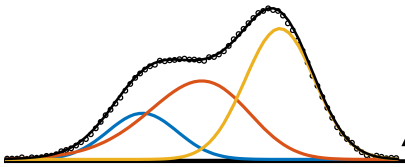

AnalySize

Software for grain size unmixing and analysis
v1.1.3

December, 2019

Contents

1 Introduction

Advances in instruments to measure particle size distribution, particularly laser diffraction particle size analyzers, has led to a increase in the number of data available and the resolution of grain size measurements. With this advance, new tools are required to processes these large data sets quickly and in a fashion that fits with the physical constraints of the data. To that end we have developed AnalySize, which is a `MATLAB` based software tool to aid Earth scientists make sense of their grain size data. AnalySize incorporates a range of powerful unmixing techniques alongside several routine methods for quantifying grain size data. AnalySize presents these tool in a clear, easy to use graphical interface that is compatible with a wide range of software platforms. AnalySize is a mathematical tool to help understand data set. Like all such tool and analyses, these mathematical procedures require physical ground-truthing with data and information outside of AnalySize. Users should strive to use physical constraints to find a balance between physical plausibility and numerical optimization.

If users encounter bugs or problems using AnalySize, or have any suggestions for improving the software, we would really like to hear from as all input is welcome.If you use AnalySize in your work, please make it clear what version was used and the what method of unmixing was used. We would also be grateful if you cited the publication that introduced AnalySize: Paterson, G. A., and D. Heslop (2015), New methods for unmixing sediment grain size data, *Geochem. Geophys. Geosyst.*, 16, 4494-4506, doi: 10.1002/2015GC006070.

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2 Version history

Pre-v0.9.0r
Draft versions during development.

v0.9.0r – August 24, 2015
The version of AnalySize released during the peer review process.

v1.0.0 – December 2, 2015
The first finalized version of AnalySize, published along side Paterson, G. A., and D. Heslop (2015), New methods for unmixing sediment grain size data, *Geochem. Geophys. Geosyst.*, 16, 4494-4506, doi: 10.1002/2015GC006070.

Changes:

1. Various adjustments to output graphics to improve compatibility with `MATLAB` 2014b and newer.
2. Updated example data sets to include the new synthetic data provided in the published paper.

v1.0.1 – December 11, 2015
Changes:

1. Fixed error when loading defined end member files.
2. Fixed sum to one of defined EMs after interpolation.
3. Added end member R^2 for defined EMs.
4. Added validity check for parametric EMA using projection to simplex. This caused quality of fit plots not to show specimen values.

v1.0.2 – January 13, 2016
Changes:

1. Improved backward compatibility extending back to `MATLAB` 2009a (v7.8).
2. Fixed error where CM plot color was incorrectly saved to user configuration file.
3. Fixed error reading in user configuration files written on Windows systems.
4. Fixed error reading text data files written on Windows systems.
5. Added clay, silt, sand, gravel fractions for specimens and end members.
6. Added linear scale plotting capability to the data and end member plots.

v1.1.0 – June 14, 2016
Changes:

1. Fixed occasional indexing error when estimating the initial distribution parameters for parametric EMA.
2. Fixed an error if a non-AnalySize *.mat file was opened when loading a saved session.
3. Increased the maximum number of iterations used in the SISAL algorithm from 100 to 200.
4. Added rounding of grain size bins to regularize data onto the same bin ranges. This simple approach is useful if data are measured on the different machines, but with the same model or manufacturer. In these cases, the bins are often near identical and differences are very small. Users are notified if this is done.
5. Added a data set size check for performing EMA (absolute bare minimum of 10 data, but more are recommended).
6. Improved graphics customization options. This includes:
    - Added symbol customization for the data plots in the main AnalySize window.
    - Clicking on individual plots now opens the plot in a separate `MATLAB` figure. This allows the user to customize each plot using the inbuilt `MATLAB` tools.
    - More functionality added to the Plot_BoxWhisker function (used for generating the "Select End Members" plots).
    - Added customization of plots used for selecting the number of end members.

v1.1.1 – October 29, 2016
Changes:

1. Fixed error in CM plots where the lower 1 percentile was used as the C values and not the upper 1 percentile.
2. Updated how Set_Data_Symbols receives the current default settings to bring it inline with other functions.

v1.1.2 – March 24, 2017
Changes:

1. Corrected error when calculating percentiles.
2. Fixed bug where the EM colors were not correct when plotting in MATLAB 2014b and higher
3. Fixed a bug where specimen names beginning with a number were not properly displayed above the data plot or when the figure was exported.
4. Adjusted lower search bound of SGG q parameter from -1 to -0.25. This ensures better fitting.
5. Fixed occasional bug when getting parametric EM initial guess. This was related to a lack of stationary points in some grain size spectra.

6. Moved the projection to simplex validity check into the optimized function. This can slow down the speed of paramedic fitting, but ensures better fits.

7. Added function for force closing all AnalySize windows (used for development and debugging).

3 System Requirements

AnalySize is written in MATLAB 2014a, and requires MATLAB v8, or higher, to run. AnalySize is self-contained and does not require any additional MATLAB Toolboxes. AnalySize will run on Windows, Mac, and Linux platforms capable of running MATLAB. Processing time of the unmixing analyses are CPU dependent and will vary from system to system, but the basic requirements to operate AnalySize are the same as those required for MATLAB The graphical elements of AnalySize require a minimum screen resolution of 1024×720. Users that experience any difficulties should contact the authors for assistance.

AnalySize may function with MATLAB versions older than 8, but users may encounter issues. Those who have older versions of MATLAB who have problems running AnalySize should contact the authors as we are more than happy to help improve backward compatibility as best as we can.

AnalySize was primarily written in MATLAB 2014a (version 8.3). The MathWorks introduced a major update to MATLAB graphics in the 2014b release (version 8.4). This completely changed the interface for manipulating figures, removing some features, while adding others (and sadly introducing some bugs). We have tried to make AnalySize as compatible as possible with both pre- and post-2014b releases, but we may have missed some issues with newer versions of MATLAB. Anyone who encounters problems exporting graphics from Analysize, or have suggestions for improvements should contact the authors for further support.

Useful Note...
As of v1.0.2, we have updated the code to improve backward compatibility of AnalySize with pre-version 8 releases of MATLAB. This has been tested on MATLAB 2009a (v7.8) and seems to work well, but let us know if you have problems.

4 Using AnalySize

4.1 Installation

All of the files required for AnalySize are available from https://github.com/greigpaterson/AnalySize. We recommend downloading the latest release of AnalySize, which is version 1.1.3 (https://github.com/greigpaterson/AnalySize/releases).

Once downloaded, the files should be put in an AnalySize folder and move to your desired destination (e.g., your MATLAB user directory).

From the "Home" tab in the main MATLAB window, select "Set Path". This will bring up a window that lists all of the directories that are currently set in the MATLAB path. Click "Add Folder..." and navigate to the location of the AnaylSize folder. Click on the folder name, then click "Open". The AnalySize folder should now appear at the top of the directory list. Now click "Save" and then "Close".

