IMAGING SPECTROMETRY FOR ECOLOGICAL APPLICATIONS

Paul J CURRAN
Department of Geography
University of Southampton
Highfield
Southampton SO17 1BJ
UK
P.Curran@soton.ac.uk

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ABSTRACT

Imaging spectrometry from aircraft or satellite borne sensors has many potential ecological applications. This paper reviews its use for the remote sensing of foliar biochemical concentration, as this is one ecological application of remote sensing that is unique to imaging spectrometry. Attention is focussed on the development of methodologies, drawing where relevant on theory and techniques from both outside and inside remote sensing. Examples from the fields of near infrared spectroscopy (NIRS) and geological remote sensing, along with an extensive reference list, provide an introduction to some of the ecological opportunities offered by imaging spectrometry.

1. INTRODUCTION

Many environmental variables influence the signals that reach a remote sensor. If we wish to use these remotely sensed signals to estimate environmental variables then we need to ensure that the number of remotely sensed signals is greater than the number of environmental variables that are causing those signals to vary (Verstraete *et al.*, 1996; Curran, 2000). The number of environmental variables can be reduced by holding some constant (e.g., restrict analysis to one geographic region, correct for atmosphere) and the number of remotely sensed signals can be increased by recording many such signals in narrow wavebands along the spectrum. We can then repeat this sampling at different locations, times, geometries of sensor and illumination and polarizations (Curran *et al.*, 1998). In ecology attention has been directed towards increased spectral sampling because of great spectral variability, in the 0.7μm to 2.5μm range, for vegetated landscapes. However, the majority of this spectral variability lies within just four or five dimensions (Curran *et al.*, 1998); two dimensions in visible (0.4-0.7 μm) wavelengths, one dimension in near-infrared (0.7-1.3 μm) wavelengths and one or two dimensions in middle-infrared (1.3-2.5 μm) wavelengths. If the remotely sensed signal in four to

five wavebands can account for most of the spectral variability in vegetated landscapes then why would we wish to record in more wavebands? From an engineering point of view surely we would be better advised to maximise the signal-to-noise ratio (Smith and Curran, 1999) or increase (i.e., make finer) the spatial resolution (Curran, 1994) of our sensor, rather than spread the remotely sensed signal over more than four to five wavebands? These concerns are reasonable if we are asking what I will call first and second level ecological questions. First level questions are a version of 'what is the vegetation there?' and once answered, second level questions are a version of 'how much vegetation is there?' Both of these questions can usually be answered using broadband sensors with wavebands positioned in the four or five locations mentioned above. For example, we may wish to use remotely sensed signals in red, near infrared and middle infrared wavebands to classify forest as a land cover class and then estimate the leaf area index of that forest (Boyd and Curran, 1998; Boyd *et al.*, 2000). Such a use of remote sensing is possible because we are detecting gross spectral features that are primarily the result of changes in pigment absorption, within-leaf scattering and water absorption respectively. If we wish to progress further and ask a third level ecological question such as 'what is the condition of that vegetation?' then the information we need does not reside within four to five broad wavebands. This information is within narrow spectral features that result from harmonics and overtones of absorptions by foliar biochemicals (Curran, 1989; Clark, 1999). To record these narrow spectral features we need a sensor with many narrow wavebands (Hill and Mégier, 1994). In other words, it is imaging spectrometry that enables us to ask ecological questions of the third kind.

