Calibration of the Felix Produce Quality Meter F750 (NIR devices)

Introduction

Near Infrared Spectroscopy (NIRS) provides a rapid and non-destructive means to predict mango dry matter which, in turn, can be used as an indicator of fruit maturity and eating quality. NIRS is an indirect analytical technique which requires calibration. These calibrations are based on the correlations of the spectra of each sample with their known dry matter content, obtained by the destructive dry matter assessment. A good model for the prediction of unknown samples should cover a wide variety of sample types and compositional values (cultivar, growing condition, management practices and level of ripeness). This ensures the dry matter predictions obtained with the Felix Produce Quality Meters are as accurate as possible.

It is important to note that each Felix machine has a unique spectrometer and that for the same sample, the spectra for each machine might vary slightly. As such, each machine requires a spectral correction by the means of a calibration.

Each NIR device includes custom-built models based on the machine's performance over the previous seasons. A well performing model will provide a good correlation between NIR dry matter prediction and the actual dry matter content. However, because every season is different, it is common to see a seasonal bias unique to each device, which needs to be corrected every year. This means that even with a well performing model, the seasonal bias will provide NIR readings that are consistently higher or lower than the actual value, and a bias correction is required.

Please note: the method below will assist in correcting the instrument's seasonal bias, as well as assessing the performance of the model in use. The seasonal bias can be calculated and corrected on your device's screen. However, if your model is not performing well enough, you might need a new custom-built model along with the bias correction. The spreadsheet template provided along with these instructions will indicate whether the model performs well enough based on statistical parameters (see details below). **If a new model is needed, it will require Central Queensland University's expertise in building F750 models and apps, and a fee will apply.**

Materials and Methods

Materials

- Cutting board
- Large knife
- Drying oven (or a dehydrator)
- Small tin foil trays or patty papers (40 per set of 20 fruit samples)
- Felix corer (same diameter as the machine spectrometer – 28mm)
- Permanent marker pen
- Balance (0.01g accuracy recommended)
- Spreadsheet to record the results (available on the AMIA website resource page)

Fruit sample selection

The method below refers to the calibration of NIR devices for mangoes in a hard green condition. If the NIR device will be used on ripened fruit, a separate calibration will need to take place for such fruit condition; the reason being that a hard green fruit and a ripened fruit will have a different internal structure, which the NIR spectrometer will interact differently with.

We recommend working with a set of samples of at least 20 pieces of fruit. This can include different varieties, but the variety should be recorded for each sample if it is a mix. For best results, the fruit selection should include fruit expected to have a dry matter range as wide as possible. The fruit needs to be in a hard green condition, and ideally picked on the day of calibration, or the day before.

Set up of the NIR instrument

- For older units (firmware version v1.1 or v1.2):
    - Ensure the NIR device is fully charged prior to calibration.
    - Load the base model that will be used for calibration purposes. **We recommend using the 2022 model**.
    - Set a new prefix.
    - Set the lot and sample number to 1, and the scans to average to 4 (8 for F751 units).
    - Set the measurements per specimen to 1.

- For upgraded units (firmware v2 and above):
    - Ensure the NIR device is fully charged prior to calibration.
    - Load the **2022Mango Bespoke app**.
    - In Options:
        - Set a Bin Prefix
        - Fruit Per Bin: 20, or as many as the number of fruit samples
        - Sides Per Fruit: 2
        - Scans Per Side: 1
        - Create a new bin.

Method

Part 1 – Preparation and dry matter prediction

1. Number each patty paper or tin foil tray from 1 to 40 (if 20 pieces of fruit in the sample set). Weigh each patty paper and record the weight into a notebook or spreadsheet (as 'pp'). Two patty papers are needed per mango for the two cheeks. The weight of each patty paper will vary, hence the importance to record all weights.

2. Number each mango cheek from 1 to 40.

3. Using the NIR device, take a measurement of each cheek and indicate with a permanent marker where the measurement was taken by drawing a circle on the fruit. The measurement should be taken from the centre of the round part of the cheek.

Figure 1. Using the NIR device, take a measurement of each cheek and indicate with a permanent marker where the measurement was taken

4. Record the dry matter predictions for each cheek number in the excel spreadsheet template provided.

5. Repeat for the other side of the fruit and for the 19 remaining pieces of fruit. You will have 40 measurements per set of 20 fruit.

Part 2 – Destructive dry matter assessment

1. Cut both cheeks of the mango and take a sample from each cheek, using the Felix corer, at the same location where the NIR prediction was taken. Peel each sample so only the flesh remains and cut to be around 1cm thick. For best results, samples should have a weight of around 7 to 10 grams. Samples taken with the corer are usually cut in four to optimise the drying process. Place into the corresponding patty paper/tray.

