LESSON
A Further Investigation of Near Infrared Reflectance Spectra

Quick Look
Grade Level: 10 – 12
Time Required: 4 hours 30 minutes (Six 45-minute class periods) with an optional two class periods
Lesson Dependency: NIR Spectra Lesson

Summary
Students further their investigation of NIR reflectance spectra. Observed colors are a combination of specific color tints (frequencies). Spectroscopes and analyzing spectra. Application of mixing specific colors to create desired colors. RGB and images. Presentations. Group work. Lesson can lead into a computer science class activity.

Engineering Connection
Breaking apart the colors emitted by an object (or reflected, in this case) with spectroscopes are an important tool in the analysis of an object's composition (a form of analysis in material sciences). The opposite, the combining specific colors is used in technology to create high efficient white lighting and color images. Analyzing patterns in data, like spectra, is an example of data analysis in machine language.

Learning Objectives
After this lesson, students should be able to:
1. Increase their familiarity with the electromagnetic spectrum
2. Understand that the light emitted by an object can be taken apart for spectral analysis
3. Understand that separate colors and their intensities can be combined to form colors and tints
4. Understand the location of NIR in the spectrum
5. Understand that colors exist in the NIR spectrum, just like they do for the visible spectrum (these are invisible to our eyes)
6. Learn how to graph a NIR spectra in Excel
7. Identify useful portions of the NIR spectra
8. Analyze spectra like a machine learning application

Worksheet Attachments
NIR Spectral Data in CSV format
Image of a NIR spectrum from Wikipedia

Pre-Req Knowledge
An understanding of how to use a spreadsheet, like Excel

Introduction/Motivation
(Ask students some initial questions to get them to think about how humans use their eyes to identify objects).
How do you identify objects visually?

What is a useful list of characteristics you might use to distinguish between two objects? What if they were very close in appearance?

Lesson Background and Concepts for Teachers

In my previous lesson plan you learned that near infrared, or NIR, is that region of the spectrum that extends just beyond the edge of the red and into the beginning of the infrared. Your camera modification illustrated just how different the world looks in NIR.

You also learned that an NIR spectrum is not produced by the electrons changing their energy levels within an atom, but by lower energy processes, mainly molecular bonds changing their energy levels. Because there are a lot more ways for molecular bonds to reconfigure themselves, the width of NIR spectral lines tend to be broader and the overall spectra tends to be more complicated than the emission spectra students observe in gas discharge tubes.

If you need a refresher on molecular bonds and NIR spectra, consult my previous lesson plan

The spectra your students will use in this lesson were collected by a SCIO (at this time, the data has not been released. Therefore, sample data was generated). The product was developed by and is available from Consumer Physics, https://www.consumerphysics.com/. Your class will not need access to a SCIO for this lesson, but you still may want to purchase one.

What we find is that much of the NIR spectrum does not have specific bands for specific molecular bonds like the MIR. That means algorithms must be developed to extract just the useful portion of the spectrum. It's as if most items in the world were a red tint in color. In that case, the fact that something is red is not helpful in identifying what a particular object is. We must therefore look at several regions and wider portions of the red spectrum for useful identifying characteristics.

Lesson Closure

Review what the students did in this lab. They used several invisible spectra to distinguish between very similar samples of asphalt. The only difference was the concentration of a binder solution added tot eh samples. While the difference between them was minor, they have major impacts on how they asphalt samples behave and whether or not they'll work in some climates. Spectra from objects is one important industrial and diagnostic tool in industry. Students practiced interpreting measurements used in career fields they may work in after graduation.

Then explain that machine learning does similar actions to what the teams did. However, machine learning runs many more tests against many more samples. Make sure students realize that they did not find a reason for why their procedure worked. Machine learning often does the same thing, there's no explanation. It only finds a relationship between the data and the desired output.

Vocabulary/Definitions

Near Infrared (NIR): The infrared spectrum that is closest to visible light
Spectroscope: A device for producing spectra for examination.

Spectrum: The band of colors produced by separation of white light by a prism or diffraction grating (the plural version is spectra)
Paper Chromatography: The separation of a dissolved mixture through a sheet of paper because different components move at different speeds (due to adhesion)

Assessment
Pre-Lesson Assessment
Discussion Questions
1. Who knows how a white LED works?
2. Who can explain what a color image on a monitor looks like if you magnify it?
3. Has anyone heard how a spectroscope is used in chemistry and astronomy?

