

TOWARDS RED-EDGE POSITIONS LESS SENSITIVE TO CANOPY BIOPHYSICAL PARAMETERS USING PROSPECT-SAILH SIMULATED DATA

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ABSTRACT

The position of the inflexion point in the red edge (680 nm to 780 nm), termed the red-edge position (REP) has been used as a measure to estimate foliar chlorophyll or nitrogen content. In this study, we assessed the utility of a new technique for extracting the REP, the linear extrapolation method recently proposed by Cho and Skidmore [Remote Sens. Environ. (in press)]. The assessment was based on synthetic canopy reflectance spectra using the PROSPECT and SAILH models. The models were parameterised to represent a wide range of canopy characteristics. REP calculated by the new method involving wavebands at 680, 694, 724 and 760 nm yielded the highest correlation with leaf chlorophyll content ($R^2 = 0.75$) and with minimal effects of leaf and canopy biophysical confounders such as LAI, leaf inclination distribution and leaf dry matter content compared to traditional techniques including the wavelength of maximum first derivative, linear interpolation, inverted Gaussian modelling and third order polynomial fitting, respectively. However, the advantage of using the new method compared to the other REP extraction techniques diminishes with increasing bandwidth. In summary, the linear extrapolation technique shows high potential for leaf chlorophyll estimation with radiative transfer models. The efficacy of the technique under field conditions needs to be established.

1. INTRODUCTION

Accurate remotely sensed estimates of leaf chlorophyll content can provide valuable information on ecosystem functioning over a wide range of scales e.g. as an indicator of vegetation stress (Collins et al., 1983; Clevers et al., 2004) or ecosystem productivity (Blackburn, 1998; Mooney, 1986; Peterson et al., 1988). Commonly used vegetation indices for chlorophyll estimation computed from visible and near infrared (NIR) bands (Gates et al., 1965; Gamon et al., 1992; Buschmann and Nagel, 1993; Peñuelas et al., 1995; Lichtenthaler et al., 1996; Gitelson and Merzlyak, 1997; Blackburn, 1998; Carter and Knapp, 2001; Haboudane et al., 2002) are also influenced by other leaf and canopy parameters such as carotenoids (yellow pigments), leaf internal structure, mass and stacking, leaf area index (LAI), leaf angle distribution (LAD) and soil reflectance (Goward and Huemmrich, 1992; Blackburn, 1998; Daughtry et al., 2000).

A spectral measure that is less sensitive to the effect of variable leaf and canopy biophysical parameters, and environmental conditions on leaf chlorophyll estimation is the wavelength of maximum slope in the region of the red edge (680 to 780 nm), termed the red-edge position (REP) (Horler et al., 1983; Curran et al., 1995; Clevers et al., 2002). The red edge represents the region of abrupt change in leaf reflectance between 680 nm and 780 nm caused by the combined effects of strong chlorophyll absorption in the red and leaf internal scattering in the NIR (Gates et al., 1965; Horler et al., 1983). Increases in the amount of chlorophyll

results in a broadening of the major chlorophyll absorption feature centred around 680 nm (Buschmann and Nagel, 1993; Dawson and Curran, 1998) causing a shift in the slope and REP towards longer wavelengths (Gates et al., 1965; Horler et al., 1983; Boochs et al., 1990; Clevers et al., 2002).

A common approach for extracting the REP has been to locate the highest peak in the first derivative spectrum (Horler et al., 1983; Boochs et al., 1990; Buschmann and Nagel, 1993; Filella and Penuelas, 1994). However, the limitation of this approach is that the first derivative of contiguous spectra may contain two or more peaks (double-peak feature) near 700 and 725 nm (e.g. (Horler et al., 1983; Boochs et al., 1990; Zarco-Tejada et al., 2003; Clevers et al., 2004). The double peak feature causes a peak jump between 700 and 725 nm and a discontinuity in the REP/chlorophyll relationship (Horler et al. 1983).

