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Review Article

Optical remote sensing and the retrieval of terrestrial vegetation bio-geophysical properties – A review

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ABSTRACT

Forthcoming superspectral satellite missions dedicated to land monitoring, as well as planned imaging spectrometers, will unleash an unprecedented data stream. The processing requirements for such large data streams involve processing techniques enabling the spatio-temporally explicit quantification of vegetation properties. Typically retrieval must be accurate, robust and fast. Hence, there is a strict requirement to identify next-generation bio-geophysical variable retrieval algorithms which can be molded into an operational processing chain. This paper offers a review of state-of-the-art retrieval methods for quantitative terrestrial bio-geophysical variable extraction using optical remote sensing imagery. We can categorize these methods into (1) *parametric regression*, (2) *non-parametric regression*, (3) *physically-based* and (4) *hybrid methods*. Hybrid methods combine generic capabilities of physically-based methods with flexible and computationally efficient methods, typically non-parametric regression methods. A review of the theoretical basis of all these methods is given first and followed by published applications. This paper focusses on: (1) retrievability of bio-geophysical variables, (2) ability to generate multiple outputs, (3) possibilities for model transparency description, (4) mapping speed, and (5) possibilities for uncertainty retrieval. Finally, the prospects of implementing these methods into future processing chains for operational retrieval of vegetation properties are presented and discussed.

1. Introduction

Vegetation bio-geophysical variable extraction, quantitatively retrieved and spatio-temporally explicit, is required in a variety of ecological and agricultural applications. Earth observation satellites in the optical domain enable the retrieval and monitoring of plant bio-geophysical variables (Moulin et al., 1998; Dorigo et al., 2007). The forthcoming super-spectral 'Copernicus' Sentinel-2 (Drusch et al., 2012) and Sentinel-3 missions (Donlon et al., 2012), as well as the planned EnMAP (Stuffler et al., 2007), HyspIRI (Roberts et al., 2012), PRISMA (Labate et al., 2009) and ESA's candidate FLEX (Kraft et al., 2012) imaging spectrometer missions will produce large data streams for land monitoring, which will soon become available to a diverse user community (Berger et al., 2012; Malenovsky et al., 2012). This vast data stream requires enhanced processing techniques that are accurate, robust and fast. The last few decades witnessed a variety of retrieval methods for vegetation attribute extraction coming into existence. Only a few made it to the status of genuine operational processing chain. Many others remained in an experimental state.

This paper provides a qualitative review of recently developed methodologies to estimate vegetation properties based on optical remote sensing (RS), covering the visible to shortwave infrared (SWIR) spectral region. By nature, bio-geophysical variables are continuous. Hence, methods which yield per-pixel estimations will be discussed, and which are potentially applicable in highly automated processing chains. Quantification of surface bio-geophysical variables with optical RS always relies on a model, enabling the interpretation of spectral observations and their translation into a surface bio-geophysical variable. Statistically, this boils down to a regression problem (Fernandes and Leblanc, 2005). Bio-geophysical variable retrievals, as described in terrestrial RS literature, are typically grouped in two categories: (1) the statistical (or variable-driven) category; and (2) the physical (or radiometric

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data-driven) category (Baret and Buis, 2008). Over the last decade, however, both methodological categories expanded into subcategories and combinations thereof. Exemplary is the increasing number of elements of both categories which have been integrated into hybrid approaches. Hence, a systematic categorization is a strong requirement. Retrieval methods can be binned in the following four methodological categories:

(1) *Parametric regression methods:* Parametric methods assume an explicit relationship between spectral observations and a specific bio-geophysical variable. Thus, explicit parameterized expressions are built, typically by relying on statistical or physical knowledge of the variable and the spectral response. Typically a band arithmetic formulation is defined (e.g., a vegetation index) and then linked to the variable of interest based on a fitting function.
(2) *Non-parametric regression methods:* Non-parametric methods directly define regression functions according to information from RS data. Hence, in contrast to parametric regression methods, a non-explicit choice is to be made on spectral band relationships, transformation(s) or fitting functions. These last ones can further be split into linear or non-linear regression methods.
(3) *Physically-based methods:* Physically-based algorithms are applications of physical laws establishing cause-effect relationships. Model variables are inferred based on specific knowledge, typically obtained with radiative transfer functions.
(4) *Hybrid methods:* A hybrid-method combines elements of non-parametric statistics and physically-based methods. Hybrid models make use of the generic properties of physically-based methods combined with the flexibility and computational efficiency of non-parametric non-linear regression methods.

This review paper aims to (1) provide a systematic overview of state-of-the-art bio-geophysical variable retrieval methods, and (2) evaluate strengths and weaknesses of these methods for operational application. This paper focuses on methods established for vegetation variable retrieval, typically leaf area index (LAI) and leaf chlorophyll content (LCC), which are very frequently applied terrestrial bio-geophysical products based on optical RS (Song, 2013). Yet, in principle the methods presented are applicable to the retrieval of other vegetation properties as well. For an overview of retrievable leaf biochemical and canopy bio-geophysical variables from superspectral or hyperspectral sensors we refer to Ustin and Gamon (2010) and Malenovsky et al. (2012). The four categories mentioned above will be reviewed in the next sections. For each of the categories, their general properties will be outlined and their use in mapping applications reviewed. Finally, the most important features of these categories will be discussed. The increasing occurrence of non-parametric methods in the recent literature makes us focus strongly on them. The review paper emphasizes on methods directly applicable to a remote sensing image. In principle, however, these methods can also be applied for time series analysis or be implemented in larger assimilation schemes. Also, the large majority of reviewed retrieval methods assumes the availability of surface reflectance, which implies an atmospheric correction prior to application of proposed methods (see Bassani et al. (2010) and Ruddick et al. (2014) for a review on atmospheric correction methods). A conclusion section will finalize this paper with recommendations fostering powerful bio-geophysical variable retrieval strategies that are applicable in next-generation operational processing schemes.

2. Parametric regression methods

Parametric regression methods explicitly determine parameterized expressions relating a limited number of spectral bands with a bio-geophysical variable of interest. This family of approaches has long been most popular in optical RS. These methods make use of subtle spectral features to reduce undesired effects, typically those related to variations of other leaf or canopy properties, soil reflectance, sun and view geometry and atmospheric composition. The principle entails mathematically defined combinations of spectral bands regressed with a bio-geophysical variable using a fitting function. The fitted function can be either linear or non-linear, e.g. an exponential, power, or polynomial fitting function. A scheme of a generalized parametric regression procedure is illustrated in Fig. 1.

2.1. Discrete spectral band approaches: vegetation indices

Parametric statistical approaches based on vegetation indices (VIs) are by far the oldest, most studied and largest group of variable estimation approaches. They are also the simplest ones. VIs are defined to enhance spectral features sensitive to a vegetation property while reducing disturbance by combining some spectral bands into a VI (Glenn et al., 2008; Clevers, 2014). The VI methods have been traditionally developed for sensors configured with only a few (broad) spectral bands. It is beyond the scope of this work to list all published VIs (see Le Maire et al., 2004, 2008, for an overview), though they can be categorized according to their mathematical definition. Some popular VI formalizations are:

- Two-band VIs, encompassing the majority of VIs, e.g., the simple ratio (SR) (Jordan, 1969), the normalized difference vegetation index (NDVI) (Rouse et al., 1974), the photochemical reflectance index (PRI) (Gamon et al., 1992), the optimized soil adjusted vegetation index (OSAVI) (Rondeaux et al., 1996), the chlorophyll index (Gitelson et al., 2003).
- Three-band VIs with, e.g., the triangular VI (TVI) (Broge and Leblanc, 2001), the modified chlorophyll absorption in reflectance index (MCARI) (Daughtry et al., 2000), the transformed CARI (TCARI) (Haboudane et al., 2002), the structure insensitive pigment index (SIPI) (Penuelas et al., 1995).
- Four or more band VIs, which are typically a combination of two VIs such as the TCARI/OSAVI (Haboudane et al., 2002).

The main advantage of VIs is their inherent simplicity. VI based methods found their origin in the first applications of broadband sensor satellites. Only a small set of spectral bands were available at that time and computational power was limited. With the advent of narrowband imaging spectrometers, with a few hundred spectrally narrow bands, paths for new extraction approaches of RS based information were developed. Optimized band information extraction algorithms based on established index formulations (e.g. simple ratio, normalized difference) were developed. By correlating all possible band combinations according to two-band indices, leading to 2D correlation matrices, it became feasible to visually identify optimal band combinations (e.g., Thenkabail et al., 2000; Le Maire et al., 2004, 2008; Mariotto et al., 2013; Rivera et al., 2014b). The so-called optimized or generic VIs permitted to select a 'best performing index'. Nevertheless, when applying this technique in studies making use of narrowband (hyperspectral) imaging, best performing identical spectral band combinations have rarely been reported. This suggests that optimized indices are strongly case specific (Gonsamo, 2011; Heiskanen et al., 2013; Mariotto et al., 2013). Hence, narrowband

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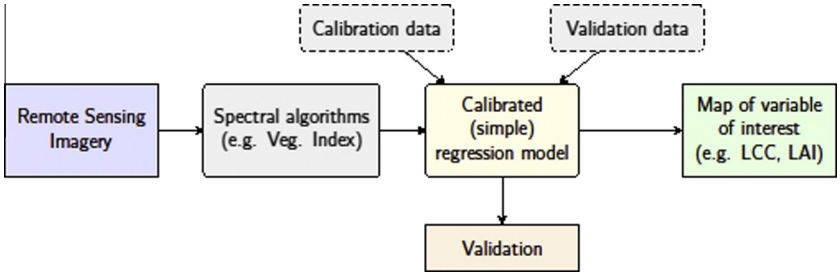

Fig. 1. Flowchart of a generalized procedure of parametric regression methods.

