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Figure01_keyStepsColourgrams.tif [Figure]

Figure02_OperantingProcedure.tif [Figure]

Figure03_mainWindow.tif [Figure]

Figure04_loadClasses.tif [Figure]

Figure05_clearModify.tif [Figure]

Figure06_selectClass.tif [Figure]

Figure07_plotSelectedCurves.tif [Figure]

Figure08_PCAsindow.tif [Figure]

Figure09_PCAselObj.tif [Figure]

Figure10_PCAloadings.tif [Figure]

Figure11_PLS_CV.tif [Figure]

Figure12_PLS_prediction.tif [Figure]

Figure13_ImageReconstruction.tif [Figure]

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Reggio Emilia, August 6th, 2019

Dear Editor,

please find enclosed a copy of the manuscript:

R. Calvini, G. Orlandi, G. Foca, A. Ulrici

Colourgrams GUI: a graphical user-friendly interface for the analysis of large datasets of RGB images

that we would like to be considered for publication in Chemometrics and Intelligent Laboratory Systems.

This article is the software description of Colourgrams GUI, a MATLAB based graphical user interface (GUI) for the analysis of RGB images through the colourgrams approach that we have developed.

The colourgrams approach allows the simultaneous analysis of a large number of RGB images altogether and it is essentially based on the conversion of each RGB image of the dataset into a one-dimensional signal, the colourgram, which acts like a fingerprint of the colour properties of the corresponding image. In this manner, a large dataset of images is converted into a matrix of signals, which in turn can be analysed with common chemometric methods for data exploration or for the quantification of colour-related properties of interest.

Among the different features, Colourgrams GUI allows to easily calculate the colourgrams matrix from a dataset of RGB images, to interactively visualize the signals coloured according to qualitative or quantitative properties of the samples and to analyse the colourgram matrix by means of Principal Component Analysis and Partial Least Squares algorithms.

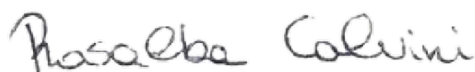
In the article, the different functionalities of Colourgrams GUI are illustrated using a benchmark dataset, which is downloadable with the software.

The software has also been independently tested by Prof. Jose Manuel Amigo (University of Basque Country, Spain) and Prof. Davide Ballabio (University of Milano Bicocca, Italy). Their comments are reported in Section 7 "Independent testing".

The article is original, unpublished and not being considered for publication elsewhere.

Best regards,

Rosalba Calvini



Colourgrams GUI: a graphical user-friendly interface for the analysis of large datasets of RGB images

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Abstract

Colourgrams GUI is a graphical user-friendly interface developed in order to facilitate the analysis of large datasets of RGB images through the colourgrams approach. Briefly, the colourgrams approach consists in converting a dataset of RGB images into a matrix of one-dimensional signals, the *colourgrams*, each one codifying the colour content of the corresponding original image. This matrix of signals can be in turn analysed by means of common multivariate statistical methods, such as Principal Component Analysis (PCA) for exploratory analysis of the image dataset, or Partial Least Squares (PLS) regression for the quantification of colour-related properties of interest. Colourgrams GUI allows to easily convert the dataset of RGB images into the colourgrams matrix, to interactively visualize the signals coloured according to qualitative and/or quantitative properties of the corresponding samples and to visualize the colour features corresponding to selected colourgram regions into the image domain. In addition, the software also allows to analyse the colourgrams matrix by means of PCA and PLS.

Keywords

Colourgrams; RGB images; Multivariate image analysis; Data exploration; Multivariate calibration; MATLAB Graphical User Interface

1. Introduction

The colour properties of an object are related to its chemical and physical attributes, which in turn characterize the whole product. As an example, the visual aspect of food commodities plays a paramount role in the final decision of consumers, since the colour of food is strongly related with quality factors, such as freshness, safety and ripening among others [1].

Colour can be defined as the perceived response resulting from the interaction between the human eye and the visible light emitted or reflected by an object [2]. Colour is not an intrinsic property of an object, since it is strongly influenced from different factors such as type and angle of illumination, and characteristics of the perceiving subject [3, 4]. For these reasons, in the past decades a great effort has been devoted towards the implementation of automated measurement systems able to give in short times an objective evaluation of the colour properties of a sample, being at the same time cheap and easily transferrable between different laboratories or production plants [5 - 8].

While colour measurement of homogeneous samples (like e.g. a tomato sauce) can be performed quite easily by means of colorimeters [9 - 11], in the case of heterogeneous samples (like e.g. not completely ripe tomatoes) it is generally not sufficient to quantify the colour of local areas or to determine the average sample colour. In the case of unevenly distributed pigments or when dealing with defect detection issues, it is in fact necessary to quantify the value and the extent of all the colours which are present on the sample surface. In addition, in some applications the evaluation of chromatic variations occurring over time may help to monitor the evolution of a given process, like e.g. in the case of ripening of fruits and vegetables.

The colour measurement systems that allow to account for colour variability are based on the use of Red-Green-Blue (RGB) sensor arrays, whose photosensitive elements are able to mimic the response of human vision. Indeed, each pixel of an RGB image contains the information about the amount of light captured by the sensor in the red ($\lambda = 700.0$ nm), green ($\lambda = 546.1$ nm) and blue ($\lambda = 435.8$ nm) regions of the visible spectrum [12], which lead to a different response of the L, M and S types of the cone cells of the human eye. When using constant and uniform illumination conditions, RGB imaging systems allow to measure the colour properties of the analysed sample for each individual pixel, giving the possibility to effectively analyse surfaces with inhomogeneous colour [13].

The acquisition of an RGB image is very quick and can be done using cheap instrumentations such as cameras, flatbed scanners, smartphones or webcams. The most complex task consists in the subsequent extraction and quantification of the useful information from the large amount of data contained in each RGB image, corresponding to the R, G and B values measured for tens of

63 millions of pixels. This issue can be obviously solved by using proper Multivariate Image Analysis
64 (MIA) methods, which should be conceived in a way to make the image analysis phase as much
65 easy and effective as possible.

66 The most widespread MIA strategies are based on a pixel-level approach, which consist in
67 considering each single pixel of the analysed image as a separate object [14 - 18].

68 However, for practical applications of computer vision systems it is often necessary to evaluate the
69 variability of large sets of samples, which implies the need to consider large datasets of images. In
70 these situations, hundreds or even thousands of images must be compared simultaneously, thus the
71 analysis at the pixel-level would require strong computation efforts, or it could be even unfeasible
72 [19].

73 In order to overcome this issue, some of us have proposed a data reduction method which consists
74 in converting each three-dimensional RGB image into a one-dimensional signal, named colourgram
75 [13]. Basically, each colourgram is obtained by merging in sequence the frequency distribution
76 curves of the R, G and B channels of the original image and of additional colour parameters derived
77 from the R, G and B values. In this manner, the whole dataset of images is converted into a matrix
78 of signals, where each row corresponds to a signal codifying the colour properties of a specific
79 image in the dataset. The basic idea of the colourgrams approach is to furnish a comprehensive
80 investigation of all the colour aspects of an image, without requiring any a priori assumption about
81 the colour parameters of interest for the problem under investigation.

82 The matrix of colourgrams can then be analysed by means of multivariate statistical methods,
83 allowing to visualize the overall structure of the dataset, to highlight clusters of similar images, to
84 identify the presence of outlier images, to calculate calibration or classification models, and to
85 select the colour features relevant to a specific problem.

86 The colourgrams approach was successfully applied to different issues, mainly related to food
87 matrices. The first application of colourgrams was aimed at discriminating different pesto brands
88 [13] and the promising results suggested to use the same strategy for the quantification of pigments
89 and sensory attributes in pesto sauce [20]. Further applications related to the quantification of
90 properties of interest include the determination of *Lactobacillus* concentration in fermented milk
91 [21], the estimate of maize nitrogen-related variables [22] and the prediction of parameters related
92 to grape ripening [23]. Thanks to its ability to preserve the information related to colour variability
93 within the images, the colourgrams approach resulted to be particularly effective when dealing with
94 the identification of spatially-resolved features, such as the presence of defects. In this context,
95 colourgrams were successfully applied for the detection of red skin defect in raw hams [24], the
96 evaluation of the effects caused by bacterial infection in citrus plant leaves [25], and the automated

identification of defective kernels in maize [26] and hazelnuts [27]. In addition, the possibility of converting the colour content of RGB images into one-dimensional signals also allowed to fuse these “electronic eye” data with electronic tongue measurements to monitor grape ripening [28].

The effectiveness of this approach induced us to adapt it also to the analysis of large datasets of hyperspectral images, leading to the hyperspectrograms approach, which allowed to obtain satisfactory results in various applications [19, 29 - 33].

In order to facilitate the analysis of large datasets of RGB images using the colourgrams approach, we have developed an easy-to-use graphical user interface, named *Colourgrams GUI*. The software includes all the features necessary to convert the images into colourgrams, and to further analyse the matrix of signals by means of PCA to gain an overview of the whole dataset of images and by means of PLS for the quantification and prediction of properties of interest.

2. The *Colourgrams* approach

The colourgrams approach basically consists in converting each RGB image into a one-dimensional signal, i.e. the colourgram, which summarizes the colour content of the corresponding image.

The main steps involved in the conversion of the image into the respective colourgram are schematically reported in Figure 1.

At first, the RGB image, with size $\{r, c, 3\}$ (where r is the number of pixel rows, c is the number of pixels columns and 3 corresponds to the R, G and B channels), is unfolded into a two-dimensional matrix with as many rows as the number of pixels ($r \times c$) and 3 columns corresponding to the R, G and B values (Step 1 in Figure 1).

Afterwards, the unfolded RGB matrix is further expanded by calculating for each pixel a series of colour-related parameters derived from the R, G and B values (Step 2 in Figure 1). These parameters include: lightness (L), calculated as the sum of R, G and B values; the relative colours (rR, rG and rB), calculated as the ratio between each RGB value and lightness; the hue (H), saturation (S) and intensity (I) values, obtained by converting the RGB colour space into the HSI colour space; the score vectors derived from three PCA models calculated on the raw (SC1R, SC2R, SC3R), mean centered (SC1M, SC2M, SC3M) and autoscaled (SC1A, SC2A, SC3A) RGB data matrix, respectively. In this manner, a matrix containing 19 variables for each pixel is obtained. Then, for each variable a 256 bins-long frequency distribution vector is calculated (Step 3 in Figure 1), and the 19 frequency distribution vectors are merged in sequence. Finally, the loading vectors and the eigenvalues of the PCA models are added at the end of the signal (Step 4 in Figure 1).

129 In this manner, the original RGB image is converted into a one-dimensional signal with size equal
130 to 4900 points [= 256 bins \times 19 variables + 3 PCA models \times 3 PCs \times (3 loading values + 1
131 eigenvalue)], which codifies the colour content of the image.
132 For further details about the algorithm the reader is referred to [13].

133 *Figure 1 near here*

134

135 **3. Software specifications and requirements**

136 Colourgrams GUI has been developed under MATLAB environment (ver. 7.11, The MathWorks,
137 USA) and it is freely downloadable from <http://www.chimslab.unimore.it/downloads/> . The
138 download package includes all the routines necessary to run the GUI and also the Fast User Manual
139 as .pdf file, which guides the user through the main features of the software.

140 Colourgrams GUI requires the MATLAB Image Processing Toolbox (The MathWorks, USA) and
141 the DataSet Object Toolbox (Eigenvector Research Inc., USA); this latter one is freely
142 downloadable from <https://www.mathworks.com/matlabcentral/fileexchange/39336-dataset-object>
143 [34]. The software works under different versions of the Microsoft Windows operating system (7 / 8
144 / 8.1 / 10) and has been tested using different MATLAB versions
145 (R2010/R2014/R2015/R2016/R2017).

146 Once all the Colourgrams GUI functions are added to the MATLAB path, the software can be
147 easily started by typing *colourgrams_GUI* in the MATLAB command window.

148

149 **4. Dataset**

150 In order to describe the use of Colourgrams GUI, the *GrapeMusts* benchmark dataset containing
151 240 images of grape must is employed, downloadable with the MATLAB code.

152 The must samples were obtained from grape berries belonging to Lambrusco Marani grape variety
153 and collected in the vineyard from 3 different plants at 5 subsequent harvest times, from veraison
154 until complete ripening. After homogenization and maceration of the grapes, the corresponding
155 must was extracted and, for each sample, 8 aliquots of 50 μ L of must were deposited on a white
156 sheet of absorbent paper. RGB images of the absorbent paper sheets were acquired with a common
157 flatbed scanner (CanoScan Lide 220, Canon). The same procedure was repeated in two different
158 measurement sessions. Then, the image area of each spot of must was cropped and saved as a
159 separate image with constant pixel size, for a total of 240 RGB images with size equal to 900 \times
160 900 pixels (= 3 plants \times 5 harvest times \times 8 aliquots \times 2 measurement sessions). Together with
161 image acquisition, the must samples were also analysed by means of reference analytical methods,

162 based on UV–Vis spectrophotometry and high-performance liquid chromatography, for the
163 determination of a series of parameters usually considered to assess phenolic maturity of grapes.
164 These parameters include colour index, total flavonoids content and total anthocyanins content,
165 among others. The goal of this study, reported in [23], was to relate the images of the must samples
166 with the level of phenolic maturity and to predict the corresponding analytical parameters of
167 interest.

168 In the present paper, this dataset is used to illustrate the main features of Colourgrams GUI.

169

170 **5. Operating procedure**

171 The operating procedure generally applied when analysing datasets of RGB images by means of
172 Colourgrams GUI is summarized in Figure 2.

