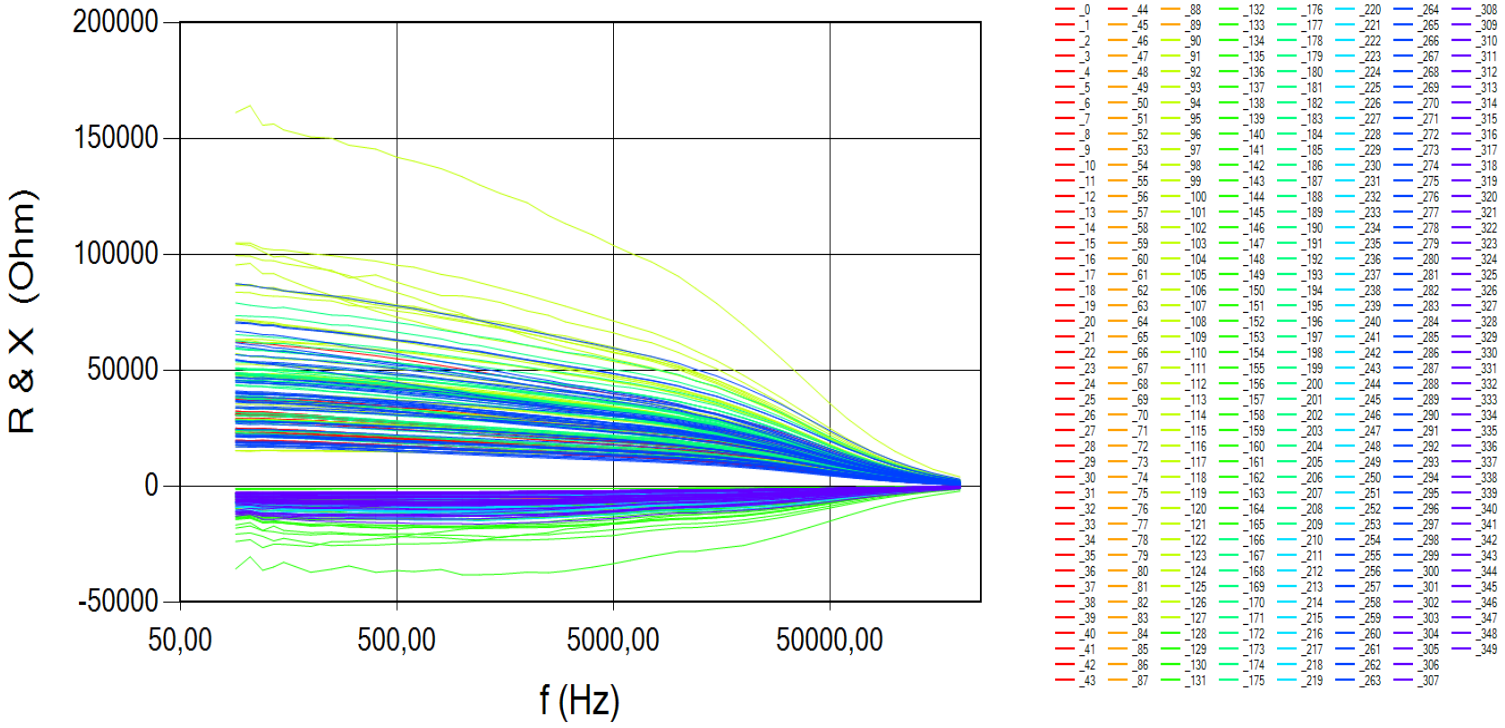
"Simitec - Revealing future of measuring"[1]

LMSSC2 -v2 for statistics of EIS data and digital classification



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Statistics

Sometimes it is useful to check the statistical properties of the EIS data before the actual classification. For this purpose, the statistical part of the EIS spectral data, such as the calculation of the mean and standard deviation of the sets and their storage in the desired file, is included in the LMSSC2 software. The statistical part is embedded in the data plotting software (see "Plot" subsection). The statistical significance of the deviation of the sets can be graphically evaluated by means of the standard deviations drawn on the averages of the sets. This activity section can be completed independently before the actual LMC and SCC classification. Added to this manual is the mathematics of how statistical calculations can be used to estimate how many measurements need to be performed to achieve a desired level of confidence. Mathematics with examples can be found in Appendix 2 of the user manual.

LMC and SSC software

The **LMC** software examines the suitability of a given test data set (test set) for a predetermined training set (training set) by a method based on a linear mapping filter, hence the term **L**inear **M**apping **C**lassification[2] used herein.

The **SSC** software examines the suitability of a given test data set (test set) for a predetermined training set (training set) using a method based on the classification of spectral distances associated with subspaces, hence the term (**S**ub**S**pace **C**lassification[3]) used herein.

For classification purposes, both the training and test set may also include subsets of these sets. For example, the electrical impedance (training) spectral set (EIS) in the cover image contains 350 spectra sorted into eight different subgroups. The first subgroup marked in red has 45 spectra (numbers 0 to 44) and the next adjacent orange grouped subgroup also has 45 spectra (numbers 45 to 89). Of these, the first subset (45) comprises the real or resistance parts of the impedance spectra (> 0) and the latter subset also has 45 spectra comprising the imaginary or reactance parts of the impedance spectra (<0). The following spectral numbers are 38/38, 44/44 and 48/48, respectively. Of course, it is clear that the spectral lengths must be the same for the calculation - and there must be no intervening numerical values. To draw the images, a variable must be entered into the program, the vector length of which must be the same as the length of the spectra. The software does not impose requirements on the compression order of the spectra, as long as the user knows against, which a subset he interprets the measurement result. The LMC and SSC software are able to read common data formats (such as txt, ascii, and csv) and determine the number of spectra of subsets internally in the program, so they do not need to be entered into the program separately.