VIs can be successfully optimized for local applications, but seem to lack generic capacity.

2.2. Parametric approaches based on quasi-continuous spectral band configurations

Since a limited number of spectral bands is used, none of the above cited VIs makes use of available information to its full extent for quasi-continuous spectral datasets. This is a disadvantage when using contiguous radiometric image information. Attempts to improve full extraction of critical information from a quasi-continuous signal led to the development of so-called shape indices. These indices, listed below, extract shape related information from atmospherically corrected spectral signatures for a specific spectral region. They are then correlated with a bio-geophysical variable.

- *Red-edge position (REP) calculations.* Mathematically, the REP is the position of a wavelength at the maximum of the first derivative of the reflectance spectrum in the red-edge region (between 670 and 780 nm). The red-edge position is known to be sensitive to bio-geophysical variable variations. On the one hand it is sensitive to LCC, influencing the reflectance of vegetation in the visible part of the spectrum (Delegido et al., 2011). On the other hand, it is sensitive to LAI, mainly influencing the reflectance in the NIR (Delegido et al., 2013). Therefore, REP related methods are typically used to derive canopy chlorophyll content (CCC) – being the product of LAI and LCC – (Clevers and Kooistra, 2012). Many approaches have been proposed to use this region as a sensitive indicator, including: (1) high-order curve fitting (Baret et al., 1992; Broge and Leblanc, 2001; Clevers et al., 2002); (2) inverted Gaussian models (Miller et al., 1990); (3) linear interpolation and extrapolation (Guyot et al., 1988); (4) Lagrangian interpolation (Dawson and Curran, 1998), and (5) Rational function application (Baranoski and Rokne, 2005).
- *Integration-based indices.* Some authors proposed to calculate finite integrals for specific spectral regions, typically covering a part of the visible and the red-edge region, into a (normalized) index (Broge and Leblanc, 2001; Oppelt and Mauser, 2004; Mutanga et al., 2005; Malenovský et al., 2006; Delegido et al., 2010).
- *Derivative-based indices.* Instead of integration, the derivative of a spectral region can be calculated and transformed into an index. Various approaches have been published (Sims and Gamon, 2002; Penuelas et al., 1994; Elvidge and Chen, 1995; Zarco-Tejada et al., 2002). A systematic evaluation of first derivative-based indices was performed by Le Maire et al. (2004). These authors made a comparison between derivative-based and conventional indices using the leaf model PROSPECT. They concluded that derivative-based indices are not necessarily better than conventional and properly elaborated indices.
- *Continuum removal.* Whereas the techniques above focus on a specific spectral region, continuum removal is typically applied over the full spectrum. This technique normalizes reflectance spectra allowing to compare individual absorption features with a common baseline (Clark and Roush, 1984). The continuum removal transformation enhances and standardizes the specific absorption features related to vegetation properties. Applications of the method in vegetation science are maps of chlorophyll (Broge and Leblanc, 2001), nitrogen content (Mutanga and Skidmore, 2004, 2007; Schlerf et al., 2010; Mitchell et al., 2012), foliar water condition (Stimson et al., 2005) and grassland biomass (Cho et al., 2007).

2.3. Experimental and generic design of parametric methods: inherent limitations

The aforementioned methods share the property of being generalized as a regression function calibrated with *in situ* experimental data. Due to their empirical nature, these regression models are developed under various experimental setups, at different scales (leaf, plant, canopy), for different sensors (e.g., broadband vs. narrowband) and under different environmental conditions. Consequently, empirical methods cannot be translated into other observation configurations without losing predictive power. Their performance can be hampered by disturbing factors, e.g., differences in surface properties and sun and viewing geometry (Verrelst et al., 2008, 2010). Hence, while being successful in the extraction of vegetation variables designed for local conditions, they are of limited applicability in a broader operational setting. The lack of a generic capacity has been partly remediated by optimizing VIs and their associated regression models through the use of large datasets generated by leaf and canopy radiative transfer models (RTMs) (Ceccato et al., 2002; Zarco-Tejada et al., 2001, 2005; Haboudane et al., 2004; Le Maire et al., 2004, 2008). Nevertheless, it is still problematic that simulated, transformed data originating from a few discrete bands do not fully reflect the complexity of real world observation conditions. Reducing simulated datasets into simple VI formulations leads to remaining spectral information left unexploited. Hence, the following aspects should be considered:

(i) *Band selection.* Typically, parametric models are mathematical functions based on discrete bands, or at best a subset of full spectral information. How do we evaluate with high enough accuracy whether the most sensitive spectral bands – with respect to bio-geophysical variable retrieval – have been selected? This question is especially relevant in view of variable retrieval from hyperspectral datasets.

(ii) *Formulation.* Transformation of spectral information according to a mathematical expression should lead to an optimal sensitivity of the spectral signal with respect to the variable of interest. Typically, established algorithms like the NDVI type of indices are used. Here again the question must be

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posed as how to assess whether an applied formulation is the most accurate one with respect to bio-geophysical variable retrieval.

(iii) *Fitting function.* A regression function expressing the relationship between a VI and a bio-geophysical variable is selected. Regression modeling is typically an exercise of least squares fitting. Here as well, the question emerges whether a selected fitting function is the most suitable one.

Consequently, it remains uncertain whether regression functions are used optimally when applying an established parametric approach (as published in the literature) to process RS imagery into a bio-geophysical product. Moreover, since parametric approaches are based on relatively simple mathematical definitions – as opposed to more advanced methods – uncertainty intervals for the retrieval on a per-pixel basis are not provided. In absence of an uncertainty estimate, the performance of a parametric regression method is hard to judge in an operational environment. Accordingly, parametric regression methods are inadequate to deliver global or operational bio-geophysical products. A strength and weakness analysis of parametric regression methods is listed in Table 1.

3. Non-parametric regression methods

Optimization of non-parametric regression methods makes use of a learning phase based on training data. The model includes weights (coefficients) adjusted to minimize the estimation error of the variables extracted. An important advantage of the more advanced methods is the use of full-spectrum information. In contrast to parametric methods, an explicit selection of spectral bands or transformations is not required. A flexible model is able to combine different data structure features in a non-linear way, conform requirements. However, model definition with a too flexible capacity may incur the problem of over-fitting the training dataset. To avoid this pitfall, model weights are defined by jointly minimizing the training set approximation error while limiting model complexity. A scheme of a generalized non-parametric regression procedure is illustrated in Fig. 2. This section only reviews experimental mapping applications based on field data. The section is subdivided into linear and non-linear non-parametric models.

Table 1
Strengths and weaknesses of parametric regression methods in view of the operational mapping of vegetation attributes.

Strengths	Weaknesses
• Simple and comprehensive regression models; limited knowledge of the user required • Fast processing • Computationally inexpensive	• Makes poor use of available information within the spectral observation interval. At most a spectral subset is used. Therefore, these methods tend to be more noise-sensitive as compared to full-spectrum ones (Atzberger et al., 2010) • Parametric regression defines boundary conditions based on the level of selected bands, formulations and regression function • Tendency for overspecialization (i.e. models are specific to the dataset used for model characterization) • Sensor-specific models (i.e. a direct transfer to other sensors is usually not possible) • A parametric function accounts for one variable at a time • There is only a limited portability with respect to different measurement conditions or sensor characteristics (Baret and Guyot, 1991) • Uncertainty estimates are not provided. Hence the quality of the output maps remains unknown • Need for collecting field data (i.e. measurement campaigns are necessary)

3.1. Linear non-parametric models

A linear non-parametric regression model is usually chosen because of optimal performance and simplicity. It may, however not be the best choice when dealing with complex datasets exhibiting non-linear attribute relationships, as is often the case with multi- or hyperspectral imagery. Canonical linear regression methods typically rely on the estimation of co-variances. This can be problematic when input data quantity is limited with respect to the dimensionality of the dataset. This is known as the 'curse of dimensionality' (Hughes, 1968). To alleviate co-linearity, often linear methods are applied after a dimensionality reduction. In what follows, a number of classical linear approaches in RS applications are reviewed:

- *Stepwise multiple linear regression* (SMLR) recursively applies multiple regression a number of times. Each step removes a variable eliciting the weakest correlation. At the end of the recursive process, a variable set is obtained that is optimally explaining the RS data distribution.
- *Principal components regression* (PCR) is a regression analysis method based on principal components analysis (PCA) estimating regression coefficients (Wold et al., 1987). Solutions from PCR are generated performing linear regression of the most relevant components (called scores) obtained after applying PCA.
- *Partial least squares regression* (PLSR) tackles the co-linearity problem differently than PCR (Geladi and Kowalsi, 1986). Applying PCR, regression is performed using PCA scores. These projections are obtained using only input patterns, not outputs. In contrast, PLSR builds the regression model on projections obtained using the partial least squares (PLS) approach. It elicits the directions of maximum input–output cross-covariance. Therefore, PLSR takes both input patterns and output variables into account.
- *Ridge (regulated) regression* (RR). As in PCR and PLSR, ridge regression is a linear least squares regression method, developed to deal with co-linearity (Hoerl and Kennard, 1970). RR deals with it by allowing a degree of bias in the estimates. Therefore, it adds a small positive value λ to the diagonal elements of the input data covariance matrix. It can be shown that RR obtains biased estimates compared to standard linear regression, but with a lower variance (Hastie et al., 2009). Hence, RR requires finding an optimal value for λ. Typically, v-fold cross validation is used to reach near optimal values.
- *The least absolute shrinkage and selection operator* (LASSO) is a regression method penalizing the regression coefficients absolute size (Tibshirani, 1996). By this penalization some of the variable estimates may be exactly zero. The larger the penalty, the more the estimates will tend toward zero. This is a convenient approach to automatically perform variable (band) selection, or to deal with correlated predictors.