The AnalySize program can now be called from any directory by typing "AnalySize" in the MATLAB command window.

Useful Note...

GitHub provides a very useful piece of software call GitHub Desktop (https://desktop.github.com/). This allows user to watch key repositories and allows them to easily synchronize with the main GitHub website. This makes it extremely easy to keep your code up-to-date with the latest releases. We strongly recommend AnalySize users to use this approach to keep their software fully up-to-date.

4.2 The main window

When AnalySize is launched the main window is opened (Figure 1). From here, all of the AnalySize functions can be accessed.

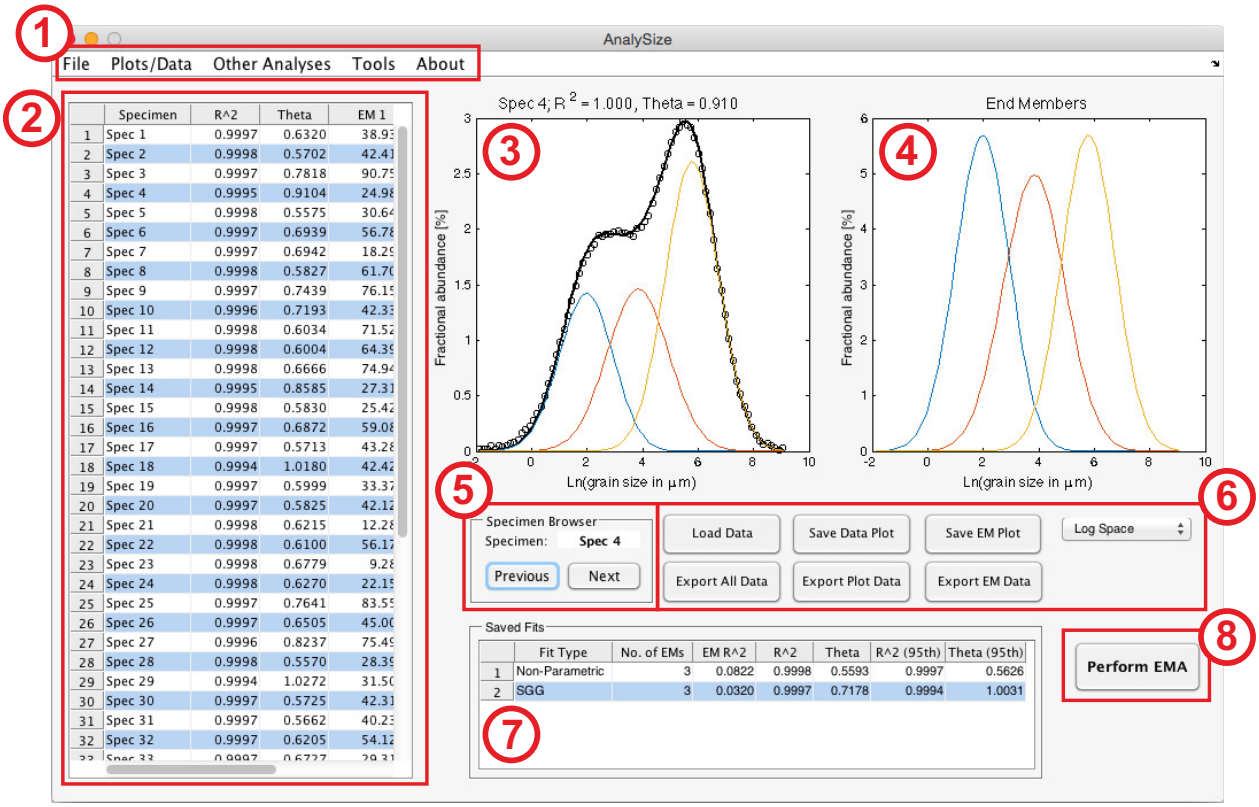


Figure 1: The main AnalySize window.

1. Menu bar

The main menu bar contains access to all the main function in AnalySize.

File:	Contains functions for loading data into AnalySize. It also includes functions for saving and loading an AnalySize session.
Plots/Data:	Contains functions for saving the main window plots and exporting data and end member fits.
Other Analyses:	Contains functions for performing other grain size analyses. This includes descriptive statistics, ternary diagrams, and CM diagrams.
Tools:	Contains functions for setting up and customizing AnalySize. This also contains function to censor grain size bins and remove specimens from the loaded data.

2. Specimen table

This table displays a list of specimen names from the loaded data. When end member fits have been made the table also includes the squared linear correlation (R^2) and angular distance in degrees

(Theta) between the measured specimen and the fitted end member reconstruction. In addition, the percentage abundance of each end member is given. By clicking on individual specimen rows the user can jump between different specimens.

3. Data plot
This plots the individual specimen data (black circle) and and end member fits that are made. The total end member fit is shown by the solid black line and the color order of the end members can be accessed from the "Tools" menu.

4. End member plot
This plots the unscaled end members of the currently selected fit (i.e., each end member sums to 100%). The color order of the end members can be accessed from the "Tools" menu.

5. Specimen browser
Controls to browse through specimens one-by-one.

6. Main control buttons
These buttons provide quick access to the main functions for loading and exporting data used to generate the plots as well as exporting the end member data. The pulldown menu allows the scale of the plots to be adjusted and can be set to a log space scale, log linear scale, or ϕ scale.

7. Saved fits
The saved fit table presents basic information about the end member fittings that have been performed on the currently selected data set. By selecting different rows of this table user can navigate between different fits that have been previous made.

Fit Type:	The type of analysis performed. Either "Non-parametric" EMA or parametric EMA (given as the distribution type).
No. of EMS:	The number of end members fitted.
EM R^2:	The maximum of the squared linear correlation between all fitted end members. This is a measure of the linear independence of the end members. If this value is too high then the data are likely over fitted and the number of end members should be reduced.
R^2:	The squared linear correlation between the measured data set and the data set constructed from the fitted end members.
Theta:	Angular distance (in degrees) between the measured data set and the data set constructed from the fitted end members.
R^2 (95^{th}):	The lower 95^{th} percentile of the squared linear correlation between an individual specimen and it's reconstruction using the fitted end members.
Theta (95^{th}):	The upper 95^{th} percentile of the angular distance (in degrees) between an individual specimen and it's reconstruction using the fitted end members.

8. Main analyses
The main button to call the End Member Analysis (EMA) routines.

4.3 Loading data

AnalySize supports a wide range of data formats, which includes both original laser particle size analyzer data files and post-processed text files and Excel spreadsheets. Data can be loaded by clicking the "Load Data" button on the main window, or by selecting "Load Data" from the "File" pulldown menu. Both of these will open up a file browser window, similar to that shown below (Figure 2), which allows the user to select their data files. Multiple files can be selected.

