

Machine Learning for Soil and Crop Management
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Lecture 21

Diffuse Reflectance Spectroscopy: Basics and Applications for Crop and Soil

Welcome friends to this week five of the NPTEL online certification course of machine learning for soil and crop management.

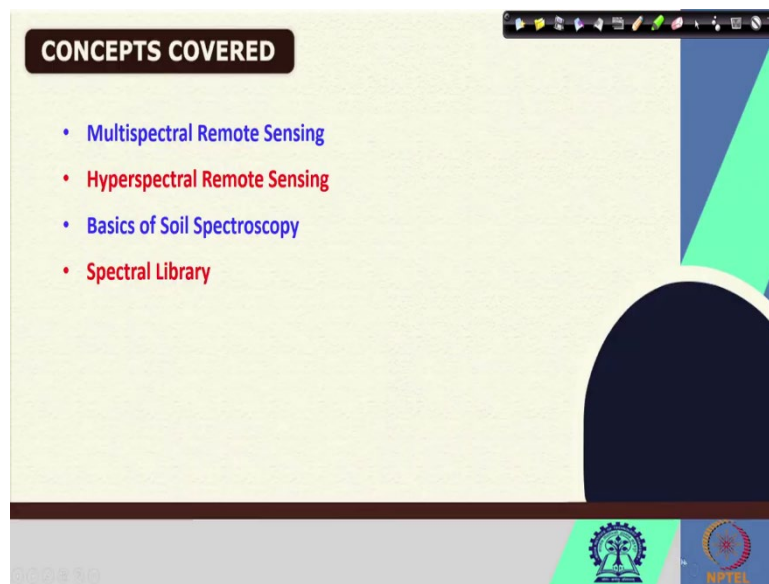
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And in this week 5, we are going to discuss a very, very important topic that is Diffuse Reflectance Spectroscopy: The Basics and Applications for Crop and Soil. Now, in the modern era of soil and crop analysis, diffuse reflectance spectroscopy has gained, a huge importance. And nowadays it became an indispensable tool for proximal soil and crop management. So, in this week, we will be especially discussing different basics of what is diffuse reflectance spectroscopy.

We will be discussing some of the specs of the diffuse reflectance spectroradiometer and also we are going to discuss some of the important soil application of course, there are 1000s and 1000s of application if you if you go and see the literature, you will see 1000s of application both for soil and crop, but we will be discussing some of the most important advancement as far as the soil and crop based monitoring are concerned based on this diffusion reflectance spectroscopy. So, this is our first lecture.

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And in this lecture, we are going to discuss on the basic concepts we will be starting with the sampling the spectrum, and then how from the electromagnetic spectrum, we can see different types of spectral reflectivity spectral values, we will be talking about the bad chromatic images, we will be talking about multispectral remote sensing, and then we will be talking about hyperspectral remote sensing and the difference between multispectral remote sensing and hyperspectral remote sensing.

We are also going to talk about the basics of soil spectroscopy and what is spectral library how to create the spectral library. Now, in our previous 4 weeks, we have discussed the basics of machine learning application for soil and crop and also we have discussed the multivariate data analytics, how to handle different multivariate data. Also, we have discussed the important regression and multivariate regression problem machine learning problems and their application for soil and crop.

We have also discussed the classification problems and different clustering problems also for predicting several important soil and crop properties or classifying several important soil and crop properties. Now, all those discussion this application of this diffuse reflectance spectroscopy came several times and today we are going to discuss what is the basic of or the fundamental concept behind this soil spectroscopy and how this diffuse reflectance spectroscopy helps in identifying or predicting several important soil and crop parameters. And so, these are the concepts which we are going to cover.

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KEYWORDS

- Soil Spectroscopy
- MIR
- Vis-NIR
- Spectral library
- Chemometrics

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And also these are the important keywords which we are going to cover. Soil spectroscopy MIR or mid infrared, then vis-NIR or visible to near infrared, then spectral library I will show you how to develop the spectral library and also chemometrics or the statistical algorithms required for measurement of a chemical parameter is known as a chemometric. So, we are going to discuss all these in our lecture.