SMLR is often used for the selection of spectral bands carrying relevant information related to vegetation attributes (Fourty and Baret, 1997; Yoder and Pettigrew-Crosby, 1995; Dorigo et al., 2007). Lately, SMLR has been compared with alternative regression techniques. For instance, Darvishzadeh et al. (2008a) found that PLSR yielded better results when estimating LAI and leaf and

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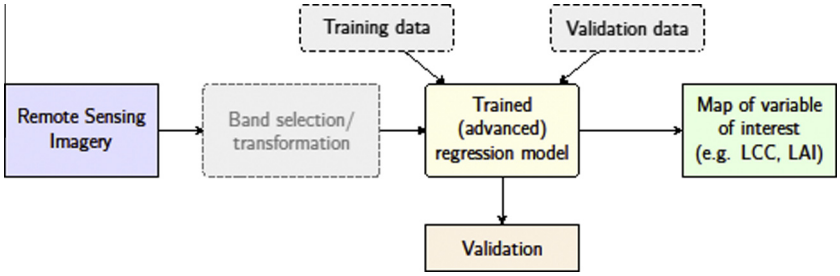

Fig. 2. Flowchart of a generalized procedure of non-parametric regression methods. Band selection/transformation is optional.

canopy chlorophyll content. Ramoelo et al. (2011) applied both regression algorithms to estimate foliar nitrogen and phosphorus in combination with continuum removal using field spectrometry. SMLR and PLSR have been found performing comparably when estimating soil properties (Bartholomeus et al., 2012). By estimating canopy nitrogen, Miphokasap et al. (2012) demonstrated that the model developed by SMLR yielded a higher correlation coefficient with nitrogen content than model applications based on narrowband VIs, suggesting that non-parametric (full-spectrum) models tend to be more powerful than parametric models.

PLSR is one of the most widely applied non-parametric approaches to map vegetation properties. For instance, Coops et al. (2003), Huang et al. (2004) and van der Heijden et al. (2007) applied PLSR to estimate foliage nitrogen content with hyperspectral data. Gianelle and Guastella (2007) used PLSR to derive grassland phytomass and its total (percentage) nitrogen content with hyperspectral data. Cho et al. (2007) and Im et al. (2009) applied PLSR to estimate bio-geophysical properties of crops (LAI, stem biomass and leaf nutrient concentrations), while Wolter et al. (2009) applied PLS to map forest structural variables (canopy diameter, tree height, crown closure). Hansen et al. (2002) and Ye et al. (2007, 2008) applied PLSR for yield prediction purposes. Mapping speed and availability in common imaging processing packages may explain the popularity of PLSR.

So far, RR and LASSO techniques hardly made it to applications for vegetation properties mapping. However, a few sparse examples are worth mentioning. Addink et al. (2007) used RR to map LAI and biomass. In another study both techniques were compared with PLSR (Lazaridis et al., 2011) and also with random forests (Zandler et al., 2015). Interestingly, RR and LASSO appeared to perform better than the other methods at least in general. Hence, it is remarkable that these techniques have not been applied more often. None of these linear non-parametric methods has even been incorporated in operational or global retrieval schemes. On the other hand, the linear methods are increasingly replaced by their non-linear counterparts. For instance, RR has been replaced by kernel ridge regression (KRR) (Suykens and Vandewalle, 1999), and PLS has been redesigned into a kernel version, i.e. the KPLSR, which proved to be more powerful than traditional PLSR for chlorophyll concentration estimation (Arenas-García and Camps-Valls, 2008). In Section 3.2.3 we will address the family of kernel methods.

3.2. Non-linear non-parametric models

For the last few decades, a diversity of non-linear, non-parametric models has been developed, going beyond linear transformation techniques. These methods, also referred to as machine learning regression algorithms (MLRAs), apply non-linear transformations. They assume that relationships between image features are non-explicit. An important methodological advantage is the capability to capture non-linear relationships of image features without explicitly knowing the underlying data distribution. Hence, they are developed without assuming a particular probability density distribution; therefore, they work well with different data types. They also offer the possibility to incorporate *a priori* knowledge and they have the flexibility to enable the combination of different data types into the analysis.

3.2.1. Decision tree learning

Decision tree learning is based on decision tree predictive modeling. A decision tree is based on a set of hierarchical connected nodes. Each node represents a linear decision based on a specific input feature. A classical decision tree algorithm cannot cope with strong non-linear input–output transfer functions. In that case, a combination of decision trees can improve results. Two approaches are available in this application field:

- *Bagging decision trees* are an early ensemble method based on building multiple decision trees by iteratively replacing resampled training data and voting for the decision trees leading to a consensus prediction (Breiman, 1996).
- The *Random Forests* (RF) approach applies a set of decision trees to improve prediction accuracy (Breiman, 2001).

Initially, only a few decision tree feasibility studies were presented in the scientific literature (e.g., Hansen et al., 2002; Im et al., 2009, 2012; Viedma et al., 2012). Nonetheless, decision trees are used more frequently in classification than in regression applications. Only lately the random forests approach gains popularity in applications with mapping of a diverse range of vegetation attributes e.g., biomass (Le Maire et al., 2011; Mutanga et al., 2012; Adam et al., 2014; Vaglio Laurin et al., 2014), canopy cover (Coulston et al., 2012; Gessner et al., 2013), LAI (Vuolo et al., 2013) and canopy nitrogen (Li et al., 2014). These studies typically demonstrate the higher efficiency of the random forests method compared with the more conventional parametric and linear non-parametric methods.

3.2.2. Artificial neural networks (ANNs)

Artificial neural networks (ANNs) in their basic form are essentially fully connected layered structures of artificial neurons (AN). An AN is basically a pointwise non-linear function (e.g., a sigmoid or Gaussian function) applied to the output of a linear regression. ANs with different neural layers are interconnected with weighted links. Hence, in case only one AN is used in an ANN, results will be similar (or only slightly better) than those obtained with linear regression (LR). An ANN is formally defined by three structural entities: (1) The interconnection pattern between the different AN layers; (2) The learning process which updates the weights of the interconnections, and (3) The activation function that converts the ANs weighted input with its output activation.

The most common ANN structure is a feed-forward ANN, where information flows in a unidirectional forward mode. From the input nodes, data pass hidden nodes (if any) toward the output

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nodes. No cycling or looping is defined in this type of ANN. This ANN type focuses on training with experimental (field) data. Feed-forward ANNs have a long track record in mapping vegetation properties based on RS data (Kavzoglu and Mather, 2003). Since the mid-90s ANNs have been applied for vegetation attribute mapping (Jin and Liu, 1997; Paruelo and Tomasel, 1997; Francl and Panigrahi, 1997; Kimes et al., 1999). The superiority of ANNs compared to linear models (e.g. those based on VIs) has been demonstrated repeatedly in experimental studies. This boosted the popularity of the method. Actually, ANNs became the most popular MLRA during the last decade leading to multiple applications in experimental and operational hybrid settings (see Section 5). Successful applications include the estimation of foliage nitrogen concentrations (Huang et al., 2004) and LAI (Jensen et al., 2012) from hyperspectral data. In both cited studies, the higher efficiency of the ANN approach compared with other linear non-parametric models (e.g. PLSR) has been demonstrated.

Alternative powerful, yet more complex, structures involve recurrent artificial neural networks (RANNs) and radial basis function neural networks (RBFNN), which only recently went into application to map vegetation properties (Chai et al., 2012; Li et al., 2013; Wang et al., 2013). Due to the complexity of ANNs, the incentive increasingly is to replace them in many applications with alternative, simpler to train MLRAs. When compared with kernel-based MLRAs (see Section 3.2.3), feed-forward ANNs perform with an unstable 'modus operandi', generating outliers and ranging from excellent to poor performance (Verrelst et al., 2012b). The problem of ANNs is that their performance is typically determined by their design. Too few or too many layers and/or ANs may significantly reduce their accuracy.