173 *Figure 2 near here*

174 Briefly, once the dataset of RGB images has been converted into the corresponding matrix of
175 colourgrams, additional information can be added to each image of the dataset, like e.g.
176 presence/absence of defects, variety, brand etc. Then, as a first approach, the whole matrix of
177 signals can be simply visualized in order to observe possible outlier signals, trends of interest or
178 differences between groups of signals. For a more comprehensive overview of the dataset, the
179 colourgrams matrix can be analysed by means of PCA, allowing to better identify groups of similar
180 images and/or to highlight outliers. In addition, the RGB images and the corresponding colourgrams
181 can be used to quantify some properties of interest of the samples using the Partial Least Squares
182 (PLS) algorithm. Finally, in order to gain a better understanding of the results of PCA and/or of
183 PLS, image reconstruction allows to visualize the relevant colour features back into the original
184 image domain.

185 Colourgrams GUI is designed in order to easily manage the operating procedure reported in Figure
186 2 by means of three windows: the main window, the PCA window and the PLS window.

187 The main window of Colourgrams GUI (Figure 3), that can be opened by typing *colourgrams_GUI*
188 in the command window of MATLAB, is subdivided into different sections according to the steps
189 of the operating procedure that will be described in the following sections.

190 *Figure 3 near here*

191

192 **5.1 Create or load colourgrams**

193 Once Colourgrams GUI is launched from the MATLAB command window, it is possible to create a
194 new dataset of signals (radio button “Create Colourgrams”) or to load an existing one (radio button

195 “Load Colourgrams”). Firstly, the user has to select the folder containing the images or a previously
196 saved dataset by clicking on the folder icon in the toolbar.

197 To create a new dataset of colourgrams, different options are available. At first, the user has to
198 select the image extension, choosing between the JPG, BMP and TIF image file formats. In
199 addition, it is possible to decide whether calculating the signals from the whole original images
200 (“Normal” mode) or from the images after background removal (“Keep only” mode). Background
201 removal is performed by a thresholding procedure based on a defined colour parameter, like e.g.
202 red, blue, hue, etc. In particular, in the “Keep only” mode the colourgrams are calculated including
203 only the pixels with values greater than (“>” mode) or less than (“<” mode) the threshold value.

204 Concerning the *GrapeMusts* dataset, colourgrams were calculated after background removal, that
205 was performed by keeping only the pixels with relative red values greater than 0.34 (i.e., selecting:
206 “Keep only” “Rel. Red” “>” “0.34”). The procedure that was followed to select this threshold value
207 consisted in a first analysis of the colourgrams calculated on the whole images (“Normal” mode).
208 Then, through the visualization of the frequency distribution curves of the single colour-related
209 parameters (see section 5.3), and by reconstructing the images corresponding to selected portions of
210 the frequency distribution curves (see section 5.6), it was possible to identify the relative red value
211 equal to 0.34 as the optimal threshold for background removal.

212 Once all the RGB images are converted into the corresponding colourgrams, the matrix of signals is
213 automatically saved as DataSet Object into a folder named “Generated_Colourgrams” and followed
214 by date and time of creation (e.g. Generated_Colourgrams_20190611_T124823). In addition, in the
215 same folder also an MS-Excel file named “Colourgrams_info.xls” is saved, which contains the
216 names of the original RGB images and that can be modified to include additional information about
217 the dataset, like e.g. class vectors.

218 Once the matrix of colourgrams is calculated or loaded, the signals are plotted on the main window
219 and all the tools for data visualization and data analysis are enabled.

220

221 **5.2 Add or modify supplementary information to the dataset**

222 The “Class Manager” section of Colourgrams GUI main window can be used to load, modify or
223 save class identifier sets (or class sets) in the current DataSet Object of colourgrams.

224 More in detail, the push button “Load class” opens a specific window which allows to load a new
225 class vector (Figure 4a). The class vector can be loaded from a MATLAB workspace variable, from
226 a .mat file or from an .xls / .xlsx / .csv file. The length of the class vectors must be equal to the
227 number of signals and class assignment can be expressed using either vectors of numbers (e.g. 1, 2,
228 3, ...) or character arrays (e.g. ‘Class A’, ‘Class B’, Class C’, ...), except for .csv files, from which

only numeric values can be loaded. When the class vector is loaded from an .xls or .xlsx file, the user is required to specify the worksheet number and the range of the class vector (Figure 4b), while if the class vector is loaded from a .csv file the user has to specify the delimiter type and the range of the class vector using an Excel-like notation (Figure 4c).

Figure 4 near here

An already existing class set can be deleted or modified using the push button “Clear/Modify”, which opens the window shown in Figure 5.

Figure 5 near here

On the left of the “Clear or Modify Classes” window, a list box reporting all the class sets saved in the current DataSet Object is displayed. When the user selects one of the class sets, a summary table reporting the corresponding information (i.e. class names and number of samples belonging to each class) is shown on the right part of the window. Furthermore, the “Clear or Modify Classes” windows also permits to delete the selected class set and to edit the class set name and the single class names.

If the class sets of the current DataSet Objects have been modified, it is possible to save the updated DataSet Object to a .mat file using the push button “Save” of the Class Manager section of the main window.

Furthermore, the Class Manager allows to select the class identifiers set to be used to define the colours of the signals in the plot of the main window, by using the “Current class” drop-down menu. For example, in Figure 6 the colourgrams shown in the plot are coloured according to the “Harvest Time” class set.

Figure 6 near here

5.3. Visualize signals

The “Visualize Signals” section has three main features:

- a) Separate visualization of the frequency distribution curves of the colour-related parameters included in the colourgrams
- b) Representation of the signals according to defined properties of the corresponding samples/images
- c) Identification of a specific signal/sample

This section has 20 check boxes, each one corresponding to one colour parameter included in the colourgrams. Each check box has a label reporting the name of the corresponding colour parameter

261 and the respective colourgram region (e.g., 1793:2048 [Hue]). When the user selects one or more
262 check boxes, the corresponding areas of the main plot are highlighted in light blue colour (Figure
263 7a) and the push button “Plot Selected Curves” allows to plot the frequency distribution curves of
264 the selected colour parameters in a separate figure (Figure 7b).

265 *Figure 7 near here*

266 In addition to plotting the frequency distribution curves coloured according to the selected class set
267 like in Figure 7b, it is also possible to colour the signals based on a continuous variable like in
268 Figure 7c, where the colour coding reflects the total anthocyanins content measured on the
269 corresponding grape samples, and the colour scale reports the total anthocyanins content value
270 corresponding to each colour. To do this, the “Colour By” push button allows to load the vector
271 containing the values of the property of interest by means of a window, named “Load Vector”,
272 similar to the one reported in Figure 4a. A new figure is then displayed, where the signals are
273 coloured according to the corresponding values of the property of interest. If one or more check
274 boxes have been previously selected in the “Visualize signals” section, only the frequency
275 distribution curves of these parameters will be displayed, as shown in Figure 7c.

276 The analysis of plots like those in Figures 7b and 7c allows to make a preliminary assessment of the
277 colour parameters that are mainly related to the problem at hand, i.e., of those parameters for which
278 the change of the shape of the corresponding frequency distribution curves corresponds to different
279 classes and/or to different values of a quantitative property.

280 Another feature of the “Visualize Signals” section is the possibility to easily retrieve information
281 about which signal corresponds to a given image and, the other way around, about which image
282 corresponds to a given signal. By selecting the name of the image of interest from the drop-down
283 menu placed on the right side of the section, the corresponding signal is represented in magenta
284 colour in the plot. Alternatively, in order to investigate which image corresponds to a given signal,
285 it is possible to select the signal directly on the plot using the “Data Cursor” button in the toolbar
286 and then, by clicking on the “Select image on the plot” button, the name of the corresponding image
287 is automatically shown in the drop-down list.

288

289 **5.4. Data exploration by PCA**

290 By clicking on the “PCA” button of the main window, the PCA window reported in Figure 8 is
291 displayed.

292 *Figure 8 near here*

293 By default, the PCA model is calculated on the colourgrams matrix considering mean center as
294 signal preprocessing method and 2 principal components. Then, the user can select the proper data
295 preprocessing method (none, mean center or autoscale) and the optimal number of PCs using the
296 corresponding drop-down menus located in the upper left part of the PCA window. The proper
297 number of PCs can be selected based on the scree plot reported in the upper right part; the drop-
298 down menu associated with this plot allows to choose between visualizing the eigenvalues, the
299 percentage of variance explained by each PC, the percentage of cumulative variance or the
300 logarithm of the eigenvalues.

301 The PCA scores are reported in the two plots placed at the bottom of the PCA window. By default,
302 the plot at the bottom left shows the Q residuals vs Hotelling T^2 plot, while the plot at the bottom
303 right shows the PC1 vs PC2 score plot. However, it is possible to change the variables displayed in
304 both plots using the “X” and “Y” drop-down menus associated with each plot. In addition, if the Q
305 residuals and/or the Hotelling T^2 values are displayed in the plots, the corresponding confidence
306 limits can be visualized by selecting the “Confidence limits” check box and typing the probability
307 value (as shown in [Figure 8](#)). If a specific colourgram has been previously selected in the main
308 window, the corresponding object is reported in the two plots as a magenta hexagram. Furthermore,
309 the objects/images reported in the two plots can be coloured according to their class membership;
310 the different class sets can be selected from the “Current class” drop-down menu.

311 Similarly to what described in Section 5.3, the objects reported in the score plots can also be
312 coloured according to a quantitative property associated to the samples, like the total anthocyanins
313 content in our example. This can be done by clicking on the “Colour by” button in the toolbar,
314 which opens a window that allows to load the vector of numeric values, as described in Section 5.3.

315 The “Select objects” push buttons associated with each plot located at the bottom of PCA window
316 allow to select directly on the plot some objects of interest, like for example outlier objects. The
317 selected objects are then represented with magenta hexagrams in both plots and, furthermore, by
318 right-clicking on the hexagrams a context menu is displayed which allows to visualize the labels of
319 the selected objects, deselect the objects or eliminate them from the dataset ([Figure 9](#)).

320 ***Figure 9 near here***

321 When the selected objects are deleted, the PCA model is automatically recalculated considering
322 only the retained samples. If necessary, it is possible to re-include the eliminated samples by
323 clicking on the “Reinclude Samples” button in the toolbar. Moreover, it is also possible to save the
324 current PCA model or the modified (i.e. without the eliminated samples) DataSet Object to a .mat
325 file, by clicking on the “Save Data” button in the toolbar.

326 By clicking on the “Only selected variables” radio button, it is possible to calculate the PCA model
327 considering only a user-defined subset of the colourgram variables. The user can choose whether
328 using the variables previously selected in the “Visualize Signals” section of the Colourgrams GUI
329 main window, using the variables employed for image reconstruction (*see* section 5.6), or typing the
330 indexes of the colourgram regions of interest.
331 The loading vectors of the current PCA model can be visualized using the “P” button in the toolbar.
332 A new window will be displayed allowing to visualize one or more loading vectors in the plot
333 (Figure 10).

334 *Figure 10 near here*

335

336 **5.5 Calibration by PLS**

337 The PLS window can be opened by clicking on the “PLS” push button in the Colourgrams GUI
338 main window. Firstly, for the calculation of the PLS model, the user is required to define the
339 training set: it is possible to use the whole colourgram matrix (radio button “Use current dataset”) or
340 a part of it. In this latter case, the training set objects can be selected either by typing the
341 corresponding row indexes (radio button “Edit dataset”) or by loading a column vector (radio button
342 “Split dataset using vector”) from a MATLAB workspace variable, from a .mat file or from an .xls /
343 .xlsx / .csv file. The vector must have values equal to 1 for samples belonging to the training set and
344 equal to 2 for samples belonging to the test set.

345 Then, the user has to define the preprocessing method of the X-block (mean centering or
346 autoscaling). The training set response variable can be loaded from a MATLAB workspace
347 variable, from a .mat file or from an .xls / .xlsx / .csv file. In the current version of Colourgrams
348 GUI, only PLS1 models can be calculated on the autoscaled response variable.

349 Regarding cross-validation, it is possible to employ predefined cross-validation schemes (i.e., leave-
350 one-out, contiguous blocks and venetian blinds) or to use a custom splitting of the samples by
351 loading the corresponding cross-validation vector; then, the user must specify the maximum number
352 of PLS latent variables and, in the case of contiguous blocks or venetian blinds CV, the number of
353 data splits.

354 After cross-validation, a plot appears in the upper right of the PLS window, reporting the RMSEC
355 and RMSECV values versus the number of LVs of the PLS model. This plot can be used to define
356 the optimal dimensionality of the regression model (Figure 11), which can be specified using the
357 “Selected number of LVs” drop-down menu.

358 *Figure 11 near here*

Then, after clicking on the “Calculate Model” button, the results of the selected PLS model appear: the software automatically shows a table with the model statistics (RMSEC, RMSECV, R^2_{Cal} and R^2_{CV}) and two graphs, reporting the Q residuals vs. Hotelling T^2 plot and the Y predicted vs. Y measured plot, respectively. Like for the PCA window, the variables displayed in the plots can be changed using the drop-down menus, and it is possible to select and remove samples.

Once the PLS model has been calculated, the model can be validated. If the option “Split dataset using vector” was previously selected to define the training set, the test set is automatically loaded and the “X ts” group is not active. Otherwise, the test set can be loaded using the “Load dataset” button or it can be defined as a subset of the current DataSet Object by specifying the row indexes of the corresponding samples.

Subsequently, the user can decide whether loading the Y measured values of the test set samples or performing the predictions with unknown Y values.