Program settings:

"Data handling"

Figure 1 shows the classification software settings, which are divided into two pages (“Data handling” and “Plot”). On the “Data handling” page, the spectrum variable is first loaded by clicking on the “Variable” button, and the program will ask for the path where the variable name can be found.

[2] Known also as Unified Pseudoinverse Algorithm; UPA (Reflectance spectra (RS) analysis; Appl. Opt., **33**(12), 2356-2362, 1994; also found to work in EIS data analysis).
[3] Known also as Class-Featuring Information Compression; CLAFIC (RS & EIS data analysis: Appl. Opt., **33**(12), 2356-2362, 1994 & Biosyst. Eng., **121**, 139-149, 2014).

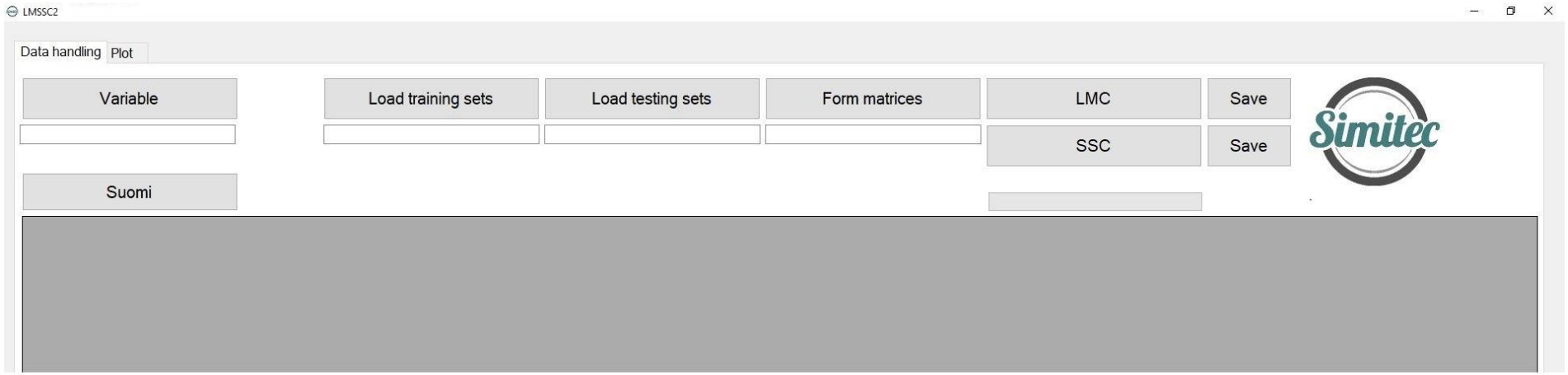


Fig. 1.

Similarly, the training/teaching and test sets are loaded by clicking the “Load training sets” and “Load testing sets” buttons, and thereafter they translated into real numbers for calculation. This is done with the “Form matrices” button. Once the conversion of the data to real numbers has been completed, either LMC or SSC calculation can be started. The green (progress) bar provides information on the progress of the calculation.
The result of the calculation appears in a blue-grey work window in tabular format, which can be saved in number format in a file if desired. If desired, the data to be classified can be viewed graphically using a drawing program by clicking the tabular page selection. The language selection (Suomi/ English) is made by clicking on the relevant selection change button.
Next the following functions will open from the buttons “Variable”, “Load training sets”, “Load testing sets”, “Form matrices”, “LMC”, “Save”, “SSC”, “Save”:

"Variable"

If the variable vector and the training set matrices are stored in the same folder, then the file view is as shown in Figure 2. When the “Variable” button is pressed, the vector f to be loaded into the variable is now displayed below the training set matrices. First paint f and press the “Open” function, whereupon the contents of f will be displayed on the desktop while logging into the calculator.

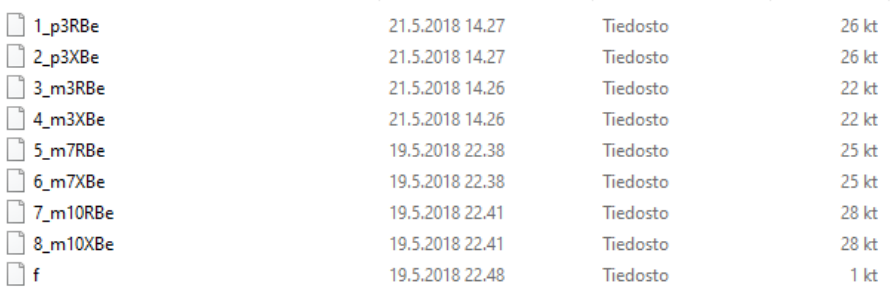


Fig. 2.

“Download Tutorials”

The next time you press the “Load training sets” button, the same view will appear as in the previous “Variable” case. The sub-matrices of the training set are painted and the “Open” button is pressed, whereby the matrices are loaded into the software. The order of the download can be viewed in the navigation window below the “Load training sets” button (Figure 3a), where the names of the subset matrices of the training set are displayed. It is also possible to view the numerical values of each subset array by clicking on the subset name in that window.