3.2.3. Kernel methods

Kernel methods in machine learning owe their name to the use of kernel functions. Kernels quantify similarities between input samples of a dataset (Shawe-Taylor and Cristianini, 2004). Similarity reproduces a linear dot product (scalar) computed in a possibly higher dimensional feature space, yet without ever computing the data location in the feature space. For the last decade, kernel methods were introduced in bio-geosciences and RS applications (Camps-Valls and Bruzzone, 2009). Its best known family member is the 'support vector machine' (SVM) for data classification. For regression and bio-geophysical variable retrieval, several kernel-based algorithms have been developed. Among them are support vector regression (SVR), relevance vector machines (RVM), kernel ridge regression (KRR) and Gaussian processes regression (GPR). These methods have recently been applied in bio-geophysical variable estimation for land, ocean and atmosphere applications (Camps-Valls and Bruzzone, 2009; Gómez-Chova et al., 2011; Camps-Valls et al., 2011). Let us briefly review the main features of these methods.

- *Support vector machines* (SVMs) are supervised learning models with associated learning algorithms. They analyze data and perform pattern recognition and are applied in classification and regression analysis as well. A support vector machine constructs a hyperplane or a set of hyperplanes in a high or even infinite dimensional space. Intuitively, one expects a good separation by application of a hyperplane, eliciting the largest distance to the nearest training data point of any class (the so-called functional margin). Generally, the larger the functional margin, the lower the generalization error of the classifier. A regression version of SVM was proposed by Vapnik et al. (1997).
- *Kernel ridge regression* (KRR), also known as least squares support vector machines (LS-SVM), is a family of supervised learning methods for data analysis and pattern recognition. The KRR and in particular the LS-SVM are applicable in classification and regression analysis. In their latest versions, solutions are found solving a set of linear equations as opposed to solving a convex quadratic programming problem for classical SVMs (Suykens and Vandewalle, 1999).
- *Relevance vector machines* (RVM) are based on Bayesian inference to find parsimonious solutions for regression and classification. The RVM has an identical functional layout as a support vector machine, but it provides probabilistic outputs. Compared with SVMs, the Bayesian formulation of the RVM avoids sets of free variables for the SVM (usually requiring cross-validation-based optimizations). However, RVMs typically provide much less support vectors than SVMs, which may lead to unstable behaviour (Tipping, 2001).
- *Gaussian processes regression* (GPR) is based on Gaussian processes (GPs), which generalize Gaussian probability distributions in a function's space. A GP is stochastic since it describes the properties of functions. As in Gaussian distributions, a GP is described by its mean (which for GPs is a function) and covariance (a kernel function) as well. This represents an expected covariance between function values at a given point (Rasmussen and Williams, 2006).

While SVMs have been introduced for classification purposes in the mid-90s, only recently support vector regression (SVR) gained popularity for the retrieval of continuous vegetation attributes. For instance, Karimi et al. (2008) applied the SVR to estimate various crop (physiological) variables (plant height, leaf nitrogen content, and LCC) with hyperspectral data. The same approach was applied by Yang et al. (2011b). They found that SVR performance was better compared to linear non-parametric methods. Verrelst et al. (2012b) compared SVR with more recent kernel-based methods (KRR and GPR) to retrieve bio-geophysical variables (LAI, LCC and vegetation cover) from simulated Sentinel-2 and Sentinel-3 data. However, SVR did not really perform as the best approach. SVR required considerably more computational training (time) than the alternative regression algorithms. Mainly the number of free hyperparameters to be tuned seemed to impact performance reduction. Although this review is restricted to retrieval methods applied to terrestrial surface variables, for RVM only one mapping application has been identified being in the field of ocean chlorophyll content estimation. Camps-Valls et al. (2006) argue that SVR entails deficiencies that can theoretically be alleviated by the RVM. Results suggest that RVMs offer a good trade-off between accuracy and solution sparsity, additionally becoming less sensitive and dependent on the selection of free-of-tuning variables. An innovative formulation of the RVM, incorporating prior knowledge of the problem, were presented and tested. This led to more exact results than with the standard RVM formulations, SVRs and ANNs.

Of the emerging powerful kernel-based regression methods, KRR is an interesting one due to its good performance. Wang et al. (2011) compared KRR for LAI estimation with linear non-parametric methods (multiple linear regression and PLSR). They concluded that KRR yielded the most accurate estimates. Peng et al. (2011) used KRR for the detection of chlorophyll content using hyperspectral imagery. KRR proved to be an efficient regression function estimator. In Verrelst et al. (2012b), KRR performed similarly to other kernel-based methods (SVR, GPR) while establishing its model considerably faster within a moderate number of training cases.

Contrary to other methods, the training phase in GPR takes place in a Bayesian framework. Verrelst et al. (2012a) compared GPR with parametric methods based on established and generic VIs. GPR not only outperformed parametric linear regression methods, but also offered interesting additional features: (1) an indication of band relevancy for each variable; (2) a weight for the most

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relevant spectra contained in the training data set; and (3) probabilistic outputs, i.e. a mean estimate and associated uncertainty interval. These features go far beyond what is typically available from parametric or non-parametric approaches. GPR has subsequently been compared with competitive MLRAs (SVR, KRR, ANN). GPR not only slightly outperformed the other MLRAs, but is also computationally more efficient since the generated models were obtained considerably faster than SVR or ANN (but slower compared to KRR) (Verrelst et al., 2012b). The associated uncertainty estimates provide information on the success of transporting a locally trained model to other sites and/or observation conditions (Verrelst et al., 2013a, 2013b). Recently, Lazaro-Gredilla et al. (2013) refined the GPR method further, proposing a non-standard variable approximation allowing for accurate inferences in signal-dependent noise scenarios. The so-called variational heteroscedastic GPR (VHGPR) appears to be an excellent alternative for standard GPR. Meanwhile GPR has found its way in more advanced vegetation trait estimations. Roelofsen et al. (2014) applied GPR to map salinity, moisture and nutrient concentrations. These in turn were used as inputs for plant association mapping. Nonetheless, GPR applications are still limited to local settings described by relatively small training datasets. The challenge for the coming years is to foster a further implementation of this methodology in operational processing schemes (see Section 5).

Table 2
Strengths and weaknesses of non-parametric regression methods in view of the operational mapping of vegetation attributes.

Strengths	Weaknesses
• Full-spectrum methods. They make use of the complete optical spectral information • Advanced, adaptive (non-linear) models • Methodologically accurate and a robust performance is possible • Some MLRAs cope well with datasets showing redundancy and high noise levels • Once trained, imagery can be processed time efficiently • Some of the non-parametric methods (e.g. ANNs, decision trees) can be trained with a high number of samples (typically > 1,000,000) • Some MLRAs provide insight in model development (e.g. GPR: relevant bands; decision trees: model structure) • Some MLRAs provide multiple outputs (e.g. PLRS, ANN, SVR, GPR and KRR) • Some MLRAs provide uncertainty intervals (e.g. GPR)	• Training can be computationally very demanding • Risk of generating over-complicated models, hence their generalization level being decreased. Sensor-specific models (i.e. a direct transfer to other sensors is usually not possible) • Some regression algorithms are difficult (or even impossible) to train with a high number of samples • Expert knowledge is required, e.g. for tuning. However, toolboxes exist automating some of the steps • Most of the methods are considered black boxes • Some regression algorithms elicit instability with datasets having statistics deviating from the datasets used for training • Need for collecting field data (i.e. measurement campaigns are necessary)

3.2.4. Bayesian networks

Bayesian networks (BNs) are a class of probabilistic models, characterized by graphical structures representing information on domains of uncertainty (Cooper and Herskovits, 1992). BNs are structured using directed acyclic graphs. Each node in the graph represents a random variable, while node edges connect the probabilistic dependencies between variables. In contrast to graphical models, which are based on uni-directional edges, this approach is known as the Markov Random Fields methodology. Results from Bayesian approaches not only demonstrate the predictive power of a Bayesian network, but also its explanatory power (or uncertainty). Since the mid-2000's, BNs have emerged as powerful retrieval algorithms. Kalacska et al. (2005) used BNs to estimate LAI using Landsat ETM imagery. Mustafa et al. (2011, 2012) used BNs to improve LAI estimates using MODIS and ASTER imagery. Both papers conclude that BNs improve the estimation accuracy for LAI by combining a forest growth model and satellite imagery. A similar approach has been applied by Qu et al. (2012) estimating LAI time series. Finally, Zhang et al. (2012) demonstrated that BNs provide improved LAI estimates compared to MODIS LAI standard product values. An overview of the strengths and weaknesses of non-parametric regression methods are listed in Table 2. To the best of our knowledge, none of these non-parametric methods based on experimental data has been incorporated into operational or global retrieval schemes.