Once the current PLS model is applied to the test set by clicking on the “Apply Model” button, the outputs displayed in the PLS window are automatically updated: the table of results includes also the RMSEP and R^2_{pred} values, and the two plots in the bottom of the window report the values predicted for the test set samples (Figure 12). By using the “Show Tr with Ts Data” button, it is also possible to compare calibration and prediction results.

Figure 12 near here

Similarly to the PCA window, by clicking on the “P” button in the toolbar of the PLS window a new window appears allowing to visualize the loading vectors, the regression coefficients and the Variable Importance in Projection (VIP) scores.

Furthermore, PLS window allows also to save the current PLS model and/or the datasets (training set and test set) used for model calculation and validation.

5.6 Image reconstruction using the colour features of interest

To better understand the colour properties codified by the different regions of the colourgrams, and to interpret the results of PCA or PLS models calculated on the colourgrams matrix, it is possible to define intervals of colourgram variables and to visualize them back into the original image domain. These intervals of interest can be identified starting from a visual inspection of the signals, from the interpretation of a PCA and/or PLS model (loading vectors, regression coefficients, VIPs) or can be automatically selected using variable selection algorithms implemented in other software packages.

The user can either type the selected intervals in the corresponding edit box of the Colourgrams GUI main window, or click on the “Select regions on the plot” button for manual selection.

392 In both cases, for each colourgram region where at least one interval has been chosen, a figure is
393 obtained where only the pixels falling in the selected interval(s) are visualized, while the remainder
394 pixels are represented in black or white colour, or in grayscale tones of the original image. For
395 comparison, also the original RGB image is reported together with the reconstructed image (Figure
396 13). Image reconstruction is performed considering the image currently displayed in the drop-down
397 menu of “Visualize Signals” section; a different image can be selected from this drop-down menu.
398 As an example, Figure 13 shows the results of image reconstruction performed considering two
399 intervals, corresponding to the relative green (Figure 13b) and relative blue regions (Figure 13c) of
400 the colourgram, respectively. In this specific example, the colourgram intervals have been chosen
401 based on the inspection of the regression vector related to the PLS model reported in Section 5.5 for
402 the prediction of the total anthocyanins content.

403 *Figure 13 near here*

404

405 6. Conclusions

406 Colourgrams GUI is a user-friendly free graphical interface which allows the analysis of large
407 datasets of RGB images through the colourgrams approach.

408 The GUI has been designed in order to easily manage in few windows the whole workflow, from
409 the conversion of the images into colourgrams, to the visualization of the colourgrams matrix, its
410 further statistical analysis by means of PCA and PLS, and the interpretation of the relevant
411 colourgram features through image reconstruction. Furthermore, thanks to the easy-to-use interface,
412 Colourgrams GUI does not need any prior knowledge of MATLAB programming language, and it
413 can be used also by beginners with a basic background in PCA and PLS.

414 Further implementations are planned, in order to add new functionalities such as classification and
415 variable selection tools. Moreover, an analogous GUI for the analysis of hyperspectral images
416 through a similar approach (hyperspectrograms) is also under construction.

417 Colourgrams GUI is freely available from the website <http://www.chimslab.unimore.it/downloads/>
418 (last accessed, July 2019) and the software package is provided along with a user manual which
419 illustrates the main features and operating procedures to run the GUI.

420

421 **7. Independent testing**

422 Prof. Davide Ballabio

423 *Milano Chemometrics and QSAR Research Group, Department of Earth and Environmental*
424 *Sciences, University of Milano Bicocca, P.zza della Scienza 1, 20126, Milano, Italy.*

425 I have tested the “Colourgrams GUI” (graphical user-friendly interface for MATLAB for the
426 analysis of RGB images) and I found that it appears to function as the authors described.

427

428 Prof. Jose Manuel Amigo

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430 *Department of Analytical Chemistry, University of Basque Country, Barrio Sarriena s/n. 48940,*
431 *Leioa, Spain.*

432 When analysing a batch of RGB images, it is important to standardize a tailored procedure and
433 retrieve results that can answer the analytical problem. This is precisely what Colourgrams GUI
434 does. Colourgrams GUI mixes different image features with some basic chemometric tools (e.g.
435 PCA and PLS) in a dynamic and clever manner. Colourgrams GUI is thought for those researchers
436 who need a fast and reliable way of handling many RGB images. Moreover, Colourgrams GUI is
437 presented in a GUI format that highlights the visual results rather than the plane numbers. This is
438 something important for what Image analysis concerns. Of course there is place for improvements.
439 Nevertheless, I truly believe that this version of Colourgrams GUI is a round version that will grow
440 with the time and with the suggestions of the users.

441 I have tried Colourgrams GUI myself in two different MATLAB versions (v 2018b and v 2019a)
442 and it does not show any relevant issue.

443

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533

534 **Figure captions**

- 535 **Figure 1.** Key steps involved in the conversion of an RGB image into the corresponding
536 colourgram.
- 537 **Figure 2.** Operating procedure of Colourgrams GUI
- 538 **Figure 3.** Colourgrams GUI main window. The different sections are numbered according to the
539 steps of the operating procedure reported in Figure 2: 1) create or load colourgrams, 2)
540 add supplementary information to the dataset, 3) visualize signals, 4) perform PCA, 5)
541 perform PLS and 6) image reconstruction using the features of interest.
- 542 **Figure 4.** “Load Vector” window (a) and windows for loading of the vector from MS-Excel files
543 (b) or .csv files (c).
- 544 **Figure 5.** “Clear or Modify Classes” window
- 545 **Figure 6.** Selection of the class set to be used for the visualization of the colourgrams.
- 546 **Figure 7.** Colourgrams GUI main window, where the regions related to red, blue and hue are
547 highlighted in light blue colour (a); frequency distribution curves of the selected
548 parameters coloured according harvest time (b) and to total anthocyanins content (c).
- 549 **Figure 8.** PCA window
- 550 **Figure 9.** PCA window with selected objects
- 551 **Figure 10.** Window for the visualization of PCA loadings.
- 552 **Figure 11.** Definition of the model parameters using PLS window
- 553 **Figure 12.** PLS window in prediction mode.
- 554 **Figure 13.** Colourgrams GUI main window in image reconstruction mode (a) and reconstruction
555 of the same image considering two colourgram intervals corresponding to portions of
556 the relative green (b) and relative blue (c) frequency distribution curves.

557

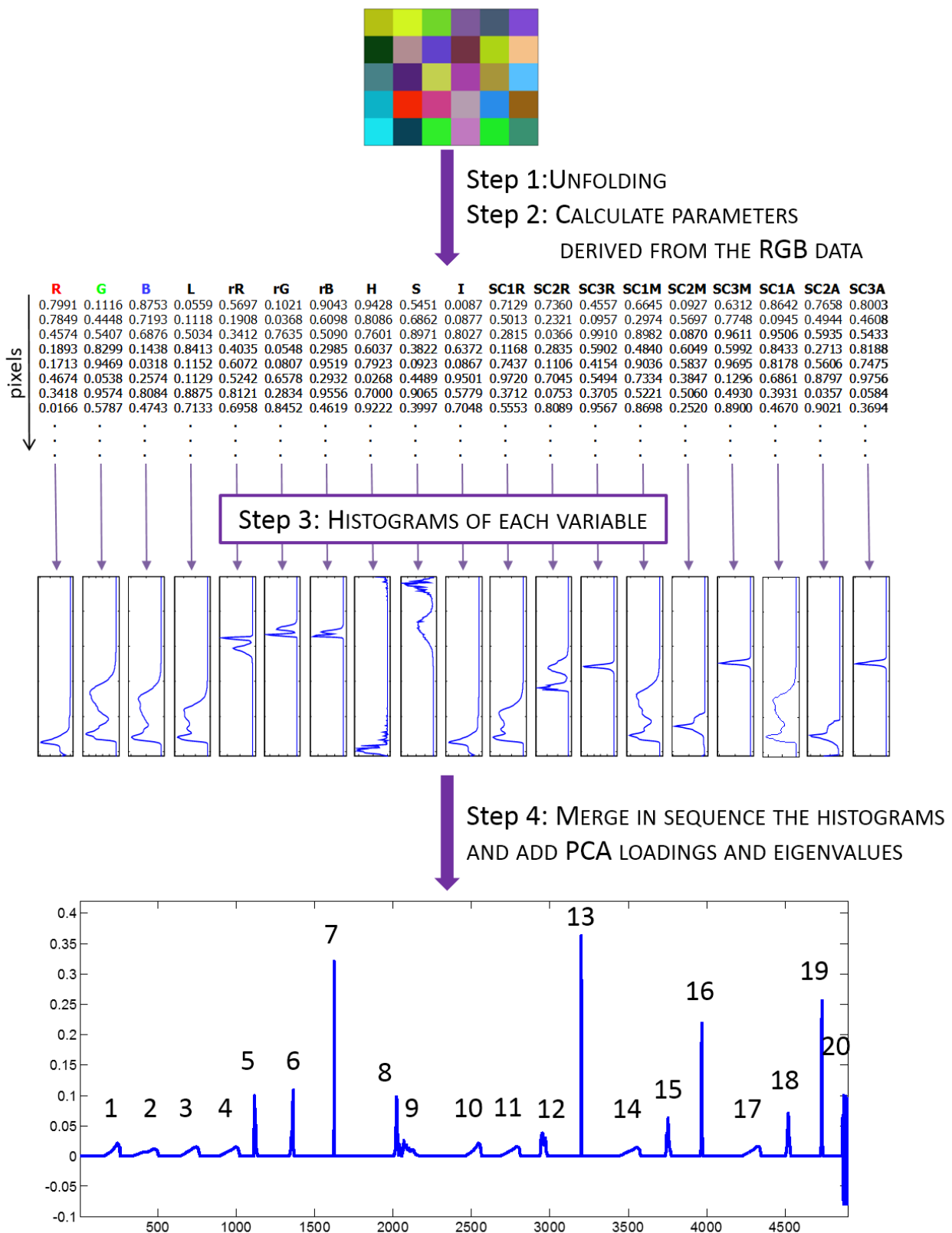


Figure 1

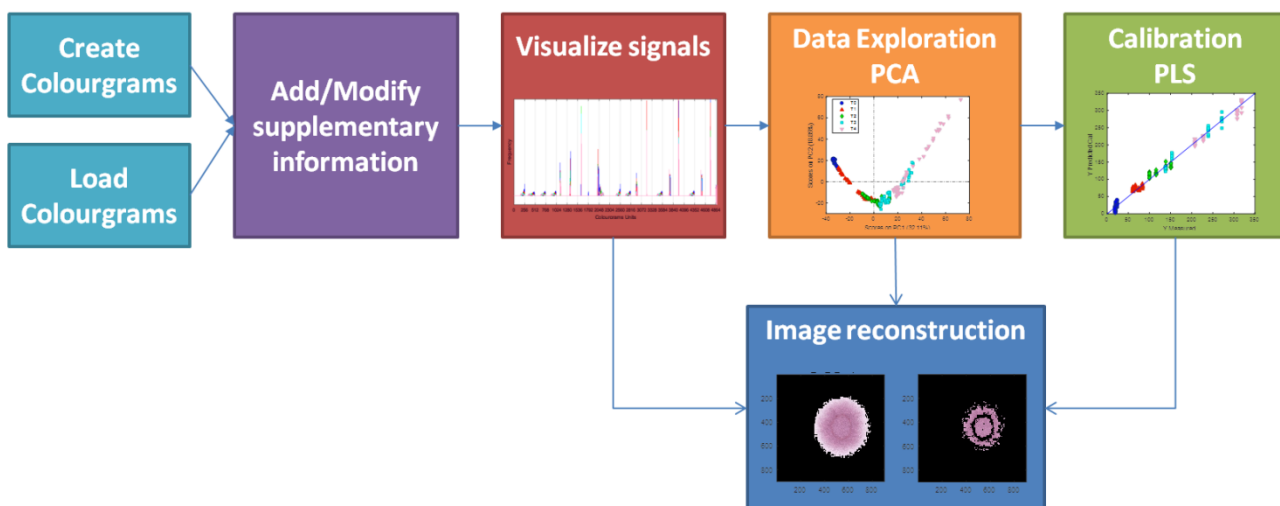


Figure 2

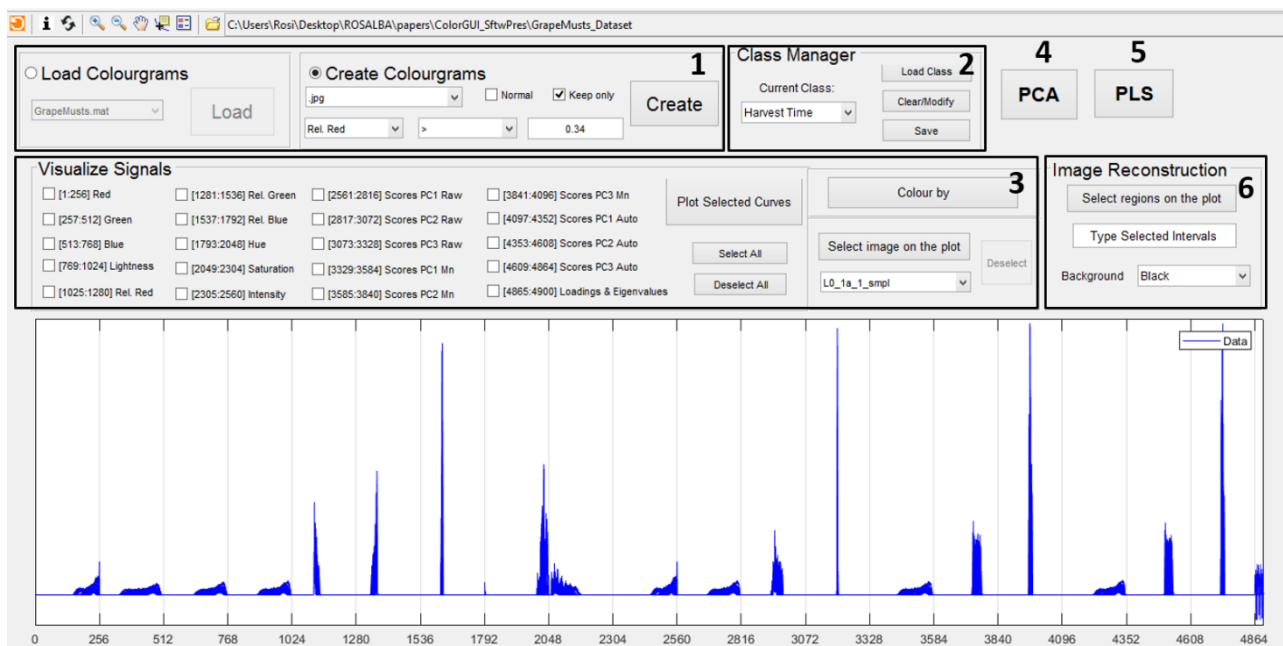


Figure 3

Load from file

E:\Paper_ColGUI_SftwPres\SoloLambruscoCorrette\Generated_Colourgrams_20161109_T122824