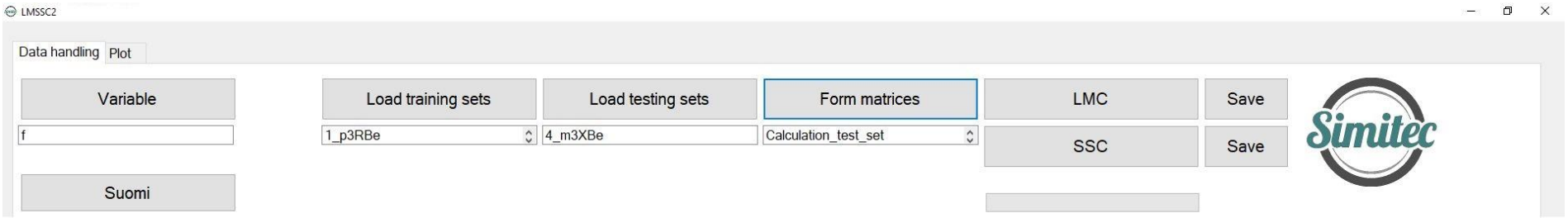


Fig. 3a.

“Download test sets”

If the test set matrices are in the same folder as the training set matrices, then paint the test set matrix/matrices and select multiple files to be imported with the “Open” button to load the matrices into the software. The load order can be viewed from the browse window below the “Load testing sets” button (Figure 3a), where the names of the test set subset matrices are displayed. It is also possible to view the numerical values of each subset matrix by clicking on the subset name in that window.

“Assemble data matrices”

Because the data is loaded as a string, the strings must be translated into real numbers for calculation. This is done with the “Form matrices” button (Figure 3a). Once the data has been converted to real numbers, you can view the conversion results from the browse window under the “Form matrices” button. If the conversion of the data from strings to double-precision real numbers has not been performed, a notification according to Figure 3b will appear in the work field. In this situation, click the “OK” button and then “Form matrices” to eliminate the problem. The aggregated data matrices can be viewed from the browse window under the “Form matrices” button, where the following items “Calculation_test_set” and “Calculation_data_set” are stored in it. If no problems are detected, then either LMC or SSC calculation can be switched. Once the LMC and/or SSC calculations are performed, both “result_LMC” and /or “result_SSC” are logged in the browse window.

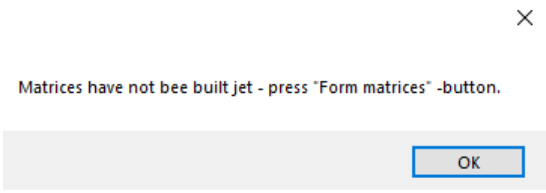
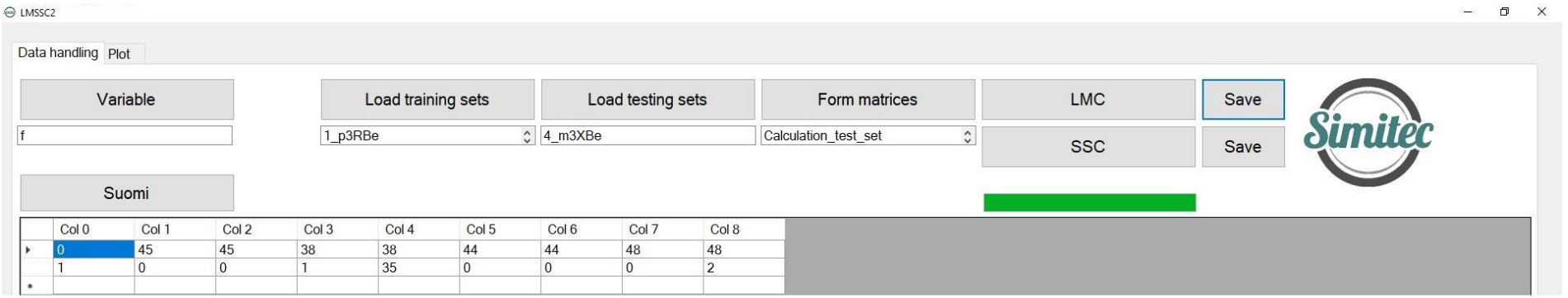


Fig. 3b.

“LMC” and “Save”

The LMC classification is based on the use of a linear mapping filter programmed in a calculation algorithm. The LMC outputs the calculation result matrix printed as form in the result window, where in this example, row 0 contains the numbers of the spectra of the subset matrices of the training set ([45 45 38 38