4. Physically-based models

Physically-based model inversion is based on physical laws and established cause-effect relationships. Inferences on model variables are based on generally accepted knowledge embedded in radiation transfer models (RTMs) and a set of RS image variables. An extensive evaluation of the physical realism of RTMs is given by ongoing Radiation Transfer Model Inter-comparisons (the RAMI exercises) as conceptualized and organized by Pinty et al. (2001, 2004) and Widlowski et al. (2007, 2013). The inversion of a canopy RTM with actual (full-spectrum) RS data is considered as a physically sound approach for the retrieval of bio-geophysical variables of terrestrial surfaces because the approach is generic and therefore generally applicable (Dorigo et al., 2007). Nevertheless, these approaches are not straightforward. First, an RTM has to be selected whereby a trade-off between the realism and inversion possibility of the RTM has to be made. Typically, complex models are more realistic, but they have many variables and are therefore hard to invert, whereas simpler models may be less realistic but easier to invert. Secondly, according to the Hadamard postulates, RTMs are invertible only when a solution is unique and dependent – in a continuous mode – on the variables to be extracted. Unfortunately, this boundary condition is often not met. The inversion of canopy RTMs is mostly under-determined and ill-posed. The number of unknowns is typically much larger than the number of independent observations. This makes physically-based retrievals of vegetation properties a challenging task. Several strategies have been proposed to mitigate the problem of ill-posedness, including iterative numerical optimization methods, lookup-table (LUT) based inversion strategies (e.g., Weiss et al., 2000; Knyazikhin et al., 1998; Darvishzadeh et al., 2008a), or hybrid approaches in which LUTs are generated as input for machine learning approaches (see Section 5). In the following section we briefly review some common RTM inversion techniques. A scheme of a generalized LUT-based inversion procedure is illustrated in Fig. 3.

Numerical optimization: Iterative optimization is a classical technique to invert RTMs in RS (Jacquemoud et al., 1995; Kuusk, 1998; Zarco-Tejada et al., 2001). The optimization consists in minimizing a cost function, which estimates the difference between measured and estimated variables by successive input variable iteration. Optimization algorithms are computationally demanding and hence time-consuming when large remotely-sensed datasets are inverted. An additional drawback when operationally applying optimization algorithms is that regularization techniques are required to achieve accurate results (Zarco-Tejada et al., 2001), though this can be expected from any inversion method.

Application of a *look-up table* (LUT) approach speeds up the inversion process. The RTM generates spectral reflectances for a large range of combinations of variable values. The inversion problem is thereby reduced to the identification of the modeled

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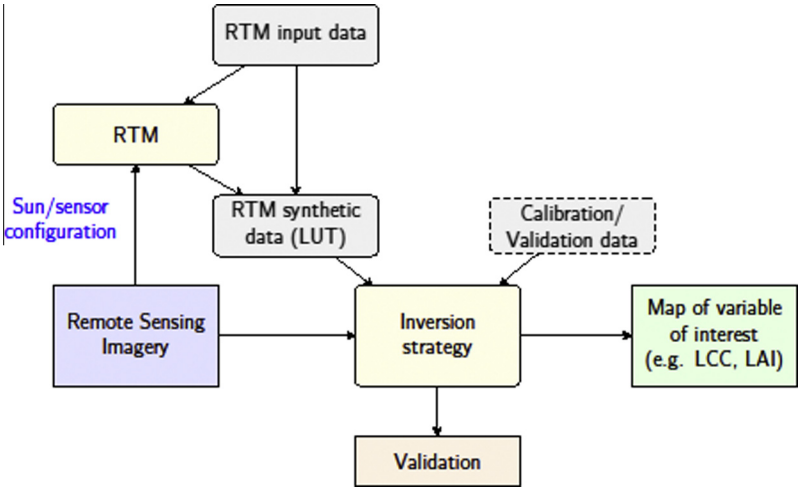

Fig. 3. Flowchart of a generalized procedure using LUT-based inversion approaches.

reflectance set that resembles most closely the measured one. This process is based on querying the LUT (Liang, 2007) and applying a cost function. A cost function minimizes the summed differences between simulated and measured reflectances for all wavelengths. LUT-based inversion has been and still is widely applied. The main advantage of LUT-based inversion routines over numerical optimization is their computational speed, since the computationally most demanding part of the inversion procedure is completed before the inversion itself (Dorigo et al., 2007). Various regularization strategies have been proposed to optimize the robustness of the LUT-based inversion routines:

- The use of prior knowledge to constrain model variables in the development of a LUT (Combal, 2002; Darvishzadeh et al., 2008a; Baret and Buis, 2008). At the local scale, prior knowledge typically involves information on the possible variable ranges for a land cover class studied (Dorigo et al., 2009; Verrelst et al., 2012c; Laurent et al., 2013).
- Selection of cost function. The inverse problem of a non-linear RTM is based on the minimization of a cost function concurrently measuring the discrepancy between (i) observed and simulated reflectance, and (ii) variables to estimate and the associated prior information (Jacquemoud et al., 2009). To avoid solutions reaching fixed boundaries, one can use a modified cost function in the LUT search that takes uncertainty of provided prior information into account (Combal, 2002; Houborg and Boegh, 2008; Jacquemoud et al., 2009). Instead, Leonenko et al. (2013a, 2013b) proposed over 60 different cost functions dealing with different error distributions. Rivera et al. (2013) and Verrelst et al. (2014) evaluated about 20 different cost functions and their interaction with Sentinel-2 data regularization options to improve the retrieval of LAI and chlorophyll content. The conclusion was that cost functions alone by default did not lead to optimized performance. The following regularization options equally play an important role in the robustness and accuracies of the inversion routine:
- The use of multiple best solutions in the inversion (mean or median), as opposed to a single best solution (Richter et al., 2009, 2011; Combal et al., 2002; Koetz et al., 2005; Darvishzadeh et al., 2011).
- The addition of Gaussian noise to account for uncertainties linked to measurements and models (Richter et al., 2009, 2011; Koetz et al., 2005).
- Several studies reported that the relationship between measured and estimated LAI perceptibly improves when only a few but well-chosen wavelengths are selected for model inversion (Meroni et al., 2004; Fang and Liang, 2005; Schlerf et al., 2005; Darvishzadeh et al., 2011).
- Spatial and temporal constraints such as the use of information from neighbor pixels in the inversion (Atzberger, 2004; Atzberger and Richter, 2012), or the use of information from a time series of observations (Koetz et al., 2005; Lauvernet et al., 2008).

Though considered as physically-sound, all cited inversion techniques rely on the existence of experimental data for calibration, which may limit their applicability in an operational setting. Furthermore, an inversion method processes imagery on a pixel-by-pixel basis. That requires intensive number crunching and hence high end computing hardware. In an ordinary LUT approach, the dimensions of the table must be large enough to achieve high accuracy, leading to a slow per-pixel LUT querying. To speed up LUT search runs, approaches have been developed to reduce the dimensions of LUTs. For instance, Gastellu-Etchegorry et al. (2003) developed empirical functions to fit LUT values, so that a table searching procedure becomes a simple calculation of local functions. Alternatively, Liang et al. (2005) developed a simple linear regression instead of a table search routine for each angular bin in the solar illumination and sensor viewing geometry. Veroustraete and Verstraeten (2005) and Veroustraete et al. (2006) proposed to simplify LUTs by parameterizing a semi-empirical bidirectional reflectance distribution function (BRDF) (Rahman et al., 1993) determined by 3 (to 4) parameters using multi-angular reflectance observations. These parameters (triplets or quartets) are stored in a LUT to be matched with the triplets (or quartets) of the BRDF of an observed pixel. This approach reduces the dimensionality of the LUT considerably, while retaining the essential angular reflectance information.

Summarizing, numerical or LUT-based inversions remain a challenge when they are implemented in an operational context: (1) additional information is required (i.e., input data, *a priori* information, regularization techniques); and (2) the method is computationally demanding. Nevertheless, LUT-based inversion is the core algorithm in the operational generation of the global MODIS LAI products (Myneni et al., 2002). The latest version of MODIS LAI is Collection 5 (C5), covering the period since 2000. Strengths

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and weaknesses of physically-based model inversion routines are listed in Table 3.

5. Hybrid methods

Having discussed the most fundamental categories of retrieval methods, this section addresses the hybrid methods. Typically, hybrid methods combine the generalization level of physically-based methods with the flexibility and computational efficiency of advanced non-parametric regression methods. The basic concept is to apply inverse mapping with a non-parametric model trained with simulated data generated with RTMs. Similarly as in LUT-based inversion, an RTM is used in direct mode to build a LUT representing a broad set of canopy realizations. Whereas a LUT approach seeks for a simulated spectrum as close as possible to the measured one, the hybrid approach uses all available data to train a (non-linear) non-parametric regression model. A scheme of a generalized hybrid procedure is illustrated in Fig. 4. First, experimental studies and subsequently operational applications (Section 5.3) are reviewed.

5.1. Artificial neural networks trained with RTM generated datasets

The awareness in the mid 90's that ANNs are excellent algorithms to deal with large datasets (e.g. >100,000 samples) led to the introduction of hybrid methods based on ANNs trained with RTM-generated data (Smith, 1993; Baret et al., 1995; Gopal and Woodcock, 1996; Kimes et al., 1998; Weiss and Baret, 1999). The hybrid approach proved to be successful in various retrieval schemes. For instance, Gong et al. (1999) and Danson et al. (2003) inverted LAI from a simulated database; Fang and Liang (2003) and Atzberger (2004) inverted LAI from Landsat ETM imagery; Kimes et al. (2002) inverted a complex 3D model (DART) for a wide range of simulated forest canopies using POLDER-like angular data. While showing promising results, these studies were still experimental. Only since the mid-2000s this method has been implemented in operational processing chains with the purpose of operational, global mapping of bio-geophysical variables (Bacour et al., 2006). In Section 5.3 operational hybrid approaches are discussed further.