☐ .mat file

☒ *.xls, *.xlsx, *.csv files

Change directory

Colourgrams_info.xls

Load from workspace

Select class vector

OK

a)

Worksheet Number

1

Excel Range

B2:B241

b)

OK Cancel

Delimiter

;

Range (spreadsheet notation)

B2:B241

c)

OK Cancel

Figure 4

Select Class Set

Harvest Time
Plant Number
Measurement Se

Class Set Name: Harvest Time

N° Objects	Class Name
48 T0	
48 T1	
48 T2	
48 T3	

Clear Class Set

Apply

Figure 5

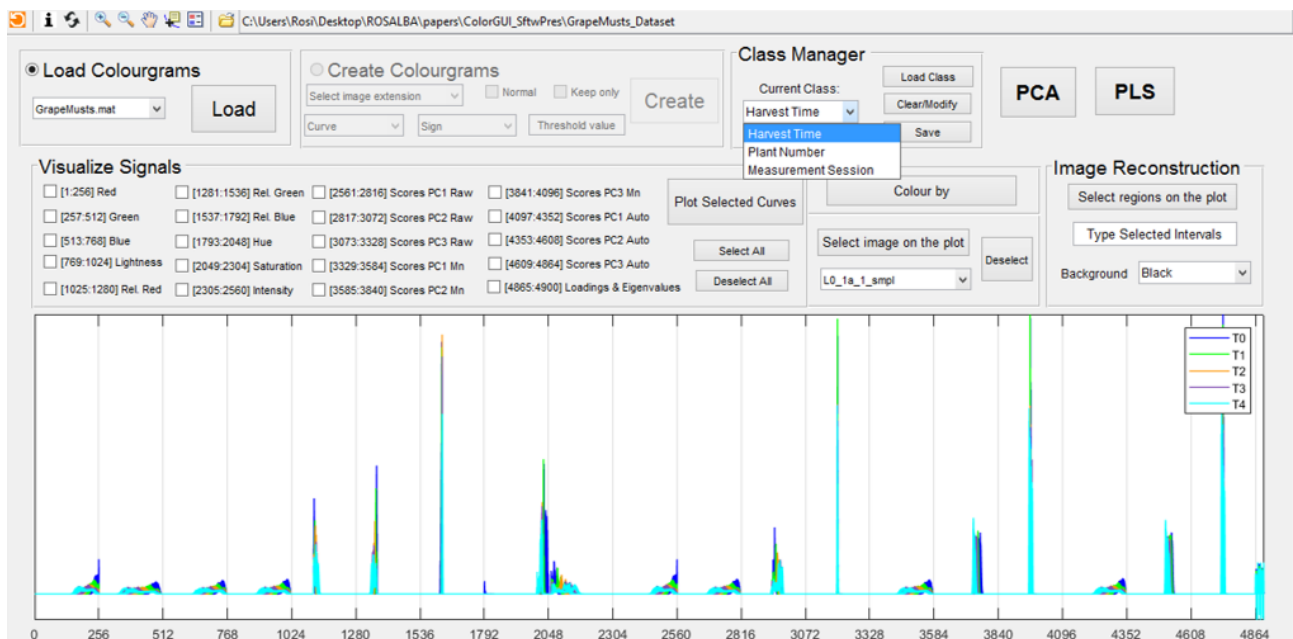


Figure 6

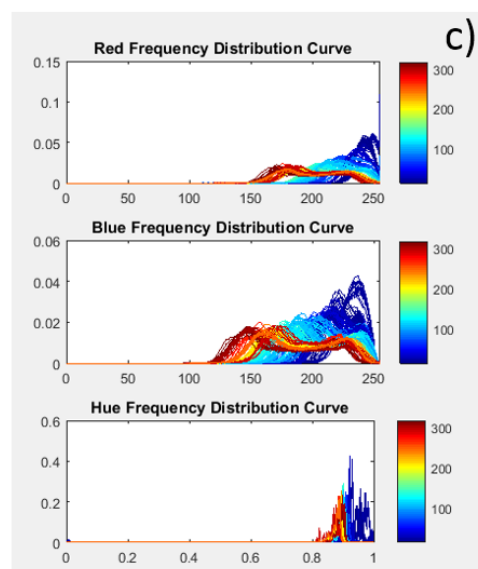
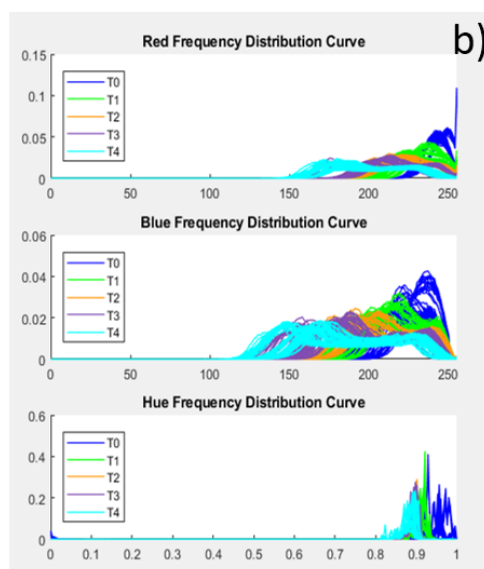
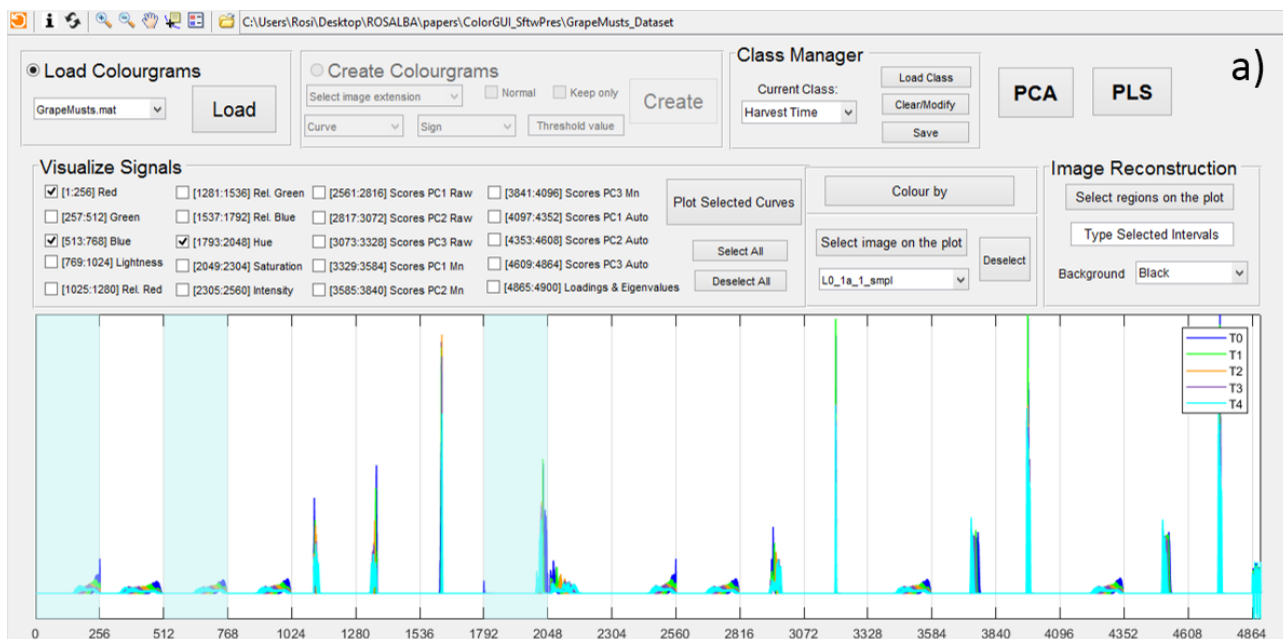