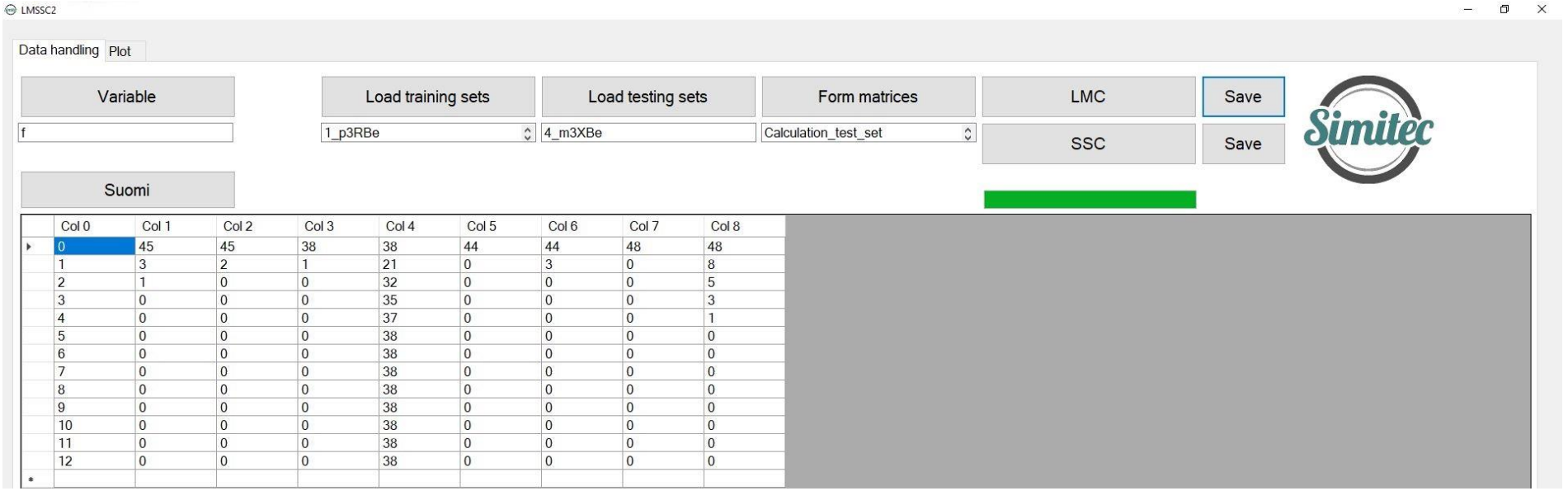
44 44 48 48]), columns 1 to 8, and row 1, the corresponding LMC classification results ([0 0 1 35 0 0 0 2]), as can be seen in Figure 4. It is also possible to save the results to a file with the “Save” button, in which case the corresponding numeric data is saved in the file. The LMC and SSC classification results (as shown in Figures 4 and 5) have been calculated from the distributions in Appendix 1.



	Col 0	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8
▸	0	45	45	38	38	44	44	48	48
	1	0	0	1	35	0	0	0	2
*									

Fig. 4.

“SSC” and “Save”



	Col 0	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8
▸	0	45	45	38	38	44	44	48	48
	1	3	2	1	21	0	3	0	8
	2	1	0	0	32	0	0	0	5
	3	0	0	0	35	0	0	0	3
	4	0	0	0	37	0	0	0	1
	5	0	0	0	38	0	0	0	0
	6	0	0	0	38	0	0	0	0
	7	0	0	0	38	0	0	0	0
	8	0	0	0	38	0	0	0	0
	9	0	0	0	38	0	0	0	0
	10	0	0	0	38	0	0	0	0
	11	0	0	0	38	0	0	0	0
	12	0	0	0	38	0	0	0	0
*									

Fig. 5.

The SSC classification is based on the classification of the distances corresponding to the different subspaces of the spectra programmed into the calculation
The SSC classification is based on the classification of the distances corresponding to the different subspaces of the spectra programmed into the calculation
algorithm. The SSC outputs the calculation result as a table in the output window, where in this example, row 0 contains the numbers of the spectra of the subset matrices of the training set ([45 45 38 38 44 44 48 48]) in columns 1 to 8 and starting from row 1 the SSC classification results corresponding to the number of subspaces used in the calculation (Figure 5).
It is also possible to save the results to a file with the “Save” button, in which case the corresponding numeric data is saved in the file.

”Plot”

The side view before starting the "Plot" function is shown in Figure 6.

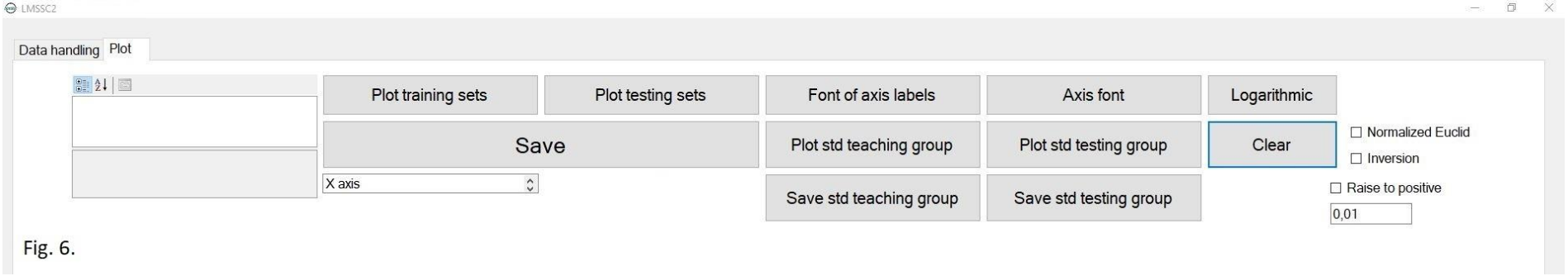


Fig. 6.

This “Plot” function can be divided into two parts as ***(A)*** *Normal spectral plotting and* ***(B)*** *Calculation of mean and standard deviation spectra with plotting.*

(A) *Normal spectral plotting*: Before starting to plot the raw or Euclidean normalized data, the data to be plotted must be loaded into the software through the "Data handling" function. You must also include a common variable as a function of which the spectra have been measured - otherwise, printing is done based on the channel number of spectrum. After this, you can alternatively draw either a training set or a testing set. Figure 7a shows a typical

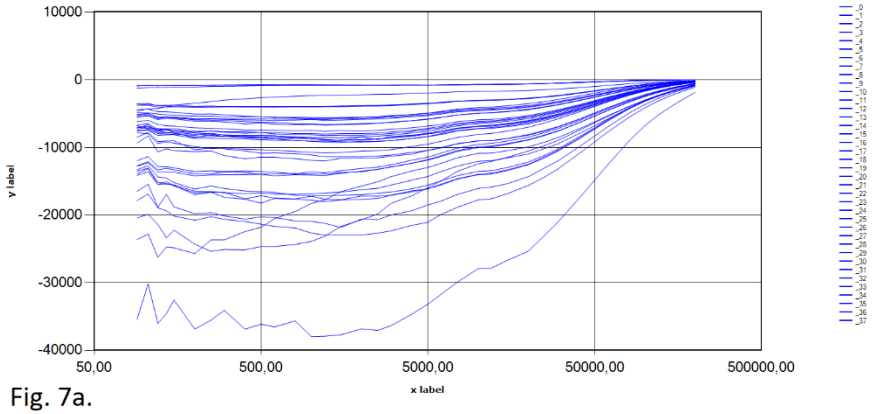


Fig. 7a.

