Chapter 6 - Spectral Data Analysis

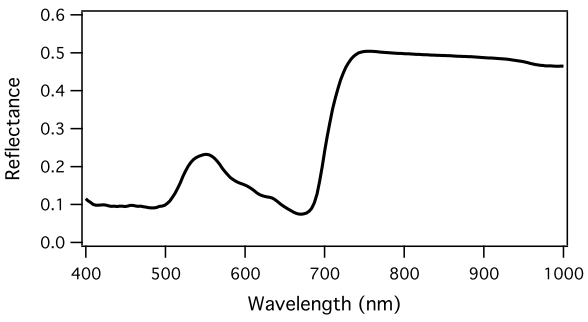
The nature of spectral data

A spectrum (plural: spectra) is large array of numbers providing rich information on any of a number of topics. The size and dimensionality of large spectral datasets provide many challenges for analysis, some of which will be briefly discussed in this chapter, which focuses on common analytical methods applied in plant spectroscopy.

A spectrum can be represented and visualized several ways:

1) Spectral plot - in this view, variation of a spectrum is shown as a function of wavelength. This can be represented graphically or in tabular form (figure 1). Multiple spectra represented in tabular form can also be considered an array or a matrix.
2) Feature (or spectral) space - this displays the value of a spectrum (or pixel) in one "band" or wavelength against the value of the same spectrum (or pixel) in another band or wavelength. Figure 2a is a 2-dimensional feature space (meaning that we are displaying the values in two bands), and figure 2b is a 3-dimensional feature space (meaning that we are displaying values in three bands). Figure 2b shows the two different spectra represented this way. In this representation, spectra can also be thought of *vectors*, and two spectra can be compared by their distance or similarity in N-dimensional feature space. While mathematics can easily represent spectra in multiple dimensions, the challenge lies in visualizing spectra beyond 3 dimensions, which lies beyond normal human intuition.
3) Image cubes (e.g., from imaging spectrometers; see figure 3). Each image pixel represents a spectrum of specific location on the surface (e.g., ground or canopy) recorded by the sensor. An *image cube* combines an image (X-Y axes) with a spectral (Z axis) representation of imaging spectrometry data from ground, airborne or spaceborne platforms in the form of images composed of elements called pixels.

Figure 1. Reflectance spectrum of a Douglas-fir (*Pseudotsuga menziesi*) needle, plotted (left) and expressed in tabular form (right) as a function of wavelength (λ).



λ (nm)	Reflectance
402.43	0.11042
405.77	0.10560
409.1	0.10013
412.43	0.09791
415.76	0.09789
419.09	0.09859
…	…
997	0.46476

Bands vs. wavelengths – These similar terms actually have slightly different meaning. Wavelengths are usually expressed in wavelength units (e.g. nm or μm). Bands (also called wavebands, spectral bands or channels) are often called by spectral region (e.g. visible, near-infrared) or by band number (e.g. MODIS bands 1 and 2), which correspond to a specified wavelength range, usually with a particular response function

and characteristic FWHM. Because many sensors cannot record data in all wavelengths, they record spectral data in specified ranges of wavelengths (bands or channels). By contrast, hyperspectral sensors sample many contiguous bands across a spectrum over a given range of wavelengths (e.g., ~400-1000 nm in the case of VIS-NIR, or ~400-2500 in the case of VIS-SWIR, or "full-range" instruments).

When expressing spectra as vectors, the direction of the spectrum conveys information about the shape of the spectrum (and thus the identity of the target) and the length of the vector conveys information about the absolute value (e.g. the brightness of the target) (figure 2). While conceptually challenging (it is hard to visualize N-dimensional space), recognizing the vector nature of spectra can assist in data management and provide many powerful tools for analyzing spectral data. To use the full power of this concept, we often use linear algebra in processing spectral data.

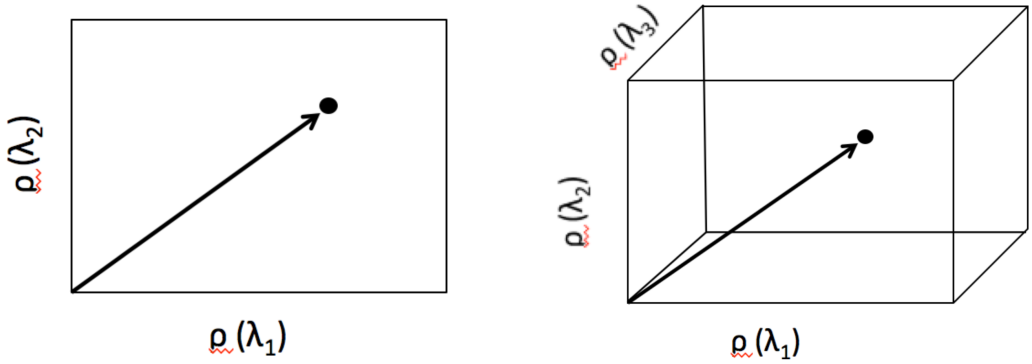


Figure 2a – A spectrum as a vector in 2-D space (left) and 3-D space (right). Axes indicate reflectance (ρ) in wavebands 1, 2, and 3 (λ_1, λ_2, λ_3).