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PANCHROMATIC BAND

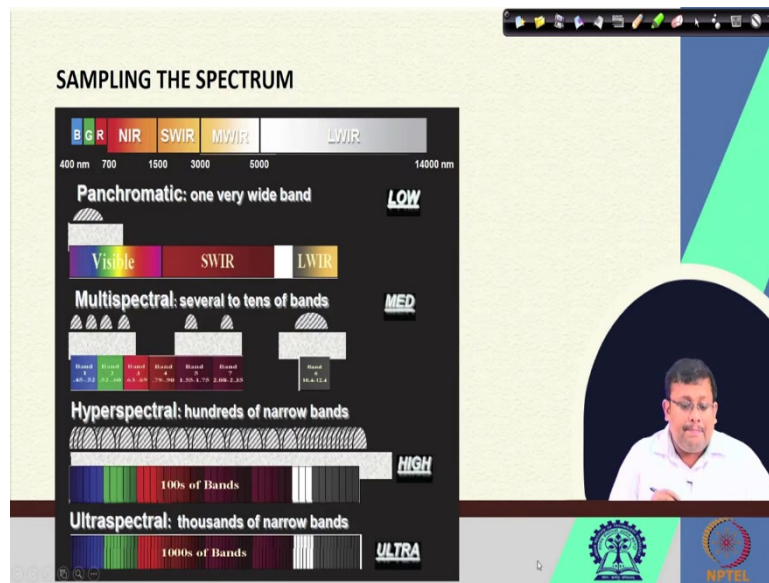
- A panchromatic band (black and white band) is one band that usually contains a couple of hundred nanometers bandwidth
- The bandwidth enables it to hold a high signal-noise, making the panchromatic data available at a high spatial resolution
- This image can be gathered with a higher resolution since the spectral range gives the smaller detectors allowance to be utilized while sustaining the high signal-noise ratio

The slide features a light green background with a dark blue and green geometric design on the right. A small inset video shows a man in a white shirt. At the bottom, there are logos for IIT Bombay and NPTEL. A URL is visible at the bottom: <https://crisp.iitb.ac.in/research/tutorial/pan.tif>

So, let us start with the panchromatic band. So, panchromatic band which is basically a black and white band is one band that usually contains a couple of 100 nanometer bandwidth. So, it is quite large the bandwidth is quite large. And the bandwidth enables you to hold high signal to noise and making the panchromatic band available at a high spatial resolution.

But in most of the cases the panchromatic band, panchromatic images are black and white images these and this image can gathered with higher resolution, can be gathered with a higher resolution since spectral range gives the smaller detector allowances to be utilized while sustaining the high signal to noise ratio. So, this is an example of a panchromatic image, black and white image of an area.

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Now, if we see that total electromagnetic spectrum, the total electromagnetic spectrum maybe differentiated into several regions, like you can see here in the visible region, we are having the blue band, green band, R band, then comes the near infrared, then comes the shortwave infrared and then the mid wave infrared and then long wave infrared. So, these are some of the terminologies generally scientists use and it varies you can see here from 400 nanometer to 14,000 nanometers.

Now, in case a panchromatic as we have discussed, it contains one very wide band. So, of course, the resolution of this panchromatic band will be comparatively lower than that or multispectral and also further lower than hyperspectral and also the ultra-spectral. So, the panchromatic that means, it contains one very large wide band to capture the information. For example, you can see these panchromatic band is containing most of the visible range.

So, the spectral resolution is lower than that of the multispectral which contains several to tens of the bands which is medium resolution you can see here these are the multispectral bands and hyper spectral bands are characterized by the hundreds of narrow bands, when the hundreds of narrow bands capturing the whole electromagnetic spectrum or the part of the electromagnetic spectrum, then we call it hyperspectral spectrum.

Now hyperspectral spectra is having high resolution because it can capture the minute details because it has very narrow bandwidth, more high resolution if we consider the higher resolution than hyperspectral we call it ultra-spectral which contains the 1000s of narrow bands 1000s of bands. So, this is called ultra-spectral spectra. So, here based on which sensor you are using either you are using panchromatic sensor or multispectral sensor, hyperspectral sensor or ultraspectral sensor this the resolution will vary.