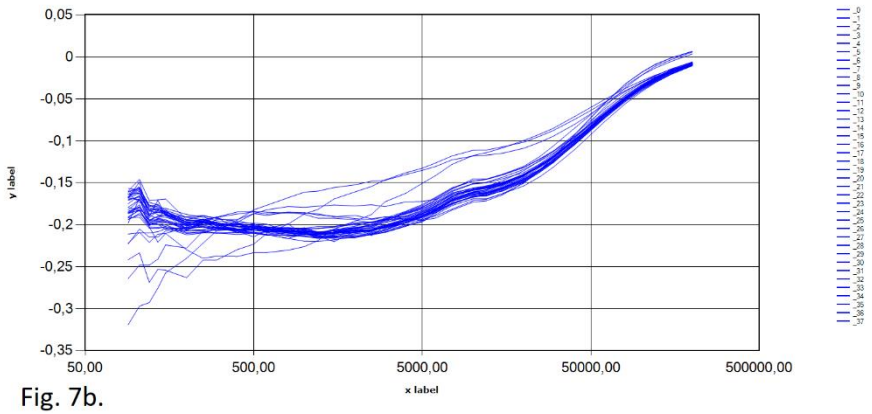


Fig. 7b.

starting graph from the test set of raw data (4_m3XBe) and Figure 7b shows the corresponding Euclidean normalization result, when the "Normalized Euclid" button is activated. This example is taken because the test set is one group and therefore the graphs are in one color (blue here). The assumed *x*-scale at the beginning of the drawing is linear.

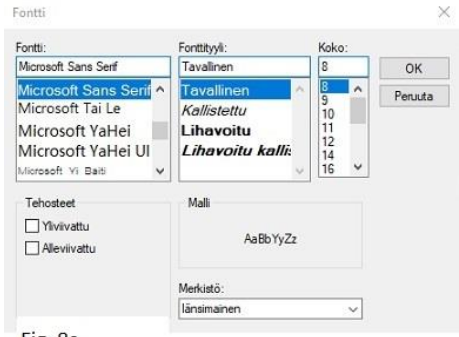


Fig. 8a.

If the spectra are measured on a logarithmic scale, it also makes the most sense to plot on the corresponding scale. Once the graphs for the selected set have been printed using either the “Plot training set” or “Plot testing set” buttons, you can set the linear or logarithmic scale of the *x*-axis to the image with the toggle button on the right. The default value is a linear scale, in which case the toggle switch has the text “Logarithmic”. An example here is again the 4_m3XBe test set (cf. Figure 2), whose spectra are considered in image format. Next, click on the “Axis font” button and select the font, font style and size for the axis numbers from the menu that opens in the working window (Figure 8a). The same is also repeated by clicking on the “Font of axis labels” button and selecting the font, font style and size for the axis names from the menu in Figure 6 that opens in the entire working window. Axis names can be pasted into a graph from the three-step scrolling menu below the “Save” button, which has the interfaces “X axis”, “Y axis” and “Axis”. Clicking on the “X Axis” interface opens a scrolling menu to the left, where you can find, among other things, the title of the axis to be named, as shown in the upper left corner of Figure 8a[4]. This bold **x label** text can be written successfully. The *y*-axis can be named in the same way. The position of the image can be aligned to the page via the “Axis” interface from the scroll menu using “Position” coordinates. Finally, by clicking the “Save” button, the image will be saved in the (pre-created) folder at the end of the path to be entered as a bmp image. The Figures 8b and 8c show the plot of the raw data of the 4_m3XBe example and the Euclidean normalized data for the logarithmic *x*-scale, respectively. For printing images, the font sizes of the *x*- and *y*-axes are also set via the "Axis font" and "Font of axis labels"

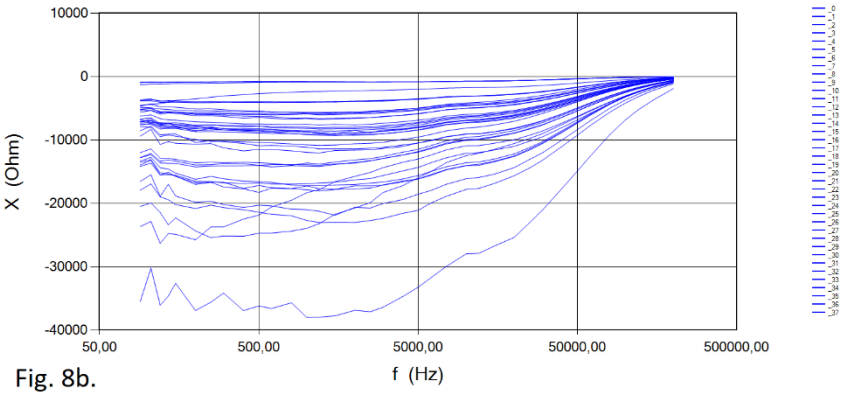


Fig. 8b.