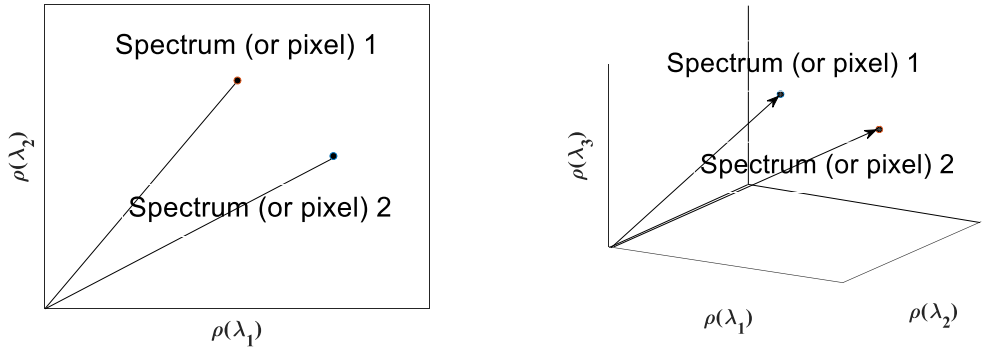


Figure 2b. Two spectra as vectors in 2-D space (left) and 3-D space (right). Axes indicate reflectance (ρ) in wavebands (or wavelength) 1, 2, and 3 (λ_1, λ_2, λ_3). Figure: H. Gholizadeh.

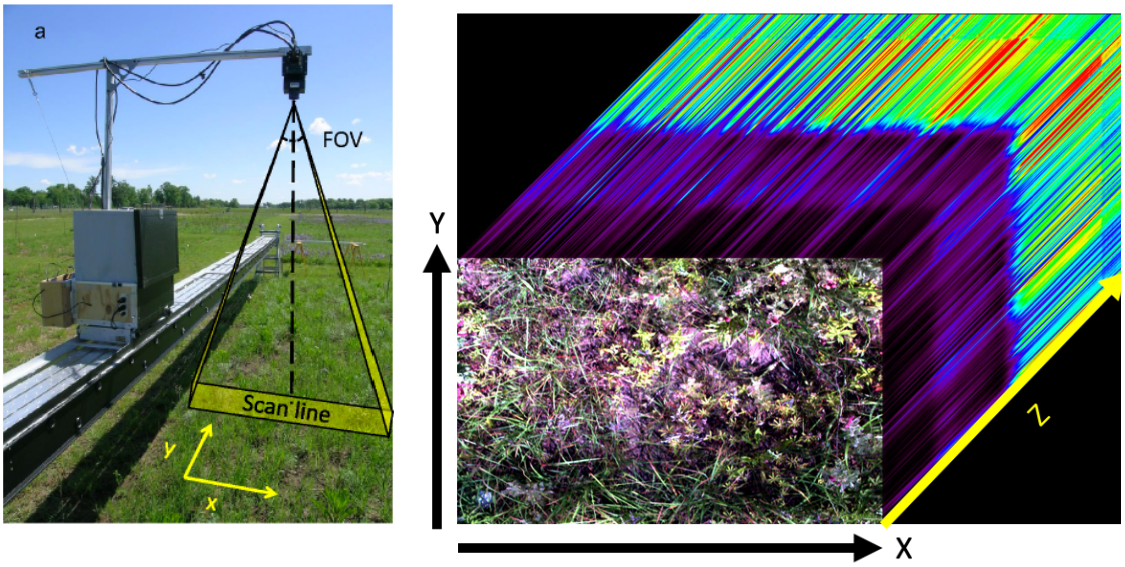


Figure 3. Pushbroom imaging spectrometer mounted on a cart and track ("tram system"). X indicates the scanline direction. The motion of the spectrometer in the Y direction builds an image line-by-line. Each pixel in the resulting *image cube* (right) is also a spectrum (reflectance values shown as different rainbow colors, purple being low, and red being high reflectance), with wavelength depicted along the Z axis. On the X-Y face of this image cube, the scene is depicted at a "true-color" RGB image, with colors approximating those seen with the eye of a human observer viewing the ground surface. Using image processing, individual bands can be assigned to RGB in multiple ways to yield a true or false color image.