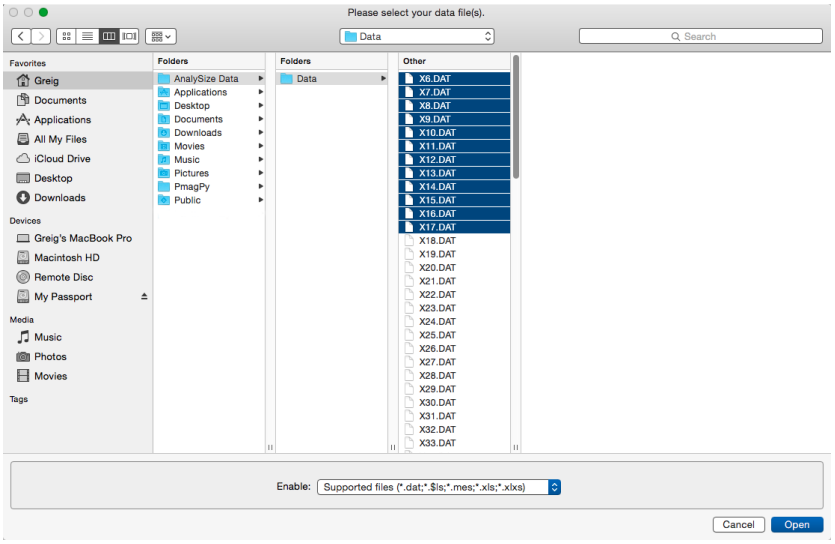


Figure 2: File browser window for loading data.

Useful Note...
OS X users should note that Beckman Coulter particle size analyzer files have the extension "*.$ls". This is not recognized by OS X as a valid extension and should be loaded by selecting the "All Files (*.*)" option from the file browser window.

Once the user has selected the file(s) to load one of two windows will open. For Excel files (*.xls, or *.xlsx) the window in Figure 3 will open. AnalySize supports different spreadsheet layouts, which can specified from this window. Specimen data can be given as either rows or columns of the spreadsheets and key columns/rows can be specified to identify the data. This allows AnalySize to process spreadsheets that may contain additional meta-data not directly required for analysis (e.g., depths or ages). An example Excel file with both layout (using the default row/column values) is provided in the "*Example_Data*" directory of AnalySize.

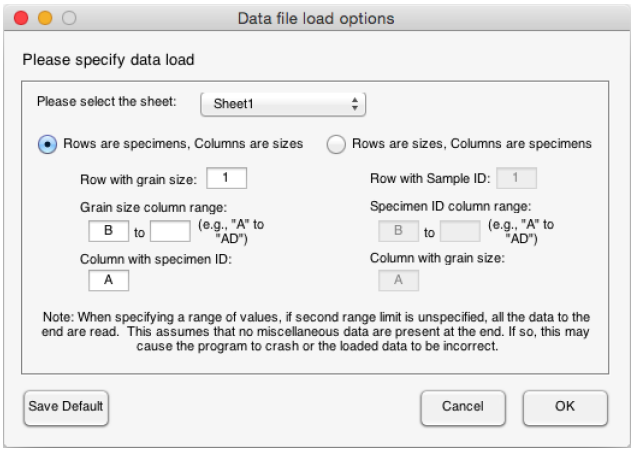


Figure 3: Load options window for Excel files.

For all other data files, AnalySize assumes that they are text files that are either delimited or direct outputs from particle size analyzer software. In this case the window in Figure 4 will open, which allows users to select the type of file they wish to load.

Beckman Coulter	Beckman Coulter *.$ls data file.
SALD-3001	SALD-3001 data files.
MicroTrac CSV	MicroTrac comma separated variable data file.
Cilas	Cilas 940 data file.
Delimited text file	Delimited text file with columns of grain size bins and data and with a single header line. The delimiter can be selected from the pulldown menu (tab, comma, or space). AnalySize assumes that the first column contains the grain size bins and that proceeding columns are specimen frequency data. Grain size values should be given in microns. Data files can contain single specimen data or multiple specimens per file ("Multiple specimens" should be checked). For single specimens, the data file name without the extension is taken to be the specimen name. For multiple specimens, AnalySize assumes that the column headers are the specimen names. An example file is provided in the "*Example_Data*" directory of AnalySize.

Useful Note...
For all currently supported file type, grain size values should be given in microns. The grain size bins don't need to be equally spaced or in ascending/descending order (AnalySize sorts the bins on read in the data). When the frequency values are read in, they are renormalized to sum-to-one, so units are arbitrary.

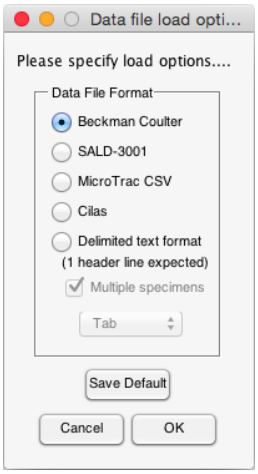


Figure 4: Load options window for data files.

Useful Note...
If a data file that you commonly are in a format that is not currently supported, please contact the authors with an example of your data format and it will be added to AnalySize.

For both of these load options windows, you can click "Save Default", which will save the data file format choices to a user configuration file. When AnalySize is relaunched these default settings will be remembered

Once the data are loaded, the specimen table and data plot will become populated (numbers 2 and 3, respectively in Figure 1). The user can browse through the data by selecting the corresponding specimen row in the specimen table, or by using the specimen browser panel (number 5 in Figure 1).

Useful Note...
Generally, AnalySize unmixing algorithms work better for laser diffraction grain size data where the number of bins is much greater than ten. However, this does not preclude other data types (e.g., sieved results), but fewer grain size bins puts a limit on the power to differentiate different end members and may lead to numerical stability and interpretability issues.

4.3.1 Censoring and removing data

From within the "Tools" pulldown menu, AnalySize contains functions to censor grain size bins and to remove individual specimens from the loaded data set. Choosing the "Censor Data" option will open the window shown in Figure 5. This window allows user to specify a grain size range to exclude from the data set. This function can be used to censor certain size bins that may be invalid (e.g., due to known measurement artifacts). Censoring the data will exclude these grain sizes from all loaded specimens. If multiple grain size ranges need to be censored the process can be repeated.

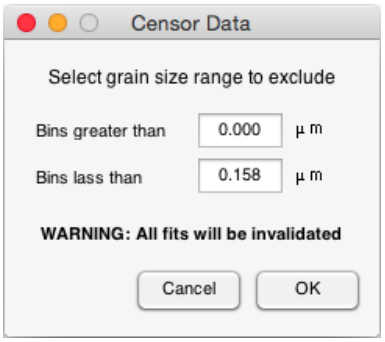


Figure 5: Censor grain size bins.

Choosing the "Remove Specimen" option will open a dialogue box confirming if the user wishes to remove the currently selected specimen. Only one specimen at a time can be removed, but the process can be repeated. When browsing through the loaded data the currently selected specimen is given in the specimen browser panel (number 5 in Figure 1).