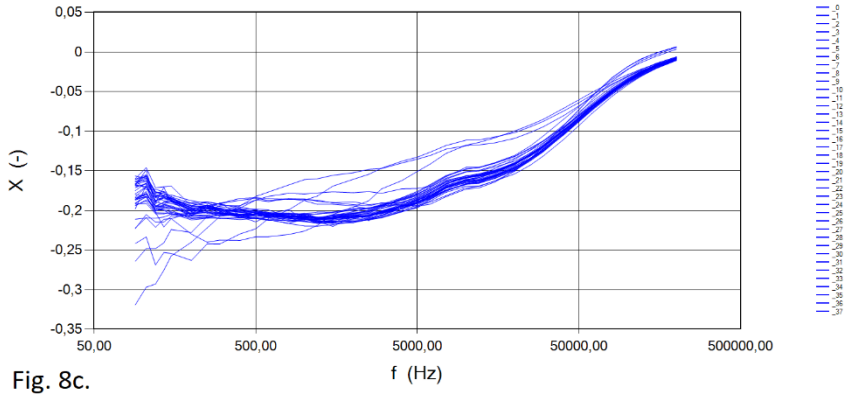


Fig. 8c.

[4] Here it is worth noting that the scrolling text of the windows can be affected by the language of the operating system you have chosen.

selection buttons. The names of the axes are written in the scrolling windows below the "Save" selection button (Figure 9). The pictures are saved with the "Save" command to a file in bmp format.

Fig. 9.

(B) *Calculation of mean and standard deviation spectra with plotting*

The calculation of means and standard deviation of raw data starts automatically when "Plot std teaching group" or "Plot std testing group" is activated, and for Euclidean normalized data, in addition to the previous ones, the "Normalized Euclid" button must be activated. The calculation prints envelope curves around the mean according to the standard deviation. The measurement points are also shown on the average curve. The picture can be saved also to a file in bmp format with the commands "Save" as shown in Figure 10a for raw data and in Figure 10b for Euclidian normalized data.

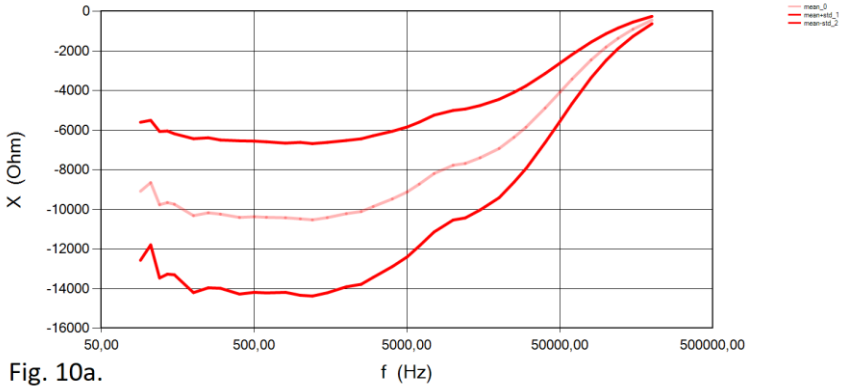


Fig. 10a.

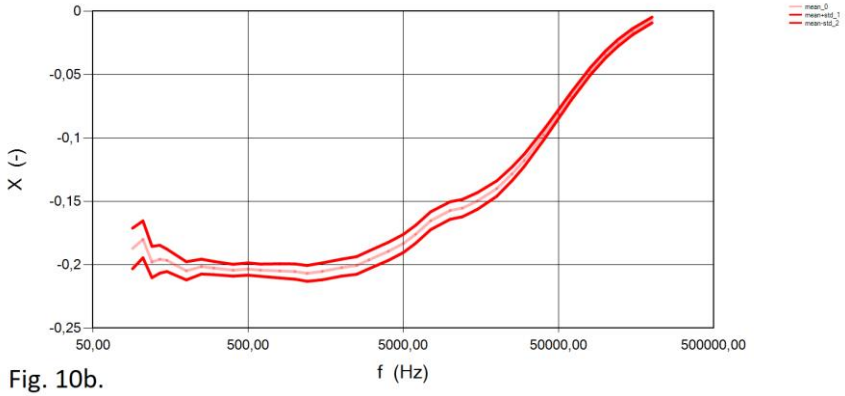


Fig. 10b.

The mean and standard deviation (mean + deviation and mean - deviation) can be saved by clicking “Save std of training group” or alternatively “Save std of testing group” button to the desired file from which this three-column matrix can be downloaded for further review[5]. If the mean and standard deviation calculation is extended to several classes at the same time, these three-column matrices are saved in parallel in the same file.

For graphical review, if the data to be printed is negative (capacitive reactance), it is possible to print the data on a logarithmic (vertical) *y*-axis by changing its polarity by activating the "Inversion" function. If the data has both negative and positive components, the data plotting threshold can be raised or lowered by a suitable factor as needed using the "Raise to positive" function. For security reasons, the "Inversion" and "Raise to positive" functions do not work in connection with the "Plot std teaching group" or "Plot std testing group" functions.