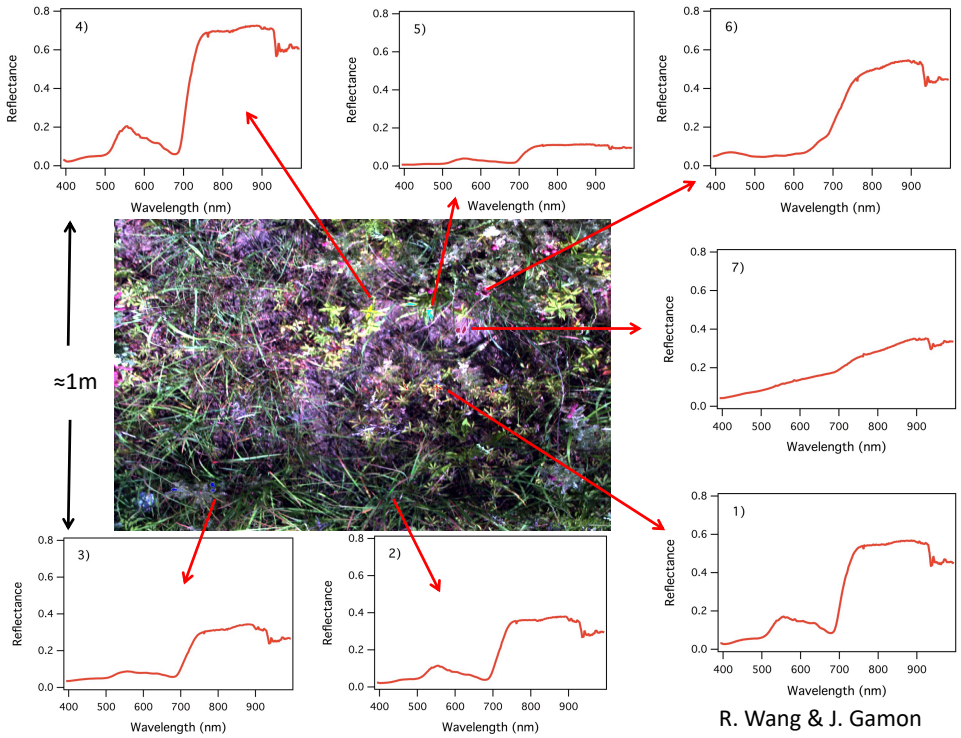


Figure 4. Alternate representation of the image cube (see Figure 3) as a 2-dimensional image, with spectra of individual scene objects (small cluster of pixels) shown as spectral plots (reflectance as a function of wavelength).

Challenge of data volume - One of the challenges of spectral data is the sheer volume of the data. Each spectrum obtained when capturing spectral data with a spectrometer (or

each pixel in an imaging spectrometer) can be comprised of hundreds or thousands of values (i.e., an array), depending upon the instrument and its spectral resolution. In a statistical sense, a spectrum of this size represents only a single independent sample. As an illustration, in a single spectrum collected with a hyperspectral instrument, the reflectance values of two adjacent bands are not truly independent and are likely to contain similar information about the target. Thus, a spectrum is best thought of as a set of related values that together contain information about shape and brightness (analogous to a vector with a direction and magnitude). When collecting multiple samples through time or space, a small spectral dataset can quickly and easily expand to include millions of numeric values, requiring consideration of large data volumes.

Data reduction (dimension reduction):

To keep datasets manageable, remove redundant data, and to help visualize data, a number of data reduction methods exist. Data reduction methods fall into two general categories: 1) band selection (choosing of a subset of bands from all available bands), and 2) feature extraction (transforming the data to extract new features and reduce the data volume). These different methods (band selection and feature extraction) each have advantages and disadvantages.

Band Selection:

Band selection preserves the original data values and is conceptually and mathematically simple. Band selection is used for selecting a subset of existing bands without a transformation; therefore, preserving the general spectral shape and greatly reducing the data volume. In band selection we try to select the best subset of original bands to get the highest possible accuracy for our desired application, for example classifying spectral data. One approach for band selection is to conduct an exhaustive search of all possible bands. In this approach, the "best" subset of bands is found by: 1) trying all possible combination of bands, and 2) evaluating all of these combinations using a criterion or fitness function (for example classification accuracy metric or correlation coefficient) to find the "goodness" of each of these subsets, until finding the best subset of bands. Other examples of well-known band selections strategies are sequential forward selection, and sequential backward selection (Devijver & Kittler, 1982).

Band selection is the first step in calculating a spectral index, which turns a spectrum into a single numeric value, or "index," that (hopefully) best represents a desired feature of the target. Band selection discards some of the spectral information, can miss fine spectral detail, and can be readily biased by preconceived notions of "what is important" in a particular spectrum.

We also perform something similar to band selection when we subset or resample a spectral data set (figure 5). While this reduces data volume, it clearly loses information present in the original spectrum.

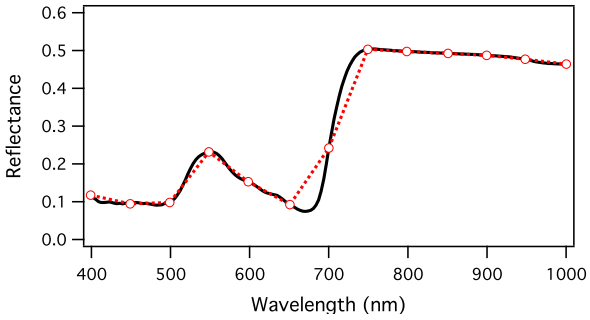


Figure 5. Douglas-fir needle spectrum before (black solid line) and after (red dotted line) subsetting. In this case, values at 50-nm intervals were retained, losing fine spectral detail (e.g. slope information), but retaining the general spectral shape and overall brightness (albedo).

Spectral Indices:

When working with spectral data, it is common to select a subset of bands for further calculation and analysis. A common example involves band selection for *spectral index* calculation (Singular: index. Plural: indices). Spectral indices (also called *reflectance indices*, or *vegetation indices*) are simply mathematical expressions of two or more bands. Two of the more common expressions are band ratios, and normalized difference indices

$$Ratio = \rho_1 / \rho_2 \qquad \text{(eq. 1)}$$

$$Normalized\ difference\ index = (\rho_1 - \rho_2)/(\rho_1 + \rho_2) \qquad \text{(eq. 2)}$$

Where ρ indicates reflectance at a given waveband or wavelength.