In our previous study (Cho and Skidmore, in press), we proposed a new technique based on locating the REP as the point of intersection between two straight lines extrapolated on the far-red and NIR flanks of the first derivative spectrum (the linear extrapolation method). We showed that the linear extrapolation method not only mitigates the destabilising effect of the double peak feature but also predicts leaf nitrogen concentration with high accuracy. Nitrogen is not only a major component of leaf chlorophyll, but also forms part of inert structural components of cell tissue (Mooney, 1986; Jongschaap and Booij, 2004). Thus, indices for chlorophyll estimation that are maximally sensitive to chlorophyll with minimal effects of leaf and canopy structure, solar zenith angle, etc. are potentially useful.

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The objective of this study was to test whether the linear extrapolation method applies equally well under different conditions including variable leaf chlorophyll, canopy biophysical parameters and sensor bandwidth. To achieve the objective, we used a numerical experiment involving well established canopy reflectance models, parameterised to represent a wide range of canopy characteristics. This allowed us to artificially create pseudo measurements that otherwise would have been difficult and expensive to obtain under field conditions.

2. METHODS

2.1 Radiative transfer models

2.1.1 PROSPECT and SAILH models

For simulation of the synthetic reflectance spectra, PROSPECT and SAILH radiative transfer models have been used. PROSPECT is a leaf optical properties model developed by Jacquemoud and Baret (1990). It simulates leaf reflectance (ρ_{leaf}) and transmittance spectra (t_{leaf}) between 400 and 2500 nm using four model inputs: leaf chlorophyll content (C_{ab} ; $\mu\text{g cm}^{-2}$), equivalent leaf water thickness (C_{w} ; cm), leaf dry matter content (C_{m} ; g cm^{-2}), and a leaf structure index (N ; arbitrary units). Specific absorption and scattering coefficients of leaf components are provided with the model. The model is widely used and well validated (Fourty et al., 1996).

SAILH is a four-stream radiative transfer model developed by Verhoef (1984). It was later modified by Kuusk (1991) to take the hot spot feature into account. For the purpose of this study, SAILH was chosen to simulate bi-directional canopy reflectance (ρ) since it requires only few input variables, while having a predictive power similar to more elaborated reflectance models (Jacquemoud et al., 1995; Jacquemoud et al., 2000; Bacour et al., 2002). SAILH assumes the canopy to be a homogeneous semi-infinite medium with Lambertian leaves characterized by their reflectance and transmittance spectra ($\rho_{\text{leaf}}, t_{\text{leaf}}$). Soil reflectance (ρ_{soil}) must be specified at the lower boundary. Canopy structure is characterized by the leaf area index (LAI ; $\text{m}^2 \text{m}^{-2}$) and the average leaf angle of an ellipsoidal leaf inclination distribution with random azimuth orientation (ALA ; degrees). The hot spot effect is modelled using the ratio between leaf size and canopy height (s ; m m^{-1}). Further variables characterise the measurement geometry (θ_z, θ_v), and the fraction of diffuse illumination (skyl).

Soil reflectance at the lower boundary of the canopy (ρ_{soil}) was modelled using a simple soil parameterization described in Atzberger et al. (2003). In contrast to many other studies, the parameterisation does not only change the overall brightness of a (standard) soil spectrum, but also allows for (small) changes in the spectral shape, for example due to variations in the chemical composition of the soil (here soil carbon content).

2.1.2 Model parameterisation

For a given measurement geometry, the full parameterisation of the radiative transfer models involves nine (structural and biochemical) variables. Their parameter ranges and distributions are described in Table 1. Within the distributions of Table 1, 1000 parameter sets were randomly chosen to simulate the synthetic

canopy reflectance spectra. The wavelength range was restricted between 450 and 800 nm (351 values in 1-nm steps) as the study focuses only on the visible and near infrared (VNIR). The distributions cover a wide range of canopy and leaf properties, including widely varying leaf angles (from planophile to erectophile), different canopy densities (from bare soil to fully developed canopies), different soil albedos and leaf optical properties, etc.

