WAVELET DECOMPOSITION OF HYPERSPECTRAL REFLECTANCE DATA FOR QUANTIFYING PHOTOSYNTHETIC PIGMENT CONCENTRATIONS IN VEGETATION.

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ABSTRACT:

The dynamics of pigment concentrations are related to vegetation photosynthetic potential and hence primary production, nutrient status, stress physiology and plant-environment interactions. Therefore, information about the spatial and temporal dynamics of pigments can provide important contributions to a range of scientific disciplines and environmental management endeavours, yet our current our capabilities for providing this information are limited. With the advent of airborne and spaceborne imaging spectrometers, there are now enhanced opportunities to acquire vegetation reflectance spectra and therefore quantify pigments over a wide range of spatial scales, repeatedly. However, of the spectral approaches that exist, none are sufficiently robust and remain sensitive to confounding factors and lack generality and extendibility. The present study examines the potential of wavelet decomposition for quantifying vegetation pigment concentrations from hyperspectral remotely-sensed data, using reflectance spectra and pigment data collected for a range of plant species at leaf and canopy scales. The research indicates that wavelet analysis holds promise for the accurate determination of chlorophyll a and b and the carotenoids, but work is needed to further test and refine the approach.

1. INTRODUCTION

Antenna pigments in leaf chloroplasts absorb solar radiation and the energy is transferred to the reaction centre pigments, which initiates the process of photosynthesis (Richardson *et al.*, 2002). Chlorophylls (*Chls*; chlorophyll *a* and *b*) are the most important of these pigments, a physiological parameter of significant interest. However, from an applied perspective, *Chls* concentration is important for several reasons: The amount of solar radiation absorbed by a leaf is largely a function of the *Chls* and low concentrations can directly limit photosynthetic potential and hence primary production; much of leaf nitrogen is incorporated in *Chls*, so quantifying their concentration gives an indirect measure of nutrient status; pigmentation can be directly related to stress physiology, *Chls* generally decrease under stress and during senescence; relative concentrations of *Chl a* and *b* change with abiotic factors such as light (e.g. sun leaves have a higher *Chl a:b* ratio) so quantifying these proportions gives information about plant-environment interactions (Gross, 1991).

Carotenoids (*Cars*) are the second major group of plant pigments, composed of carotenes and xanthophylls. *Cars* can absorb incident radiation and contribute energy to photosynthesis. The fraction of photosynthetically active radiation absorbed by a plant canopy (APAR) has been related to net primary productivity as a function of a light use efficiency (LUE) coefficient defining the carbon fixed per unit radiation intercepted. Such studies assume that the contribution of each pigment to the energetics of photosynthesis is equal, but this is an insufficient interpretation, as the concentration of *Chl a* is the limiting factor in the utilisation of light for photosynthesis, because it receives energy absorbed by *Chl b* and *Cars* (Kim *et al.*, 1994). Thus, the photosynthetic potential of two plants may differ even though their APAR is equal, depending upon the concentrations of individual pigments. Furthermore, when incident radiation exceeds that needed for photosynthesis, *Cars* that compose the xanthophyll cycle dissipate excess energy and

protect the reaction centres. Thus, while changes in *Chls* are indicative of stress and phenological stage, *Cars* concentration provides much complementary information on vegetation physiological status (Young and Britton, 1990).

Information about the spatial and temporal dynamics of plant pigments can, therefore, provide important contributions to scientific investigations and applied environmental / agricultural management, yet our current our capabilities for providing this information are limited. Traditional techniques for measuring foliar pigment concentrations involve extraction with a solvent and spectrophotometric analysis using standard procedures. This is possible because pigments have differing spectral absorption properties and even though the absorption features overlap, simple combinations of absorbance values at a number of wavelengths can be used to accurately determine individual pigment concentrations from mixed extracts. However, these wet laboratory techniques are time and labour-intensive thus for whole canopies pigments must be quantified by extrapolation from a limited number of samples, which introduces inaccuracies. Spectral absorbance properties of pigments are manifest in the reflectance spectra of leaves and this offers the opportunity of using measurements of reflected radiation as a non-destructive method for quantifying pigments. Moreover, with the advent of airborne (e.g. AVIRIS, CASI) and, more recently spaceborne imaging spectrometers (e.g. HYPERION), with high spectral and radiometric resolutions and signal:noise ratios, there are now enhanced opportunities to acquire vegetation reflectance spectra and therefore quantify pigments over a wide range of spatial scales, repeatedly.