Figure 7

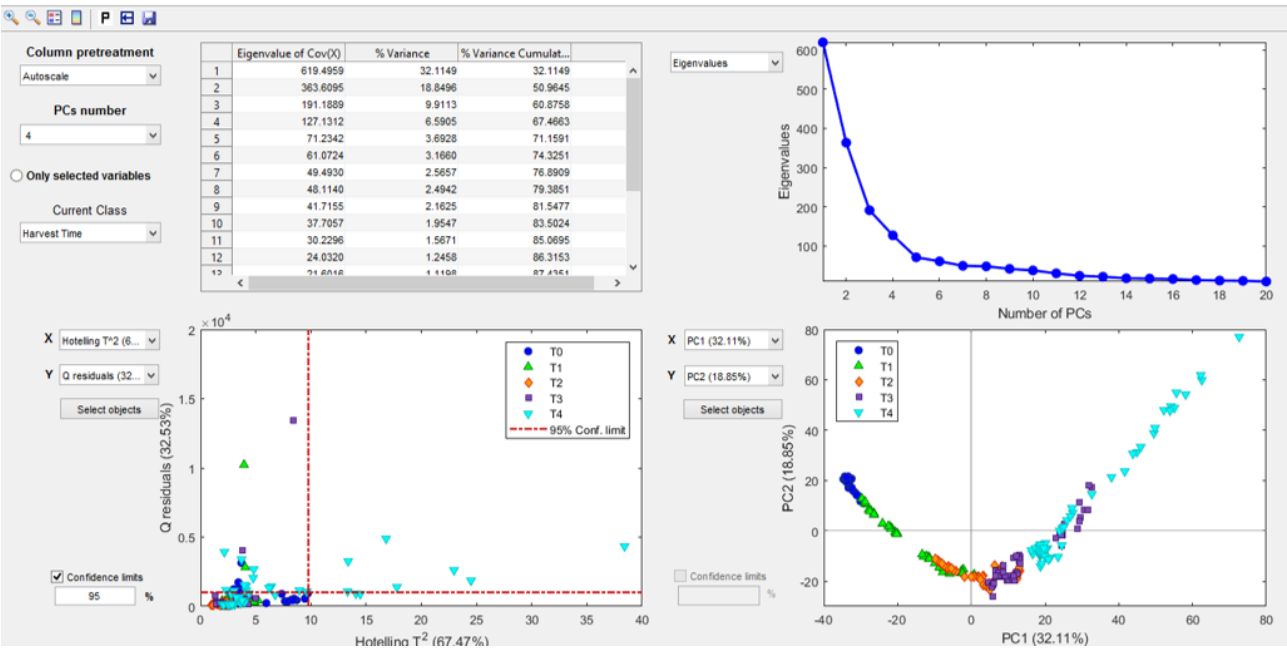


Figure 8

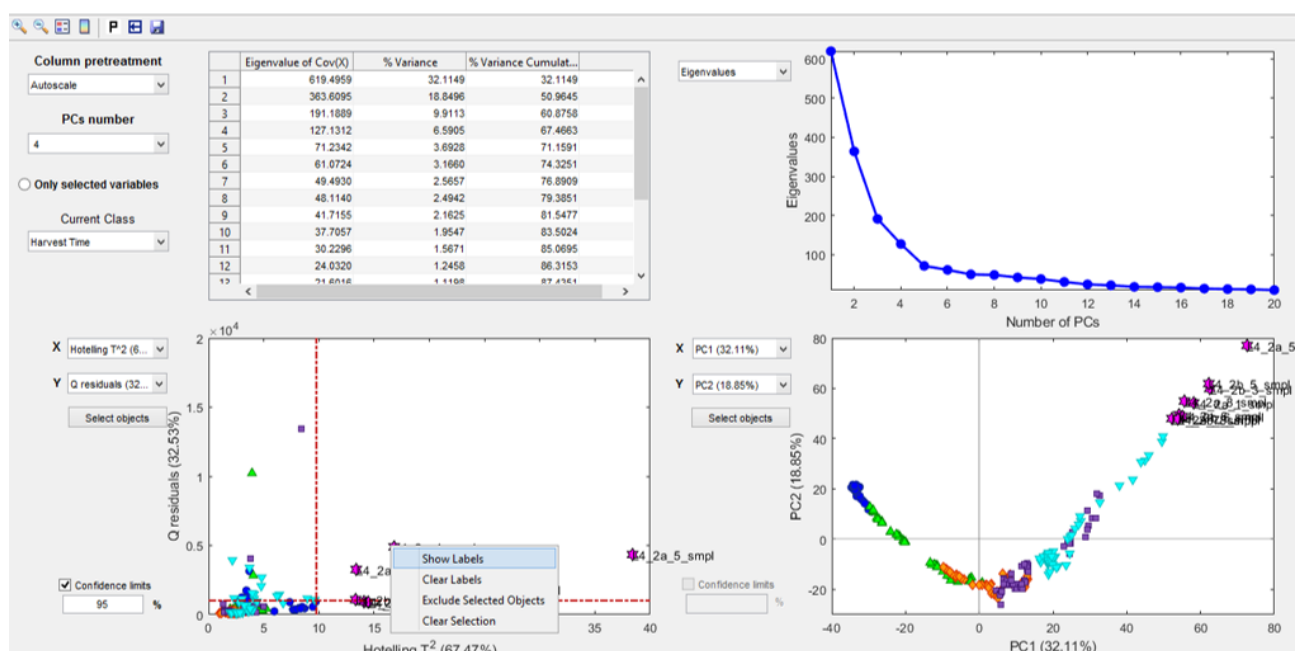


Figure 9

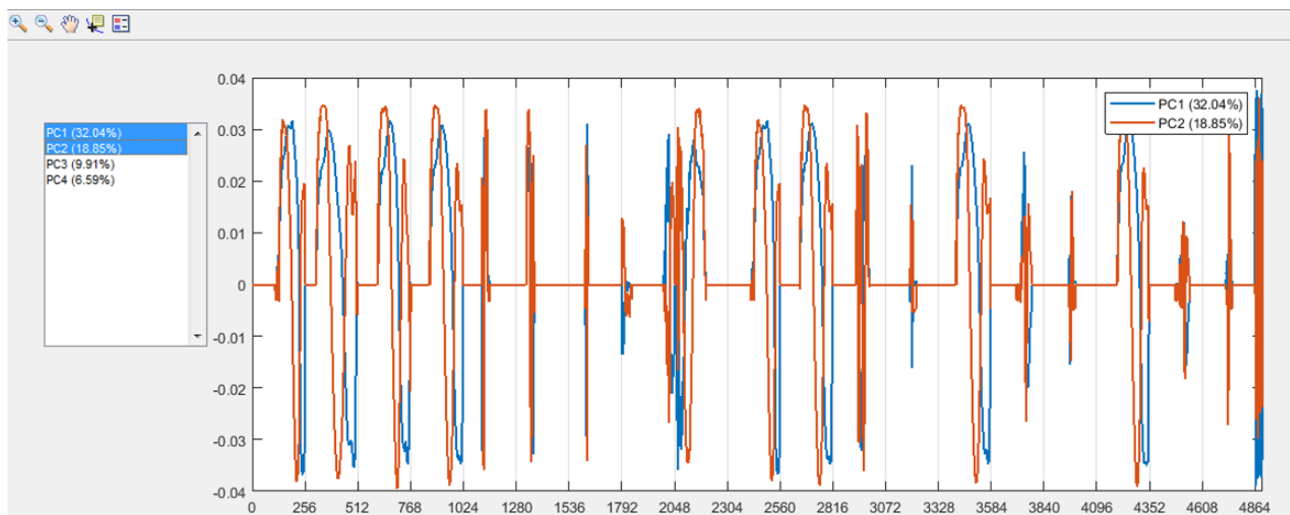


Figure 10

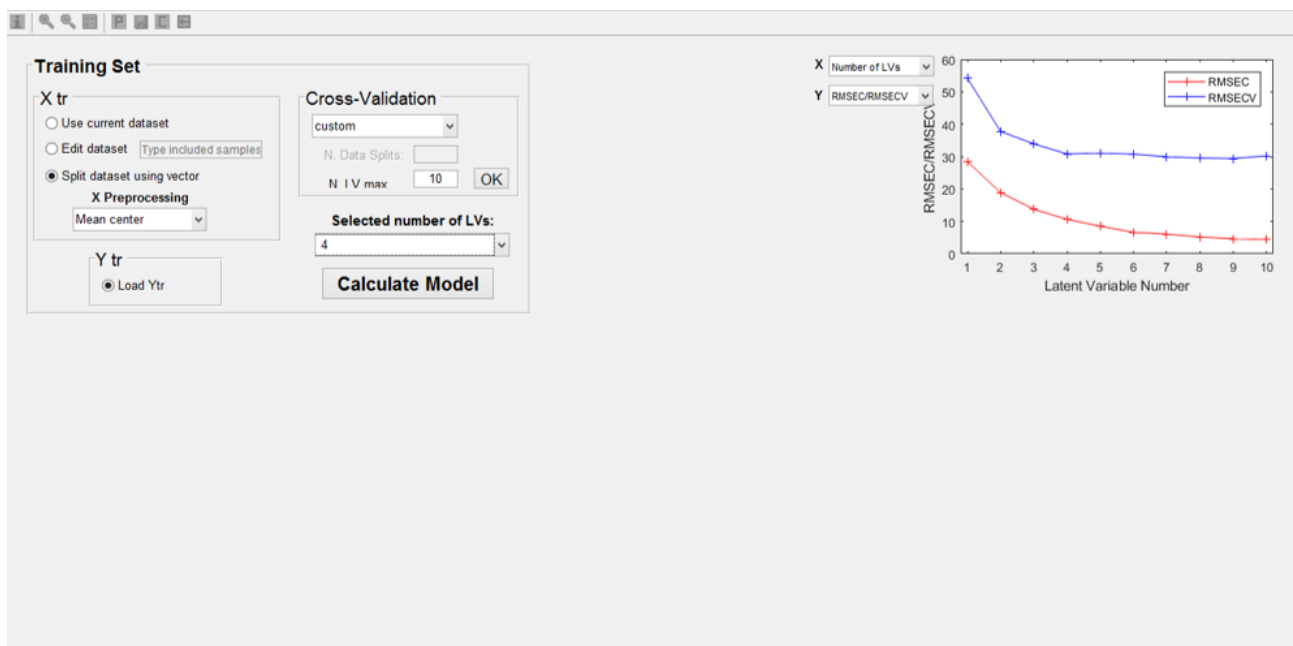


Figure 11

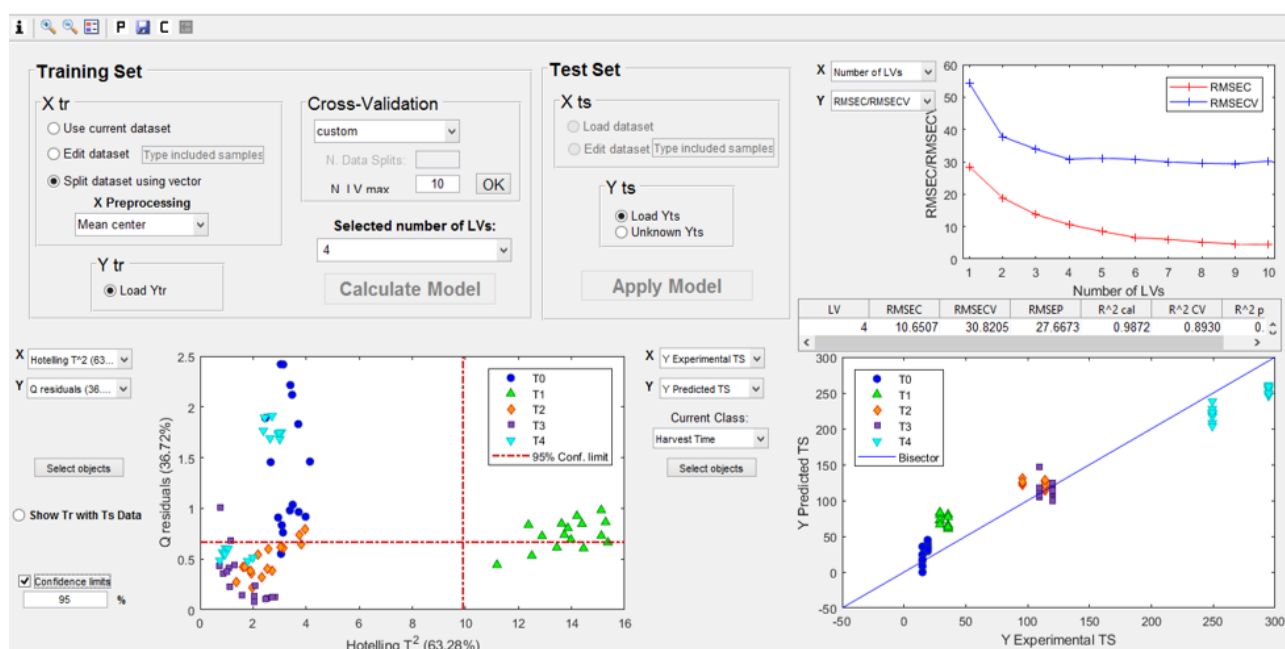


Figure 12

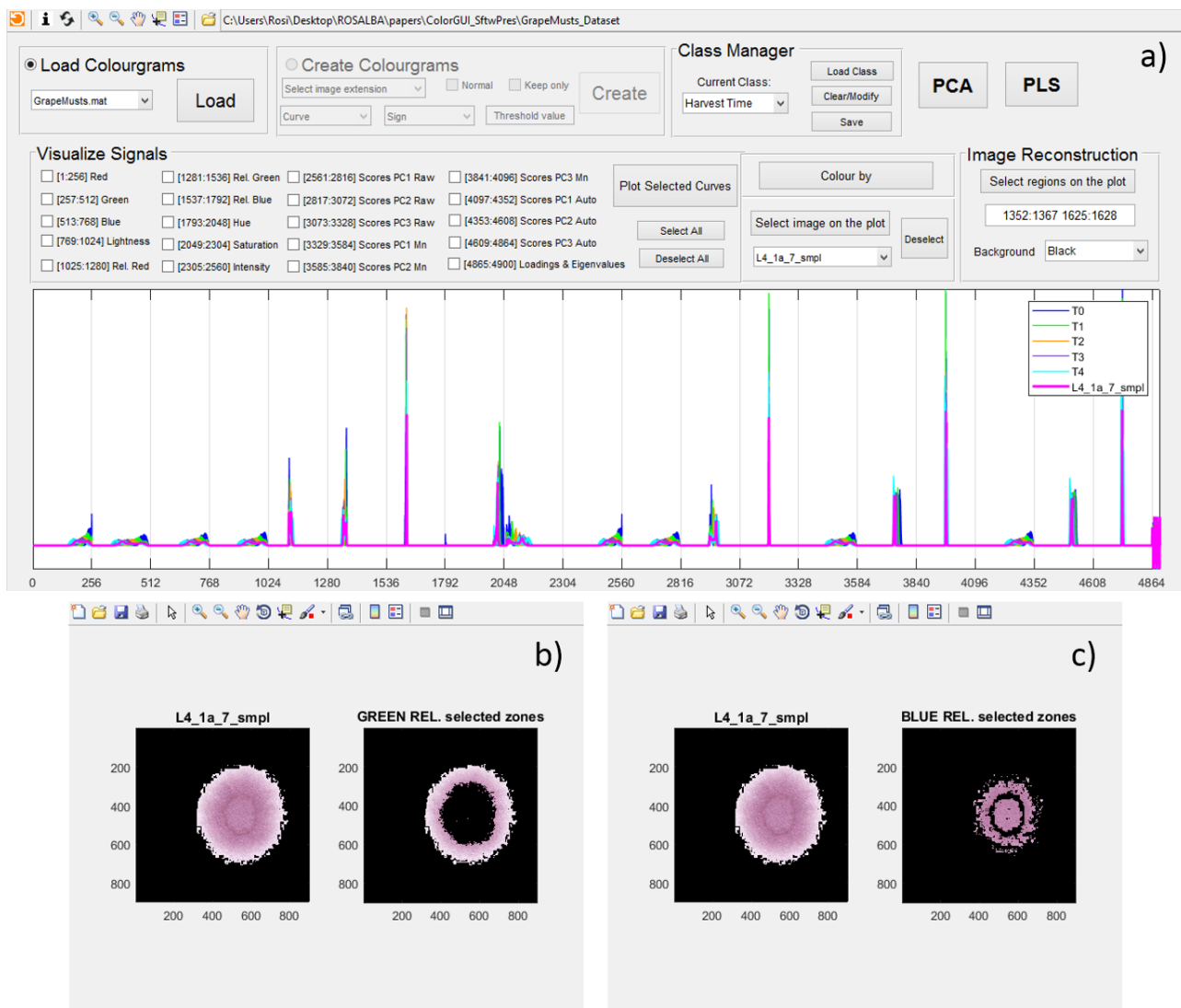


Figure 13



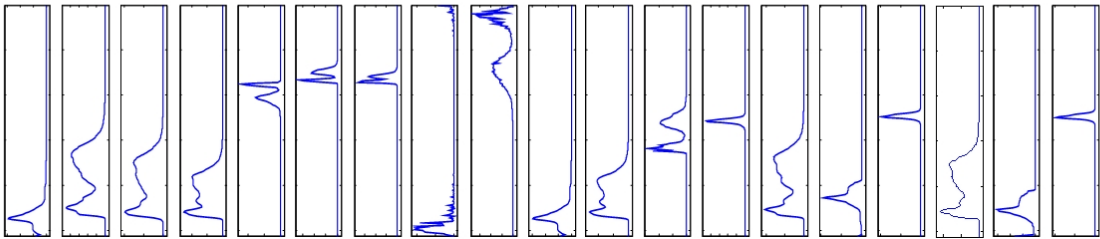
Step 1: UNFOLDING

Step 2: CALCULATE PARAMETERS

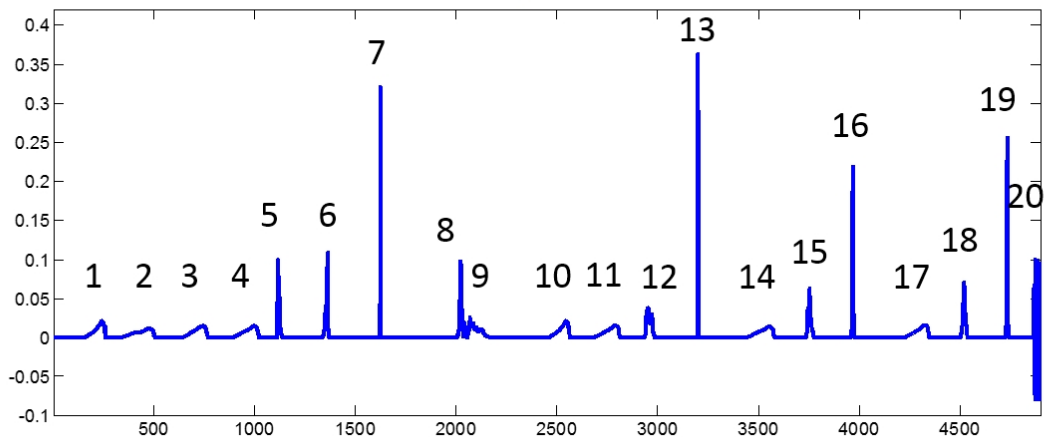
DERIVED FROM THE RGB DATA

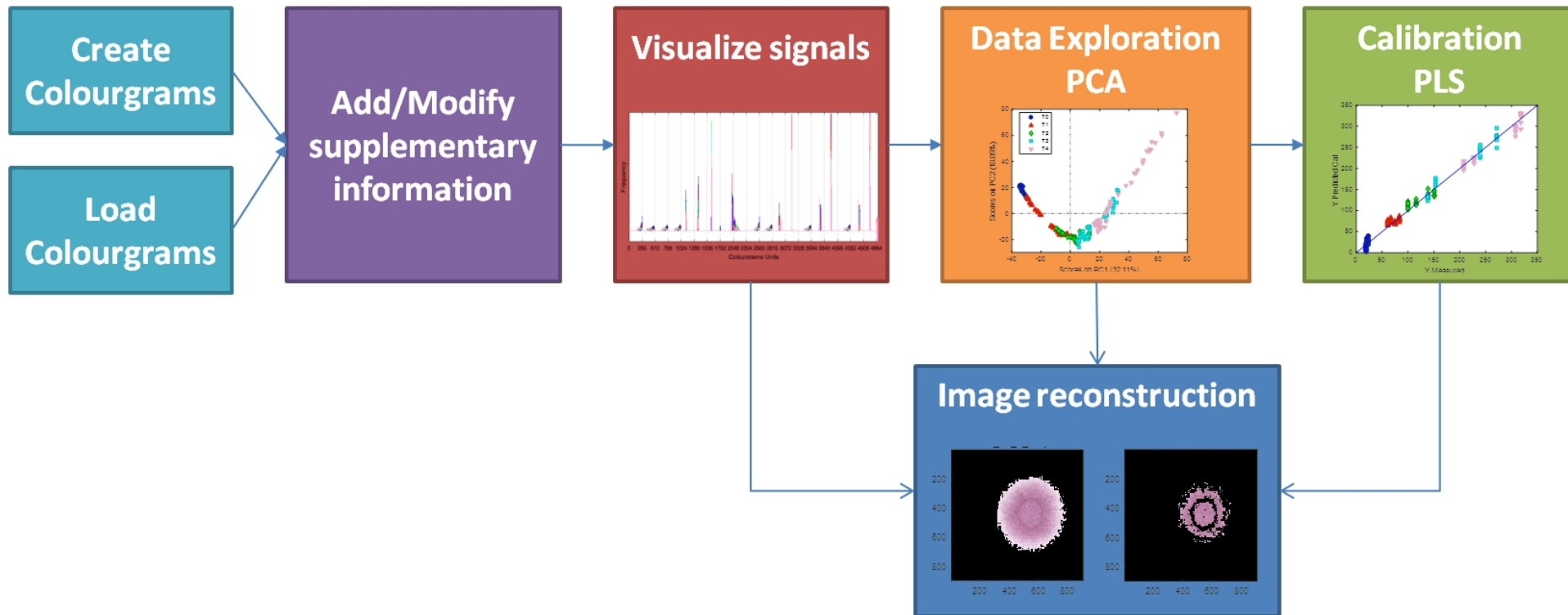
	R	G	B	L	rR	rG	rB	H	S	I	SC1R	SC2R	SC3R	SC1M	SC2M	SC3M	SC1A	SC2A	SC3A
pixels	0.7991	0.1116	0.8753	0.0559	0.5697	0.1021	0.9043	0.9428	0.5451	0.0087	0.7129	0.7360	0.4557	0.6645	0.0927	0.6312	0.8642	0.7658	0.8003
	0.7849	0.4448	0.7193	0.1118	0.1908	0.0368	0.6098	0.8086	0.6862	0.0877	0.5013	0.2321	0.0957	0.2974	0.5697	0.7748	0.0945	0.4944	0.4608
	0.4574	0.5407	0.6876	0.5034	0.3412	0.7635	0.5090	0.7601	0.8971	0.8027	0.2815	0.0366	0.9910	0.8982	0.0870	0.9611	0.9506	0.5935	0.5433
	0.1893	0.8299	0.1438	0.8413	0.4035	0.0548	0.2985	0.6037	0.3822	0.6372	0.1168	0.2835	0.5902	0.4840	0.6049	0.5992	0.8433	0.2713	0.8188
	0.1713	0.9469	0.0318	0.1152	0.6072	0.0807	0.9519	0.7923	0.0923	0.0867	0.7437	0.1106	0.4154	0.9036	0.5837	0.9695	0.8178	0.5606	0.7475
	0.4674	0.0538	0.2574	0.1129	0.5242	0.6578	0.2932	0.0268	0.4489	0.9501	0.9720	0.7045	0.5494	0.7334	0.3847	0.1296	0.6861	0.8797	0.9756
	0.3418	0.9574	0.8084	0.8875	0.8121	0.2834	0.9556	0.7000	0.9065	0.5779	0.3712	0.0753	0.3705	0.5221	0.5060	0.4930	0.3931	0.0357	0.0584
	0.0166	0.5787	0.4743	0.7133	0.6958	0.8452	0.4619	0.9222	0.3997	0.7048	0.5553	0.8089	0.9567	0.8698	0.2520	0.8900	0.4670	0.9021	0.3694

Step 3: HISTOGRAMS OF EACH VARIABLE



Step 4: MERGE IN SEQUENCE THE HISTOGRAMS AND ADD PCA LOADINGS AND EIGENVALUES





Load Colourgrams

GrapeMusts.mat

Load

Create Colourgrams

.jpg

☐ Normal ☒ Keep only

Rel. Red

>

0.34

Create

Class Manager

Load Class

Current Class:

Harvest Time

Clear/Modify

Save

PCA

PLS

Visualize Signals

- ☐ [1:256] Red ☐ [1281:1536] Rel. Green ☐ [2561:2816] Scores PC1 Raw ☐ [3841:4096] Scores PC3 Mn