1. REMOTE SENSING OF FOLIAR BIOCHEMICAL CONCENTRATION

Accurate remotely sensed estimates of the foliar biochemical concentration of vegetation canopies have been used to aid the understanding of ecosystem function over a wide range of scales (Peterson *et al.*, 1988; Gholz *et al.*, 1997; Dawson *et al.*, 1999). This is because many biochemical processes, such as photosynthesis, respiration, evapotranspiration and decomposition are related to the foliar concentration of biochemicals such as chlorophyll, water, nitrogen, lignin and cellulose (Running, 1990; Peterson, 1991, Goetz and Prince, 1996). Such remotely sensed estimates have also found application in a wide range of ecosystems for estimating vegetation stress (Jago *et al.*, 1999); identifying species (Martin *et al.*, 1998) and driving ecosystem simulation models over large areas (Lucas and Curran, 1999; Lucas *et al.*, 2000). The remote sensing of foliar biochemical concentration developed rapidly during the 1980s and 1990s (Peterson and Hubbard, 1992; Wessman, 1994; Curran and Kupiec, 1995; Wülder, 1998; Treitz and Howarth, 1999). Emphasis during the 1990s was on the use of airborne imaging spectrometers (Staenz, 1992; Curran, 1994) to estimate the biochemical

concentration of tree canopies (Matson *et al.,* 1994; Johnson *et al.,* 1994*;* Dungan *et al*., 1996; Johnson and Billow, 1996; Martin and Aber, 1997). The research was stimulated by both the NASAs Accelerated Canopy Chemistry Programme (ACCP) (Aber, 1994; Wessman, 1994; Smith and Curran, 1995; 1996; Curran *et al*., 1997) and parallel activities aimed at understanding the interaction of radiation with leaves (Fourty *et al*., 1996; Fourty and Baret, 1998), forest canopies (Danson and Curran, 1993; Danson, 1995) and leaves in forest canopies (Yoder and Pettigrew-Crosby, 1995; Kupiec and Curran, 1995). In retrospect, a large component of this understanding seems to have come from modelling (Ustin *et al*., 1999), where leaf models containing a biochemical component (Jacquemoud and Baret, 1990; Dawson *et al*., 1998a) have been used on their own (Baret and Fourty, 1997; Ganapol *et al*., 1998) or have been coupled with canopy models (Jacquemoud *et al*., 1996; Dawson *et al*., 1999; Ganapol *et al*., 1999). For example, such an approach has been used to determine the seasonality of leaf chlorophyll content (Demarez *et al*., 1999) and the potential of radiation measured by the Medium Resolution Imaging Spectrometer (MERIS) on Envisat for the estimation of canopy chlorophyll content (Dawson, 2000).

If the remote sensing of foliar biochemical concentration is to flourish then ecologists who use imaging spectrometer data will need to be alert to (i) the very many challenges that still lie ahead (Peterson and Hubbard, 1992; Peterson, 2000) and (ii) techniques being developed for the processing of spectra both outside and inside the field of remote sensing.

1. DEVELOPMENTS OUTSIDE REMOTE SENSING: AN EXAMPLE OF NIRS

The well-established research field of laboratory-based near infrared spectroscopy (NIRS) involves the operational use of *spectrometry* in near-to middle-infrared wavelengths (AOAC, 1990). NIRS methods were brought to the attention of the remote sensing community by the United States Department of Agriculture (USDA) who used NIRS for the spectrometric assay of biochemicals in forage crops (Williams and Norris, 1987; Marten *et al.,* 1989). NIRS methods utilise an empirical multivariate approach which assumes that a foliar spectrum is the difference between 100% reflectance and the sum of the absorption features of each biochemical, weighted by their concentration (Peterson *et al.,* 1988; Curran *et al.,* 1992). At its simplest this method uses stepwise regression to select wavelengths from across the whole of several reflectance, or more usually, derivative reflectance spectra (Dixit and Ram, 1985; Tsai and Philpot, 1998) that are most strongly correlated with the biochemical concentration of foliar samples (Curran, 1989; Martin, 1994). However, NIRS is far more than this, as can be seen in NIRS textbooks (Burns and Ciurczak, 1992;

Osborne *et al.*, 1993), proceedings of the various *International Conferences on NIR Spectroscopy* (e.g., Davies and Williams, 1996), the *Journal of Near Infrared Spectroscopy* and *NIR News*. Many of the applications reported in the NIRS literature relate, in some way, to the food industry (Thyholta and Isaksson, 1997; Batten, 1998; Büning-Pfaue *et al.*, 1998). For example, quantifying cheese condition (Sørensen and Jepsen, 1997), detecting faecies on chicken carcasses (Peterson, 2000), measuring sugar in sugar beet (Salgo *et al.,* 1998), or estimating kiwifruit softness (McGlone *et al.*, 1997). However, it is not a great leap of imagination to move from the analysis of spectra produced by say, a laboratory-based imaging spectrometer with a spatial resolution of 0.5 mm (Martinsen *et al.*, 1999) to the analysis of spectra produced by an airborne or spaceborne imaging spectrometer.

