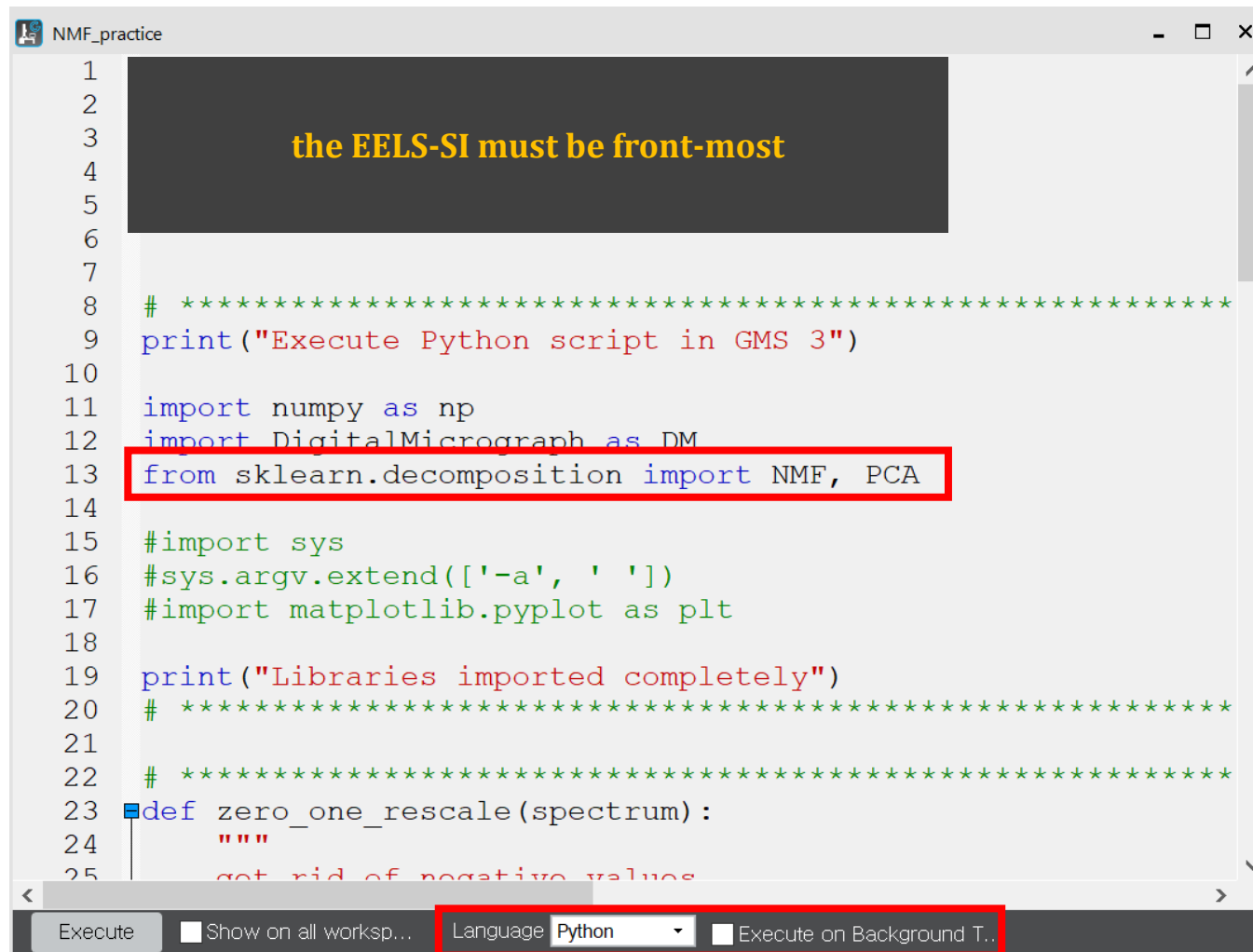


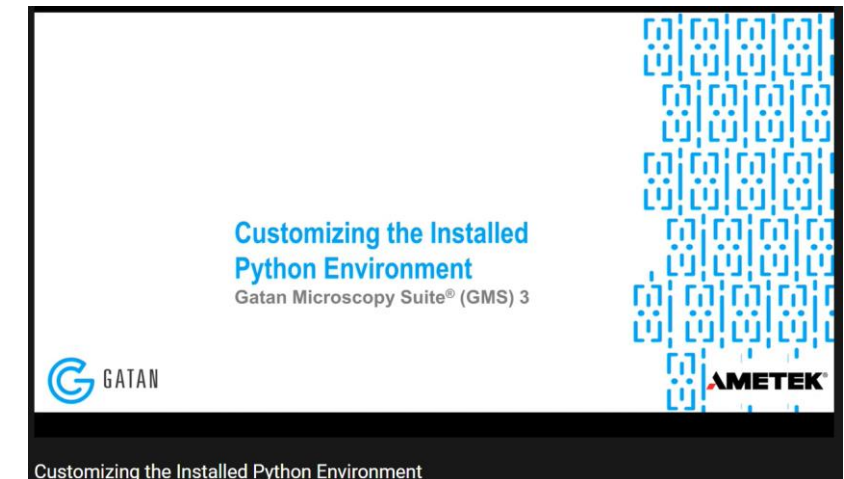
Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

Requirements: Python-integrated GMS 3, Numpy, Scikit-learn



```
1
2
3 the EELS-SI must be front-most
4
5
6
7
8 # *****
9 print("Execute Python script in GMS 3")
10
11 import numpy as np
12 import DigitalMicrograph as DM
13 from sklearn.decomposition import NMF, PCA
14
15 #import sys
16 #sys.argv.extend(['-a', ' '])
17 #import matplotlib.pyplot as plt
18
19 print("Libraries imported completely")
20 # *****
21
22 # *****
23 def zero_one_rescale(spectrum):
24     """
25     get rid of negative values
```

uncheck "Execute on Background Thread"



<https://www.youtube.com/watch?v=-pQMytgaRVg>

$$\begin{pmatrix} v_{11} & \cdots & v_{1m} \\ \vdots & \ddots & \vdots \\ v_{n1} & \cdots & v_{nm} \end{pmatrix} \approx \begin{pmatrix} w_{11} & \cdots & w_{1r} \\ \vdots & \ddots & \vdots \\ w_{n1} & \cdots & w_{nr} \end{pmatrix} \times \begin{pmatrix} h_{11} & \cdots & h_{1m} \\ \vdots & \ddots & \vdots \\ h_{r1} & \cdots & h_{rm} \end{pmatrix}$$