An example of the first is the "Simple Ratio," a vegetation greenness index that is the ratio of NIR reflectance (ρ_{NIR}) to red reflectance (ρ_{red}). An example of the second is the Normalized Difference Vegetation Index (NDVI), a vegetation greenness index that is the most widely used vegetation index, which uses the difference divided by the sum of a red and near-infrared (NIR) band. Not surprisingly, the Simple Ratio and NDVI provide identical information about vegetation, but in two slightly different ways (Gamon et al. 1995)

Literally hundreds of indices have been defined and published for vegetation, measuring any of a number of features including plant "greenness" (e.g. simple ratio or NDVI), plant water content (e.g. water index), plant pigment content, and biochemical content. Table 1 lists a few commonly used vegetation indices and their uses. Many indices are intended to measure a particular physiological or structural feature of vegetation, many of which can be thought of as characteristic "plant traits."

Table 1 – Examples of some commonly used vegetation indices, their formulas, applications and sources.

Index	Formula	Application	Reference
Normalized Difference Vegetation Index (NDVI)	$(\rho_{NIR}-\rho_{red})/(\rho_{NIR}+\rho_{red})$	Vegetation greenness	Gamon et al. 1995
Simple Ratio	ρ_{NIR}/ρ_{red}	Vegetation greenness	Gamon et al. 1995
Enhanced Vegetation Index (EVI)	$G\frac{\rho_{NIR}-\rho_{red}}{\rho_{NIR}+C_1\times\rho_{red}-C_2\times\rho_{blue}+L}$	Vegetation greenness	Huete et al. 2002
Chlorophyll Index	$(\rho_{750}-\rho_{705})/(\rho_{750}+\rho_{705})$	Chlorophyll content	Gitelson & Merzlyak 1994, Sims & Gamon 2002

MERIS Terrestrial Chlorophyll Index	$(\rho_{753.75}-\rho_{708.75})/ (\rho_{708.75}+\rho_{681.25})$	Chlorophyll content	Dash & Curran 2007
Photochemical Reflectance Index (PRI)	$(\rho_{531}-\rho_{570})/ (\rho_{531}+\rho_{570})$	Xanthophyll cycle & photosynthetic efficiency (fast response); chlorophyll/carotenoid ratios (slow response)	Gamon et al. 1992, 1993, 1997
Water Index	ρ_{900}/ρ_{970}	Plant water content	Peñuelas et al. 1993
NDWI	$(\rho_{NIR}-\rho_{SWIR})/ (\rho_{NIR}+\rho_{SWIR})$	Plant water content	Gao, 1996
Soil-Adjusted Vegetation Index (SAVI)	$(1+L)(\rho_{NIR}-\rho_{Red})/(\rho_{NIR}+\rho_{Red}+L)$	Vegetation greenness, after correction for soil	Huete 1988

Since a waveband can be narrow or broad, the same formula can have different numerical values depending upon the exact instrument (and band definition) used. For example, a red band at 670 nm with a full-width-half-maximum (FWHM) of 1 nm yields a slightly different NDVI value than another red band centered at the same wavelength but with a FWHM of 10nm. For these reasons, it is always good to define not only the wavelength of a particular band center, but the FWHM or the spectral response function (if available) of that band.

To make the spectra or indices from two instruments more readily comparable, it is often helpful to first *convolve* the band responses of the two instruments, which involves matching the spectral responses of the two instruments mathematically. A good convolution will make the resulting index values of the two instruments more similar when sampling the same target. With instruments having several broad bands with gaps in between, it can be difficult or impossible to closely match index values. With hyperspectral instruments having narrow bands, convolution can be a necessary but easy task (many image processing and mathematical or statistical software have built-in routines for spectral convolution). Band convolution can also be a useful step in simulating a broadband (e.g. satellite) index from hyperspectral sensors

Feature extraction:

In contrast to band selection, feature extraction uses mathematical transformations to extract useful information about a spectral dataset while greatly reducing the original data volume. As an example of feature extraction, *principal component analysis* (PCA) transforms a spectral dataset by "rotating" the spectra in multi-dimensional data space, to re-express the data according to a smaller number of orthogonal "principal components" that represent the axes of greatest variability of the spectrum (Figure 6) (Jolliffe 2002). Before transformation, the data are highly dependent (Figure 4 - left) and after PCA transformation, they are completely independent (orthogonal) meaning that the values of PC1 change independently from values of PC2 (Figure 6 - right).

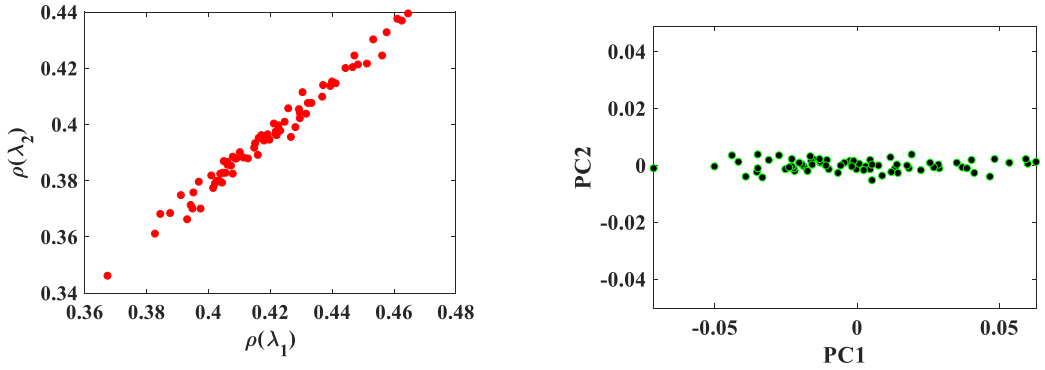


Figure 6. Data before (left) and after (right) PCA transformation. Each data point represents a single spectrum (or vector) before (left) and after (right) rotation, as represented in 2-D. Figure: H. Gholizadeh.