Table 1.

Specification of parameter ranges and distributions for SAILH+PROSPECT reflectance modelling. In all cases, a nadir looking sensor has been assumed. The solar zenith angle was set to 45° .

model parameter	Abbreviation	units	Distribution	range ⁽¹⁾
canopy parameter				
Leaf Area Index	LAI	$\text{m}^2 \text{m}^{-2}$	uniform	0-10
Average Leaf Angle	ALA	$^\circ$ (degree)	uniform	30-80
Hot spot parameter	hot	no dimension	normal	0.1 ± 0.01
leaf parameter				
Leaf chlorophyll content	C_{ab}	g cm^{-2}	uniform	20-80
Leaf water content	C_{w}	cm	uniform	0.004-0.044
Leaf dry matter content ⁽²⁾	C_{m}	g cm^{-2}	uniform	$1.25 \times C_{\text{w}}$
Leaf structure parameter	N	no dimension	normal	2 ± 0.2
soil parameter				
Soil brightness	SCALE	no dimension	normal	1 ± 0.14
Carbon content	C_{c}	g cm^{-3}	uniform	0-6

⁽¹⁾In cases where *distribution* is *normal*, *range* indicates mean \pm std.

⁽²⁾ C_{m} is varied proportional to C_{w} as proposed by Combal et al. (2002)

2.2 Red-edge position algorithms

We have assessed the correlation between leaf chlorophyll content and REPs determined by the simple maximum derivative, linear interpolation (Guyot and Baret, 1988), inverted Gaussian modelling (Bonham-Carter, 1988; Miller et al., 1990), high order polynomial fitting (Pu et al., 2003) and linear extrapolation (Cho and Skidmore, in press) techniques. We have not considered the three-point Lagrangian interpolation technique (Dawson and Curran, 1998) because, Clevers et al. (2002) show that it is only suitable for coarsely sampled spectra.

2.2.1 Maximum first derivative

The REP is defined by the wavelength of the maximum first derivative of the reflectance spectrum in the region of the red edge. The first derivative was calculated using a first-difference transformation of the reflectance spectrum (Dawson and Curran, 1998) as follows:

$$\text{FDR}_{(\lambda_i)} = (R_{\lambda_{(i+1)}} - R_{\lambda_{(i)}}) / \Delta\lambda \quad (1)$$

where FDR = first derivative reflectance at a wavelength λ
midpoint between wavebands j and $j+1$
 $R_{\lambda(j)}$ = reflectance at the j waveband
 $R_{\lambda(j+1)}$ = the reflectance at the $j+1$ waveband, and
 $\Delta\lambda$ = difference in wavelengths between j and $j+1$.

2.2.2 Linear interpolation technique

The linear interpolation method (Guyot and Baret, 1988) assumes that the reflectance curve at the red edge can be simplified to a straight line centred around the midpoint between the reflectance in the NIR at about 780 nm and the reflectance minimum of the chlorophyll absorption feature at about 670 nm. It uses four wavebands (670, 700, 740 and 780 nm), and the REP is determined by using a two-step calculation procedure.

(a) Calculation of the reflectance at the inflexion point (R_{re})

$$R_{re} = (R_{670} + R_{780}) / 2 \quad (2)$$

where R = reflectance

(b) Calculation of the red edge wavelength or red edge position (REP)

$$REP = 700 + 40 \left(\frac{R_{re} - R_{700}}{R_{740} - R_{700}} \right) \quad (3)$$

where 700 and 40 = constants resulting from interpolation in the 700-740 nm interval.

2.3.3 Inverted Gaussian fitting technique

An inverted Gaussian (IG) model (Bonham-Carter, 1988; Miller et al., 1990; Dawson and Curran, 1998; Pu et al., 2003) was fitted to the spectral reflectance in the 660-780 nm band range. Accordingly, the IG model (Eq. 4) represents the red edge by the reflectance equation:

$$R(\lambda) = R_s - (R_s - R_o) \exp\left(-\frac{(\lambda_0 - \lambda)^2}{2\sigma^2}\right) \quad (4)$$

where R_s = maximum spectral reflectance
 R_o = minimum spectral reflectance
 λ_0 = wavelength of minimum reflectance
 σ = Gaussian function variance.