Figure 11 shows the effects of heat treatment on the averages and corresponding standard deviations of the reactance of the sample set (red +3°C, n=18; yellow -3°C, n=25; cyan -7°C, n=24 and blue -10°C, n=24). From the graphs in the picture, it can be concluded that heat treatments +3C and -3C have no significant effect on each other. The same conclusion can also be drawn from the mutual effect of heat treatments -7°C and -10°C, because the standard

[5] As when making, for example, a comparison between classes, as can be seen in Figures 11 and 12.

deviations drawn on the average spectra intersect each other. On the other hand, the effects of thermal treatments (+3°C & -3°C) and (-7°C & -10°C) on the spectrum reactances can be considered significant because the standard deviations drawn on the average spectra of these categories do not really intersect. In the case of the normalized spectra, a similar trend can be seen, albeit in a certain frequency range, as crossed distributions for resistance (figure 12 a) and reactance (figure12 b). In Figure 12b, the spectra have been inverted and increased by a factor of 0.01, so that the phenomenon could be These functions such as "Inversion" and "Rise to positive" and coincidentally the value of the coefficient 0.01 in the picture, can be seen in Figure 6.

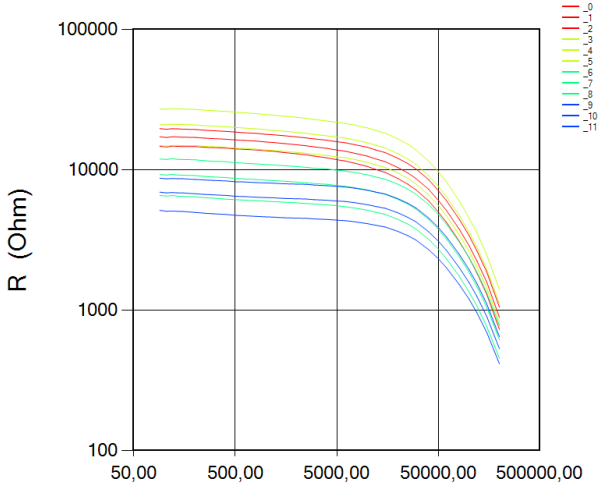


Fig. 11a.

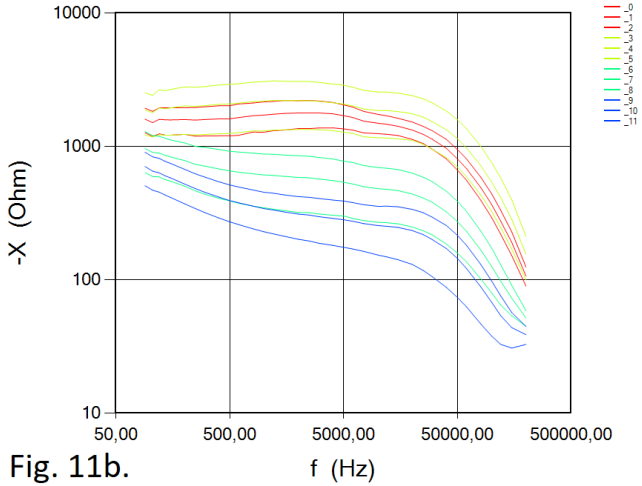


Fig. 11b.

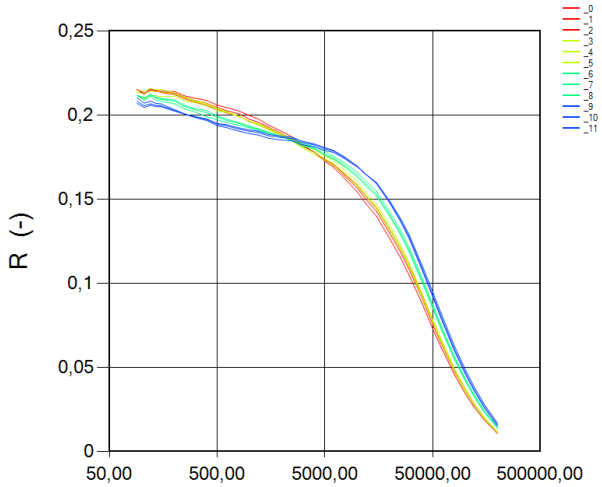


Fig. 12a.

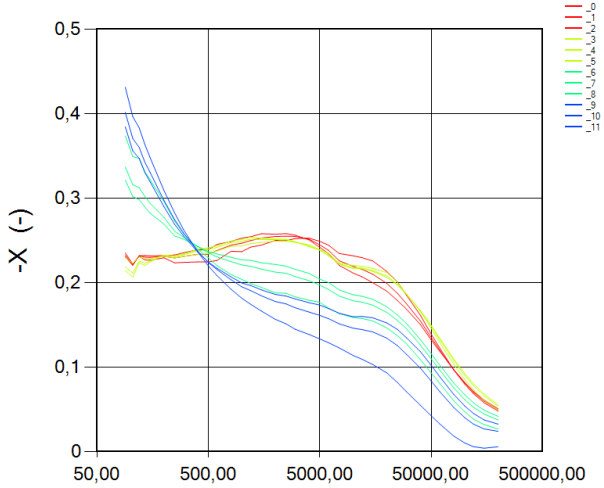


Fig. 12b.

Appendix 1.