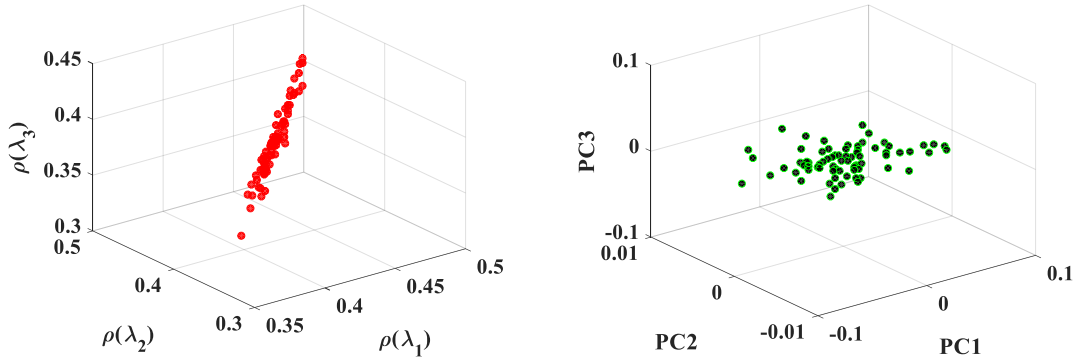


Figure 6. The same transformation of spectra (figure 4), illustrated in 3D. In this case, a set of spectra (represented as a set of data points in wavelength space, left) are transformed (rotated) to obtain the transformed dataset shown in "principal components space" (right). Figure: H. Gholizadeh.

PCA is often applied to a set of reflectance spectra to identify the primary components of variability within the data. To do this, PCA mathematically "rotates" a spectrum in feature space to find the primary (principal) axes of variability. The first axis represents the direction of primary variability or maximum variance (the first *eigenvector*). The second axis is, by definition, orthogonal to the first and represents the direction of secondary variability (the second *eigenvector*). In PCA this process is repeated until the desired number of components (*eigenvectors*) are identified. Typically, 3-5 components define well over 90% of the variability, so it is often common to use only the first few components (See figure 6) in data reduction. However, sometimes useful information is present beyond the first few components, so the exact number of components can depend upon the application. The human brain easily visualizes two or three dimensions and cannot readily perceive multi-dimensional data volumes above three dimensions, so the top two or three PCs are typically visualized, often capturing most of the variation in the data (figure 7).

It is worth noting that PCA can in principle obtain as many components (or eigenvectors) as the number of wavebands (bands). It is possible that meaningful information can be "buried" way past the third component. This is often true when considering plant traits that can be detected with subtle absorption features in reflectance spectra. The first few components of a PCA typically provide information on illumination (brightness) and canopy structure (e.g. greenness), with subsequent

components yielding progressively more information on subtle absorption features. Thus, the exact method and which components to use will depend in part upon the goal.

Determining which PCs to use and how can be a difficult judgement due to the abstract nature of the data transformation. One way to assign meaning to PCs from a spectral dataset is to plot the component "loadings" or "weightings" for each wavelength as a coefficient spectrum. Also called factor score coefficients, these loadings represent the correlations between the transformed (rotated) axes, and the original axes (wavelengths). This allows the expression of each component in the original (wavelength) space, sometimes facilitating the identification of the cause of variability. For example, in developing the formula for the Photochemical Reflectance Index, Gamon et al (1992) used PCA and concluded that the first PC was primarily associated with brightness, and the second component with greenness, based on their spectral shape and location. The third component contained information on the relative levels of xanthophyll cycle pigments and helped reveal the wavelength of interest. By relating transformed data back to the original wavelengths in this way, meaning can be attributed to transformed data. Particularly if PCA provides a similar answer to that from independent methods, it can be a powerful tool for spectral data exploration.

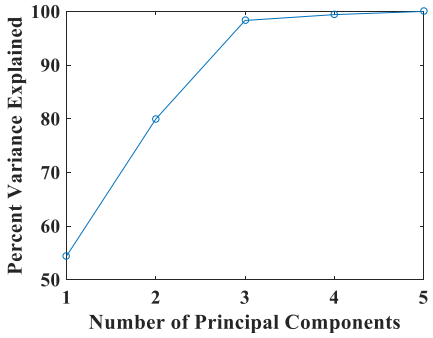


Figure 7.

Cumulative percent variance explained by the first 5 components. Notice how most of the variance can be explained by a small number of PCs. Figure: H. Gholizadeh

PCA is a good example of a transformation that reduces data volume and allows feature extraction. However, because PCA alters the original data, the transformed data cannot always be easily related to observable properties of a target or it's spectrum. The abstract nature of the data transformation associated with feature extraction can present special challenges in visualization. Another limitation of PCA is that it requires more cases (replicate samples) than wavelengths to function properly and avoid overfitting. Consequently, it sometimes requires very large datasets (many spectra) or band subsetting (restricting the spectra to fewer bands than the number of spectra).