Table 3
Strengths and weaknesses of physically-based model inversion methods in view of the operational mapping of vegetation attributes.

Strengths	Weaknesses
• Full-spectrum methods • Reputation of physically-based methods (however, note the impact of regularization factors) • Generally and globally applicable (e.g. MODIS products) • Capability to provide multiple outputs • Yields additional information about uncertainty of the retrievals (e.g. through spectral residuals)	• Computationally demanding due to the per-pixel based approach (however, solutions based on *a priori* information have been developed) • Retrieval quality depends on the quality of the RT models, prior knowledge and regularization • Quite complex approach: requires parameterization and optimization procedures • The imposed upper/lower boundaries in the LUT have a logical consequence in that estimated variables cannot go beyond the boundaries imposed. This contradicts somewhat the physical approach as the prior information has an overwhelming influence (Baret and Buis, 2008) • LUT-based inversion methods are often strongly affected by noise and measurement uncertainty (Liang, 2007)

Meanwhile a diversity of ANN-based hybrid methods has been developed. Most of them use simulations from the canopy RTM SAIL (Verhoef, 1984). The PROSPECT-SAIL model, further referred to as PROSAIL, has been applied to provide simulations for the development of an ANN model. For instance, PROSAIL was applied for the retrieval of vegetation canopy water content across the continental United States using MODIS data (Trombetti et al., 2008). Richter et al. (2009) trained an ANN based on PROSAIL simulations to estimate LAI using simulated Sentinel-2 data. Noteworthy is the work of Vohland et al. (2010). These authors compared a numerically optimized ANN with a LUT-based inversion using PROSAIL simulations. Prediction accuracies generally decreased in the following sequence: numerical optimization > LUT > ANN. This indicates that an ANN may not always be the best choice for inversion applications. Yang et al. (2012) compared a PROSAIL-ANN hybrid approach with a PCA approach for hyperspectral data. The authors concluded that a PCA transformation into a regression function can mitigate the known reflectance saturation effect of dense canopies to some extent. Also other types of RTMs have been applied. Yang et al. (2011a) trained an ANN with the canopy RTM INFORM (Schlerf and Atzberger, 2006) to estimate LAI from multi-source and multi-angular data. It was concluded that the inversion accuracy of LAI with multi-angular image data improved by 30% compared with the average accuracy of the LAI estimated with an inversion based on mono-angular data. Similarly, Malenovsky et al. (2013) trained an ANN based on PROSPECT-DART simulations to estimate leaf chlorophyll content (LCC) from hyperspectral AISA data.

5.2. Alternative MLRA methods trained with RTM generated datasets

Although hybrid strategies traditionally rely on the application of an ANN, recently the results of feasibility studies have been presented in which ANNs were replaced by more novel kernel-based MLRAs. Durbha et al. (2007) retrieved LAI from a MISR dataset using a support vector regression (SVR) model trained with PROSAIL data. The same strategy was applied to estimate LCC based on imaging spectroscopy data (Preidl and Doktor, 2011) and to estimate LAI from a HJ-CCD image (Pan et al., 2013). Doktor et al. (2014) used a PROSAIL dataset to train a random forests model to predict LAI and LCC. While some of the MLRA methods elicit advantages compared to ANN structures (e.g. in models in a Bayesian framework), they are nonetheless still experimental and none of them have made it to operational applications yet.

5.3. Operational hybrid approaches

Nowadays, ANNs are commonly used in operational bio-geophysical variable retrieval schemes. The majority of these algorithms exhibit a comparable design. This was presented for the first time by Bacour et al. (2006). Since then, the strategy based on ANN algorithms has been implemented as a core routine in various processing chains. A brief overview of operationally generated products is provided here.

- The MERIS vegetation algorithm is based on the training of ANNs with a database containing simulations from canopy and atmosphere RTMs. The ANN estimates LAI, *f*APAR (fraction of absorbed photosynthetically active radiation) and *f*Cover (vegetation cover fraction) products. PROSAIL was used to simulate canopy reflectance according to MERIS spectral band specifications. The data were used to train back-propagation ANNs for each variable considered. The architecture has been

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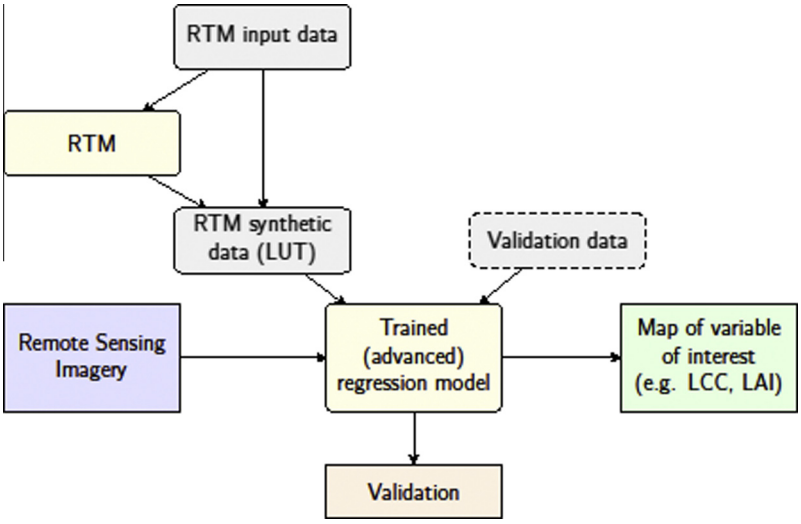

Fig. 4. Flowchart of a generalized procedure of the hybrid approaches.

optimized by two hidden layers of tangent-sigmoid artificial neurons, corresponding with a total of roughly 340 coefficients to be adjusted (Bacour et al., 2006).

- The CYCLOPES products are processed in a similar way for the SPOT-VEGETATION sensor at a resolution of 1/112° (about 1 km at the Equator) every 10 days for the period 1999–2007 (Baret et al., 2007).

5.3.1. Validation of the CYCLOPES products and beyond

The MERIS and CYCLOPES products have been extensively validated with experimental data as well as compared with other global products, e.g. from MODIS (Bacour et al., 2006; Weiss et al., 2007; Garrigues et al., 2008; Fang et al., 2012b). MODIS and CYCLOPES LAI products have been improved over time. Therefore we refer to the latest findings of Fang et al. (2012b) only. It was reported that the overall mean difference between the best MODIS C5 and CYCLOPES V3.1 products are within an interval of ±0.10 LAI. Though the LAI product is recommended to the user community, results indicate that the uncertainty in LAI products (around ± 1.0 LAI) does not meet the quality requirements (±0.5 LAI) proposed by the Global Climate Observing System (GCOS) (GCOS, 2011). It has also been elicited that CYCLOPES does not provide LAI values that are high enough to properly characterize forests (Garrigues et al., 2008).

Apart from validation exercises using field data, theoretical uncertainties can be used for evaluation purposes as well. Theoretical uncertainties originate from uncertainties inherent to input data as well as from model imperfections. They are usually estimated during the variable retrieval process (Baret et al., 2007; Knyazikhin et al., 1998; Pinty et al., 2011). An independent method has recently been proposed by Fang et al. (2012a), in which the authors apply an uncertainty calculation based on a triple collocation method (i.e. a method to estimate root-mean-square errors based on three independent estimates). The uncertainties of MODIS, CYCLOPES, and GLOBCARBON LAI products were evaluated based on this method. The main conclusion drawn was that particularly CYCLOPES generally meets GCOS quality requirements. However, some well-known fundamental limitations remain to be tackled:

- While ANNs are proven to be robust algorithms in various operational processing chains, the retrieval schemes are far from perfect. For instance, LAI estimates from CYCLOPES are less accurate in the higher value range (LAI > 4). This is suggested to be due to the saturation effect in the radiative transfer simulation and the ANN inversion algorithm (Bacour et al., 2006; Weiss et al., 2007; Garrigues et al., 2008).
- ANNs are black box models. These tend to behave relatively unpredictable when used with input spectra deviating from what has been input during the training stage (Atzberger, 2004; Baret and Buis, 2008; Rivera et al., 2014a).