Censoring data will invalidate all fits and all fits will be cleared from the AnalySize session. Removing a single specimen will also effect EMA fits, but since the effects are often small, after removing a specimen, no fits will be cleared from the session. Before final interpretation, however, it is recommended that any fits are re-run after specimens have been removed.

Useful Note...
Removing specimens can often be useful to reduce the effects of outlying specimens on EMA fitting. For example, when a data set contains a specimen with an end member that appears in no other specimens (e.g., a sandy layer in a sequence dominated by clay and silt variations), the resultant EMA end members will often fit poorly to this specimen. In some cases this effect can be large and will affect the fitting of the whole data set. In these cases, removing the outliers and re-running the EMA fitting can improve the overall quality of fit with minimal loss of information.

4.4 Unmixing analyses

After data have been loaded into AnalySize EMA can be performed by selecting the "Perform EMA" button highlighted in panel 8 of Figure 1.

Choosing "Perform EMA" open up the window shown in Figure 6 and allows the user to undertake the EMA analyses as outlined by *Paterson and Heslop* (2015). The user has three end member options for EMA:

Non-Parametric	The form of the end members is determined from the data set. This routine uses the HALS-NMF algorithm of *Chen and Guillaume* (2012).
Parametric	The form of the end members is based on parametric distributions (e.g., log-normal or Weibull). This routine uses a search algorithm to find the best fit distribution parameters. For each tested set of parameters the simplex projection algorithm of *Heylen et al.* (2011) to determine end member abundances.
Defined	The form of the end members is taken from a used defined input file containing the end members to unmix. This uses the fully constrained least squares algorithm of *Heinz and Chang* (2001) to determine end member abundances.

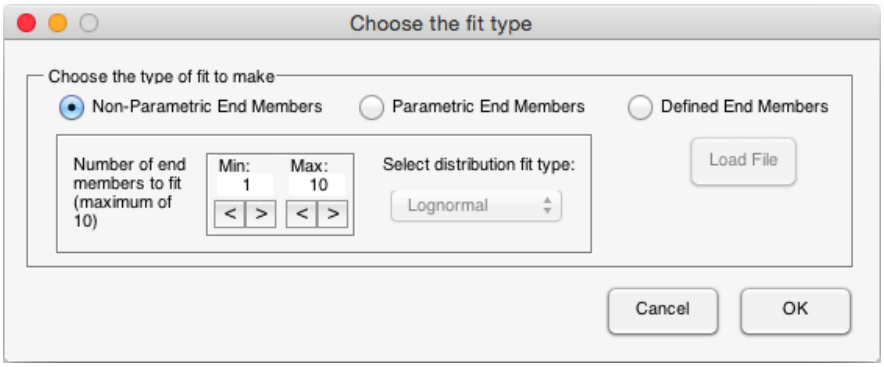


Figure 6: EMA fitting options.

For non-parametric and parametric end members, the user can set the minimum and maximum number of end members to test. The maximum number of end members support by AnalySize is 10, which more than is usually required to model a typical data set. For the parametric end members, users can choose from 4 parametric distributions given in Table 4.4.

Table 1: Parametric distributions supported in AnalySize.

Type	Parameters to fit	Comment
Lognormal	2	Parameters control the location and scale of the distribution. Lognormal distributions are fitted in linear space.
Weibull	2	Parameters control the shape and scale of the distribution. Weibull distributions are fitted in bin number space, where each size bin is number consecutively.
Gen. Weibull	3	General Weibull distribution. Includes an additional location parameter to the Weibull distribution. General Weibull distributions are fitted in bin number space, where each size bin is number consecutively.
SGG	3	Skewed Generalized Gaussian (SGG) distribution (*Egli*, 2003). The SGG is a 4 parameter distribution, but a maximum entropy approximation is used to reduce the number of free parameters to fit to 3 (*Egli*, 2004). When the parameters are saved or exported, all 4 parameter are output. Parameters control the location, scale, and skewness/kurtosis of the distribution. SGG distributions are fitted in log space.

When using defined end members, the user must first load an end member file by clicking on "Load File". This will open a file browser where the user can select the desire end member file. The end member file should be a tab delimited text file with one header line. The first column must be the grain size bins in microns. The proceeding columns can be in any order and can contain additional data not needed for the unmixing (e.g., grain size bins in different units). The end member columns must be headed with "EMx", where x is an integer number denoting the end member number.

Once the end members options have been setup, simply click on "OK" to perform the fitting. For defined end members, AnalySize will determine the unmixing proportions and return to main

window where the results will be presented. The goodness-of-fit statistics will be shown in the fit table (part 7 in Figure 1). If the R^2 value is low and theta is high, this is an indication of a poor fit. This may be because the given end members do not fit the data well, or that additional end members are needed to model the data.

For non-parametric and parametric end members, AnalySize will determine the best end members and unmixing proportions for the range of end members given by the maximum and minimum number of end members to fit (Figure 6). The number of end members that best represents the data set must then be selected. To facilitate this, the window shown in Figure 7 is displayed after all the fits have been determined.

This window presents the fitting statistics for the different number of end members tested. The left hand plot displays various squared linear correlations as a function of the number of end members. The right hand plot displays angular differences (in degrees) between the reconstructed and observed data sets as a function of the number of end members. The lower panel displays some quantitative statistics for the selected number of end members, which can be controlled from the left hand side of this panel. These two plots can be saved to an EPS format file by clicking "Save Plot". When the number of end members has been selected AnalySize will return to main window where the results will be presented.