Vector normalization:

If the goal is to focus on subtle spectral features, such as absorption associated with plant biochemical traits, it is sometimes useful to first remove (normalize for) the effects of brightness, which typically appears as the first component of PCA. *Vector normalization* is sometimes used to normalize spectra by their intensity (brightness). By reducing the variation in overall reflectance (or radiance) due to illumination, vector normalization can enhance spectral differences due to small features (e.g. absorption features associated with plant traits), often making it easier to detect differences in trait values between two individuals or in a landscape against a complex background of widely varying illumination and canopy structure, as is often found in nature. The potential drawback of vector normalization is that, by altering the original spectral

information, it can sometimes miss important features or introduce artifacts into the subsequent analysis. For example, vector normalization of vegetation canopy spectra removes variation due to sunlit and shaded canopy regions and can lose information related to illumination and plant structure but emphasize more subtle plant traits (Wang et al. 2022).

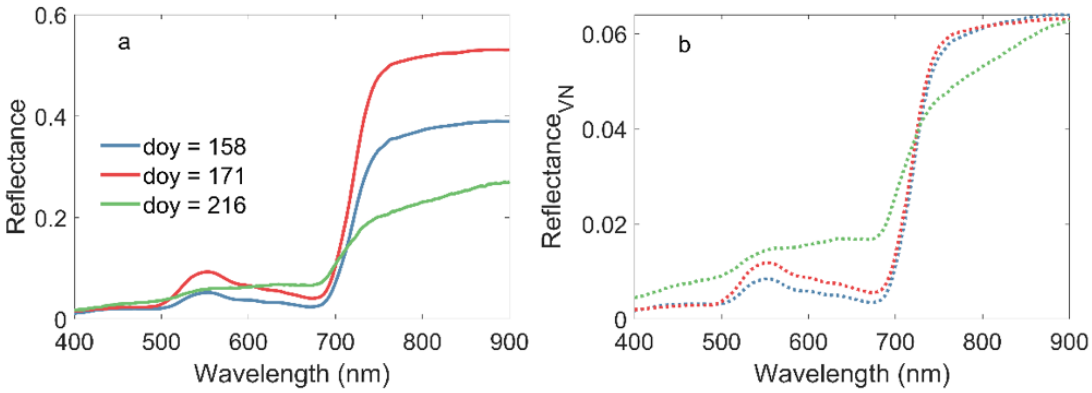


Figure 8. VIS-NIR vegetation canopy spectra before (a) and after (b) vector normalization (VN). Note how large differences in brightness (best seen as reflectance in the NIR above 700 nm) are reduced, enhancing some of the subtle differences in spectral shape associated in part with pigmentation. Figure: Wang et al. (2022).

Partial Least Squares Regression:

Because each of the analytical methods applied to spectra offers advantages and disadvantages, it is sometimes good to combine methods for additional insight. For example, partial least squares regression (PLSR), which is a combination of principal component analysis and multiple linear regression (Wold et al. 2001), is a powerful statistical method. Unlike PCA, PLSR is not compromised by overfitting. PLSR can transform reflectance spectra into a set of coefficients (a "coefficient spectrum") that represents the weightings or relative strength of each wavelength in predicting a variable of interest. Wavelengths that are positively correlated with the variable will have positive coefficient values, and wavelengths that are negatively correlated will have negative coefficient values. Wavelengths lacking useful information will have coefficient values near zero. A regression coefficient spectrum plot can provide quick insight into which wavelengths might have useful information and provide statistical power for a given analysis, and can help select wavelengths that might be good bands for a spectral index or for revealing key plant traits. If PLSR reveals that the same bands as those used in a spectral index are important predictor variables, it can provide additional, independent confidence in that spectral index.

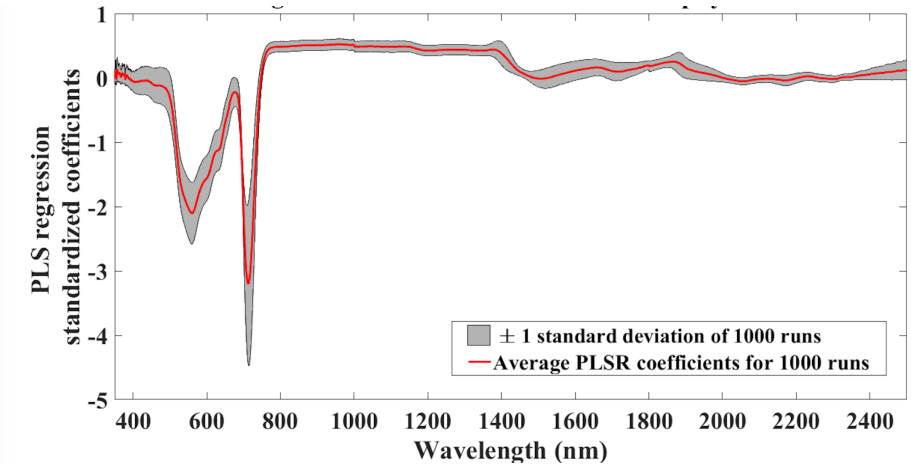


Figure 9. Standardized coefficients for PLSR regression (reflectance vs. chlorophyll content). Wavelengths with large absolute values have a strong weighting (strong predictive power for chl). Figure: H. Gholizadeh.

Continuum removal:

To analyze a particular absorption feature in a reflectance spectrum, it is sometimes useful to isolate that feature from the overall spectrum ("continuum"). *Continuum removal* (Clark and Roush) provides one method to characterize the depth of a particular *absorption feature*. In this method, a line is fit to either side of the feature, and the depth can then be measured as the distance from the bottom of the absorption feature to that line (figure 10). Widely used in mineral identification and quantification, this method can also useful for quantifying plant biochemical absorption features.