- ☐ [257:512] Green ☐ [1537:1792] Rel. Blue ☐ [2817:3072] Scores PC2 Raw ☐ [4097:4352] Scores PC1 Auto
- ☐ [513:768] Blue ☐ [1793:2048] Hue ☐ [3073:3328] Scores PC3 Raw ☐ [4353:4608] Scores PC2 Auto
- ☐ [769:1024] Lightness ☐ [2049:2304] Saturation ☐ [3329:3584] Scores PC1 Mn ☐ [4609:4864] Scores PC3 Auto
- ☐ [1025:1280] Rel. Red ☐ [2305:2560] Intensity ☐ [3585:3840] Scores PC2 Mn ☐ [4865:4900] Loadings & Eigenvalues

Plot Selected Curves

Select All

Deselect All

Colour by

Select image on the plot

L0_1a_1_smpl

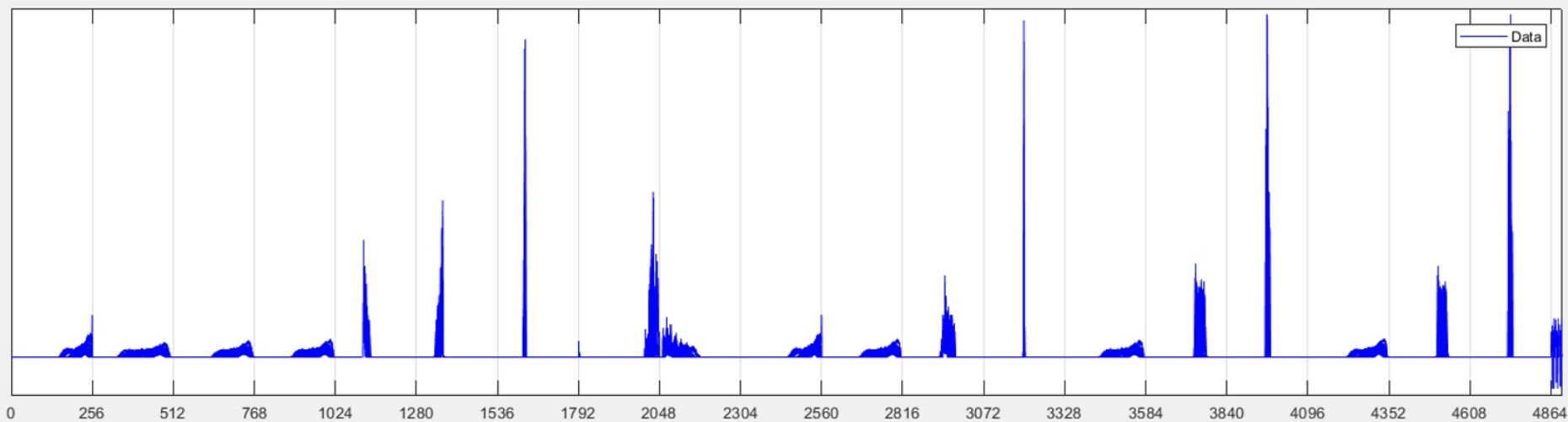
Deselect

Image Reconstruction

Select regions on the plot

Type Selected Intervals

Background Black



☒ **Load from file**

E:\Paper_ColGUI_SftwPres\SoloLambruscoCorrette\Generated_Colourgrams_20161109_T122824

☐ .mat file

☒ *.xls, *.xlsx, *.csv files

Change directory

Colourgrams_info.xls

☐ **Load from workspace**

Select class vector

OK

a)

Worksheet Number

1

Excel Range

B2:B241

b)

OK Cancel

Delimiter

;

Range (spreadsheet notation)

B2:B241

c)

OK Cancel

Select Class Set

Harvest Time
Plant Number
Measurement Se

Clear Class Set

Class Set Name: Harvest Time

N° Objects	Class Name
48 T0	
48 T1	
48 T2	
48 T3	

Apply

Load Colourgrams

GrapeMusts.mat

Load

Create Colourgrams

Select image extension

Normal

Keep only

Create

Curve

Sign

Threshold value

Class Manager

Current Class:

Harvest Time

Harvest Time

Plant Number

Measurement Session

Load Class

Clear/Modify

Save

PCA

PLS

Visualize Signals

- ☐ [1:256] Red
 ☐ [1281:1536] Rel. Green
 ☐ [2561:2816] Scores PC1 Raw
 ☐ [3841:4096] Scores PC3 Mn
- ☐ [257:512] Green
 ☐ [1537:1792] Rel. Blue
 ☐ [2817:3072] Scores PC2 Raw
 ☐ [4097:4352] Scores PC1 Auto
- ☐ [513:768] Blue
 ☐ [1793:2048] Hue
 ☐ [3073:3328] Scores PC3 Raw
 ☐ [4353:4608] Scores PC2 Auto
- ☐ [769:1024] Lightness
 ☐ [2049:2304] Saturation
 ☐ [3329:3584] Scores PC1 Mn
 ☐ [4609:4864] Scores PC3 Auto
- ☐ [1025:1280] Rel. Red
 ☐ [2305:2560] Intensity
 ☐ [3585:3840] Scores PC2 Mn
 ☐ [4865:4900] Loadings & Eigenvalues