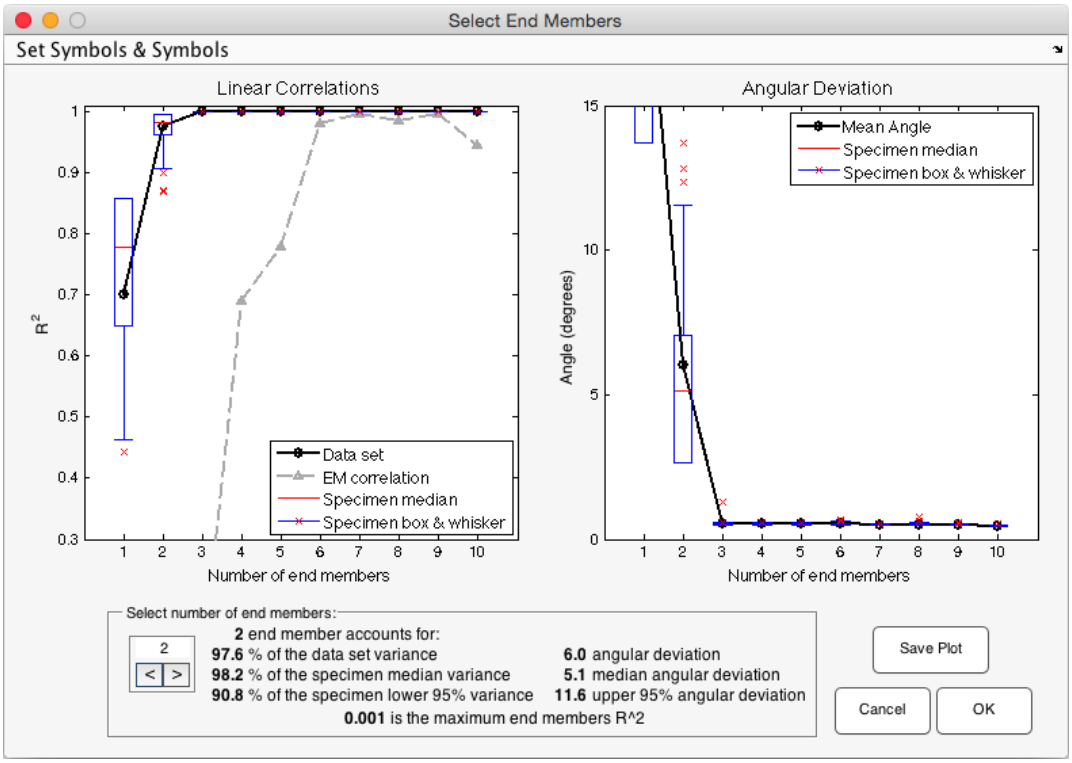


Figure 7: The end member selection window.

In both plots, the solid black lines and circles are the model misfit to the whole data set, the blue box and whiskers represent the values determined from individual specimens. The red bars are the median values, the blue boxes are the interquartile range, and the blue whiskers mark out the one-sided 95^{th} percentiles (i.e., the 95% coverage interval). For R^2 this is the lower 95^{th} percentile and for angular deviation it is the upper 95^{th} percentile - these represent a measure of the lowest

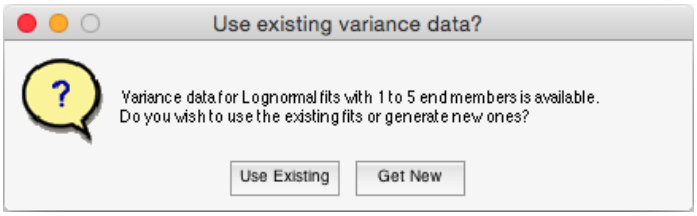
quality fits. The red crosses represent outlying specimens (i.e., specimens that lie outside of the 95% coverage interval). The grey dashed line and triangles on the left had plot is the maximum squared linear correlation between the different fitted end members. This is a measure of the linear independence of the end members.

Useful Note...
A low linear correlation between end members is desirable, but there are physically reasonable situations where some correlation will occur (i.e., cases where end members contain a common source component). High end members correlations (i.e., $R^2 \gtrsim 0.7 - 0.8$), however, are a strong indication of overfitting where one end member is a near duplicate of another. As will all goodness-of-fit statistics, physical considerations of the data at hand are needed to make an informed decision.

Useful Note...
Increasing the number of end members to fit should decrease the number of outlying specimens. In situations where increasing the number of end members notably improves the model fit to the data, but does not notably reduce the number of outlying specimens, this is an indication that these outliers likely contain an end member that is poorly represented in the data set (i.e., an end member that is an outlier end member). Identifying and removing these specimens (using the information from the table in the main AnalySize window and the "Remove specimen" function) and re-running the EMA fitting can often improve the overall quality of fit with minimal loss of information.
In such cases, it is always advisable to seek physical justification for excluded data and not to rely soley on numerical considerations.

If parametric unmixing is performed, AnalySize remembers the previous fits that were tested to generate Figure 7. If the parametric unmixing with the same distribution is repeated, AnalySize will asked if the exiting tested fits should be reused (Figure 8a). The user can choose to use the existing ones or generate new ones. After the analysis, the user will then be asked if they wish to keep the exiting fits, overwrite the existing fits with the new ones, or to merge the two sets (Figure 8b). This allows users to perform piecewise analyses, which can be useful for large data sets where parametric fitting can be slow.

(a)



(b)

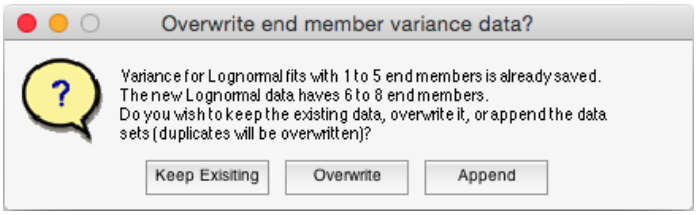


Figure 8: Prompt widows allow the user to reuse and save the parametric EMA fit data for different numbers of fitted end members.

After EMA fitting has been performed the fitted end members are plotted in the main window (panels 3 and 4 in Figure 1) and the fit statistics shown in the "Saved Fits" table (panel 7 in Figure 1). For non-parametric EMA, the end members are sorted by their median grain size. For parametric EMA, end members are sorted by their modal grain size.

When unmixing defined end members, a file with the known end members must be loaded. This is a simple tab delimited text file that must contain at least two columns with one header row. The column that contains the grain size bins must be headed "Grain size" and the bins should be in microns. The end member frequency values must be headed "EM 1", "EM 2". "EM 3", etc, and the values can have arbitrary units (AnalySize renormalized each to sum-to-one). Additional columns may be present, but these will be ignored. This format is the same as the format generated when saving unmixed end member data (see *Export EM Data* below) and an example is given in the Example Data directory.

4.5 Saving and exporting plots and data

All of the data and plots in the main AnalySize window (i.e., the measured grain size data and unmixed end members; Figure 1) can be exported through either the "Plots/Data" pulldown menu or the relevant button in the main control button panel (number 6 in Figure 1).

Save Data Plot	Save the currently selected specimen plot to a publication ready EPS file (number 3 in Figure 1).
Save EM Plot	Save the currently selected end member fit plot to a publication ready EPS file (number 4 in Figure 1).
Export Plot Data	Exports the data associated with the currently selected specimen (number 3 in Figure 1) to a tab delimited text file. This includes the measurement data, individual end members, and the total end member fit.
Export EM Data	Exports the data associated with the currently selected end member fit (number 4 in Figure 1) to tab delimited text files. This exports two files; a file containing the end member densities and a file containing the end member abundances and the goodness of fit statistics for all specimens.
Export All Data	Exports all of the measurement data into a tab delimited text file readable by AnalySize. The first column is the grain size in microns, which is followed by frequency data (sum to 100%) with each column representing a specimen.

Useful Note...
When saving the data plot AnalySize checks the version of `MATLAB` being used and adjusts the data symbols accordingly. For 2014a and earlier releases (version 8.3 and previous), AnalySize outputs circular symbols to the saved file (as shown on the GUI plot). For 2014b and later releases (version 8.4 and after), AnalySize outputs square symbols to the saved file. This is to overcome a graphical bug introduced in `MATLAB` 2014b, which distorts circular symbols to octagons when being saved to a file.