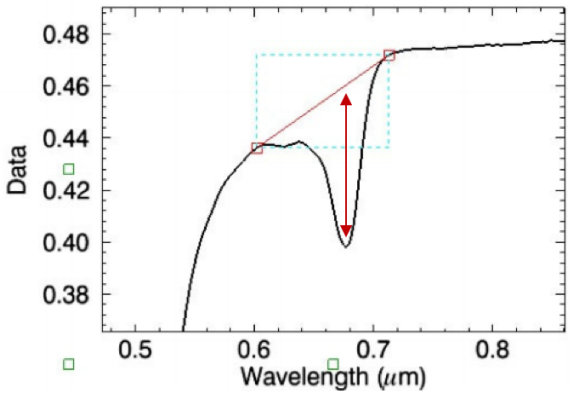


Figure 10. Illustration of continuum removal by fitting a line to either side of an absorption feature. The vertical distance (red arrow) from the bottom of that feature to the fitted line provides a measure of band depth. From Kokaly 2008.

Chlorophyll fluorescence:

Chlorophyll fluorescence is a tiny amount of radiation that is first absorbed by plant pigments, then re-emitted at a slightly longer wavelength by plant chlorophyll, and provides a useful measure of photosynthetic activity (see Chapters 2, 3& 5). The fluorescence signal from plant leaves and canopies can be measured along with the reflected radiance, where is evident as a tiny, dynamic additional contribution to the detected radiance (or reflectance). Because it is so tiny, it is often ignored and considered part of the radiance or reflectance signal. Strictly speaking, including fluorescence and calling it "reflectance" is incorrect as fluorescence arises from a

different mechanism (emission) from reflected radiance (scattering) (see Chapter 2). Due to the slight contamination of the reflectance signal by the fluorescence signal it may be technically more correct to call reflectance that contains this signal *apparent reflectance*. Because the fluorescence signal is so small, analyzing and quantifying the fluorescence signal against the larger signal of scattered radiation represents a special challenge. A number of methods have been derived for doing this, and some are briefly reviewed here.

Kinetic analysis – Because fluorescence is closely related to plant photosynthetic light regulation (see Chapter 5) measuring the radiance over time from leaves or canopies exposed to rapidly changing light can reveal the pattern and amount of fluorescence emitted. A simple way to do this is to take a dark-adapted leaf (or canopy), and suddenly exposed it to full sunlight or artificial, bright white light. The change in apparent reflectance upon sudden illumination reveals a double-dip near the red edge due to chlorophyll fluorescence quenching (relaxation of the sudden fluorescence signal) which can be used to quantify both the spectral shape and size of the chlorophyll fluorescence peaks (Figure 11; see also Figure 7 in Chapter 5). This can also be analyzed kinetically to probe the response of photosynthesis when the plant is under stress (see Chapter 5).

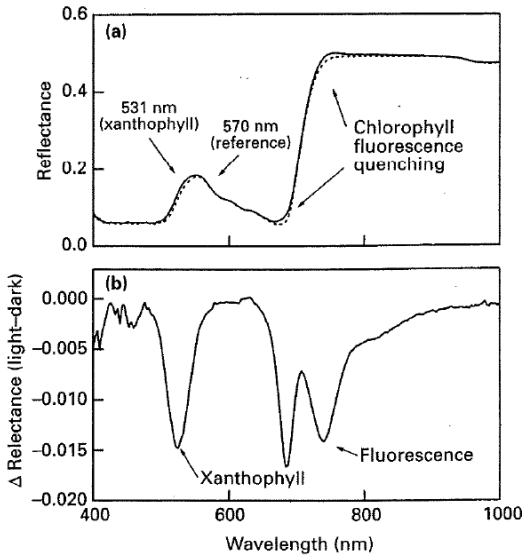


Figure 11

Apparent reflectance spectra (top panel) and difference spectrum (Δ reflectance, dark minus light state), of dark-adapted sunflower (*Helianthus annuus*) leaf following exposure to ten minutes of bright light. These difference spectra exhibit dips centered at 531 nm due to conversion of the xanthophyll cycle pigments from violaxanthin to zeaxanthin, and a double dip near 685 and 740 nm due to chlorophyll fluorescence quenching. These rapid changes in apparent reflectance due to fluorescence can also be analyzed kinetically (as a time-series) a way to probe the light regulatory processes of photosynthesis under stress (Gamon and Surfus 1999).

Filters - Because fluorescence is emitted from a different process than reflectance, and involves a red shift (*Stokes shift*) in the spectrum (see Chapter 2), filters can be used to isolate the emitted fluorescence radiation, against a larger background of scattered radiation. One way to do this is using a leaf clip (e.g. *FluoWat* leaf clip; Van Wittenberghe 2014) that includes a *cutoff filter*, blocking any scattered radiation beyond a given wavelength (typically 650 nm) (figure 12). Under these conditions, the signal measured above the cutoff wavelength is, by definition, fluoresced radiation (along with a small amount of light leakage through the filter). Usually, this radiation is expressed in absolute radiance units (Watts m^{-2} nm^{-1} sr^{-1}), which requires conducting a radiometric calibration (converting relative machine units to absolute energy units).