Plot Selected Curves

Select All

Deselect All

Colour by

Select image on the plot

L0_1a_1_smpl

Deselect

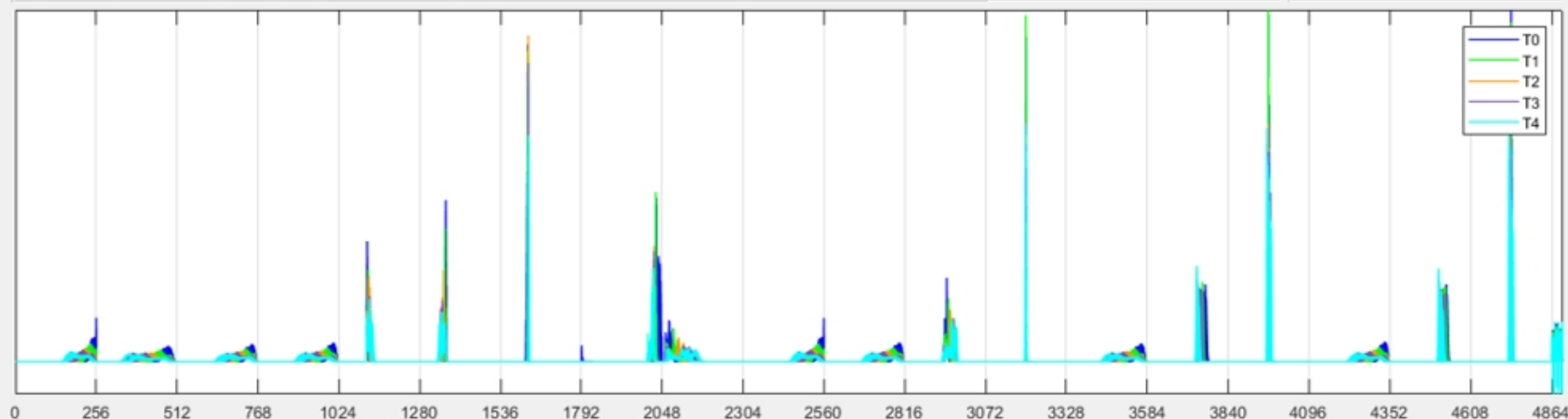
Image Reconstruction

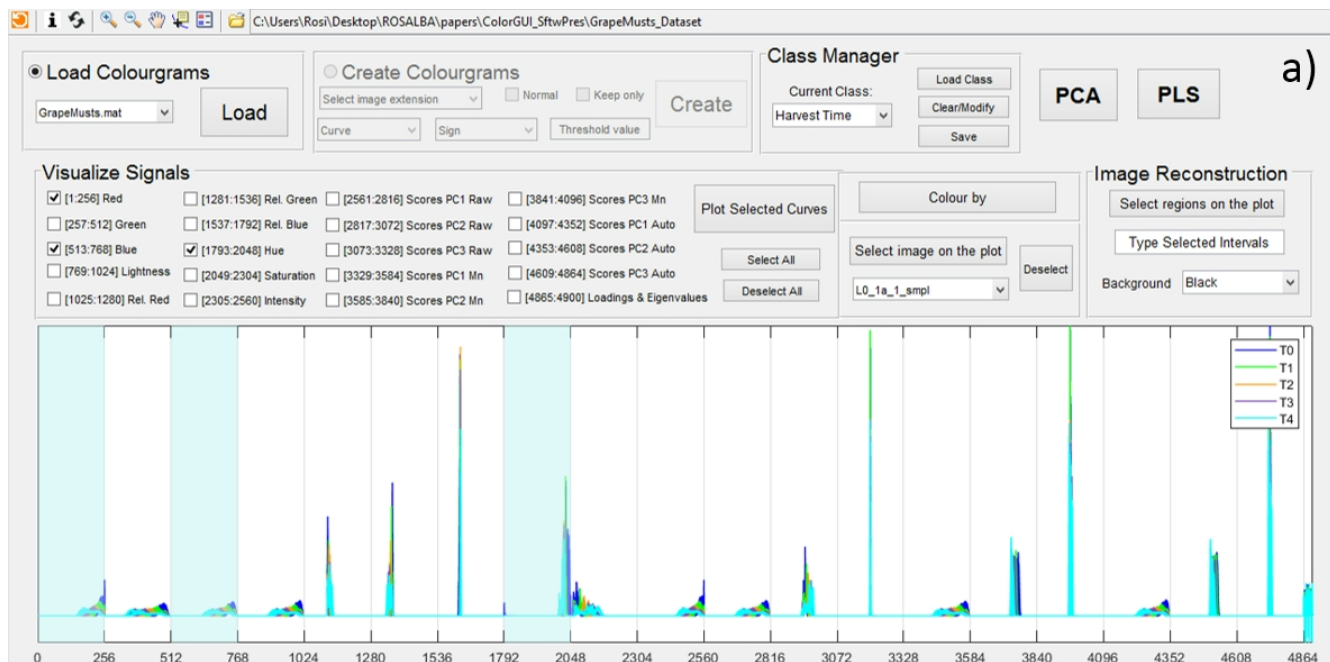
Select regions on the plot

Type Selected Intervals

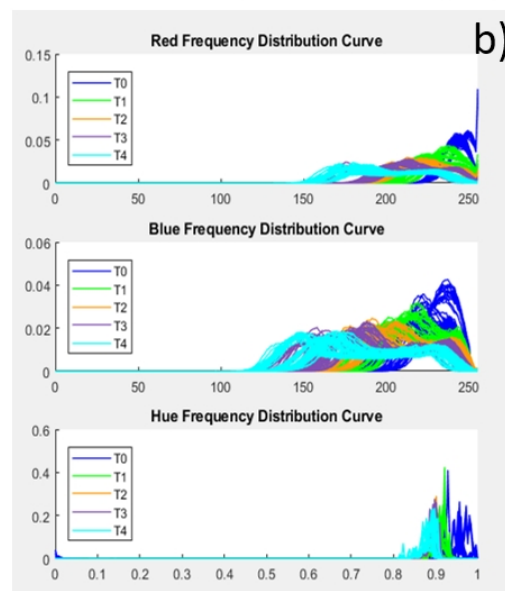
Background

Black

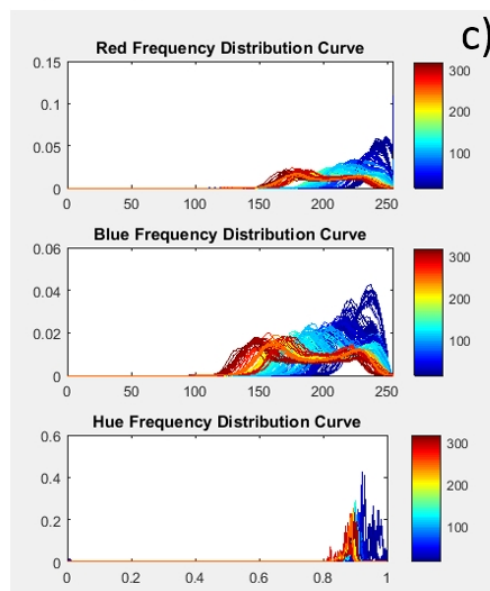




a)



b)



c)



Column pretreatment

Autoscale

PCs number

4

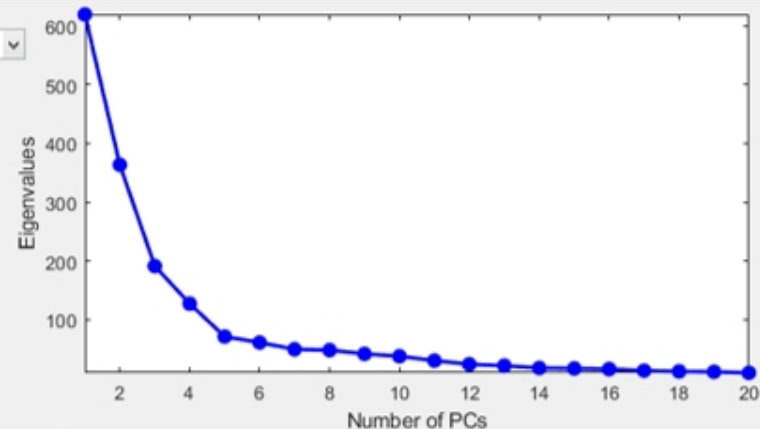
☐ Only selected variables

Current Class

Harvest Time

	Eigenvalue of Cov(X)	% Variance	% Variance Cumulat...
1	619.4959	32.1149	32.1149
2	363.6095	18.8496	50.9645
3	191.1889	9.9113	60.8758
4	127.1312	6.5905	67.4663
5	71.2342	3.6928	71.1591
6	61.0724	3.1660	74.3251
7	49.4930	2.5657	76.8909
8	48.1140	2.4942	79.3851
9	41.7155	2.1625	81.5477
10	37.7057	1.9547	83.5024
11	30.2296	1.5671	85.0695
12	24.0320	1.2458	86.3153
13	21.6016	1.1108	87.4261

Eigenvalues



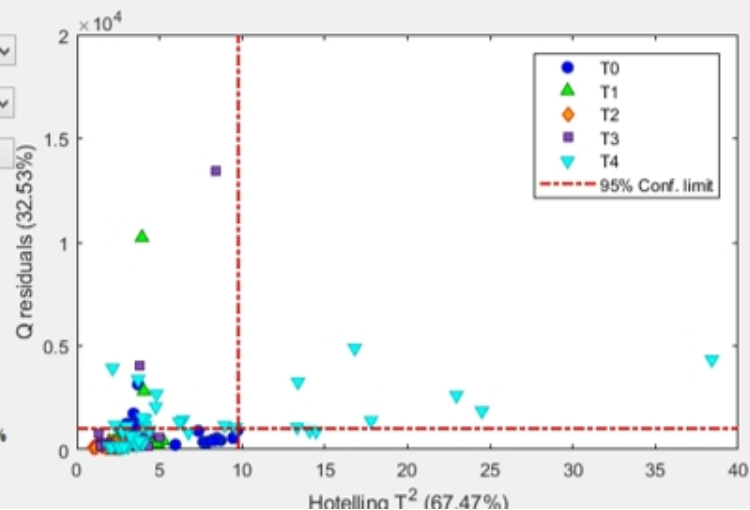
X Hotelling T² (67.47%)

Y Q residuals (32.53%)

Select objects

☒ Confidence limits

95 %



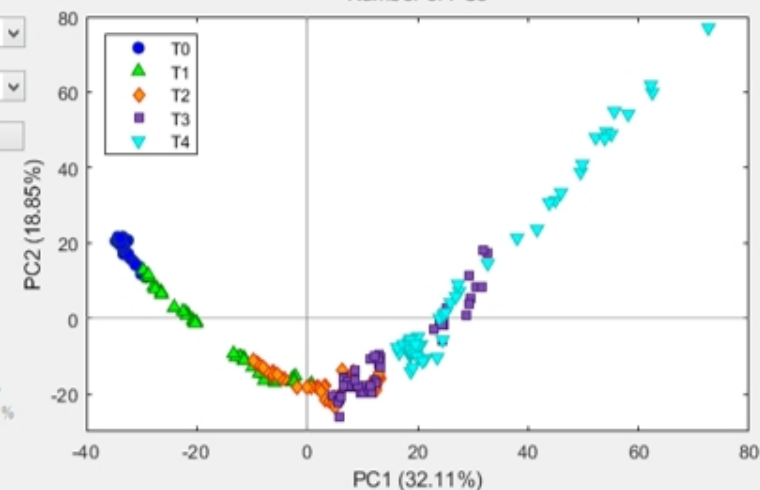
X PC1 (32.11%)

Y PC2 (18.85%)

Select objects

☐ Confidence limits

%





Column pretreatment

Autoscale

PCs number

4

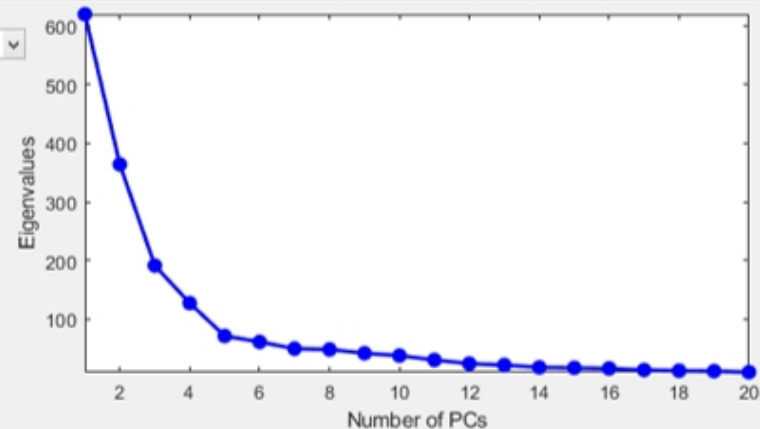
☐ Only selected variables

Current Class

Harvest Time

	Eigenvalue of Cov(X)	% Variance	% Variance Cumulat...
1	619.4959	32.1149	32.1149
2	363.6095	18.8496	50.9645
3	191.1889	9.9113	60.8758
4	127.1312	6.5905	67.4663
5	71.2342	3.6928	71.1591
6	61.0724	3.1680	74.3251
7	49.4930	2.5657	76.8909
8	48.1140	2.4942	79.3851
9	41.7155	2.1625	81.5477
10	37.7057	1.9547	83.5024
11	30.2296	1.5671	85.0695
12	24.0320	1.2458	86.3153
13	21.6016	1.1108	87.4251

Eigenvalues



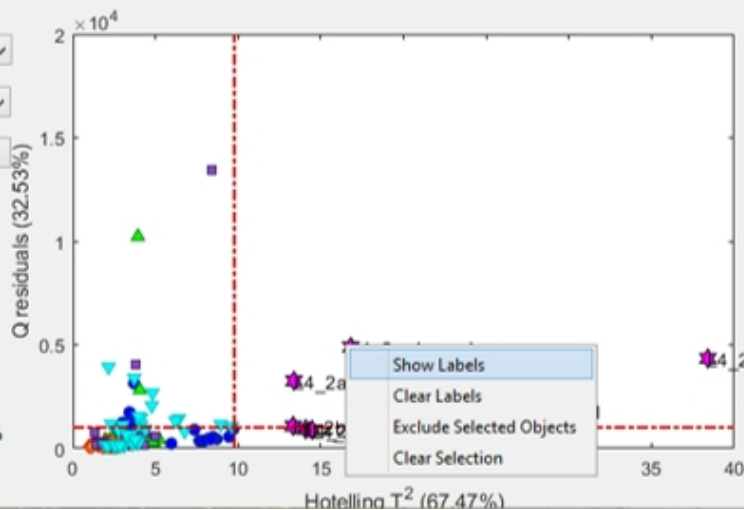
X Hotelling T² (67.47%)

Y Q residuals (32.53%)