Lesson Summary Assessment
Evaluate student presentations for the following items
1. Correctness: 70%
2. Effectiveness of the solution: 10%
3. Student team self-evaluations: 10%
4. Clarity and appeal of presentation: 10%

Daily Procedure
Day 1

Materials
Access to paper and pens for a presentation or to PowerPoint

Teacher Prep
None

Divide students into teams and give each team a name. Students will remain in these teams for the duration of the unit.
Ask teams how they can identify objects visually, what list of characteristics could they would use.
Teams then give examples of how they would apply these techniques in a short class presentation.
After presentations, ask other teams if they can come up with examples where another team's techniques might fail?
Based on what they learned, update your presentation

Day 2

Materials
Different colors of construction paper and colored markers

Teacher Prep
Create cardboard cut outs of five different shapes (circle, triangle, square, rectangle, and pentagon), all of the same color (called cutouts 1)

Create cardboard cut outs of five of the same shapes, but in different colors (called cutouts 2)
Create cardboard cutouts of five of the same shape and in the same color (called cutouts 3)
Create cardboard cutouts of five of the same shape, same color, but apply a light coating of different water colors. Be sure to make the tinting subtle. (called cutouts 4)

Reinforce what was presented on Day 1 with a short presentation.
Hold up and show cutouts 1. How are teams going to identify the shapes?
Hold up and show cutouts 2. How are teams going to identify the shapes?
Hold up and show cutouts 3. How are teams going to identify the shapes?
Hold up and show cutouts 4. How are teams going to identify the shapes?

It's easy to identify objects based on their shape. But often, shape is not a characteristic of the objects we want identify. A lot of the techniques presented on Day 1 probably involved the color of objects (shape is another, but it's not important for this lesson). That's because we have color vision and we use the visible portion of the spectrum to make measurements about the world. The color we see in an object is normally based on a mixture of colors the object reflects. Therefore, some things can appear the same color and therefore more difficult to distinguish between. But if we separate out the individual tints, we'll find additional information useful to distinguish between them. To see this, have each team complete the paper chromatography lab on day 3. This will show that the pigment in ink markers is based on the total sum of colors the ink reflects and the intensity of each color. The less intense the particular pigment, the less effect it has on the overall color we see. But its presence can be detected. And in the case of leaves, it can be useful for distinguishing between similar leaves or between healthy and unhealthy leaves (and plants).

Day 3
Materials
Paper chromatography kit
Several color markers to analyze their color mix
Tree leaves (optional)
Mortar and pestle (optional)

Teacher Prep
Read how to use the paper chromatography kit

Review how to perform the paper chromatography lab with students. Then give them color markers to use in the lab. If there's available time, let students crush leaves with a pestle and try using plant pigments.

Day 4

Materials
White LED and 3.3V coin cell
Magnifying glass and cell phone screen
Prism
PC monitor

Teacher Prep
Place materials in to separate piles so teams can pick them up in order
Practice connecting an LED to a coin battery and the proper orientation of the leads

The fact that an overall appearance of a color is due to the combination of separate colors and their intensities can be put to use in technology. First, show teams how to connect the leads (wires) of the white LED to the coin cell. If the LED does not illuminate, make sure the leads are not connected backwards. If the connection is fine, then the LED may be bad or the coin cell discharged. Be prepared to switch out LEDs and coin cells. The LED is white, correct? Now disconnect the LED and look inside the plastic case with a magnifying lens. Students should notice there's a yellow-colored cup inside the LED. Do not look directly at the light that the LED emits with a magnifying glass, it's too bright. What's happening is the LED chip inside the metal cup emits blue light. Some of the light escapes the plastic case. The rest shines of the metal cup and excites phosphors surrounding the LED chip. When the phosphors are excited, they emit yellow light. The mix of yellow and blue appears as white to our eyes. As an experiment, see if teams can use a prism to split the light. They may have better luck if they look at the LED through the prism or reflect its light off a tilted plastic CD.

Let's look at one more use of this technique. Have each team use a magnifying glass to look at the LCD screen of their cell phones. Put up a school appropriate image. Notice how each pixel in the image is made up of three different colors. In reality, each pixel is made up of four cells, one red and blue, and two green (look up Bayer Filter if you want more information).

So we have seen that the colors we perceive in nature are based on the mixture of colors an object reflects (each shade and its intensity). This fact can be applied to technology to create colored images.

But do we only see three colors? Is there only one red color? No, there are shades or tints of each color. The rods and cones in our eyes detect three colors and our brains can combine what they see to create the color of an object we are looking at. However, our ability to distinguish between colors is limited to about 100 shades. If we could detect a greater number shades, we could distinguish between more colors and even see subtle differences in the shade or tint of objects. That increased ability could even be useful in choosing between objects. As an example, as a fruit ripens, its color changes. The color difference of an unripe and ripe fruit decreases as the fruit achieves the prefect ripeness. With a greater sensitivity to color tint, we could pick the perfectly ripe fruit. Also, farmers could select fruits that are at the perfect level of ripeness and ship them to the grocery store just in time. But what can we use to separate the individual colors and make the different tints obvious to us? A spectroscope or spectrometer.

Day 4 (optional lab)

Materials
Spectrometer lab
DVD or CD

Teacher Prep
Practice using the spectrometer on gas discharge tubes
Practice holding up a CD (nearly on-edge) to see the spectrum of a gas discharge tube

Do optional spectrometer lab to acquaint students to spectroscopes the electromagnetic spectrum. If time constrained, this could be a quick demonstration rather than a lab.