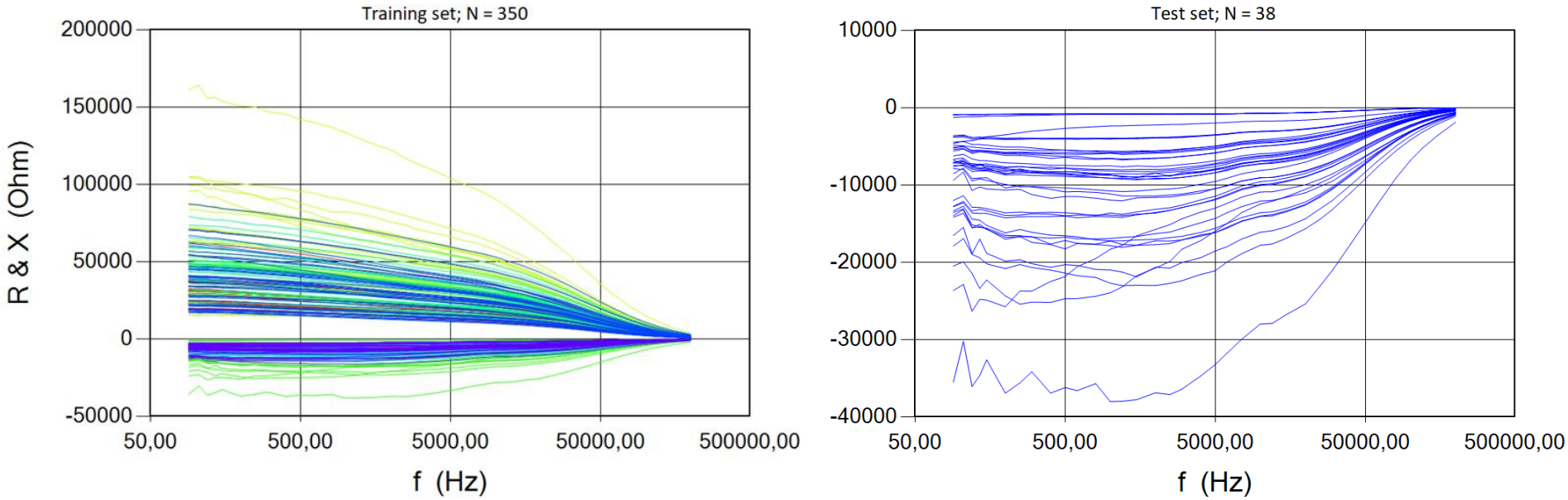


Fig. A1. The LMC and SSC classification results (in Figures 4 and 5) have been calculated from these distributions.

RECOMMENDED CUSTOMER GROUP

- Industry and companies
- Universities and Research Institutes

PRICE

1) LMSSC2 – v2 software incorporates two classification algorithms (LMC and SSC) and a print part suitable for preliminary data review. The LMC (Linear Mapping Classification) software examines the suitability of a given test data set (test set) for a predetermined training set (training set) by a method based on a linear mapping filter, whereas the SSC software uses a method based on the classification of spectral distances associated with subspaces. The LMS, SSC, and print partition work on the laptop.
2) LMSSC2 – v2 installation media and operating license. The LMSSC2 – v2 software is stored on a USB memory stick for delivery to the customer, and after installation on the computer, the stick acts as a license key. Therefore, it must be connected to the USB port while using the program.
3) Laptop (option)

   Key features (minimum requirements)

   - anti-glare 15.6 "HD Full HD or better
   - 5th Generation Intel Core i7 processor or equivalent
   - integrated Intel UHD Graphics or better
   - 8GB DDR4 memory or more
   - 256GB hard disk or larger
   - WLAN and Bluetooth 4.0
   - min. 2pcs USB 3.0 and 1pc USB 2.0 connectors
   - Gigabit Ethernet (RJ-45) network interface
   - operating system Windows 64bit (e.g. Win11)

IN TOTAL: 4 375 € (VAT 0%)[6]; EXW Joensuu

Delivery Terms & Conditions

Equipment FCA JOENSUU (Incoterms 2020). Other terms and conditions according to TK Services 2010. The ownership of the supplied equipment will be transferred to the subscriber when the entire trade amount has been paid to the supplier. Equipment and work not mentioned in this offer and its annexes and other components are treated as additional work.
Delivery terms in the following order: 1. LMSSC2-v2 offer, 2. TK Services 2010.

[6] Changes in prices are reserved. Customers who already have the previous LMSSC2 software can get an update to their old version for 1 250 € (VAT 0%).

Transfer of risk

The risk is transferred to the Subscriber when the goods are handed over to the subscriber or transported by an independent carrier in accordance with the contract, subject to the delivery clause.

If the item is not handed over at the right time and this is due to the fact that the Subscriber or the Subscriber is involved, the Liability shall be transferred to the Subscriber when the Supplier has done what he or she is required by the contract to enable the transfer.

Delivery time

Delivery time is agreed separately. The Agreement enters into force when the Subscriber's written order confirmation (including e-mail is accepted) has been received and confirmed from the Supplier's side to the Subscriber.

Payment terms

The terms of the offer are as follows. Late interest rate 10.5%.

The total price of the product when ordering, 14 days net

Additional work and any other supplies and equipment not included in the delivery will be billed after delivery, 14 days net.

Warranty and maintenance

The warranty for the devices to be delivered is 12 months from the time the equipment is ready for EXW. The warranty does not include travel and accommodation costs. This offer includes LMSSC2 for email and phone support for the warranty period without any charge. If the Subscriber makes his own changes to the LMSSC2 system, the warranty will expire. The repair of the program is done by Simitec Ltd and the costs are invoiced according to the company's service price list and they are charged 100% afterwards, 14 days net.

After the warranty period, the training, support and installation services and repair work will be billed according to the current Simitec Ltd service price list and will be charged afterwards at 100%, 14 days net.

For example, the cost of repairing a bug or installing an update will be charged on the basis of work hours and parts used for repair after work.

Fee for additional work

Additional and modifications must be agreed in advance and are based on a service price list. Other costs will be charged to actual amounts based on the Supplier's selling prices and terms and conditions set out in the Job Charging Pricing Schedule.