The REP is then defined as:

$$REP = \lambda_0 + \sigma \quad (5)$$

We used an iterative optimisation fitting procedure to determine parameters of the IG model (Miller et al., 1990). Initial guesses of the model parameters were made after review of each data set. Typically, R_o was set at 670 and 30 nm was selected for σ . The IG model employs a least-square criterion to fit a normal curve to the reflectance red edge. The values of λ_0 , R_o , R_s and σ are then determined by the fitting procedure.

2.2.4 Polynomial fitting technique

A polynomial (Pu et al., 2003) function (e.g. 3rd order polynomial - Eq. 6) was fitted to the reflectance spectrum between the wavelengths, corresponding to the minimum reflectance in the red and the maximum NIR (shoulder) reflectance.

$$R(\lambda) = a_0 + \sum_{i=1}^3 a_i \lambda^i \quad (6)$$

where λ = band between 670 nm to 780 nm.

Subsequently, REP was determined from the maximum first derivative spectrum.

2.2.5 Linear extrapolation technique

The linear extrapolation technique (Cho and Skidmore, in press) is designed to (i) mitigate the destabilising effect of the double peak feature on the correlation between chlorophyll and REP and (ii) track changes in slope near 700 nm and 725, where derivative peaks (Fig. 1) occur.

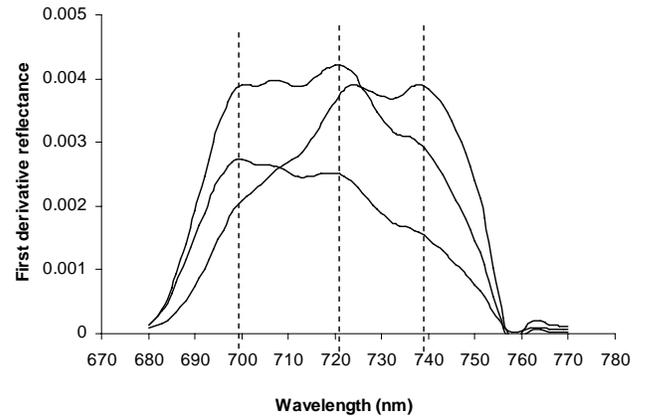


Fig. 1. First derivative curves for three SAILH+PROSPECT simulated spectra showing multiple peak regions near 700, 720 and 740 nm.

The REP is calculated as the wavelength at the intersection of two straight lines (Eq. 7 & 8) extrapolated through two points on the far-red flank and two points on NIR flank of the red edge (680 – 760 nm) first derivative reflectance spectrum (Fig. 2).

$$\text{Far-red line: } FDR = m_1 \lambda + c_1 \quad (7)$$

$$\text{NIR line: } FDR = m_2 \lambda + c_2 \quad (8)$$

where m and c = slope and intercept of the straight lines; c_1 and m_1 for the far-red line and c_2 and m_2 for the NIR line. At the intersection, the two lines have equal λ and FDR values. Therefore, the REP, which is the λ at the intersection, is given by:

$$REP = \frac{-(c_1 - c_2)}{(m_1 - m_2)} \quad (9)$$

Cho and Skidmore (in press) identified two combinations of wavebands for calculating leaf nitrogen-sensitive REPs. We shall call them linear extrapolation I involving far-red 680 and 694 nm

in combination with NIR 724 and 760 nm, and linear extrapolation II involving far-red 680 and 694 nm in combination with NIR 732 and 760 nm.