1.1 Evaluation of previous spectral approaches

To extract pigment information we must first account for the range of other factors which also influence vegetation reflectance spectra. The internal structure of leaves, with large numbers of refractive discontinuities between cell walls and intercellular air spaces, scatters incident radiation and allows a large proportion to pass back through the upper epidermis to be

observed as reflected radiation. Pigments, water and other biochemicals absorb certain wavelengths of radiation which reduces reflectance in these regions. However, because of the overlapping absorption features of the pigments, it is difficult to relate reflectance at a single wavelength to the concentration of an individual pigment. Furthermore, leaf reflectance can vary independently of pigment concentrations due to differences in internal structure, surface characteristics (hairs/waxes) and moisture content. The reflectance spectrum of a whole canopy is subject to even more controlling factors, notably, effects of variations in number of leaf layers (leaf area index; LAI), orientation of leaves (leaf angle distribution; LAD), presence of non-leaf elements, areas of shadow and soil/litter surface reflectance. This range of factors, at leaf and canopy scales, obscures relationships between spectral reflectance and concentrations of individual pigments and there has been an increasing intensity of research aimed at overcoming these problems. Four groups of spectral variables have been identified as being of value:

(i) Reflectance in individual narrow wavebands have been employed (e.g. Fillela *et al.*, 1995). While there is little agreement on the optimal wavelengths, there is good evidence that at wavelengths where absorption coefficients of pigments are high, reflectance is more sensitive to low concentrations, while spectral regions with low absorption are more sensitive to higher pigment concentrations (Carter and Knapp, 2001);

(ii) Ratios of reflectance in narrow bands have been proposed as a means of solving the problems of the overlapping absorption spectra of different pigments and the effects of leaf structure, leaf surface interactions and canopy structure (Peñuelas *et al.*, 1995). Most workers propose pigment indices which employ ratios of narrow bands in the visible and near-infrared (e.g. Blackburn, 1998a), while some identify only visible wavelengths and others use combinations of narrow wavebands in the red edge region (e.g. Tarpley *et al.*, 2000);

(iii) Characteristics of first and second derivatives of reflectance spectra have been investigated. It has been suggested that spectral derivatives have important advantages over spectral reflectance, such as their ability to reduce variability due to changes in illumination or soil/litter reflectance. The majority of workers have used derivatives to define the wavelength position of the red edge (λ_{RE}) and illustrated relationships between λ_{RE} and total chlorophyll (Chl *tot*) concentration for both leaves and canopies. The amplitude of first and second derivatives of reflectance at particular wavelengths (and combinations of wavelengths) has also been found to be closely related to pigment concentrations as has the amplitude of the first derivative of pseudo absorbance (Blackburn, 1999);

(iv) Measurements of absorption feature depths have been obtained by fitting a continuum to vegetation reflectance spectra (Kokaly and Clark, 1999). This approach was extended by normalising to the band depth at the centre and the area of the absorption feature and using stepwise regression to identify optimal combinations of band depths which were used to estimate accurately Chl *tot*, *a* and *b* in dried and ground pine needles (Curran *et al.,* 2001).

Most research has focussed on *Chls* and only recently has attention been paid to quantifying *Cars* and anthocyanins from reflectance spectra, using simple adaptations of the above approaches (Gitelson *et al,* 2002). Even for *Chls*, no single spectral approach is emerging as a generic solution. Often developers of spectral approaches do not test their methods on a range of vegetation types and this has lead to many species- or site-specific techniques. Recent literature suggests that of the spectral approaches that exist, none are sufficiently robust and remain sensitive to confounding factors such as variations in chlorophyll fluorescence, leaf surface reflectance, water stress and specific leaf mass. Moreover, studies testing many spectral approaches under a range of circumstances have reported a lack of generality and extendibility (Richardson *et al.*, 2002) and even that hyperspectral approaches offer no improvements over traditional broadband indices for canopy *Chl* estimation (Broge and Mortenson, 2002). Indeed, recent work by the author (Blackburn, 2002) demonstrated limited applicability of approaches across leaf/canopy/stand scales. Within the same scale, there was a need for locally derived regression relationships (e.g. between λ_{RE} and Chl *tot*) and even these were not transferable between different vegetation types. Furthermore, papers claiming evidence of robust spectral approaches (Sims and Gamon, 2002) fail to identify methods to estimate independently *Chl a* and *b,* or *Cars* and only demonstrate convincing results for Chl *tot* at the leaf scale.