Select objects

☒ Confidence limits

95 %



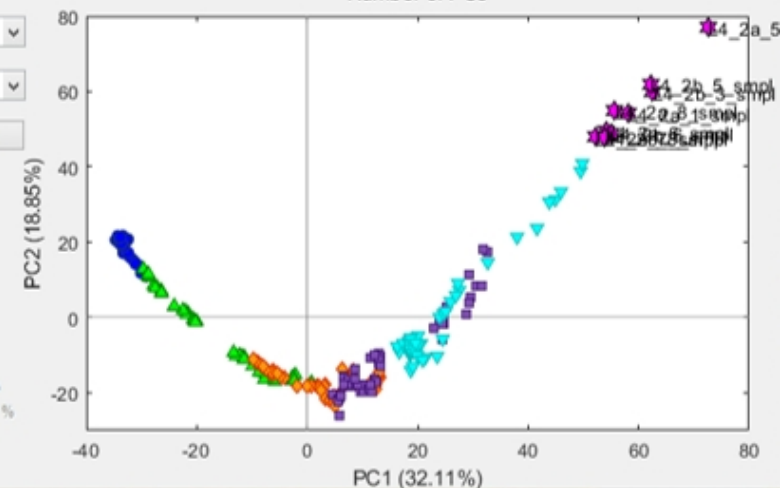
X PC1 (32.11%)

Y PC2 (18.85%)

Select objects

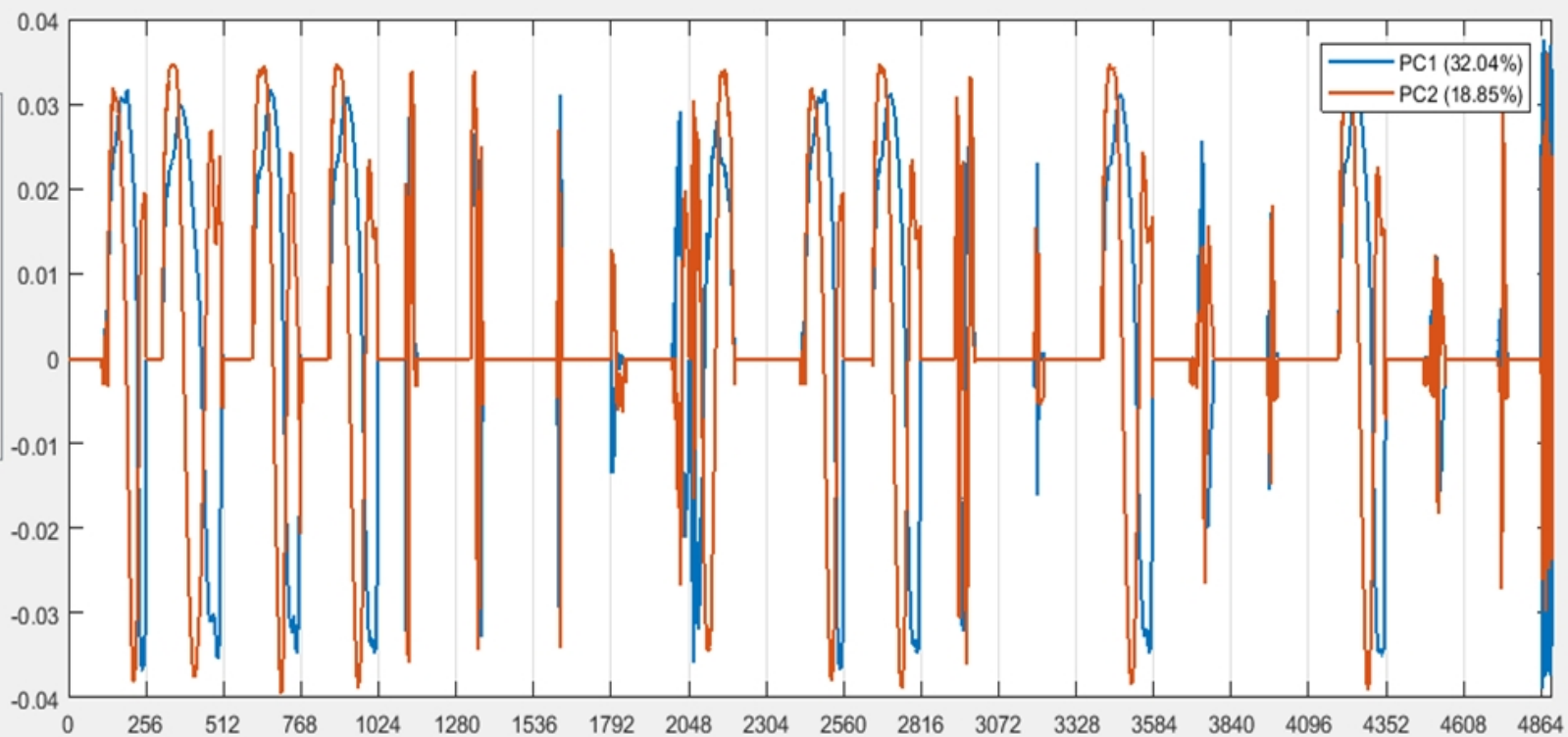
☐ Confidence limits

%





- PC1 (32.04%)
- PC2 (18.85%)
- PC3 (9.91%)
- PC4 (6.59%)





Training Set

X tr

- ☐ Use current dataset
- ☐ Edit dataset
- ☒ Split dataset using vector

X Preprocessing

Mean center

Y tr

- ☒ Load Ytr

Cross-Validation

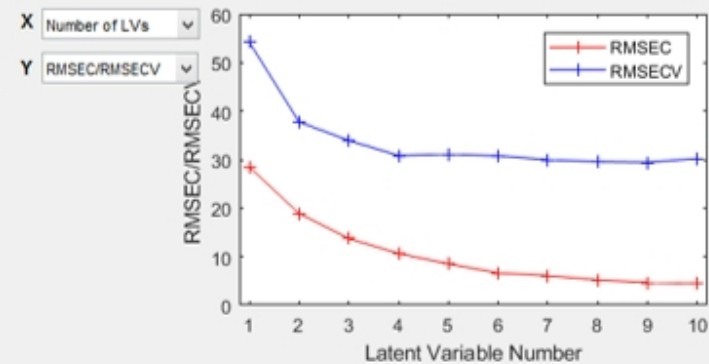
custom

N. Data Splits:

N I V max

Selected number of LVs:

4



Training Set

X tr

- ☐ Use current dataset
☐ Edit dataset
☒ Split dataset using vector

X Preprocessing

Mean center

Y tr

- ☒ Load Ytr

Cross-Validation

custom

N. Data Splits:

N I V max

10

OK

Selected number of LVs:

4

Calculate Model

Test Set

X ts

- ☐ Load dataset
☐ Edit dataset

Y ts

- ☒ Load Yts
☐ Unknown Yts

Apply Model

X Hotelling T² (63.28%)

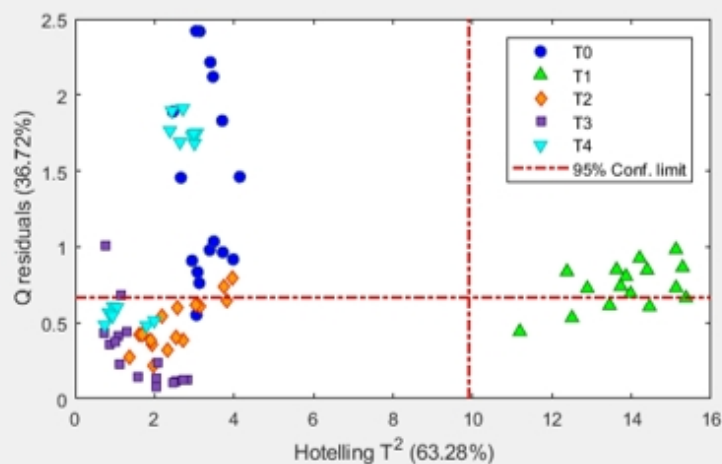
Y Q residuals (36.72%)

Select objects

☐ Show Tr with Ts Data

☒ Confidence limits

95 %



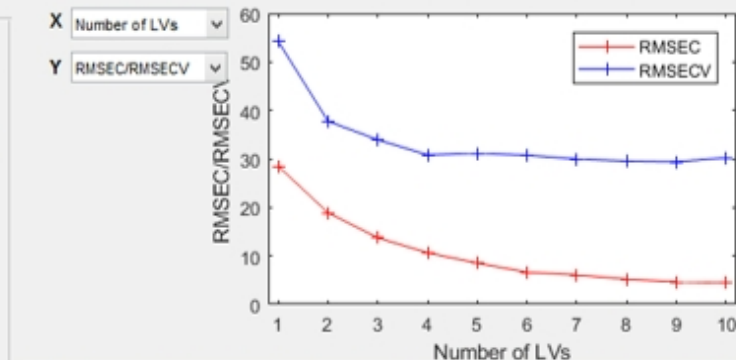
X Y Experimental TS

Y Y Predicted TS

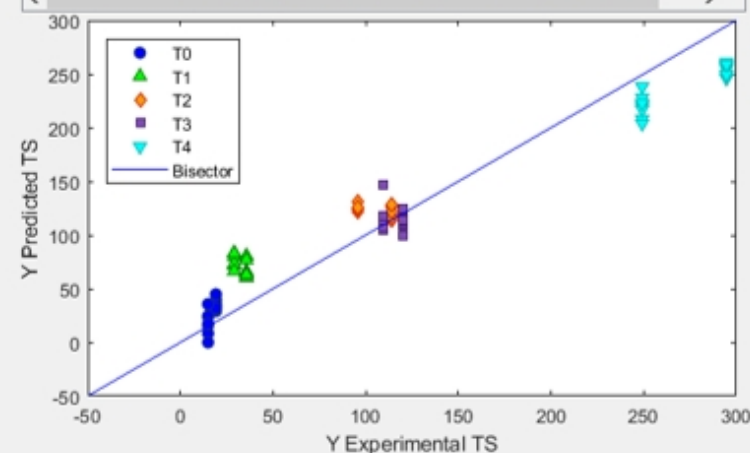
Current Class:

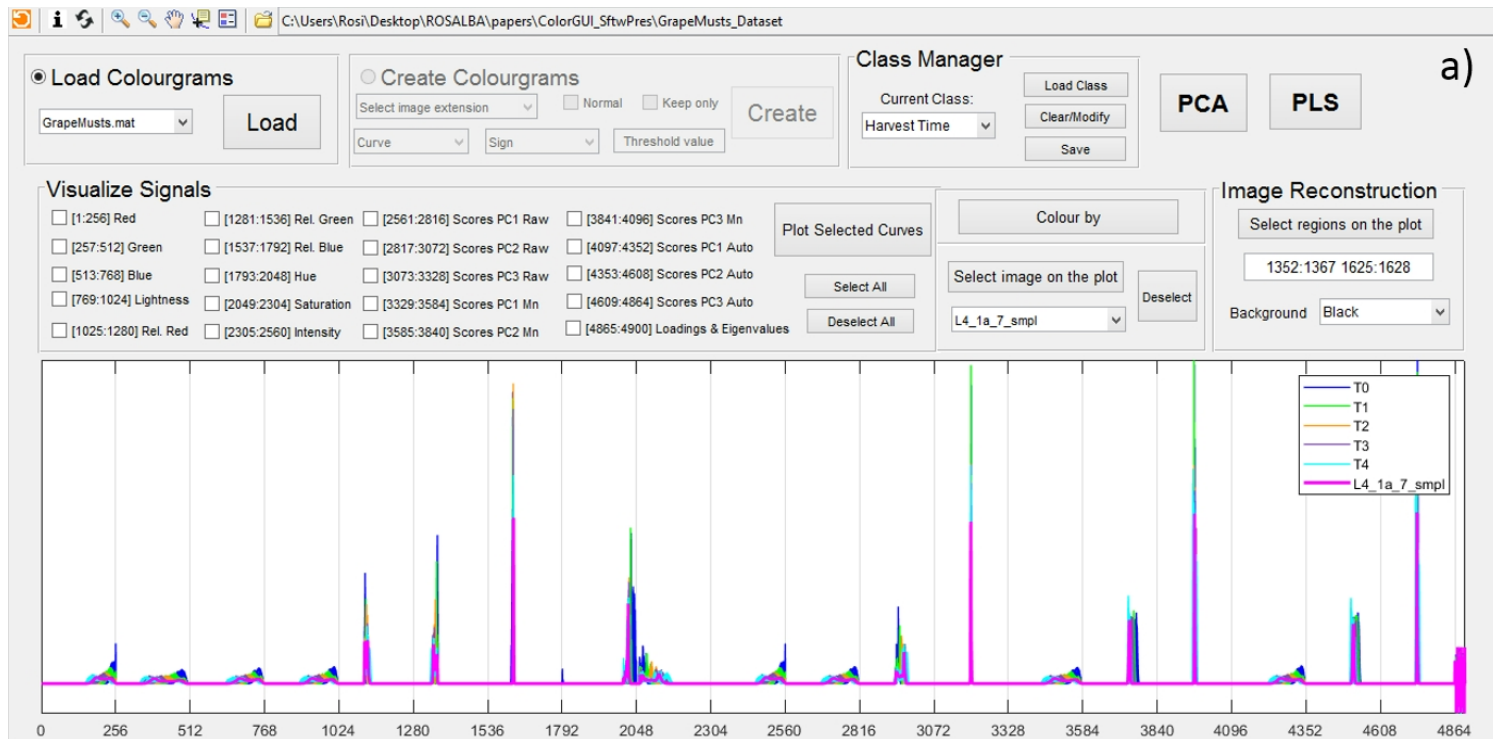
Harvest Time

Select objects



LV	RMSEC	RMSECV	RMSEP	R ² cal	R ² CV	R ² p
4	10.6507	30.8205	27.6673	0.9872	0.8930	0.9





a)