So, what we can see? Ultraspectral has the highest resolution followed by hyperspectral, multispectral and panchromatic. So, this diffuse reflectance spectroscopy or the soil spectroscopy basically deals with this hyperspectral data which contains the hundreds of narrow bands. Now, why this why we are considering this hyperspectral, why it is beneficial, we are going to discuss in our coming slides.

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The slide, titled "MULTISPECTRAL AND HYPERSPECTRAL", contains the following text and diagrams:

- Multispectral imaging measures light in a small number (typically 3 to 15) of spectral bands
- Hyperspectral imaging is a special case of spectral imaging where often hundreds of contiguous spectral bands are available

The diagram illustrates a hyperspectral sensor system. Light from a "Telescope" passes through a "Slit" and a "Spectrometer" to a "Detector Array". A graph shows "100s of Parallel Spectrometers" with reflectance curves for different wavelengths (400-2000 nm). The output is a "Calibrated Image Cube" which is processed into a "Material Map". Logos for IIT Bombay and NPTEL are visible at the bottom.

So, let us first discuss or discriminate between the multispectral and the hyperspectral. So, multispectral imaging measures the light in a small number typically 3 to 15 of spectral bands. So, the number of width bands are in case of multispectral remote sensing or multispectral images are very low as compared to hyperspectral because, in case of hyperspectral often hundreds of contiguous spectral bands are available and remember that these bands are contiguous.

So, if you see the hyperspectral mapping of an area, this will be much more clear to you. So, you can see it is an hyperspectral sensor. So, hyperspectral spectrometer and using a detector which detects a whole area and using the detected array, you can see that it can capture the spectra of hundreds of, it can be considered these detectors array can be considered as hundreds

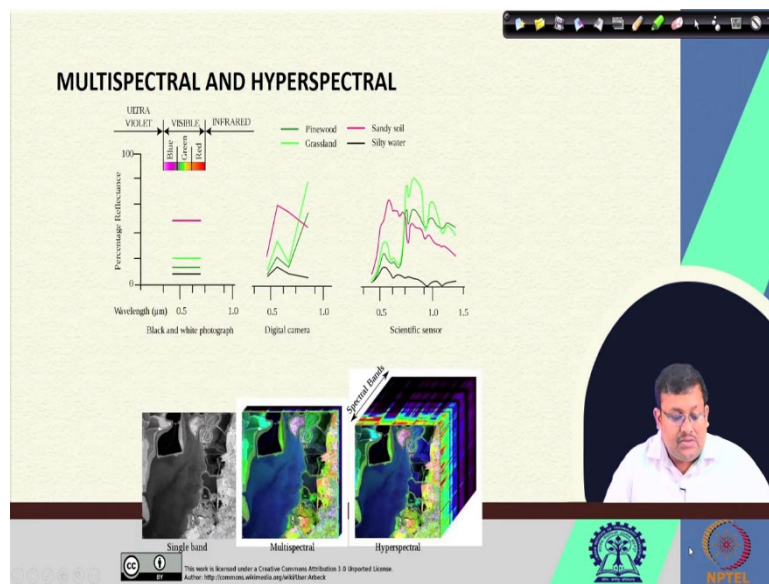
of parallel spectrometers and when we have these suppose from 400 nanometers to 2500 nanometer wavelength for each of the for the for each of these wavelengths from 400 to 2500 nanometers, which generally we consider as visible to near infrared.

So, for each of the wavelength it will capture an image. So, you can consider this is a image cube, ultimately, when you stack all these images captured using the individual wavelengths, contiguous wavelengths, in the visible to near infrared or any range, it will be considered as a image cube or hyperspectral data. You can consider as a book the whole data you can consider as a book or image cube you can consider as a book and individual pages of that book as an image captured by individual wavelength.

So, this is called the image cube and of course, when we are capturing these are individual images using the individual and we are capturing the images using the individual wavelength and we are stacking them together ultimately getting the high resolution, very high resolution map of an area using this hyperspectral sensor. So, again hyperspectral sensor uses a detector arrays.