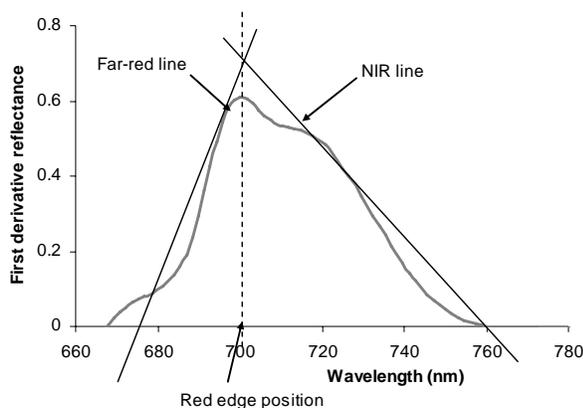


Fig. 2. Schematic representation of the linear extrapolation technique for extracting the red edge position (REP) – wavelength of the meeting point between two straight lines extrapolated on the far-red and NIR flanks of the first derivative spectrum.

2.3 Data analysis

First, to evaluate the predictive value of the linear relationship between leaf chlorophyll content and REP extracted by various methods, the relationship was calculated for 750 randomly selected samples (calibration data set) and used with the REPs to estimate leaf chlorophyll content for the remaining 250 samples (test data). Secondly, we quantified the main effects of chlorophyll content and LAI, ALA or leaf dry matter content and their interaction on the REPs extracted by various methods. The contribution of each factor to the total variance in the REP was calculated by dividing its sum of squares by the total sum of squares. Lastly, we assessed the effect of degrading the bandwidth (re-sampled spectra) on the correlation between REP and chlorophyll content. The synthetic 1nm-data (simulated ASD data) was re-sampled to the spectral coverage of Hyperion (~10 nm bandwidth) and HyMap (~15 nm bandwidth). The re-sampling was conducted using the ENVI (Environment for Visualising Images, Research System, Inc.) software.

4. RESULTS AND DISCUSSION

4.1 Relationship between leaf chlorophyll content and red edge position

The linear regression between leaf chlorophyll content and REP derived by the linear extrapolation method (I and II) yielded higher coefficients of determination (R^2) with the calibration data set and lower standard errors of prediction with the test data compared to the traditional methods (maximum first derivative, linear interpolation, inverted Gaussian and polynomial fitting techniques) (Table 2).

In our previous study (Cho and Skidmore, in Press), we obtained the same correlation coefficient between leaf nitrogen concentration and REP extracted by linear extrapolation I and II

for each of the following data sets; rye (*Lolium perenne*) canopy, maize leaf and mixed grass/herb leaf stack spectra. But this study shows that linear extrapolation I performs better than linear extrapolation II for leaf chlorophyll estimation.

Table 2. The relationship between leaf chlorophyll content and red edge position (REP) extracted by various methods.

REP method	R^2 (calibration data set)	Predictive equation	¹ RMSE (test data set, n = 250)
Maximum first derivative (748 df)	0.50	- 647.56 + 0.97*REP	12.75
Linear interpolation (748 df)	0.60	- 2494.31 + 3.53*REP	10.76
Inverted Gaussian modelling (723 df)	0.61	- 1707.99 + 2.46*REP	13.87
3 rd order polynomial fitting (748 df)	0.62	- 595.28 + 0.88*REP	10.36
Linear extrapolation I (746 df)	0.75	- 1111.01 + 1.63*REP	8.98
Linear extrapolation II (746 df)	0.70	- 866.41 + 1.28*REP	9.77

¹RMSE=root mean square error

Table 3.

Main and interaction effects (quantified by the coefficient of determination – R^2) between leaf chlorophyll content and canopy biophysical parameters on the red edge position extracted by the wavelength of the maximum slope (max FDR), linear interpolation (LI), inverted Gaussian (IG), polynomial fitting (PF) and linear extrapolation methods (LE)