To mitigate some of the above-identified limitations, Baret et al. (2013) recently presented the global GEOV1 products, available from 1999 to present, at a 1/112° spatial grid size, and a decadal time step. When capitalizing on the development and validation of existing products, improvements of the global estimates of LAI, *f*APAR and *f*Cover have been obtained. Specifically, the best-performing estimations of MODIS and CYCLOPES products have been selected, fused and scaled to generate a new ANN training dataset. This training dataset has subsequently been applied to SPOT-VEGETATION top-of-canopy (TOC) directionally normalized reflectances. The resulting GEOV1 products are labeled with quality control flags and uncertainty estimates. These products have been validated by Camacho et al. (2013). These authors reported that GEOV1 products show a reliable spatial distribution, smooth temporal profile, stability from year to year, and a good dynamic range with a reliable magnitude for bare soil areas as well as dense forests. GEOV1 outperforms the quality of reference global products (e.g., MODIS C5, CYCLOPES V3.1, GLOBCARBON V2 LAI, and JRC SeaWIFS *f*APAR) and constituted a step forward in the development of consistent and accurate global bio-geophysical variables within the land monitoring core service of Copernicus (Camacho et al., 2013). Worth noting is that these products are no longer based on simulated training datasets, but are based on data derived from existing products. While this approach tends to mitigate the limitations of PROSAIL (e.g. saturation at LAI > 4), the core retrieval ANN algorithm nonetheless remains unchanged. Therefore, it is questionable whether ANNs are the most flexible tool for the estimation of biophysical variables. Training ANNs involves accurate tuning of several model parameters. This tuning process strongly affects the final robustness of the model. Therefore, alternatives overcoming this limitation in ANN training are most welcome.

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6. Discussion

The estimation of vegetation properties with optical RS data is a broad and steadily expanding field of research and development. In this review paper an updated summary and discussion on a wide range of retrieval methods dedicated to the quantification of continuous bio-geophysical variables has been compiled. In general, RS retrieval methods can be categorized into four main domains: (1) *parametric regression*; (2) *non-parametric regression*; (3) *physically-based models*; and (4) *hybrid methods*.

These four categories have been qualitatively compared and evaluated in this paper. They can be compared on the basis of the following general criteria, i.e.:

(1) The retrievability of vegetation bio-geophysical properties.
(2) Their ability to generate multiple outputs.
(3) The possibility to describe model transparency.
(4) The mapping speed for specific bio-geophysical variables.
(5) Their ability to provide retrieval uncertainties.

The evaluation of these five criteria is summarized in Table 4 and discussed below.

6.1. Retrievability of vegetation bio-geophysical variables

Regarding retrievability of vegetation bio-geophysical variables, strategies relying on RTM simulations are inherently limited by the input variables of the RTM. They are known to play a prominent role in radiative transfer theory and are therefore considered as so-called state variables (Verstraete et al., 1996). The relationships between state variables and the spectral reflectance are physically well understood. Therefore, the argument is often raised that only state variables can be retrieved with optical RS data (e.g., Knyazikhin et al., 2013). Alternatively, state variables are sometimes combined and hence give rise to newly defined variables. A typical example are leaf biochemical constituents scaled up to the canopy level by multiplication with canopy LAI (Weiss et al., 2000; Combal, 2002; Bacour et al., 2006; Dorigo et al., 2009; Darvishzadeh et al., 2012).

On the other hand, statistical approaches possess the flexibility to relate reflectance data with any measured bio-geophysical variable – state variable or not. This includes typically leaf biochemical constituents such as nitrogen or cellulose content. The strength of the correlation with validation data typically determines the validity of the statistical model. While this approach may be criticized because of the absence of a physical basis (Knyazikhin et al., 2013), statistical approaches are powerful methods to extract bio-geochemical variables through complex and often indirect relationships. Particularly (non-linear) non-parametric models are powerful in extracting information from subtle variations in reflectance through adaptive, non-linear models. With statistical models not only variable-specific absorption features can be used for information extraction, but also secondary relationships with variables that co-vary with the variable of interest. Using GPR for instance, secondary relationships can be revealed by the identification of relevant spectral bands. To illustrate this, some GPR models developed (Van Wittenberghe et al., 2014) showed a strong relationship between spectral data and chlorophyll content at leaf level (R^2 of 0.78–0.84) and at canopy level (R^2 of 0.92–0.99) (Verrelst et al., 2012a, 2012b). In either case, GPR identified important spectral bands within the chlorophyll absorption region (e.g., 620, 665, 710 nm). Interestingly, also bands in the NIR (e.g., 950 nm) and SWIR (e.g., 1430, 1730 nm) – which are located outside the chlorophyll spectral absorption region – were identified to play an important role. Typically, these spectral regions are related to leaf water content, cellulose and lignin (Thenkabail et al., 2000, 2004; Van Wittenberghe et al., 2014). Consequently, the sensitivity to chlorophyll in the NIR and SWIR may be driven by the covariance of chlorophyll with leaf water content and cell biochemical compounds. This has been observed by Filella and Penuelas (1994) and Stagakis et al. (2010). At the same time, chlorophyll is to some extent correlated with plant structural variables such as LAI and fractional vegetation cover, imposing additional spectral variations in the NIR and SWIR (Darvishzadeh et al., 2008b; Verrelst et al., 2010; Ollinger, 2011). The co-variation between, e.g., leaf biochemicals such as pigments, starch and lignin content and plant structural traits and their respective spectral responses can therefore be used to predict leaf biochemical constituents along a spectral range even beyond their specific spectral absorption range. In turn, the estimation of canopy structural variables can also be supported by co-varying leaf biochemical constituents (Verrelst et al., 2012a, 2012b).

Summarizing, the inversion of RTMs can essentially lead to the retrieval of state variables only. Although these variables are well defined in radiative transfer theory, their successful retrieval is largely determined by the physical realism of the model used and the inversion strategy applied. Alternatively, non-state variables can be mapped by applying (non-linear) statistical methods, which indirectly exploit co-variance relationships hidden in the reflectance data.

6.2. Multiple outputs

The capability to produce multiple outputs is an interesting possibility offered by both statistically and physically-based methods. In general, multiple outputs can be provided in two ways: (i) by training independent models, which is convenient and easily performed; and (ii) by training a single model which directly generates multiple outputs. The first way, however, does not take into account relationships between dependent variables. On the other hand, a single model approach leads to more complexity, but co-varying relationships between multiple dependent variables are taken into account. For non-linear (and non-parametric) regression, examples of multiple output regression algorithms include PLSR, ANN, SVR, KRR and GPR (Tuia et al., 2011; Rasmussen and Williams, 2006; Rivera et al., 2014a; Camps-Valls et al., 2012a). The use of multiple-output models has been reported to lead to improved results. The main reason for this is that the input is evidently the same for the dependent variables (Tuia et al., 2011). Nevertheless, including variables with little or no

Table 4
Synthesis of the evaluation with respect to five criteria of the three main retrieval approaches. Best features are boldfaced.

Method	Parametric regression	Physically-based methods	Non-parametric regression	Hybrid methods
Surface variables	**Any**	Only RTM state variables	**Any**	Only RTM state variables
Multiple outputs	No	**Yes**	**Some MLRAs** (e.g. PLSR, NN, KRR, GPR)	**Some MLRAs** (e.g. PLSR, NN, KRR, GPR)
Model transparency	Yes	Partly	In part some MLRAs (e.g. RF, GPR)	In part some MLRAs (e.g. RF, GPR)
Mapping speed	**Instantly**	Slow	**Fast**	**Fast**
Uncertainties	No	**Yes** (e.g. residuals)	**Some MLRAs** (e.g. GPR)	**Some MLRAs** (e.g. GPR)

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relation amongst them may degrade the performance of the model. The main reason being that its training is more complex and the risk of ending in a local minimum becomes higher. For instance, Baret et al. (2007) reported for a ANN single output model that the output is more robust than for multiple output models.

RTM inversion routines are essentially iterative minimization calculations applied per pixel to estimate RTM input variable values. In principle, this allows all state variables to be mapped. Examples of these multiple output inversion mapping routines have been described by Lauvernet et al. (2008) and Laurent et al. (2013). Its success depends on the number of variables and their cross-relationships across the spectral domain. Some variables can be retrieved more successfully than others (Lauvernet et al., 2008; Mousivand et al., 2014). Inversion routines optimized for a single variable tend to perform slightly better than generic multiple output inversion algorithms (Rivera et al., 2013; Verrelst et al., 2014). Probably the prime advantage of multiple output routines is the gain in processing speed. This may be an important property in operational processing chains, particularly for global applications.

6.3. Model transparency

Model transparency, i.e. insight in a model's formulations, is optimally provided by parametric regression models. Usually this type of models is based on relatively simple calibrated regression functions. Transparency in model functioning can also be elicited by RTM inversion routines. These are typically forced by a cost function. The inversion performance, however, is less transparent. It depends on the realism of RTM simulations and the role of the input variable space on output reflectances. Consequently, the functional transparency of RTMs requires expert knowledge.

Non-parametric, non-linear regression algorithms (such as ANN) are often criticized because they represent a black box approach that represents a stochastic and not a physical approach (Haykin, 1999). Hence, the outputs may be very useful, but do not help the user to interpret the results in physical terms. The terminology 'black box' refers to an important drawback of this type of retrieval technique. It has therefore earlier been concluded that the full potential of machine learning techniques is unlikely to lead to new breakthroughs as long as these developments do not have a physical meaning (Liang, 2007).