So, basically using this detector array, it capture the images of any surface for each of these contiguous wavelength and then overlay each other and stack each other ultimately creating a image cube or data cube and this data cube is known as hyperspectral data cube and this hyperspectral data cube has much more information than that of multispectral as well as panchromatic sensor.

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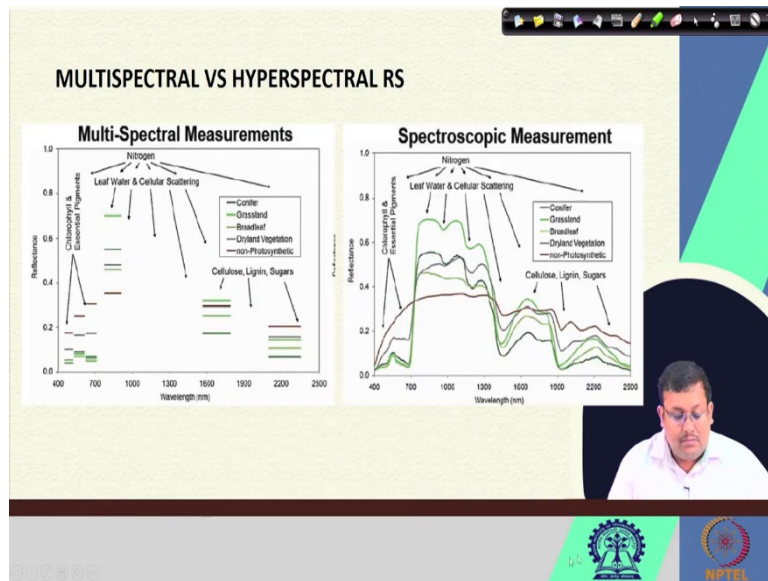


So, if you can see the difference in these images also, this will be much more clear. So, you can see here the black and white photograph can be used by can be utilized by using these visible bands. So, black and white photographs can be can be taken using this visible range and in the digital cameras the different digital cameras can also use the, you can also use the multispectral data. So, here you can see there is a single band image, this is a multispectral image and this is a hyperspectral image.

In case of hyperspectral image, you can see how these are there are different types, pinewood, grassland, sandy soil and silty water, how they will appear in different types of sensor. So, you can see here in the visible sensor, there will be difference, but you cannot identify the spectral signatures. In case of multispectral, you can see the spectral variation, but these bands and spectral features are quite broad. So, minor features cannot be discriminated.

However, when you plot them using is the scientific sensor which are mostly hyperspectral sensor, you can see the much more details of the spectral signatures. You can see this is the spectral signatures of these individual pinewood grassland sandy soils anywhere and silty water and you can see the clear differences as far as the spectral signatures are concerned. So, spectral signatures, so, high resolution. So, the crux of this whole discussion is when you move from a single band to multispectral to hyperspectral, we are getting much higher information than that of using the multispectral data as well as the single band data. So, let us move ahead and see.

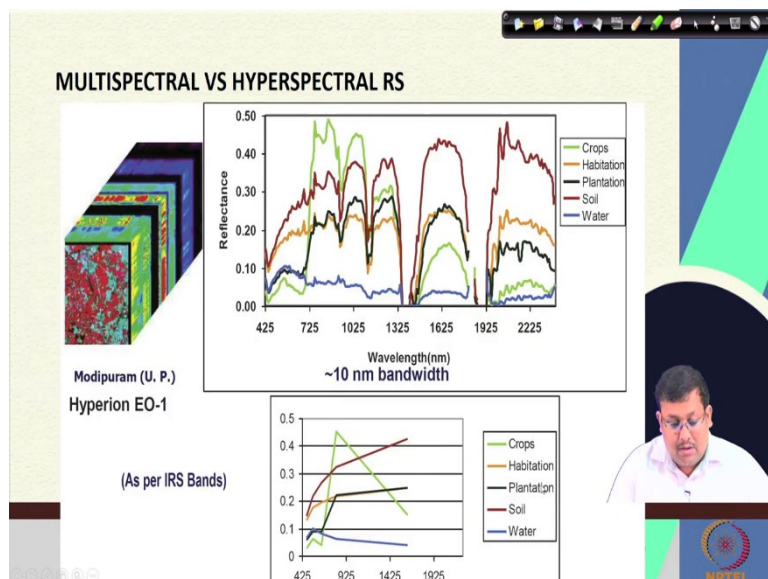
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So, you can see these a multispectral measurement of different types of vegetation, coniferous, grassland, broadleaf, dry land vegetation and non-photosynthetic vegetation and you can see, when we are using the hyperspectral sensor, how we are getting much more information, much higher signal to noise ratio, I would say and also when we are we are getting much more spectral information, when you are using the spectroscopic measurement as compared to the multispectral measurement.