Most research in this field has used individual leaves, collections of leaves or small plants growing in the laboratory under controlled conditions. Canopy scale studies have either derived statistical relationships between ground-measured pigment data and canopy-measured reflectance, or applied leaf-scale relationships between optical indices and pigment content directly to canopy-measured reflectance. Relatively few studies have examined the applicability of different spectral approaches as we move from individual leaves to whole plant canopies and stands. Empirical work by the author on vegetation with a relatively simple or spatially homogenous canopy architecture has indicated that some spectral variables are robust predictors of pigment concentrations from leaf to stand level (Blackburn, 1998b), however, such variables are unsuitable for vegetation with a more complex structure (Blackburn and Steele, 1999). Recent work using coupled leaf and canopy radiative transfer (RT) models has examined the predictive capabilities and robustness of different spectral approaches for quantifying canopy Chl *tot* (Haboudane *et al.*, 2002). While these scaling-up studies are able to identify spectral indices that are insensitive to factors such as canopy structure, illumination geometry and soil/litter reflectance, there is little consensus on the optimal spectral approaches for estimation of Chl *tot*. The numerical inversion of RT models based on measured reflectance spectra has been used to quantify leaf and canopy Chl *tot* (Weiss *et al.,* 2000). Such models afford greater insight into the underlying functionality of reflectance-based pigment quantification and the inversion approach promises greater generality, however, parameterisation of RT models requires considerable *a priori* knowledge of the leaves and canopies under investigation which can render this approach impractical for operational use. Nevertheless, a technique that offers greater potential for extendibility combines the rigour of (bio)physically-based RT models with the normalising capabilities and pigment-specificity of a hyperspectral index which is used as the merit function in the inversion (Zarco-Tejada *et al.*, 2001). However, there is a need to substantially improve the predictive accuracy of this approach and to test it over a range of vegetation types. In summary, hyperspectral remote sensing has the potential to satisfy the increasing demand for information on plant pigments over a range of spatial scales, yet, a standard analytical approach remains absent.

1.2 Potential for a new approach

The limitations of previous methods call for the evaluation of novel spectral analytical approaches. Within laboratory spectroscopy methods for decomposing spectra and modelling component absorption features have recently emerged which hold considerable promise for quantifying plant pigments. One approach that appears to be particularly appropriate is wavelet analysis (WA).

WA was developed independently in several scientific fields but interchanges between these during the last decade have led to a diverse range of applications of this signal processing technique. The potential of WA in image processing has been recognised with new techniques in image compression, classification, archiving and enhancement. Recent studies in laboratory spectroscopy have shown that WA offers several advantages over previous spectral approaches. Wavelets are functions that satisfy certain mathematical requirements and are used in representing data or other functions. Approximation using superposition of functions is the basis of Fourier Analysis (FA), however, in WA data is processed data at different scales or resolutions. Observing a spectrum through a large 'window' identifies gross features and through a small 'window' small features. The sines and cosines of FA are, by definition, non-local and poor at approximating spectra with sharp discontinuities (such as vegetation reflectance). WA is able to use more appropriate functions to capture local spectral features as it can decompose into components that are well localised in both time and frequency domains, while FA can only characterise frequency information (Strang and Nguyen, 1996). WA of a spectrum yields a vector of wavelet coefficients that are assigned to different frequency bands. Each band expands over the complete wavelength domain and responds to a certain frequency range of the spectrum. By selecting appropriate wavelet coefficients a spectral model can be established by regression of the coefficients against component chemical concentrations.

