lambda)} \tag{9}$$

Eq. (9), identical in form to p-theory (Eq. (2)), will allow us to interpret p-theory as the expansion of the scattered radiation field into a sum of eigenvectors and ignoring all but the first few terms. The first term with a spectral dependence described by the photon recollision probability p_1 describes total canopy scattering and other terms may be either correction terms for taking into account the deviation of true scattering from p-theory, or other "spectral invariants" describing the spectral behavior of the angular distribution of exiting radiance but without altering total scattering. However, the spectral behavior of all correction terms or spectral invariants is described by Eq. (9).

3.2. Merging via RTE

A more "physical" approach may be used to derive the p-theory from the equation of radiative transfer, Eq. (3). The details of the derivation are too long to be presented here, only the general traits of the derivation are described below. Merger is achieved by integrating the radiative transfer equation, Eq. (3), over all directions and the whole canopy volume V_{CAN}. If we know a solution of the eigenvalue problem, Eq. (7), i.e. an *eigenvector*, we can calculate 1) total canopy-leaving irradiance s and 2) total (internal) radiative energy contained inside the canopy E (also called *canopy interaction coefficient* by [6]). We can now calculate the ratio s/E and use it to characterize the structural complexity of the vegetation canopy. If we assume that the same s/E ratio is valid also for the solution $I'(\mathbf{r},\Omega)$ of a realistic canopy radiative transfer problem, we arrive at the p-theory, Eq. (2).

The spectral dependence of an eigenvector is exactly described by the p-theory, Eq. (2). Thus, if also the spectral dependence of a solution of the RTE, Eq. (3), $I(\mathbf{r},\Omega)$ is exactly described by the p-theory, integrating $I(\mathbf{r},\Omega)$ has to result in the s/E ratio of to an eigenvector of the RTE for all wavelengths. For stationary solutions, this leads to the conclusion that I' is itself an eigenvector of the RTE.

The spectral dependence of the first eigenvalue can be written as

$$\gamma_1 = p_1\omega. \tag{10}$$

Thus, choosing p_1, the p-value corresponding to the first eigenvalue γ_1, will give us a spectrally invariant parameter relating the first eigenfunctions $\phi_1(\mathbf{r},\Omega)$ for all wavelengths ω. Assuming that the eigenfunctions describe reasonably well the distribution of radiative energy $I(\mathbf{r},\Omega)$ inside the canopy, we may use the parameter p_1 to relate canopy scattering at different wavelengths.

4. SPECTRAL INVARIANTS IN REMOTE SENSING

The ability of spectral invariants to quantify the structural characteristics of a vegetation canopy should be beyond question. However, the usability of p depends also on whether the invariants provide additional information on canopy structure and if this structure can be related to real-life phenomena. Further, spectral invariants can successfully applied to vegetation remote sensing only if they can be related to the reflectance measured by a satellite- or airborne sensor.

The first spectral invariant p_1 corresponding to the first eigenvector ϕ_1 describes the spectral variation in canopy scattering in the form of Eq. (2). Although Eq. (2) is an approximation, simulation studies have indicated that the approximation works very well for many natural vegetation canopies [6, 7, 4, 11, 12, 13]. The largest shortcoming of Eq. (2) lies in its lack of any directional information. Indeed, the radiation is scattered both upwards and downwards (i.e., reflected or transmitted by the canopy) with the ratio of reflectance to transmittance changing considerably with the wavelength ω [12].

All remotely sensed vegetation reflectance retrievals are performed in only a limited number of directions, most commonly just one. Thus, for realistic retrievals, auxiliary information or supplemental (physically-based) models have to be used to relate reflectance to p_1. Fortunately, more information than just a single parameter p_1 should be retrievable from spectroscopic data. Such iformation may be used in models that range from simple parameterizations based on leaf area index or kernel-based approaches to full canopy reflectance models. The spectral invariants theory, however, proposes the use of additional spectral invariants corresponding to other eigenvalues and eigenvectors (ϕ_i, γ_i, $i \geq 2$). Although different spectral invariants have peen proposed, only the photon recollision probability p has been directly related to an eigenvalue of the RTE.

As discussed above, only the first eigenvector which is positive for all directions and the whole canopy volume can be used independently of other eigenvectors. The physical requirement of positive radiation field restricts the use of all other eigenvectors, and thus all other eigenvalues, without the first one. Indeed, Eq. (8) prescribes the use of all other eigenvectors ϕ_i ($i \geq 2$) as "correction terms" in the expansion of the radiation field into eigenvectors. Therefore, when retrieving eigenvalues from directional canopy scattering measurements, retrieval of several (at least two) eigenvalues should be attempted simultaneously: the first eigenvector cannot describe the directionality of canopy scattering; the remaining eigenvalues cannot describe the amount scattering. Unfortunately, no such algorithm exists today, it is also unclear how many eigenvalues and eigenvectors are required to predict the directionality of canopy reflectance with reasonable accuracy.

However, simultaneous use of more than one spectral invariant in describing basic directionality (up or down) of scattering, in addition to quantifying total scattering, has been recently demonstrated. The scattering asymmetry parameter proposed by [12] can be shown to be related to the ratio of first to second eigenvalues for simple canopy configurations. The extent of the practical usefulness of spectral invariants in remote sensing is still to be demonstrated. Such a demonstration requires, besides clear empirical evidence (which can already be found in the literature cited in this article), also strong physical and mathematical support.

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