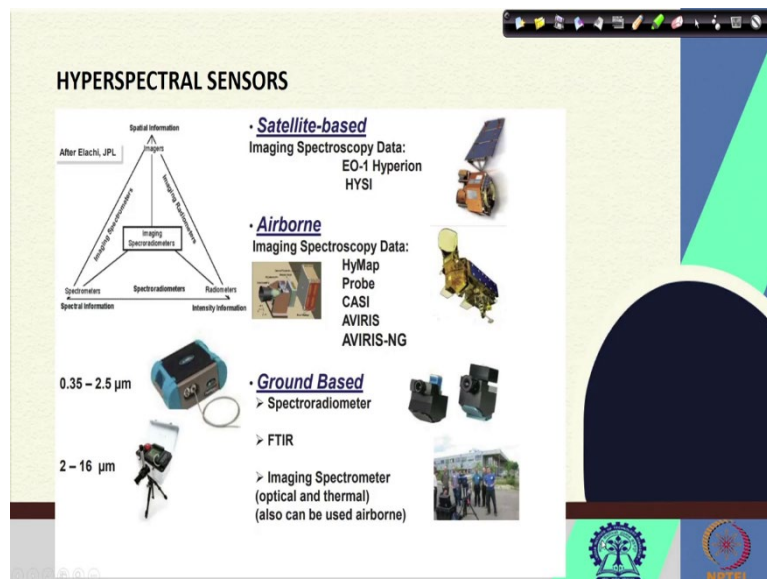
Because the multispectral measurement, we can see the lines, but you cannot see these important spectral features. So, these important spectral features can be only resolved when you are using the scientific sensors or hyperspectral sensors like spectroscopic sensors.

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Again, this is an example you can see here how the difference between the multispectral and hyperspectral remote sensing data you can clearly see that these are from different crops, habitation, plantation, soil and water, these are from hyperspectral data and this is the same surface with the multispectral data. So, you can clearly see the difference between the multispectral data and the hyperspectral data. So, of course, that reflects in the differences between the multispectral and hyperspectral remote sensing.

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So, if we consider all of these, there are different types of hyperspectral sensors. Now, the hyperspectral sensors which are, there are different types of hyperspectral sensors and based on the some of the features we have discriminated them for example, if you see these, this diagram you can see. If we have the spectroradiometers, it will capture only the, it is a combination of spectrometers as well as the radiometers because the spectrometers it captures the spectral information and in case of radiometers it capture the intensity information.

So, when a instrument combines both spectrometer and radiometer, that means, it captures both spectral information as well as the intensity information or radiance then it will be considered as a spectroradiometer and also when there is a combination of radiometers and images. Because the spectroradiometers cannot give you the special values or it cannot be specially applied it is a point spectroradiometer but, when these radiometers can be utilized, when the radiometers and images are also combined, because images can give you the special information and radiometers give you the intensity information.

So, combining these you will be getting the imaging radiometers and when there is a combination between spectrometers and images that will be considered as an imaging

spectrometers. So, when we combine all images, spectrometers, and radiometers then ultimately we will be getting the imaging spectroradiometers. These imaging spectroradiometers are there in different types of sensors, satellite sensor, airborne sensors, but generally when you talk about field spectroscopy, we will be focusing today's discussion on the point spectroradiometers which cannot capture the special information.

However, the same principle will be followed in case of satellite base and airborne hyperspectral remote sensing. The difference is in there, there will be imager which will capture the special information. So, there are different types of satellite based sensors hyperspectral sensors, airborne (()) (18:08) sensors, hyperspectral sensors and ground based hyperspectral sensors. Some of the satellite based hyperspectral sensors are observatory one, Hyperion and then HYSI these are satellite based sensors.