4.6 Saving and loading an AnalySize session

For large data sets, some analyses can be time consuming and users may need to stop a fitting session or wish to save their fitting session for future work. To facilitate this, AnalySize includes a "Save Session" function (accessed from the "File" pulldown menu), which saves the current fitting session to a `MATLAB` data file. Users can then load this data file at a later time (using the "Load Session" function in the "File" menu) and continue their analyses where they left off. This also allows user transfer their results and data to others user or computers and maintain the integrity of their analyses without having to repeat the time consuming steps.

4.7 Other plots and analyses

AnalySize contains other basic functions for processing and quantifying grain size data. These can be accessed from "Other Analyses" pulldown menu in the main AnalySize window.

4.7.1 Descriptive statistics

The "Descriptive Statistics" option generates tables of descriptive statistics and percentiles for the loaded data set, which can be readily exported to tab delimited text files. The available statistics include mean, standard deviation, skewness, and kurtosis determined by geometric and logarithmic methods of moments and geometric and logarithmic graphic analysis, as well as commonly used percentiles (*Krumbein and Pettijohn*, 1938; *Folk and Ward*, 1957; *Blott and Pye*, 2001).

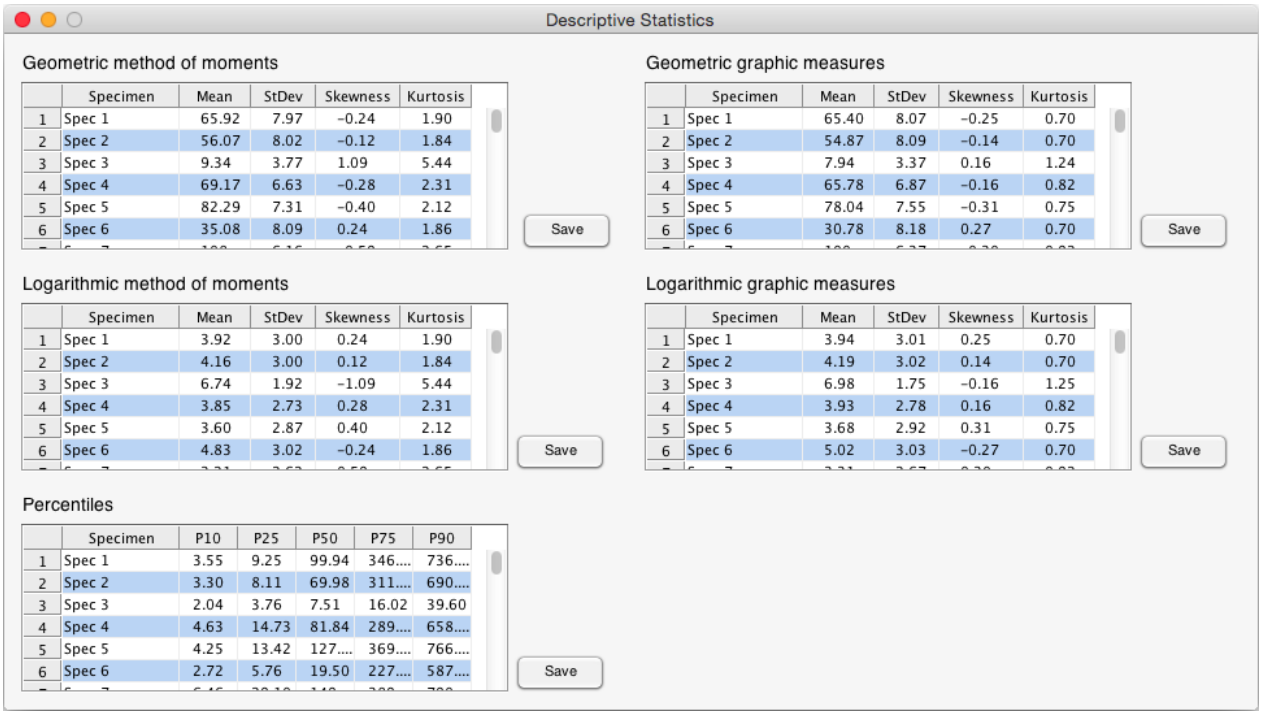


Figure 9: Descriptive statistics for the measured data.

4.7.2 End member statistics

The "End Member Stats" function generates tables of the descriptive statistics for the fitted end members, as described above. An example of the tables for EMA end members is given below in Figure 10.

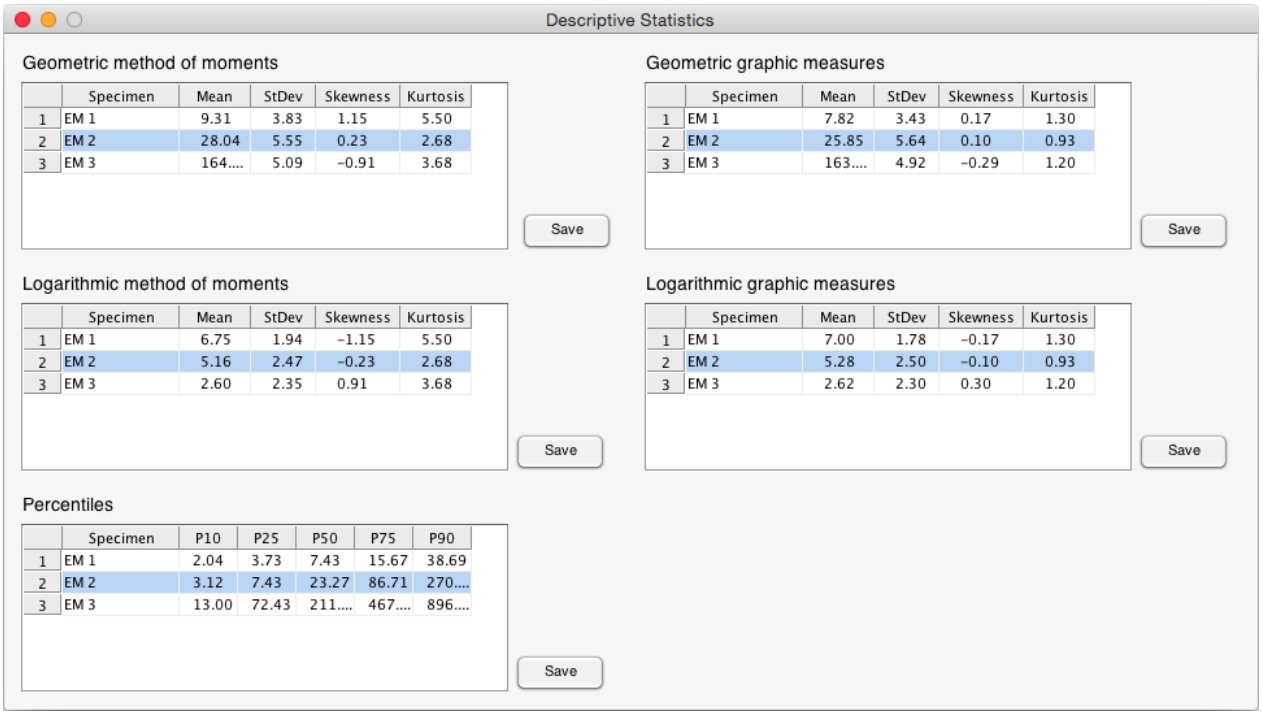


Figure 10: Descriptive statistics for EMA end members.