WA was initially applied in laboratory spectroscopy for quantifying glucose concentrations in solutions of varying protein (present in larger quantities with more dominant absorption features than glucose) and temperature (McNulty and Mauze, 1998). The results were comparable to Partial Least Squares regression (PLS) when calibration and prediction data sets contained the same protein concentration, but WA outperformed PLS when protein concentrations differed. The study highlighted the potential of WA to quantify concentrations based on localised absorption features from a mixture of compounds and that the approach is extendible beyond the calibration data set. It also showed how appropriate wavelet basis functions (or 'mother wavelets') can be selected from the multitude available based the correspondence between their shape and that of absorption features of components of interest, this gives the procedure a sound physical basis and chemical (pigment) specificity. The ability of WA to remove the effects of background spectral variation when quantifying concentrations of components with fine absorption from mixtures has also been demonstrated (Mittermayr et al., 2001). This offers potential for removing the effects of broader absorption features from the narrower features of specific pigments and for dealing with factors which affect broader regions of vegetation reflectance spectra such as leaf or canopy structure and soil/litter response. Importantly, the resilience of

WA to low frequency background noise can be tuned by choosing the appropriate number of vanishing moments in the wavelets and WA can deal with difficult situation where background varies between calibration and prediction data sets (Mittermayr et al., 2001). Furthermore, due to the localisation of wavelets, the wavelet coefficient can be chosen by chemical knowledge, e.g. the position and width of absorption bands. Conversely chemical knowledge can be discovered by selecting wavelet coefficients according to statistical measures (e.g. correlation, prediction errors etc.) and the localisation of coefficients indicate wavelength regions related to the analyte under investigation (Mittermayr et al., 2001). This is important in the context of plant pigments which display differing absorption spectra in vivo and in vitro.

Further evidence of the robustness of the approach is provided by spectroscopic studies that have used WA to remove background signals, noise and specular reflectance to produce accurate estimates of chemical concentrations by preserving fine spectral features of components, unlike other filtering/smoothing algorithms which attenuate and distort the absorption features of interest (Cai et al., 2001). The capacity of WA for noise suppression and insensitivity to background spectral variations has recently been exploited in quantitative remote sensing for the extraction of significant spectral features in AVIRIS data for vegetation type discrimination and the selection of width of smoothing and operator used for calculating spectral derivatives (Bruce and Li, 2001). Moreover, work on the classification of canopy reflectance spectra to discriminate crops and weeds has shown that WA is accurate and robust with respect to variations in % canopy cover and soil/litter properties (Huang et al., 2001).

1.3 Aims

The work reported in this paper forms part of a wider project aimed at developing a generic technique for quantifying vegetation pigment concentrations from hyperspectral remotely-sensed data. Specifically, the research will investigate the ability of WA to provide a method that is able to determine accurately *Chl a* and *b*, and *Cars*.

2. METHODS

The initial evaluation reported here, focussed on the application of WA to data sets collected by the author for previously published research – thereby facilitating a comparison with previous spectral approaches.

2.1 Data sets used

The data sets used were acquired using a common set of principles. Reflectance spectra of leaves and canopies were acquired with a spectroradiometer then immediately after the pigment determinations were conducted by extraction using an organic solvent followed by spectrophotometric analysis. In the case of canopies, pigment concentrations obtained from leaf samples were scaled up to the canopy level using leaf area index data collected *in situ*. The vegetation types used were broadleaved deciduous tree leaves (and stacks thereof) at various stages of senescence (see Blackburn, 1998a + 1999), bracken canopies (Blackburn, 1998b) and matorrral bushland canopies (Blackburn and Steele, 1999). Details of the methods and instrumentation used can be found in these papers.

2.2 Analytical methods

WA was implemented within Matlab 6.1 using the Wavelet Toolbox (v.2.1). Multilevel 1-D wavelet decompositions were performed on reflectance spectra using the range of different wavelet basis functions available in this package. Approximation and detail coefficients were extracted for each spectrum and a stepwise multiple linear regression was performed on the wavelet coefficients and pigment concentrations of the leaves and canopies under investigation. A 95% confidence interval was used in the stepwise procedure and up to 9 terms were permitted in the regression model (however, in most cases the number of terms selected ranged between 3 and 6). The predictive capabilities of the regression model were evaluated by calculating the coefficient of determination for prediction - the averaged coefficient of determination with one observation removed from the model (leave-one-out cross validation).