Airborne sensors are HyMap, Probe, CASI, AVIRIS, AVIRIS New Generation or AVIRIS-NG and also ground based or spectroradiometers are the these the spectroradiometer as well as Fourier transform infrared spectroradiometers, so spectrometers so and also some imaging spectrometers are also their optical and thermal which can be also used in airborne but generally our discussion in this week will be focusing on these point spectroradiometer which we generally use for ground trothing as well as point measurement.

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SOIL SPECTROSCOPY

- Can characterize soil properties efficiently
- Defined as the study of the spectral signature of a soil material
- The spectral signature relates to soil characteristics such as organic and mineral components
- Measurements are fast, cost-effective and nondestructive and can be made both in the laboratory and in situ in the field
- Soil composition and characteristics are encoded in the spectrum at specific wavelengths of the electromagnetic spectrum
- For example, mid-infrared spectra have encoded information on soil mineralogy or soil organic matter composition, which can be assessed quantitatively or qualitatively using the absorption or reflectance at specific wavelengths

So, what is soil spectroscopy? Soil spectroscopy can characterize soil properties efficiently it is defined as the study of the spectral signatures of the soil material and the spectral signatures relate to the soil characteristics such as organic and mineral components and what are the

advantages of this soil spectroscopy because this is very fast using a spectrophotometer you can capture a scan, a whole scan of the single soil within only a couple of seconds.

So, it is very fast and beauty of it is it is high throughput that means, using a single spectrum, you can capture so many spectral information, you can relate with the, you can, which you can relate to the soil and crop components. So, the measurements are very fast it is cost effective, because you can see how many samples you can cover within a very short period of time and also it is nondestructive that means, it does not destroy the sample since it is an optical instrument, it does not destroy the samples and it is field portable, so, you can carry it in your in your field to do the measurement.

So, it can be used both inside the laboratory as well as in the field. So, you can see these are, so, these are the advantages of using the soil spectroscopy. Now, soil composition and characteristics, that the soil composition and characteristics are encoded in the spectrum at specific wavelengths of the electromagnetic spectrum. I will show you how these important spectral features appear in the soil from different sources. Of course, individual clay minerals as well as functional groups in the organic matter and also the function groups which are present in soil moisture can show their presence in the spectrum of hyperspectral spectrum or VisNIR spectrum.

So, using those information and also the chemometric algorithm or the multivariate prediction algorithm, we can predict the presence of those individual components. So, we know that the soil composition and characteristics are encoded in the spectrum at specific wavelengths of the electromagnetic spectrum. For example, the mid infrared spectra, which varies from 2500 nanometers to 25,000 nanometers.

So, these mid infrared spectra has encoded most information most of the information of soil mineralogy or soil organic matter composition which can be accessed or assessed qualitatively and quantitatively using the absorption of reflectance at specific wavelengths.

So, mid infrared spectroscopy is more capable of capturing the information of spectral features which are appearing from the clay minerals as well as the soil organic matter. So, may if we use the mid infrared spectra followed by different types of chromatic algorithm, we can, predict the presence of clay as well as the clay minerals as well as the presence of soil organic matter.

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ELECTROMAGNETIC SPECTRUM

- Visible : soil colour
- The γ rays, X rays and infrared spectra : especially elemental composition and soil mineralogy

Lillesand et al. (2015)

So, if you see the electromagnetic spectrum of course, when we go from the low frequency to the higher frequency from right to left, we are increasing the frequencies and of course, from higher frequency to lower frequency you can see different areas like gamma rays, X rays, UVs, then visible, then infrared microwaves and radio waves. So, that the gamma rays, X rays and infrared spectra, they are much more sensitive to the elemental composition or soil mineralogy. So, generally using this information, the fundamentals of soil spectroscopy has been laid out and we will see some of the applications.