4.7.3 Multi-Specimen Spectra plot

The "Multi-Specimen Plot" option generates line plots for the grain size spectra for all loaded specimens. Users can select which specimens to plot using the checkboxes in the table provided and change the x-axis scale using the pulldown menu (Figure 11). The final plot can be exported to a publication ready EPS file by selecting "Save Plot".

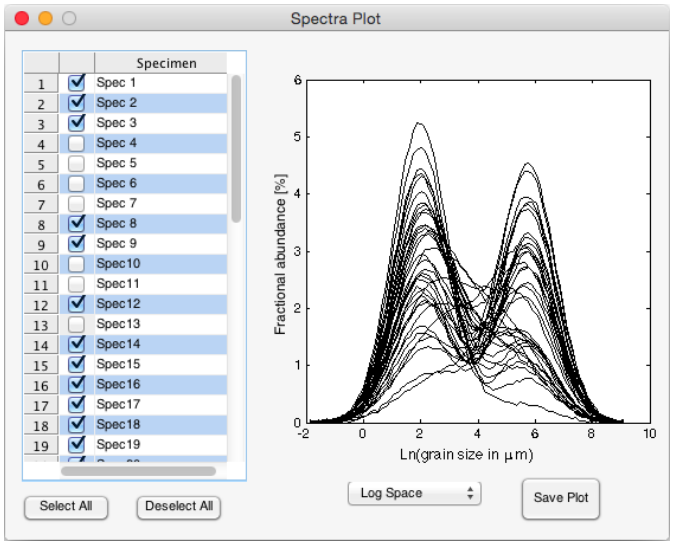


Figure 11: Multi-Specimen spectra plot.

4.7.4 Ternary plots

The "Ternary Plots" options plots the loaded data onto a range of ternary diagrams (Figure 12). AnalySize supports fine and coarse ternary plots of *Shepard* (1954), as modified by *Schlee* (1973), and *Folk* (1954). Clay, silt, sand, and gravel proportions follow the definitions of *Wentworth* (1922). On fine plots, AnalySize warns if significant gravel is present and excludes these specimens from the plot (e.g., lower left panel in Figure 12). Significant gravel is $> 0.01\%$ for Folk's classification (*Folk*, 1974) and $> 10\%$ for Shepard's (*Shepard*, 1954). All grain size proportions can be exported to a tab delimited text file by selecting "Export Data" and the diagrams can be saved to publication ready EPS files by selecting "Save Plot". Plot symbols can be customized by selecting "Set Symbols" (described further in Section 4.8).

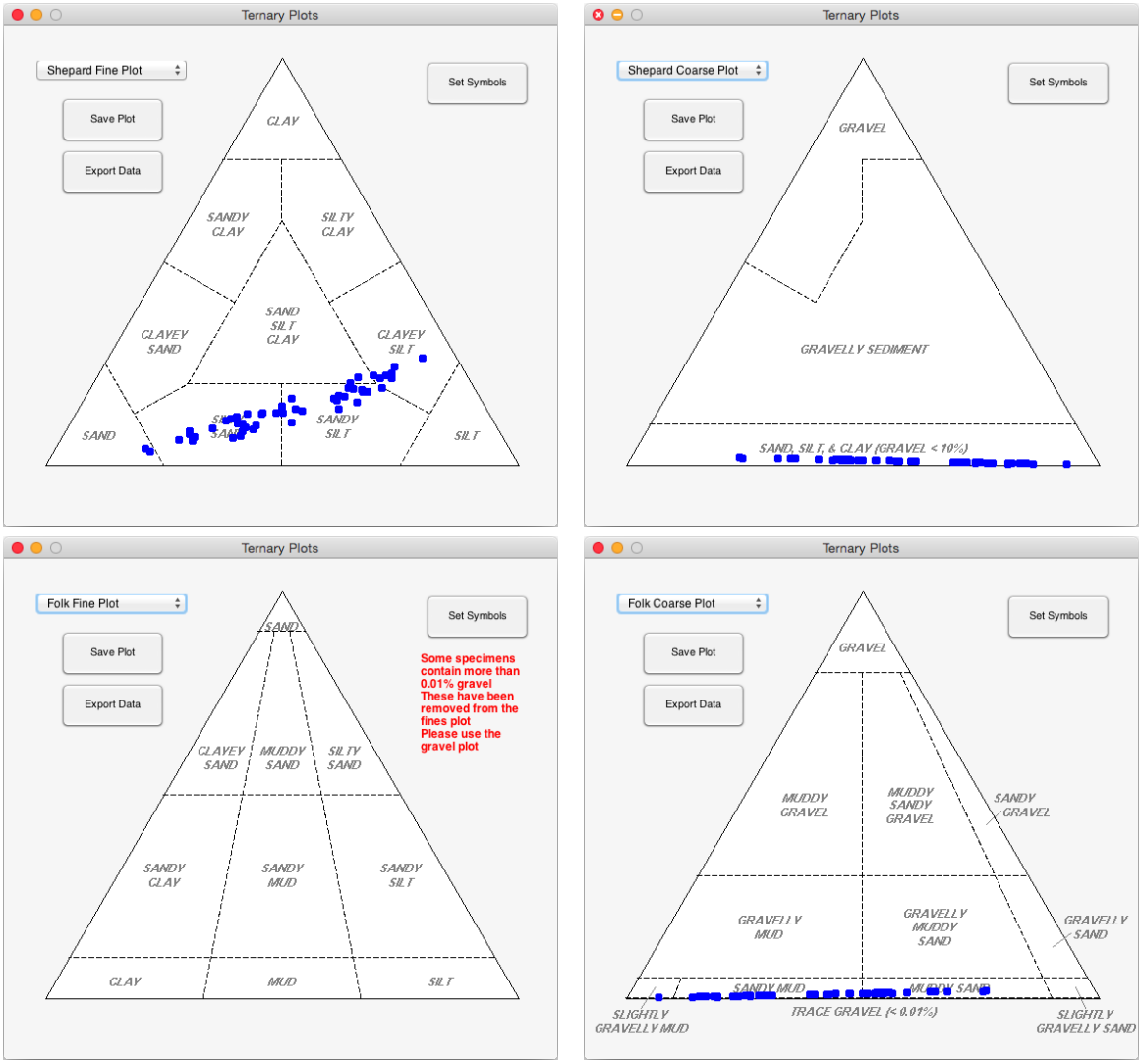


Figure 12: Ternary plots generated by AnalySize.

