

## Near-Infrared Spectroscopy

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## Verification of Coffee Roast Using Fourier Transform Near-Infrared Spectroscopy

### Introduction

With approximately 100 million people drinking coffee daily, it is no surprise that \$18 billion are spent on coffee, frappes, and cappuccino annually in

the United States. Grown around the world, coffees from different nations each have a distinct flavor. In most regions, beans are grown on small local farms then brought to market to sell. At the market, a buyer carefully inspects the beans before purchase and sends them off to be processed.

Processing coffee includes roasting the beans, as specific beans are roasted at different levels. The roast can be a dark, medium, or light with different levels within each. To determine what level of roast the coffee is while roasting, the master roaster has to listen for cracking noises or remove sample beans to distinguish the roast by color. When master roasters use the cracking method, there are two distinct noises they listen for. The first crack is caused by water and carbon dioxide bursting out of the bean; it also signifies the beginning of the bean becoming a light roast. The second crack is created by the cellulose matrices in the bean beginning to fracture. This also represents the beginning of the dark roast level. Near-Infrared (NIR) spectroscopy is shown here to be a fast and simple technique for measuring the roast levels of coffee beans and ground coffee.

## Method

A coffee shop named Cool Beans™, which roasts its own coffee, donated eight samples of Columbian Coffee™ at multiple stages of roast. The stages included: the green beans, pale beans, early tan, late tan, into first crack, first crack plus, into second crack, and second crack plus. A PerkinElmer Frontier Fourier Transform Near-Infrared (FT-NIR) Spectrometer equipped with a Near-Infrared Reflectance Accessory (NIRA II) using a petri dish spinner were used to scan the coffee as whole beans. The beans were then ground to similar particle size by visual inspection in a coffee

grinder and scanned again with the FT-NIR. Spectra were collected from 10,000 to 4,000  $\text{cm}^{-1}$  using 32 scans at 8  $\text{cm}^{-1}$  resolution.

## Results

Two methods were created to see if the spectra of each level of roast were different in both the whole beans and grounds. The methods for each were created with a Soft Independent Model by Class Analogy (SIMCA) algorithm using an offset baseline correction and a noise weighting filter.

Table 1. Table of the inter-material distances in whole beans.

Inter Material Distances								
Material	Roast Level 1	Roast Level 2	Roast Level 3	Roast Level 4	Roast Level 5	Roast Level 6	Roast Level 7	Roast Level 8
Roast Level 1	-	3.94	11.4	15.5	23.7	57.5	123	99.4
Roast Level 2	-	-	5.36	8.66	16.9	40.3	81.4	67.3
Roast Level 3	-	-	-	7.57	16.9	46.9	129	106
Roast Level 4	-	-	-	-	12	32.3	74.4	72.9
Roast Level 5	-	-	-	-	-	10	27.8	33.3
Roast Level 6	-	-	-	-	-	-	10.1	20.6
Roast Level 7	-	-	-	-	-	-	-	18.4

Table one is a display of the inter-material distance between each whole bean coffee type and from each other.

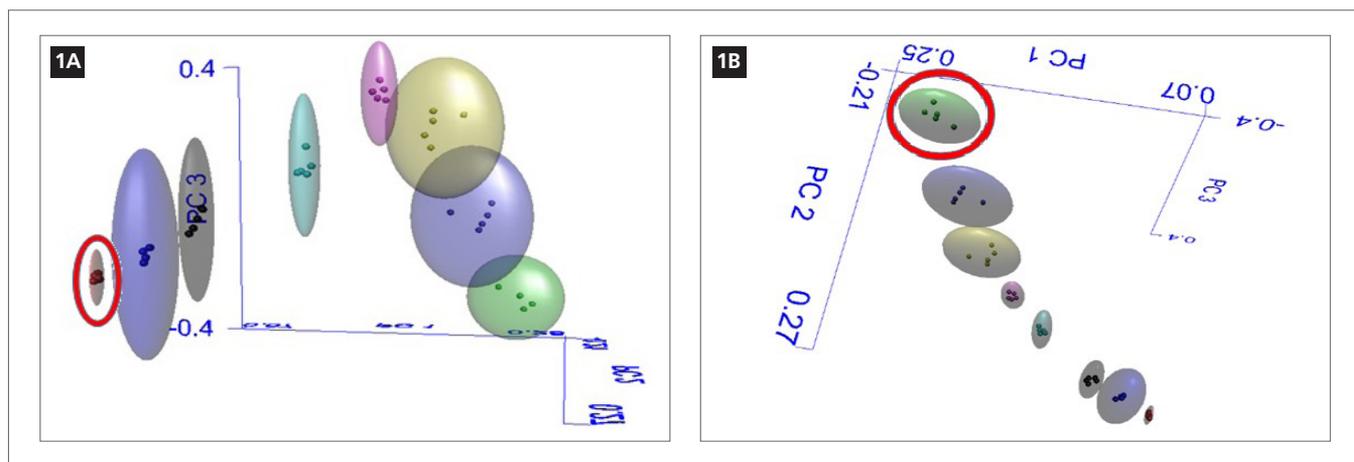


Figure 1A (left) and Figure 1B (right). Three dimensional representation of the SIMCA model for whole bean samples from different viewing angles.

Notice how the separation grows greater between each level of roast and from the initial green beans. The three bubbles in Figure 1A are the dark, medium, and light roasts (in that order from the right). Each is distinct with no overlap. The complete separation of each bubble is also present in Figure 1B. Dark roasted beans are highlighted in Figure 1A and the green beans highlighted in Figure 1B.

Table 2. Table showing the inter-material distances between ground coffee samples.