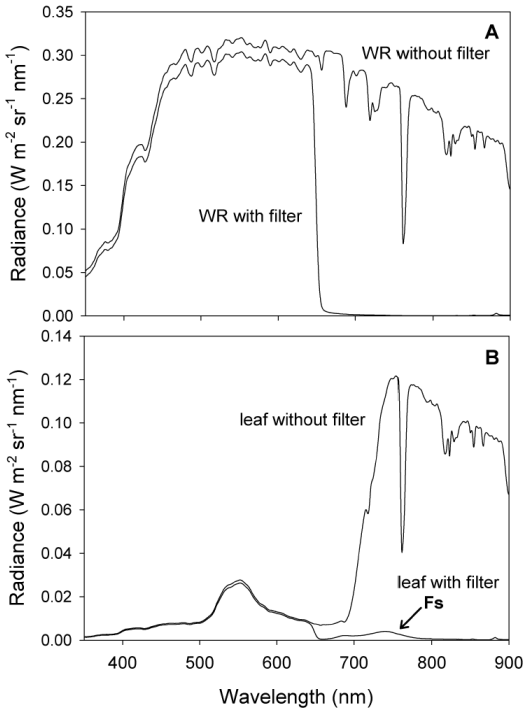


Figure 12

Top: Radiance spectra of a white reflectance standard with and without a 650 nm cutoff filter.

Bottom: Apparent radiance of a leaf with or without a 650 nm cutoff filter. Note that a small part of the apparent radiance (mostly composed of reflected radiation scattered back from the leaf surface) consists of a double-peaked fluorescence signal, which is only visible when the cutoff filter blocks the scattered light.

Figure 2.3 from vanWittenberghe (2014)

Spectral fitting methods - The fluorescence signal present as slight "contamination" of the reflected radiance from green vegetation can also be isolated using various spectral fitting methods when using ultraspectral sensors (sensors with extremely high spectral resolution). These sensors can resolve narrow absorption features of gases present the Sun's and Earth's atmosphere (Fraunhofer and telluric lines, see top panel, Figure 13). These features can be resolved with *ultraspectral* sensors covering the range of a chlorophyll fluorescence spectrum (red to near-infrared region). Because the solar radiation in these *Fraunhofer* and *telluric* features is blocked by atmospheric absorption, but the radiation present in these features includes the fluorescence signal, the fluorescence values can be extracted with spectral fitting methods. A number of spectral fitting methods have been developed to extract this tiny fluorescence signal in a larger radiance spectrum of reflected radiation. One method (Fraunhofer Line Discrimination, FLD) measures the fluorescence signal in the oxygen A band (760 nm) by comparing the signal in this oxygen absorption band against the signal outside and immediately adjacent to that band (Meroni et al. 2010, Alonso et al. 2008). Another method (Spectral Fitting Method, SFM), isolates the fluorescence spectrum by fitting across multiple atmospheric absorption features across the apparent radiance spectrum (Meroni et al. 2010), Cogliati et al. 2015).

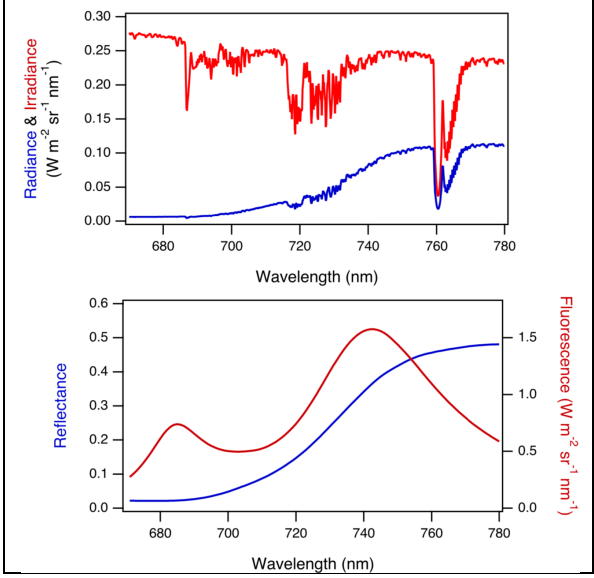


Figure 13

Radiance and irradiance spectra collected over a corn (*Zea mays*) field, August 4, 2021, using ultraspectral spectrometers (FLoX, JB Hyperspectral, Dusseldorf Germany) (top panel). The Spectral Fitting Method (SFM Cogliati et al. 2015) was applied to these spectra to derive the fluorescence and idealized reflectance spectra shown in the bottom panel. Data courtesy Ran Wang.

Fluorescence metrics - Because fluorescence is emitted as a signal across multiple wavelengths (as a spectrum), and there are several methods of extracting this signal, there are also several ways of analyzing and expressing this signal. Common fluorescence metrics include the height of the fluorescence peaks in the red (around 694 nm) or the near-infrared (around 740 nm), the integrated area under the entire fluorescence spectrum, or any of these metrics divided by the amount of incoming (or absorbed) *photosynthetically active radiation* (PAR). This last method, called fluorescence yield provides a normalized measure that tells us how much of the incident or absorbed radiation is converted to fluorescence, revealing key information about photosynthetic light regulation (see Chapter 5). When analyzed in concert or with other reflectance metrics (including PRI, as discussed above), these fluorescence metrics provide a particularly potent way to evaluate plant photosynthetic responses in response to environmental conditions.

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