Other methodological models are referred to as 'gray boxes'. This is especially true for developments during the last few decades, wherein the machine learning community developed a complete family of techniques to scrutinize this type of models. This includes model pruning, advanced sensitivity analyses, weight visualization techniques, etc. The problem of the lack of physically-relevant explanatory capacity of non-parametric models also signifies that artifacts propagating in such a model may remain unnoticed. This re-initiates the discussion whether the incorporation of effective regularization and invariances in the models is an opportune methodological development track. Recent MLRAs in a Bayesian framework (e.g. GPR) have overcome this limitation. These MLRAs offer the possibility to train flexible self-explanatory kernel models, i.e. through the ranking of relevant spectral bands during model development, and the possibility to generate confidence intervals for the bio-geophysical variable estimates (Verrelst et al., 2012a). Also other non-parametric regression methods provide insight in band relevancy, such as SVR, PLSR and random forests (Feilhauer et al., 2015).

Typically, one can generalize that the higher the complexity of a model, the lower its transparency will be. In a probabilistic paradigm, nevertheless, this has changed with the new generation of Bayesian MLRAs. Importantly, the inclusion of physically-relevant constraints in model training partly overcomes the lack of transparency.

6.4. Mapping speed

Regarding mapping speed, it can be suggested that the lower the complexity of a model the faster it will be able to produce maps. This highly favors the application of parametric regression approaches since only few coefficients have to be estimated. Also non-parametric regression algorithms, once trained, can be applied to process an RS image virtually instantaneously. Training of non-parametric models is frequently related to the tuning of several free variables with costly cross-validation approaches. These scale poorly with the number of samples (such as in kernel machines) or with the data dimensions (such as in ANNs). A trained ANN converts an image into a map quasi-instantly. Kernel-based methods require more processing time since the similarity between each test pixel in the image and those used to train the model has to be estimated. This process can be computationally costly when using a big dataset for training purposes, e.g. in the case of RTM inversion (Camps-Valls et al., 2011). One of the major advantages of hybrid processing chains is that the training step takes place only once and outside the processing chain. A considerably lower processing speed is observed with the LUT-based inversion routines. Since the evaluation takes place on a per-pixel basis with iterative calls of LUT entries, inversion routines are computationally expensive leading to relatively slow mapping speeds. Despite attempts to optimize processing algorithms in terms of mapping speed (Gastellu-Etchegorry et al., 2003; Liang et al., 2005) the RTM inversion routines are not competitive when compared with statistical methods.

6.5. Model portability by deriving retrieval uncertainties

Statistical methods have often been criticized for their low portability leading to poor estimations when applied under other conditions (e.g., Baret and Guyot, 1991). However, only a meaningful interpretation of the portability of a method can be given when the per-pixel estimation performance can be quantified. In this respect, theoretical uncertainties are of interest, as they can be quantified on a per-pixel basis during the retrieval process (Fang et al., 2012a). Uncertainty intervals provide the reliability of a given estimation with regard to what has been presented during the training phase.

An operational definition of transportability can be formalized as follows. If retrieval uncertainties are low in space and time (e.g. below a threshold), then a method can be considered as a transportable one. The quantification of variable-associated uncertainties is a strong requirement when vegetation products are ingested in higher level processing, e.g. to estimate ecosystem respiration, photosynthetic activity, or carbon sequestration (Jägermeyr et al., 2014). Hence, to evaluate the portability of a method, first its ability to deliver low uncertainties should be addressed. Several excellent reviews of probabilistic uncertainty quantification and specification for environmental, geo-scientific and RS applications have been published (Peter et al., 2009; O'Hagan, 2012; Richardson et al., 2012). GCOS proposed an uncertainty threshold below 20% for many bio-geophysical variable value estimation problems (GCOS, 2011). One can estimate uncertainties for parametric functions by adopting perturbation or bootstrapping approaches (Efron, 1979), though these techniques are not yet common in the broader RS community. With regard to LUT-based inversion routines, uncertainties are provided as spectral residuals (Rivera et al., 2013) or standard deviations, when

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mapping multiple solution means (Yang et al., 2006). In case of non-parametric regression models, uncertainty estimation is a complex exercise but nonetheless one can rely on bootstrap or ensembles of predictors for uncertainty estimation. ANN can generally provide uncertainty intervals for the estimations, but their value is compromised by the risk of overfitting. Recently, Bayesian non-parametric models such as GPR provided uncertainties by applying a solid and elegant mathematical framework (Verrelst et al., 2012a, 2012b). The Bayesian interpretation provides the probability interval of an estimation relative to the samples used during the training phase. By analyzing the uncertainties as delivered by GPR, Verrelst et al. (2013b) demonstrated that for the large majority of pixels within an image a locally developed regression model could be successfully transported in space and time. Despite the importance of Bayesian non-parametric models for higher level products and the advances in quantifying and constraining uncertainty estimations in regression models during the last decade, this field is still in its infancy.

6.6. Recommendations for next-generation operational bio-geophysical variable retrieval methods

So far only a few vegetation variables are routinely mapped on a global scale and for long time periods. MODIS and CYCLOPES products provide LAI datasets and maps for over a decade now. Both products have been refined over time, gradually leading to more accurate estimates. For instance, the CYCLOPES' successor GEOV1 no longer directly makes use of PROSAIL-simulated training data but capitalizes on existing products such as the less recent CYCLOPES and MODIS LAI products. Nevertheless, GEOV1 relies on the same conventional ANN, while the MODIS LAI product (based on a LUT-based inversion) still uses an empirical NDVI-based backup algorithm in case the inversion algorithm fails.

Of the four presented model categories, during the last decade most progress has been made in the field of non-parametric regression, and more specifically in machine learning. This has led to advanced MLRAs, such as kernel-based regression algorithms. Though these methods have not yet made it to operational processing schemes, they possess attractive new properties. For instance, several studies indicated that kernel-based MLRAs perform more robustly than feed-forward ANNs (Camps-Valls et al., 2006; Verrelst et al., 2012b). Moreover, kernel-based MLRAs developed in a Bayesian framework enable the delivery of probabilistic outputs (i.e., with associated uncertainties). These novel methods can be applied as a stepping stone toward a next generation of operational satellite image processing strategies. When comparing the qualitative features of the main retrieval approaches of Table 4, some MLRAs such as GPR seem flexible in coping with the ability to retrieve multiple vegetation variables simultaneously. They provide model transparency and uncertainty estimates as well. Moreover, mapping occurs computationally faster than for pixel-by-pixel inversion approaches. The same conclusion was reached in a related paper (Verrelst et al., 2015) where a multitude of parametric, non-parametric and physical methods were systematically and quantitatively evaluated on LAI retrieval accuracy and processing speed based on experimental data. GPR was performing best and processed a simulated Sentinel-2 image within about a minute (compared to an hour when using an inversion scheme). However, further R&D and prototype algorithm testing is required in view of full operational implementation. Especially, the issue of how advanced MLRAs cope with large datasets during the training phase in a hybrid setting has to be tackled. For the sake of performance optimization, the training dataset itself has to be validated as well, whether or not it is globally applicable and of high enough quality. Simulated data generated with relatively simple RTMs may not provide the best match with reality, especially in case of CAVS RTMs (Coupled Atmosphere – Vegetation – Soil RTMs). The development of more realistic and easily invertible RTMs with fast and powerful inversion procedures is required for operational processing in order to provide high level products. Currently, the approach pursued by GEOV1, i.e. selecting the best retrievals from existing products as a new training set, is a promising approach since it bypasses known RTM-related shortcomings (e.g., the PROSAIL saturation at an LAI > 4).

7. Conclusions

With the forthcoming superspectral and imaging spectrometer satellite missions, an unprecedented stream of datasets on the terrestrial biosphere will become available. On the short term this will require powerful processing techniques enabling a spatio-temporally explicit quantification of vegetation attributes in an operational and global setting. Four categories of retrieval methods have been discussed in this review paper: (1) *parametric regression*, (2) *non-parametric regression*; (3) *physically-based* and (4) *hybrid methods*. For each of these categories strengths and weaknesses have been qualitatively assessed to judge their implementation in operational processing schemes.

It is our opinion that the weaknesses of parametric regressions outweigh their strengths. Their empirical backbone, suboptimal use of available spectral bands, sensitivity to disturbing factors and lack of uncertainty estimates, makes us decide that parametric regression methods cannot be considered as state-of-the-art for operational mapping applications. Non-parametric methods, on the other hand, are powerful regression algorithms due to their non-linear and adaptive fitting capacities. They cope well with full-spectrum inputs, which is a considerable advantage compared with parametric methods. Especially powerful are the non-linear MLRAs, and particularly those that generate probabilistic outputs in a Bayesian framework.

Though the inversion of physically-based RTMs is generally possible, the approach is more challenging compared to parametric and non-parametric methods. Inversion is computationally demanding and ancillary information is required as an input or to regulate the inversion algorithm. This information may not always be accurate, available or up-to-date.

Hybrid methods are based on the coupling of an RTM with a non-parametric method. This approach has long been restricted to the training of an ANN with simulated data from an RTM (e.g., PROSAIL). While ANNs have proven to be successful on an operational basis, the question whether an ANN is the best choice as core algorithm for new operational retrieval schemes of vegetation properties remains open. Alternatively, (Bayesian) kernel-based MLRAs possess promising features to replace ANNs, because they combine speed, flexibility and the provision of uncertainty estimates. Though these methods are still in their infancy, this paper recommends to further explore the feasibility and implementation of this category in next-generation hybrid processing chains for the retrieval of vegetation properties in view of future RS missions.

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