	Max FDR	LI	IG	PF	LE I	LE II
<i>Cab and LAI</i>						
Cab	0.490*	0.608*	0.604*	0.625*	0.751*	0.701*
LAI	0.025*	0.015*	0.025*	0.015*	0.008	0.016*
Cab*LAI	0.000	0.008*	0.000	0.000	0.000	0.000
Total R^2	0.515	0.631	0.629	0.641	0.759	0.717
<i>Cab and ALA</i>						
Cab	0.490*	0.608*	0.605*	0.620*	0.750*	0.698*
ALA	0.009*	0.020*	0.013*	0.009*	0.012*	0.011*
Cab*ALA	0.001	0.002*	0.000	0.002	0.000	0.000
Total R^2	0.500	0.630	0.618	0.632	0.767	0.709
<i>Cab and Dm</i>						
Cab	0.490*	0.608*	0.608*	0.621*	0.755*	0.704*
Dm	0.207*	0.250*	0.222*	0.159*	0.142*	0.181*
Cab*Dm	0.004*	0.000	0.004*	0.027*	0.001*	0.001*
Total R^2	0.701	0.858	0.834	0.807	0.898	0.886

*= $p < 0.05$, LAI = leaf area index; ALA = average leaf angle of an ellipsoidal leaf inclination distribution with random azimuth orientation; DM = leaf dry matter content.

4.2 Influence of canopy biophysical parameters on red edge positions extracted by various methods

Among the investigated perturbing canopy biophysical variables (LAI, ALA and leaf dry matter content), leaf dry matter content

showed the highest influence on the REP (Table 3). However, the influence of dry matter content was lowest on the REP derived by the linear extrapolation I method. The contribution of LAI to the total variance of REP was low (R^2 ranges from 0.008 to 0.025) but statistically significant for all the REP techniques with the exception of the linear extrapolation I. Furthermore, the effect of ALA was equally low but significant for all REP techniques. The interaction effects between the chlorophyll content and biophysical parameters on REP were generally low. We should note that there was no significant ($p>0.05$) correlation between leaf chlorophyll content and LAI or ALA or leaf dry matter. Results reported in literature on the relationship between REP and LAI are mixed. Some studies using one or at most a few closely related species suggest that REP is influenced by both chlorophyll content and LAI (Filella and Penuelas, 1994; Danson and Plummer, 1995; Pu et al., 2003). On the contrary, Boegh et al. (2002) found no relationship between REP and LAI across eight crop fields consisting of both winter-sown and spring-sown crops but observed a high positive relationship between REP and leaf nitrogen concentration. Broge and Leblanc (2000) using PROSPECT and SAIL simulated data observed that REP poorly relates to LAI.

4.3 Effects of degrading the bandwidth on the linear extrapolation method

Degrading the bandwidth from 1nm in the original data to the spectral coverage of Hyperion (~10 nm) and HyMap (~15 nm) lowered the correlation between REP and chlorophyll content for all REP extraction methods (Table 4). The advantage of using the linear extrapolation I method compared to the various alternatives diminishes with decreasing spectral resolution, confirming results obtained by Cho and Skidmore (in press).

Table 4.
Correlation (R^2) between leaf chlorophyll content and red edge position derived from ASD, Hyperion and HyMap band settings for various red-edge position (REP) extraction methods.

	LE	IG	PF	LE I	LE II
ASD (1 nm)	0.61	0.604	0.62	0.75	0.70
Hyperion (~10 nm)	0.63	0.61	0.60	0.66	0.59
HyMap (~15 nm)	0.55	0.44	0.53	0.55	0.50

linear interpolation (LI), inverted Gaussian (IG), polynomial fitting (PF) and linear extrapolation methods (LE)

5. CONCLUSION

This study has shown that REPs extracted by the linear extrapolation method involving wavebands at 680, 694, 724 and 760 nm have the potential for maximally explaining variations in leaf chlorophyll content with minimal effects of leaf and canopy biophysical confounders such as LAI, leaf inclination distribution and leaf dry mass content, compared to traditional techniques including the linear interpolation, inverted Gaussian and polynomial fitting techniques. However, the advantage of using the linear extrapolation method compared to the various REP algorithms diminishes with decreasing spectral resolution. The

efficacy of the technique under field conditions needs to be established.

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