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SOIL SPECTROSCOPY

- Infrared spectra: sensitive to both organic and inorganic soil materials
- The mid-infrared (MIR) spectra: direct information on soil organic and mineral components of the soil than the visible and near-infrared (VisNIR) range
- Various components of the soil organic matter have very distinct spectral signature in the mid-infrared range. The reason is that the fundamental molecular vibrations occur in the mid-infrared range, while the overtones and combinations occur in the VisNIR
- The absorption features detected in the vis-NIR: fewer, broader and more complex than those recorded in the MIR
- Development of chemometrics: advanced soil spectroscopy

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So, we know that the infrared spectrum is sensitive to both organic and inorganic soil minerals at the mid infrared spectra generally contains more direct information on soil organic and mineral components, then the soil that the visible and near infrared range and various components of the soil organic matter have very distinct spectral signatures in the mid infrared range as I have already told you. And the reason is that the fundamental molecular vibration generally occur in the mid infrared range.

However, for we in the visible to near infrared range, we generally see the overtones and combination bands. So, that is why the direct spectral features or the most important spectral features or the fundamental spectral features of soil components can be seen in the mid infrared region. However, their overtones and combination bands can be seen in the visible to near infrared region and the absorption features detected in the VisNIR are basically very few, they are fewer, broader and more complex than that those which are recorded in their mid-infrared regions.

So, we need to develop the chemometric models to extract those information, we need to go for the spectral preprocessing which I am going to talk about. So, spectral preprocessing followed by the chemometric algorithm is useful for predicting several soil properties because in the visible near infrared range the spectral features are fewer, broader and more complex than those recorded in the MIR.

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SOIL SPECTROSCOPY: POINTS TO BE REMEMBER!

- Infrared spectral bands are largely non-specific: they are not linearly related to a single soil property and overlap between properties
- This is particularly true for vis-NIR range of the spectra
- To extract these complex patterns and obtain quantitative estimates of a soil property, mathematical transfer functions are used to correlate spectral wavelengths to soil properties
- The transfer function is calibrated using the spectral wavelengths as independent variables and the laboratory measured values of the soil properties as the dependent variable
- Once calibrated on the spectra, the soil property can be predicted using the spectral information only
- PCR, PLSR, RF, SVR etc.

The slide includes a video inset of a man in a white shirt speaking, and logos for IIT Bombay and NPTEL at the bottom.

So, what are the points which we should remember that infrared spectral bands are largely nonspecific, they are not linearly related to a single soil property and overlap between the properties. And this is particularly true for the visible in near infrared range, the spectra is highly complex and we need several spectral preprocessing to increase the signal to noise ratio to resolve this complex pattern of the spectra.

And to extract the complex pattern and obtain the quantitative estimation of the soil property, mathematical transfer functions are used to correlate spectral wavelength to soil properties and this transfer function is calibrated using the spectral wavelength as independent variables and laboratory measured values of the soil properties as the dependent variable. So, once calibrated on the spectra, the soil property can be predicted using the spectral information only. There are different types of spectral spectro transfer, we call them spectro transfer function.

So, this spectral transfer function or spectro transfer function can be executed using different types of chemometric algorithm like principal component regression, partial least squares regression, random forest regression, support vector regression, we have already covered all of these. So, these are known as the chemometric algorithm, why chemometric because, these will be these are required to measure or predict the chemical component. So, that is why it is called chemometric algorithm.

So, you should remember these important points before we go for discussing the new topic. So, the infrared spectral bands are very much nonspecific, they are not linearly related to the single soil properties. So, we need to have we need to extract this complex pattern using some

kind of mathematical transfer functions we call them spectro transfer or spectral transfer function, which are generally executed by different types of chemometric algorithm.

So, once we take the spectrum, we first preprocess the spectra. After we do the preprocessing, then we calibrate the spectra against the target soil property using different types of chemometric algorithm. So, mostly applied the highest applied chemometric algorithm for diffuse reflectance spectroscopy is the partial least squares regression which we have already discussed.

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SOIL SPECTROSCOPY: POINTS TO BE REMEMBER!