The application of NIRS is wider than the food industry and includes for example, operational tasks such as monitoring production lines, to more interesting tasks such as assay of blood outside and inside a patient, identifying a cars make and model from paint left at the scene of an accident, to predicting the trees that will be chewed by elephants (Lister *et al.*, 1997; Sollinger and Voges, 1997; Cassis *et al.*, 1998; Heise *et al.*, 1998). Further examples of NIRS applications are given in table 1 and broadly-based spectroscopy texts (e.g., Clark, 1991; Duckworth, 1998; Workman and Springstein, 1998).

- **Estimation of a biochemical/chemical**

  Salt in water; ammonia and propane in air; nitrogen in soil, sheep guts and potatoes; sugar/starch in bananas, fruit juice and oranges; nicotine in tobacco and 'foreign substances' in milk.
- **Biochemical assay of**

  Beer, cereals, rapeseed, flax, goats milk, blood, faeces, silage and compost.
- **Differentiation between**

  Olive oils, kiwi fruit berries, high acid fruits, apple juices, tree pulps, tobaccos, meats, plastics and crude oils.

Table 1 A selection of near infrared spectroscopy (NIRS) applications as reported in the *Journal of Near Infrared Spectroscopy* volumes 1 (1993) to 8 (2000) inclusive. (Source: http://www.nirpublications.com)

Some of the techniques and applications of NIRS are made possible by the large signal-to-noise ratio of laboratory spectrometers and the homogeneity of the samples. However, there are three areas of NIRS that have an immediate relevance here. The first is the biochemical assay of leaves (Thygesen,

1994; Hallett *et al.*, 1997; Méthy *et al.*, 1998), where laboratory-based spectra of leaves have been used both for the estimation of key foliar biochemicals, such as a nitrogen (Aber *et al.*, 1994; Newman *et al.*, 1994) and for the development of methods relevant to remote sensing (Card *et al.*, 1988; Curran *et al.*, 1992; Peñuelas *et al.*, 1995; Gitelson and Merzlyak, 1997; Ponzoni and Gonçalves, 1999).

The second is the formulation of theory (Wonzy *et al.*, 2000) and the development of techniques (Berzaghi *et al.*, 2000) for spectral analysis. Many NIRS techniques can be transferred with little modification to the analysis of remotely sensed spectra, whether it be for calibration (Sinnaeve *et al.*, 1994), variable selection (Westad and Martens, 2000), mixture modelling (Hlavka *et al.*, 1997) or some aspect of regression analysis (Montalvo *et al.*, 1994).

The third is the development of NIRS as part of the field of chemometrics (Otto, 1999; Kayes *et al.*, 2000). The interface between NIRS and issues such as signal processing, artificial intelligence, spectral databases and genetic algorithms provides an area of particular interest for a remote sensing audience (Morgan, 1991; Geladi and Dåbakk, 1995; Massart *et al.*, 1998). The most fertile of these is probably the use of neural networks to train spectral classifiers (Hana *et al.*, 1997; Dawson *et al.*, 1998b).

However, a note of caution:

> *'Even though NIR began as a classical spectroscopy, its growth was marked by pragmatism. That is its characteristics or effects were observed and exploited long before we ever truely understood why it really worked'* (McClure *et al.*, 1991, p. 14A).

NIRS will continue to be a valuable source of techniques for ecological remote sensing but to understand the processes involved we will undoubtedly need to return to first principles and leaf and canopy reflectance models (Ustin *et al.*, 1999).