4.7.5 CM plot

The CM-plot of *Passega* (1964), which plots the first percentile (C) of grain size against the median grain size (M) can be accessed by selecting "CM Plot". The data for this plot can be exported to text file and the plot can be saved to a publication ready EPS file. Plot symbols can be customized by selecting "Set Symbols" (described further in Section 4.8).

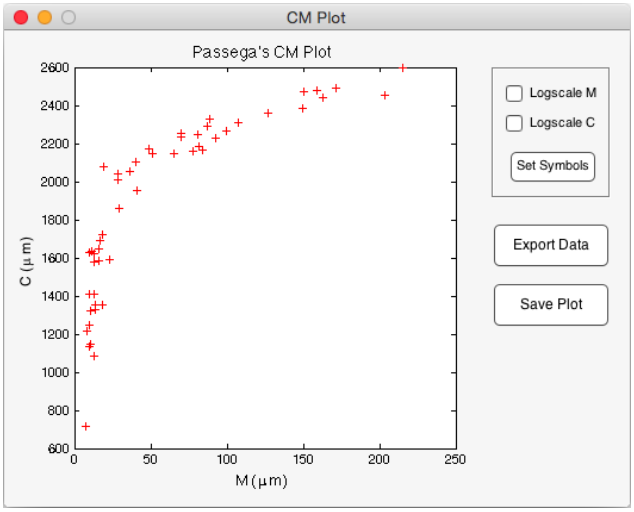


Figure 13: A CM plot from AnalySize.

4.8 Customizing plots

The "Tools" menu of the main AnalySize window (Figure 1) contains options to allow users to customize the plots generated by AnalySize. For the grain size distribution data presented in the main window (panel 3 in Figure 1), ternary plots, and CM plots the symbols are fully customizable and can be adjusted by selecting "Set Symbols" button in the relevant window (i.e., Figure 12 or Figure 13) or from the "Tools" menu in the main AnalySize window (Figure 1). The symbol style, size, and color can be adjusted. Clicking "OK" will change the symbols for the current AnalySize session only. "Save Default" will save the choice of symbol style and color for all future AnalySize sessions.

Useful Note...
The graphics updates introduced in `MATLAB` 2014b (version 8.4) changed how many plotting functions are handled. However, this has resulted in some bugs that affect the appearance of the graphics files saved from AnalySize. In particular, plot symbols saved in 2014b and later can have a distorted shapes in the final encapsulated postscript files. This is most pronounced for symbols with curved edges, such as circles, which appear as octagons. Unfortunately, this is a `MATLAB` bug, which cannot be readily solved in AnalySize.
This issue is present in the following `MATLAB` releases: 2014b (v8.4), 2015a (v8.5), 2015aSP1 (v8.5.1), 2015b (v8.6). As of release 2016a (version 9.0) this bug has reportedly been fixed.
It is recommend that users of the affected `MATLAB` versions choose straight edged markers for their plots, but the new plot customization features of AnalySize v1.1.0 and above should allow users to bypass most of these issues.

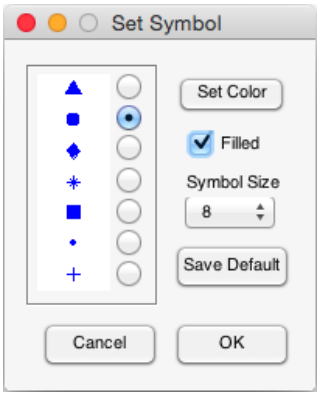


Figure 14: Data plot, Ternary, and CM plot symbol options.

"Set End Member Colors" opens up the window shown in Figure 15, which allow the colors of the different end members to be modified. Clicking on each end member button opens MATLAB's color palette tool, which provides a wide range of colors to choose from. Clicking "OK" will change the colors for the current AnalySize session, but these will revert to the standard default colors when AnalySize is closed. By selecting "Save Default", AnalySize will save the choice of color to a user default configuration file, which allows AnalySize to recall user preferences each time it is run.

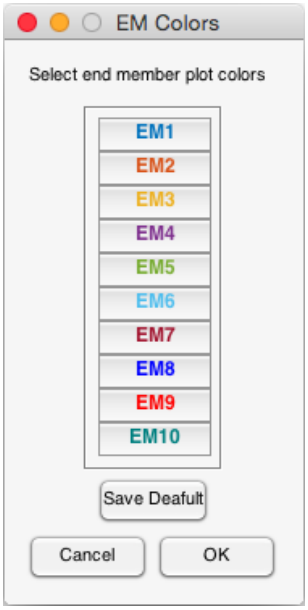


Figure 15: End member color options.

Useful Note...
By clicking on an empty space on any plot in AnalySize, the selected plot will open in a new MATLAB figure window. From here, users can use all of the inbuilt MATLAB functionality to fully customize Analysize plots. For ternary plots, users must elect the "New Figure" button to access this function.

The "Set Select End Member Plot" opens up the window shown in Figure 16 and allows user to customize the look the box-whisker plots used to select the number of end members. The functionality of this window is the same as described above for customizing colors and symbols

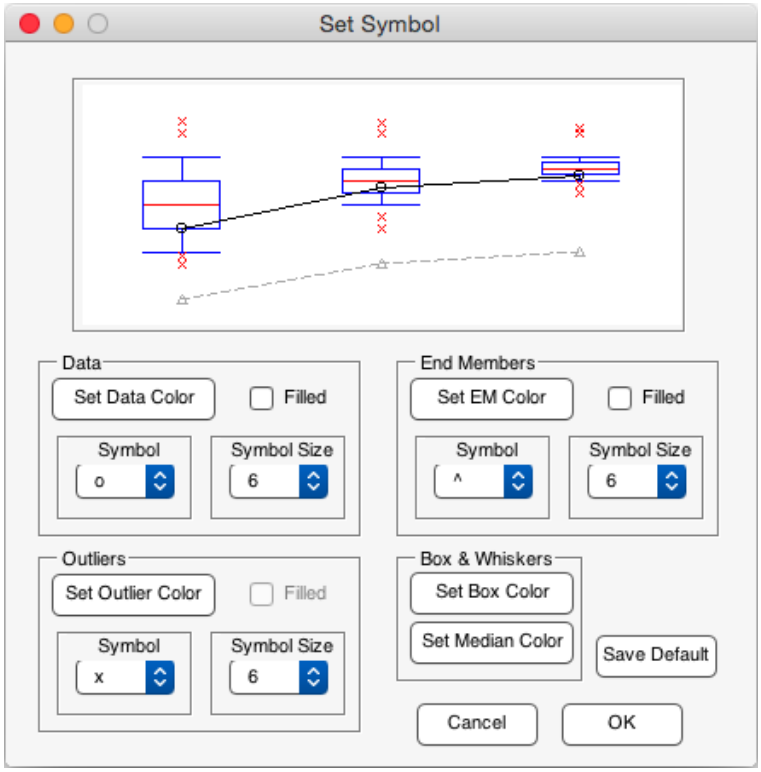


Figure 16: Options for customizing the box-whisker plots used to select the number of end members.

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