Inter Material Distances								
Material	Roast Level 1	Roast Level 2	Roast Level 3	Roast Level 4	Roast Level 5	Roast Level 6	Roast Level 7	Roast Level 8
Roast Level 1	-	6.5	15.7	25	46.5	89.5	90.9	134
Roast Level 2	-	-	18.8	36.2	86.3	178	161	259
Roast Level 3	-	-	-	14.1	59.8	140	138	209
Roast Level 4	-	-	-	-	47.4	128	133	201
Roast Level 5	-	-	-	-	-	97.1	116	190
Roast Level 6	-	-	-	-	-	-	38	112
Roast Level 7	-	-	-	-	-	-	-	56.4

Notice how the separation grows greater between each level of roast and from the initial green beans, as compared to the whole beans (Table 1).

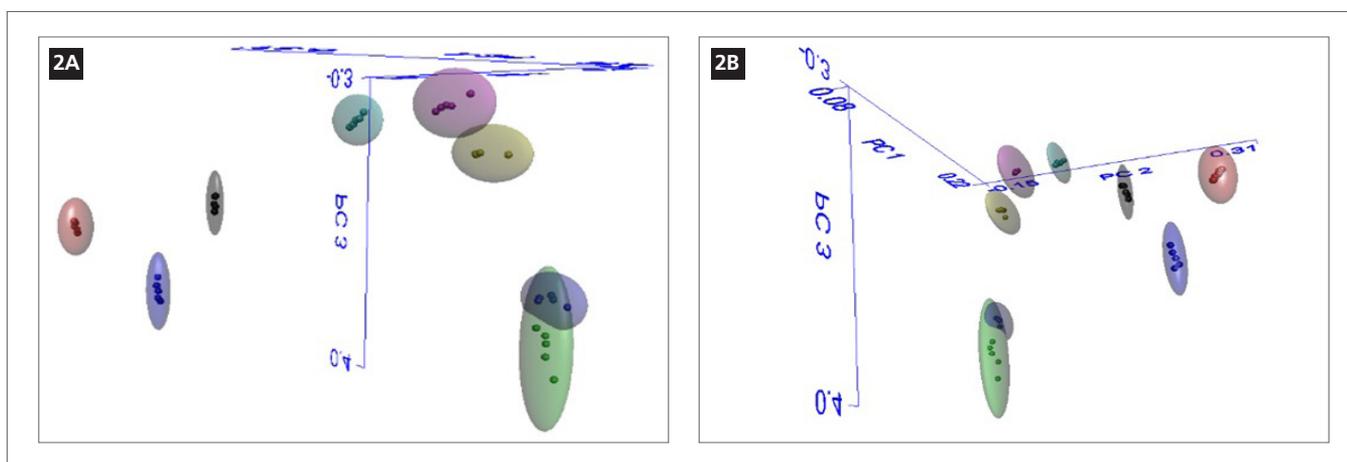


Figure 2A (left) and Figure 2B (right). Three dimensional representation of the SIMCA model from different viewing angles.

Figures 2A and 2B are Principal Component Analysis plots of where each coffee spectrum lies. All of the above figures demonstrate the separation seen in Table 2 between levels of roast. Note that the farthest right green and purple bubbles in figure 2A (green beans and pale beans) do overlap where they did not in Figures 1A and 1B. Conversely, the farther left bubbles in figure 2B (dark, medium, and light roasts) have a greater separation than they do in Figures 1A and 1B. This would suggest that although the whole beans data is suitable for the analysis, ground beans allow for greater separation between the levels of roast. This can be visualized by looking at Figure 3, the level of separation for the ground coffee samples appears to be much greater than for the whole beans.

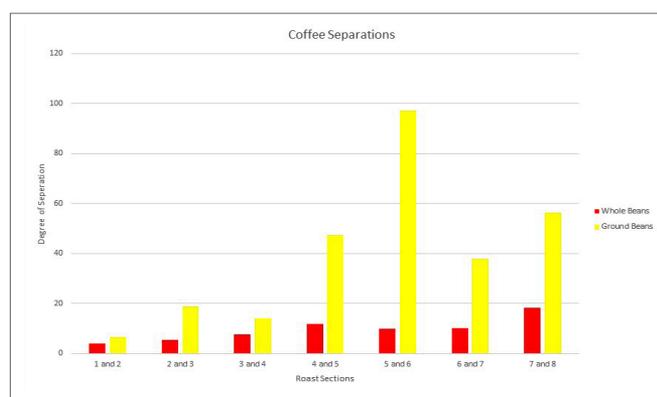


Figure 3. Bar graph plotting the inter-material differences between whole beans and ground beans.

An example execution of the method through Spectrum Touch™ is demonstrated in Figure 4. In this example, a sample of medium roast coffee, which was not included in the SIMCA model, was tested. The sample was set to identify the material, as opposed to verifying it. The model was able to correctly assign the sample as a medium roast.



Figure 4. Results table verifying a medium coffee roast using SIMCA analysis.

## Conclusion

Due to the variety of large and small companies roasting their coffee beans with different techniques as well as the numerous types of coffee, it is hard to come up with an industry standard for each roast level. NIR provides a quick and easy way to distinguish between different roast levels, making it possible for coffee roasts to be compared. Regardless of whether the beans are whole or ground, there is a distinction among the dark, medium, and light roasted coffees. Using the Workflow application, companies will be able to rapidly test their samples (less than 30 seconds) and see if their product matches the required roast level.

## References

- <http://www.statisticbrain.com/coffee-drinking-statistics/>
- <http://www.ncausa.org/i4a/pages/index.cfm?pageid=74>
- [Coolbeanscoffeeroasters.com](http://Coolbeanscoffeeroasters.com)

## Special Thanks:

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