4 DEVELOPMENTS INSIDE REMOTE SENSING: AN EXAMPLE FROM GEOLOGICAL REMOTE SENSING

NIRS techniques based on stepwise regression are robust and effective; however, they are not ideal due to (i) the risk of overfitting (usually when many more wavebands than samples are used); (ii) the selection of wavelengths that are non-causal (Baret and Fourty, 1997), or are located in the absorption feature of a biochemical to which the biochemical of interest is correlated (Curran *et al.*,

1992; Grossman *et al.*, 1996) and the (iii) lack of generally accepted procedures for both data preprocessing to enhance absorption features and standardisation to minimise the effect of spectral variability that is independent of biochemical concentration. To overcome at least some of these problems we need look no further than geological remote sensing (Clark, 1991; Kruse *et al.*, 1993; Schowengerdt, 1997), in particular the methodologies proposed by Kokaly and Clark (1999) that benefited from *continuum-removal, calculation of band depth* and *normalisation*. In these methodologies a continuum was fitted to the reflectance spectra in order to represent absorptions other than the one of interest (Clark and Roush, 1984). The value associated with a wavelength was then expressed, not as reflectance or the first derivative of reflectance, but as band depth normalised to the waveband at the centre of the absorption feature (BNC) or the area of the absorption feature (BNA).

Band depth normalised to band depth at the centre of the absorption feature (BNC)

This measures the depth of the waveband of interest from the continuum line, relative to the depth of the waveband from the continuum line at the centre of the absorption feature.

$$BNC = (1-(R/R_i))/(1-(R_c/R_{ic}))$$

where BNC is band depth normalised to the centre; R is reflectance of sample at waveband of interest; R_i is reflectance of continuum line at waveband of interest; R_c is reflectance of sample at absorption feature centre and R_{ic} is reflectance of continuum line at absorption feature centre.

Band depth normalised to area of absorption feature (BNA)

This measures the depth of the waveband of interest from the continuum line, relative to the area of the absorption feature.

$$BNA = (1 - (R/R_i))/A)$$

where BNA is band depth normalised to area and A is area of absorption feature.

These are illustrated for waveband λ in figure 1, where R is 48.9%, R_i is 52.4%, R_c is 41.5% and R_{ic} is 49.5%. Therefore, band depth is 0.07 relative reflectance at wavelength λ and 0.16 relative reflectance

at the centre of the absorption feature. Given that the area of the absorption feature (A) is 19.13 relative reflectance nm^{-1} then for waveband λ BNC is 0.41 and BNA is 0.004.