Day 5

Materials
Prism
SCiO NIR spectra in CSV format
PC with Excel for student teams

Teacher Prep
Practice tilting the prism to draw out the solar spectrum
Practice importing a CSV file into Excel
Practice making a chart in Excel

The one thing to know about spectrometers is that they use a prism (or today they can use a diffraction grating) to split the colors of the visible spectrum apart (similar to how water separated the different colored pigments of the leaf in the paper chromatography lab).

Have teams hold up a prim to the sunlight to illustrate how the prism separates the "white" light of the sun into its components colors (don't look directly at the sun through the prism – try looking at its reflection off of a white surface). Notice that each color appears to have different tints as you move across the spectrum. Our eyes are good at detecting colors of light. But they can only distinguish between 100 shades. So we could "theoretically" sense the intensity of 100 shades of color in a spectrum. That's plenty for distinguishing ripe and unripe fruit, but not well enough for our technological society.

Electronic devices called spectrometers have been designed to scan the spectrum. They can measure just how bright each tint is in a quantitative sense. In addition, their image sensors are so sensitive that they can detect over 300 different tints in the spectrum. That gives the electronic spectrometer the ability to measure far more subtle differences in a spectrum than our eyes and brains. In addition, they can do it repeatedly, accurately, and precisely. This makes a device like an electronic spectrometer very useful in science and engineering.

Share the NIR spectrum with the teams.
This is an example of what spectrometer data looks like. When near infrared (NIR) light is shone on a material, it absorbs some of the light and reflects the rest. What portions it absorbs is complicated and the result of many factors in the sample. The spectrum is great, but having the numeric values of each wavelength is more useful for analysis. So you will get a comma delimited files (CSV file) to analyze in a spreadsheet.

Each cell in the spreadsheet shows the intensity of 300 colors in the NIR spectrum. We can't see this light (the human eye can actually see some NIR, but visible light overwhelms the NIR). Notice each wavelength of NIR is listed at the top of the spreadsheet and samples are listed down the rows. Each cell gives a digital measurement of how intense that particular shade of NIR was for that particular sample.

Explain a little about how the data comes from the NIR reflected from samples of asphalt. The samples of asphalt contain different concentrations of a chemical called a binder agent. This compound makes asphalt stick together more strongly.

For the rest of this lab, we want to use the given NIR spectrum to distinguish between each percentage of binder in each sample. There's a lot of data here. Some of it is useful, much of it is not. Our goal is to determine which portions are most diagnostic of the percentage of binder. That means this, we need to determine where the spectrum changes the most for the smallest changes in percentage of binder. Normally, something like this is done by machine learning, or programs or algorithms that look at the spectrum data and compare each sample. Your task for this lab is to replicate what machine learning does, but on a much smaller scale.

Day 6

Materials
SCiO NIR spectra in CSV format
PC with Excel

Teacher Prep
Same as the day before

Review importing CSV data into Excel
Review graphing spreadsheet data
Make the learning SCIO asphalt data (0.0 to 1.0% binder, but don't teams analyze the 0.6% and the 1.2% test data yet) available in digital form
Now give the teams their challenge. They are to import and graph the SCIO data. There are learning NIR spectra of asphalt with 0.0% to 1.0% (but not the 0.6% and 1.2% test NIR spectra) binder. Note that once the full dataset is released, there will also be several samples for each percentage.

Compare (graphing) the original SCIO samples. Based on what they see, what range of wavelengths (740 to 1040 nm) are best at indicating the percent of binder in the asphalt sample? The evidence can be based on the intensity of particular wavelengths, the overall shape, comparison between two spectral values, etc.

At the completion, teams will do the following

1. Describe the steps they used to develop their procedure.
2. Show how their procedure can distinguish between the percent binder in the learning data.

After all the presentations are complete, give teams an opportunity to critique each other's procedures. Can the entire class determine which procedure works the best?

As a final test of the algorithms or procedures, give teams the test data (spectra for asphalt samples containing 0.6% and 1.2% binder compound). None of the routines have been tested against these particular values. See whose procedure works best.

Unit Extension

Explain that machine learning does similar actions to what the teams did. However, machine learning runs many more tests against many more samples. Make sure students realize that they did not find a reason for why their procedure worked. Machine learning often does the same thing, there's no explanation. It only finds a relationship between the data and the desired output.

This is an introductory video for the class to watch,
https://www.youtube.com/watch?v=ukzFI9rgwfU
A more in depth MIT class is located here, https://www.youtube.com/watch?v=h0e2HAPTGF4
Students who know Python and would like to expand their boundaries, will find this video interesting, https://www.youtube.com/watch?v=7eh4d6sabA0

Ask if there are any students interested in learning/applying machine language as an after school project? The videos are a good place to start. In addition, you may want to find someone at a local university using machine learning to present to the class. Perhaps the interested students can participate in university-level research after classes. This project would make a good science fair project.