Figure 2. For best results, samples should have a weight of 7 to 10 grams.
Samples taken with a corer are usually cut in four.

2. Weigh the tray containing the fresh (wet) sample and record the weight (as 'wet').

3. Repeat the process for the second cheek and for the remaining 19 pieces of fruit.

4. Place all patty papers/trays into a drying oven or dehydrator pre-set at 65°C for 48 hours. Higher temperatures will cause burning, lower temperatures might not remove all the water contained. It is also important to respect the drying time.

5. After drying, weigh the patty papers with the dried samples and record the weight (as 'dry').

Figure 3. Dried samples after 48 hours at 65°C.

6. Dry matter is calculated as follows:

$$Dry\ matter\ (\%) = \frac{Dry\ weight}{Wet\ weight}\ x\ 100\% = \frac{'dry' - 'pp'}{'wet' - 'pp'}\ x\ 100\%$$

This calculation is included in the spreadsheet template provided on the AMIA website resource page, along with these instructions.

Results

Enter your results in the spreadsheet template in the first tab "Dry matter predictions":

- Felix dry matter predictions (column D)
- Patty paper weight 'pp' (column E)
- Wet weight 'wet' (column F)
- Dry weight 'dry' (column G)

The actual dry matter (calculated by means of the destructive dry matter assessment) is automatically calculated in column H. Please do not overwrite the calculation in column H.

Remember to record the variety of each piece of fruit if using a mix.

The data entered in the first tab will automatically feed the second tab "Statistical analysis". Please do not overwrite anything in that tab. Model performance will be defined by the values below:

RMSEP	Below 1.5
R^2	Above 0.8

The lower the RMSEP and the closer to 1 the R^2 is, the better the model performs. The graph also shows how NIR predictions correlate to the actual dry matter content. Further details on the statistical parameters can be found below.

Please note that the R^2 is also dependent on the variation of maturity of the fruit used as samples; as such, lower R^2 are expected if fruit maturity is limited to one stage, and it is best to collect wider maturity ranges where possible, for example from 12.0% to 17.0%.

R^2, Coefficient of Determination - Describes how well the data points fit the statistical model (the line of regression). Values range from 0 to 1. A 100% accurate model would have an R-Squared of 1 with all samples lying on the regression line. This statistic needs to be used with caution since it is sensitive to the sample range.

RMSEP, Root Mean Square Error of Prediction - This measures the average accuracy of the prediction (i.e. the difference between the true and estimated dry matter). In this instance, this statistic is a better measurement of model accuracy as it specifically describes the error in individual measurements.

Bias - This is defined as the average difference between the NIR-predicted value and the real value. A positive value means that, on average, the model is over-estimating the composition by this amount whilst a negative value represents an underestimation.

SEP, Standard Error of Prediction refers to the error term if all measurements have the bias subtracted.

An example of results with statistical analysis can also be found in the tab "Example".

If your RMSEP and R^2 are within the recommended value, your current model performs well. Only a bias correction is needed to adjust for the seasonal bias. The bias is calculated in the spreadsheet (cell C42 or K4) and will need to be adjusted on the NIR device's screen.

How to adjust the bias on the NIR device:

- For older units (firmware version v1.1 or v1.2):
  In the 2022 model, go to: Advanced settings > Intercept coefficient. Each NIR device and each model will have a unique value already specified as the intercept coefficient, to which the seasonal bias needs to be underlined subtracted.
  Ex: if the current intercept coefficient is -8.00 and the seasonal bias is 1.5, the value needs to be amended to -9.50.
  Save the new intercept coefficient by going right past the value and exit.

- For upgraded units (firmware v2 and above):
  In the **2022Mango Bespoke** app, go to: Options > Measurement Offsets > Select the model > Enter the bias as a **negative value** then go right past the value to save and exit.
  Ex: if the bias calculated in the spreadsheet template is 1.32, enter -1.32.
  If the bias calculated in the spreadsheet is a negative value, ex -0.7, then it will need to be entered as a positive value 0.7.

Please note: we recommend writing down the previous value (existing "intercept coefficient" or "measurement offset") for your own records and/or if you ever wish to revert to the previous settings.

If your RMSEP and R^2 are outside of the recommended values, your model might not provide accurate results and you might need a new custom-built model. This requires experience with the Felix model/app builder software. Central Queensland University (CQU) is able to assist with building a new model based on your data. You will need to send your spreadsheet results and a copy of your SD card. Please note that a fee will apply to cover CQU's services. For further information, please get in touch with the AMIA.