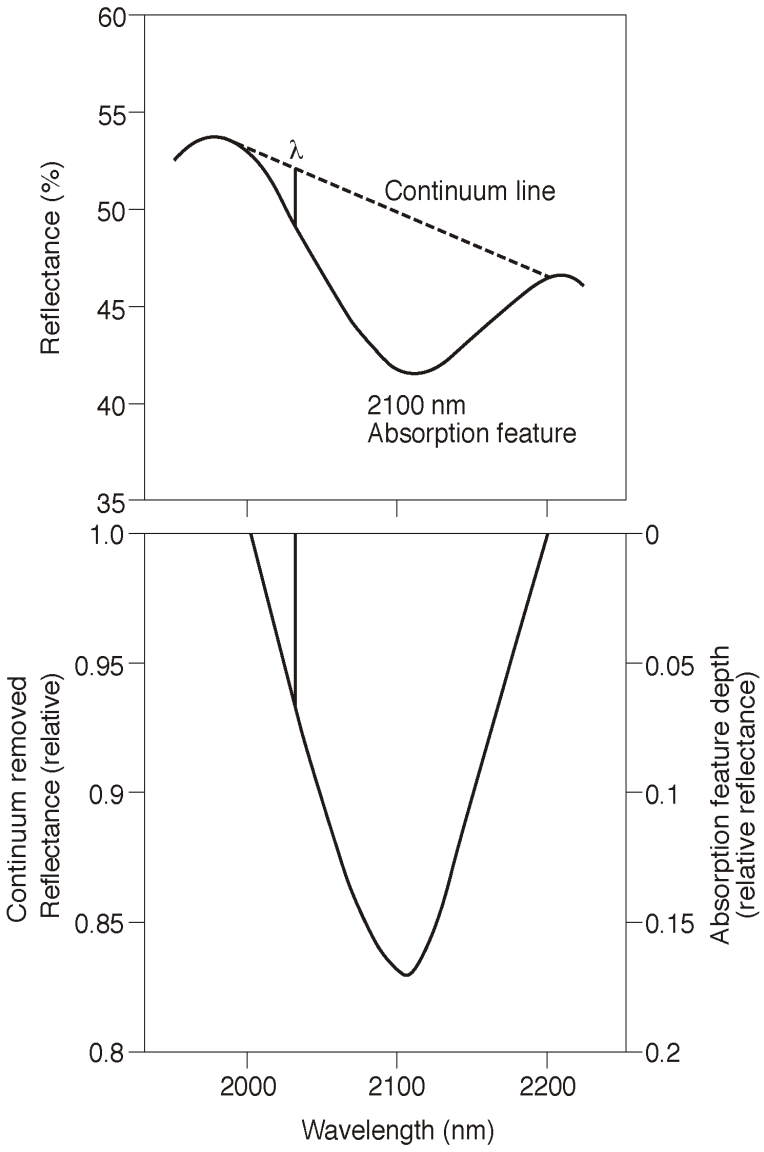

Figure 1 Diagrammetric illustration of continuum-removal and band depth calculation for waveband (λ) in the 2100 nm absorption feature.

Kokaly and Clark (1999) developed and tested their methodologies on a large data set collected as part of the ACCP. This comprised laboratory spectra and biochemical assays of three biochemicals (nitrogen, lignin, cellulose) for seven sites and a total of 744 samples. They used three absorption

features (centred around 1730 nm, 2100 nm and 2300 nm) and the procedures outlined above. With this approach they obtained high values of R^2 between spectral data and biochemical concentration (for example, R^2 for nitrogen ranged from 0.75 to 0.94).

These methodologies have been tested independently on a smaller foliar dataset (n=68-70) from one site but for twelve biochemicals (Curran *et al.*, 2001). Stepwise regression on first derivative spectra resulted in large R^2 (maximum 0.90, average 0.74) and a small root mean square error (RMSE) as a percentage of the mean (minimum 0.46, average 8.24) between estimated and observed foliar biochemical concentrations. Stepwise regression on bands normalised to band depth at the centre of the absorption feature (BNC) or the area of the absorption feature (BNA) resulted in even larger R^2 (maximum 0.94 and 0.96, average 0.80 and 0.84 respectively) and small RMSE as a percentage of the mean (minimum 0.24 and 0.12, average 6.68 and 4.86 respectively) between estimated and observed foliar biochemical concentrations. In this case the most accurate methodology for the estimation of foliar biochemical concentration is well-known in geological remote sensing (Clark, 1999) and was stepwise regression normalised to the area of the absorption feature.

The original scientific rationale for imaging spectrometry was geological (Peterson, 2000) and throughout the 1990s the geological agenda drove many developments in imaging spectrometry (Hill and Mégier, 1994; Green *et al.*, 1998; Kruse, 1999). Ecological remote sensing has developed considerably during this time but can still look with benefit at the leads being taken by those working in geological remote sensing (Clark, 1999).

5 SUMMARY

We are currently seeing a transition from airborne to spaceborne imaging spectrometry (Curran, 1994; Denniss, 1999). This offers opportunities to ecologists who will have a tool capable of determining the amount of given biochemicals, the degree of environmental pollution, or the rate of biogeochemical cycling at scales from the local to the global (Curran and Kupiec, 1995; Guyot and Phulpin, 1997). We need to pose questions that will capitalise on this technology and these questions need to be not just "what is the vegetation there?" or "how much vegetation is there?" but "what is the condition of that vegetation?" To answer questions of the 'third kind' we will need to be alert to developments outside and inside remote sensing. In particular, we will need to take advantage of techniques in NIRS and

geological remote sensing that compliment recent developments image processing and leaf and canopy modelling.

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