3. RESULTS

For all leaves and canopies sampled a number of wavelet basis functions (wavelet families) produced coefficients from which multiple regression models could be derived that were correlated with pigment concentrations: Daubechies wavelets (shortened to 'db' subsequently); Symlets ('sym'); Coiflets ('coif'); Biorthogonal wavelets ('bior'); and, Reverse biorthogonal wavelets ('rbio'). Generally the higher order wavelets within each family produced the highest correlation with pigments– hence the results for these wavelets are displayed below.

3.1 Individual leaves and stacks of leaves.

The range of pigment concentrations generated using the individual leaves and leaf stacks was large: 13 to 3235 mg.m^{-2} for Chl *a*, 8 to 2168 mg.m^{-2} for Chl *b* and 80 to 1447 mg.m^{-2} for Cars. Even over this large range of concentrations the multiple regression models derived from wavelet decomposition of reflectance spectra displayed high correlation with pigment concentrations.

	sym8	db8	coif5	bior6.8	rbio6.8
Chla	0.863	0.935	0.925	0.899	0.872
Chlb	0.863	0.863	0.891	0.886	0.847
Cars	0.637	0.743	0.486	0.761	0.715
Chltot	0.863	0.908	0.903	0.892	0.865

Table 1. R^2 values for multiple regression models, deciduous broadleaves.

Table 1. shows the coefficients of determination derived from multiple regression models based upon spectral decomposition using five particular wavelets. In all cases the coefficient of determination for prediction was slightly lower than the values depicted in the table. Other wavelets within each family produced lower correlations. As the table, for most wavelets, there were lower correlations for *Cars* than for the chlorophylls – this concurs with previous findings in investigations of other spectral approaches.

3.2 Bracken canopies

Table 2. demonstrates that for bracken canopies the wavelet decomposition can produce regression models with high correlations with pigments. Again, correlations are lower for *Cars* than *Chls*.

	sym8	db8	coif5	bior6.8	rbio6.8
Chla	0.910	0.915	0.901	0.809	0.782
Chlb	0.902	0.873	0.882	0.812	0.798
Cars	0.686	0.732	0.505	0.675	0.701
Chltot	0.905	0.908	0.891	0.810	0.791

Table 2. R^2 values for multiple regression models, bracken canopies.

3.3 Matorral canopies

As table 3 demonstrates, correlations derived for the matorrral canopies are lower than those for bracken and deciduous broadleaves.

	sym8	db8	coif5	bior6.8	rbio6.8
Chla	0.760	0.785	0.801	0.695	0.608
Chlb	0.755	0.764	0.789	0.687	0.599
Cars	0.656	0.710	0.678	0.600	0.502
Chltot	0.758	0.772	0.792	0.692	0.600

Table 3. R^2 values for multiple regression models, matorral canopies.

4. CONCLUSIONS.

This initial investigation of wavelet decomposition has revealed that this technique can produce results that are comparable with, and in some cases superior to, existing spectral approaches to pigment quantification from reflectance spectra. This provides support for further work on the technique, particularly in the context of testing the robustness and extendibility of the approach. In the first instance this can be done by combining the data sets of the various leaf and canopy samples used in the present study, then by employing additional data sets pertaining to a wider range of vegetation types. Radiative transfer models will be of particular value in providing an experimental platform to investigate issues which are difficult to address comprehensively in lab or field investigations – notably, the effects of viewing and illumination geometry and canopy architecture (i.e. LAD) on the robustness of the wavelet decomposition techniques, together with the consequences and emergent properties of many different combinations of biochemical and biophysical leaf and canopy characteristics, differing sensor characteristics and atmospheric effects. Refinements to the wavelet decomposition technique will be made through the development of automated approaches for the selection of appropriate wavelet basis functions, application of

the technique to spectral derivatives and for quantifying other plant biochemicals in addition to photosynthetic pigments.

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