- Fast
- Cost-effective (almost zero recurring cost)
- Needs minimum or no sample pretreatments
- High Throughput and **Non-invasive**
- Portable

Parameters:

- OC, Available N, P, K
- pH and clay
- Moisture and heavy metals

Figure (a): $y = 0.94x + 1.5$, $r^2 = 0.73$, RMSD = 4.6 g kg⁻¹

Figure (b): $y = 0.91x + 2.1$, $r^2 = 0.77$, RMSD = 4.1 g kg⁻¹

Figure (c): $y = 0.70x + 2.4$, $r^2 = 0.64$, RMSD = 5.4 g kg⁻¹

Figure (d): $y = 0.82x + 4$, $r^2 = 0.47$, RMSD = 5.4 g kg⁻¹

Morgan et al. (2009)

So, you remember this slide this is so, as these gives you a snapshot of whatever we have covered. So, soil spectroscopy you should remember this point that it is fast it is cost effective, because it has almost 0 recurring cost, it is minimum or no sample pretreatments it is high throughput and non-invasive and it is also portable. So, you can see you can literally carry the spectroradiometer in your backpack and you can scan the soil on site by this handheld probe.

And then you can take the scan and you can send the scan to the PDA or the any computer and then through Bluetooth and then you can do you can predict the soil properties using several spectro transfer function or a calibration algorithm which you have developed using the chemometric algorithms.

So, what are the parameters you can measure? You can measure organic carbon, you can measure available nitrogen, phosphorus, potassium, some people has shown the application of DRS for prediction of pH and clay and also moisture and heavy metals. Heavy metals cannot

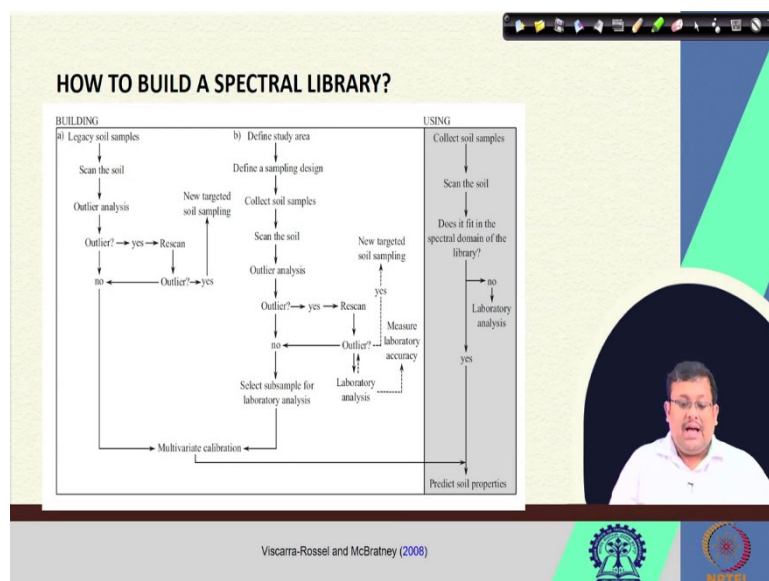
be directly measured, but due to his co-variation with organic matter which can be also measured, we will see some examples.

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So, these are some of the important spectrometers which are available in the market. This is ASD FieldSpec 4, High Resolution spectroradiometer, another one is from spectral evolution which is called the PSR 3500 spectroradiometer, these are widely used for different spectro soil spectroscopic research and crop spectroscopic based research and we are going to discuss their specs our coming lectures.

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SOIL SPECTRA

Reflectance

Wavelength /nm

Geeves et al. (1994)

NPTEL

SOIL SPECTRA

Reflectance

Wavelength /nm

● Low clay content
● High clay content

Reflectance soil spectra from Geeves et al. (1994) where the colour represents the amount of clay (low to high clay content) derived from conventional laboratory soil analysis Wadoux et al. (2021)

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So, guys, let us wrap up our lecture here, this lecture we cannot complete the soil spectral library. We will start from here in our next lecture and I will show you how to build the soil spectral library and then we will be discussing from here. So, so far, so, in our next lecture we are going to discuss how to build the soil spectral library and also we are going to see the soil spectra.

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Thank you

And these are the references which I have used so far and so, you can use it you can conceive you can consult these references for more informations and so, let us wrap up our lecture here. In the next lecture we will be starting from the discussion of soil spectral library. Thank you.