$V (n \times m) \approx W (n \times r) \times H (r \times m)$

loading vectors coefficients

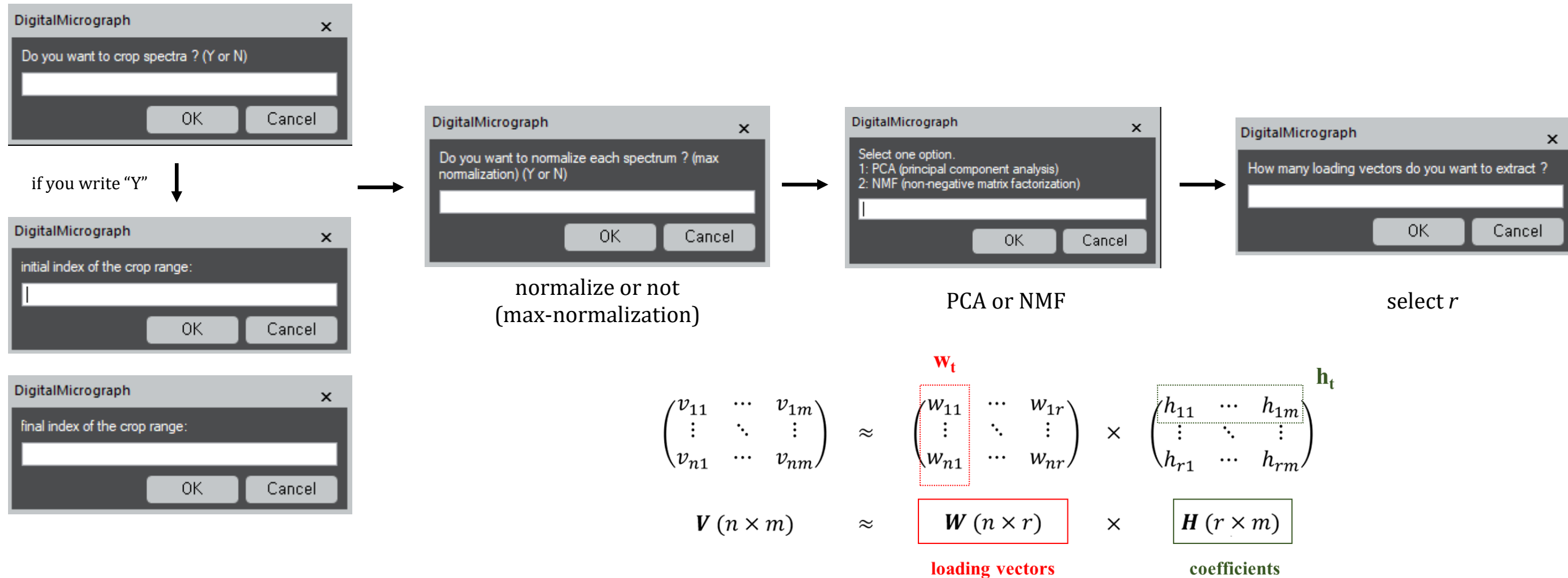


[SI]_dimensionality_reduction.py

Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

Requirements: Python-integrated GMS 3, Numpy, Scikit-learn

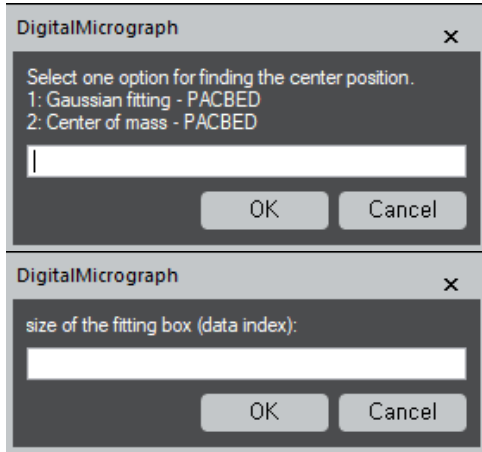
Case 1: 3D spectrum image



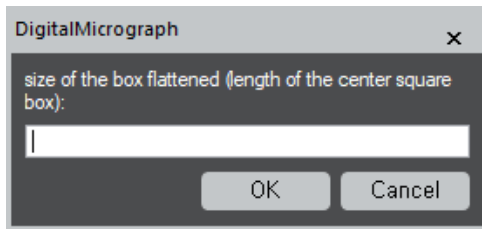
Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

Requirements: Python-integrated GMS 3, Numpy, Scikit-learn

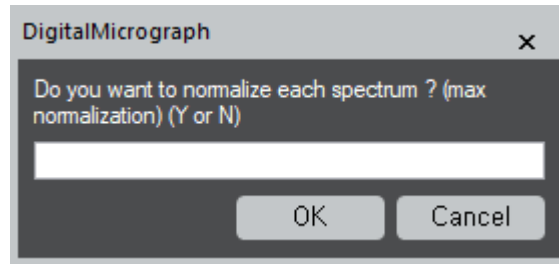
Case 2: 4D-STEM data



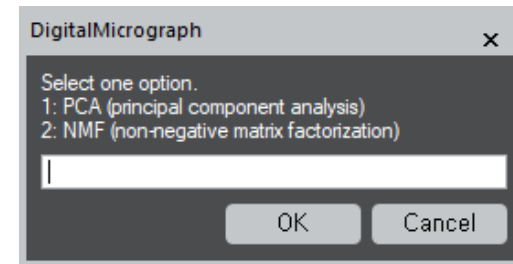
find the center position



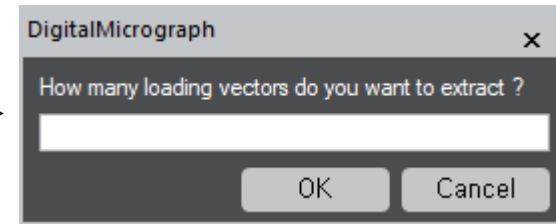
flatten the data
for a square region



normalize or not
(max-normalization)

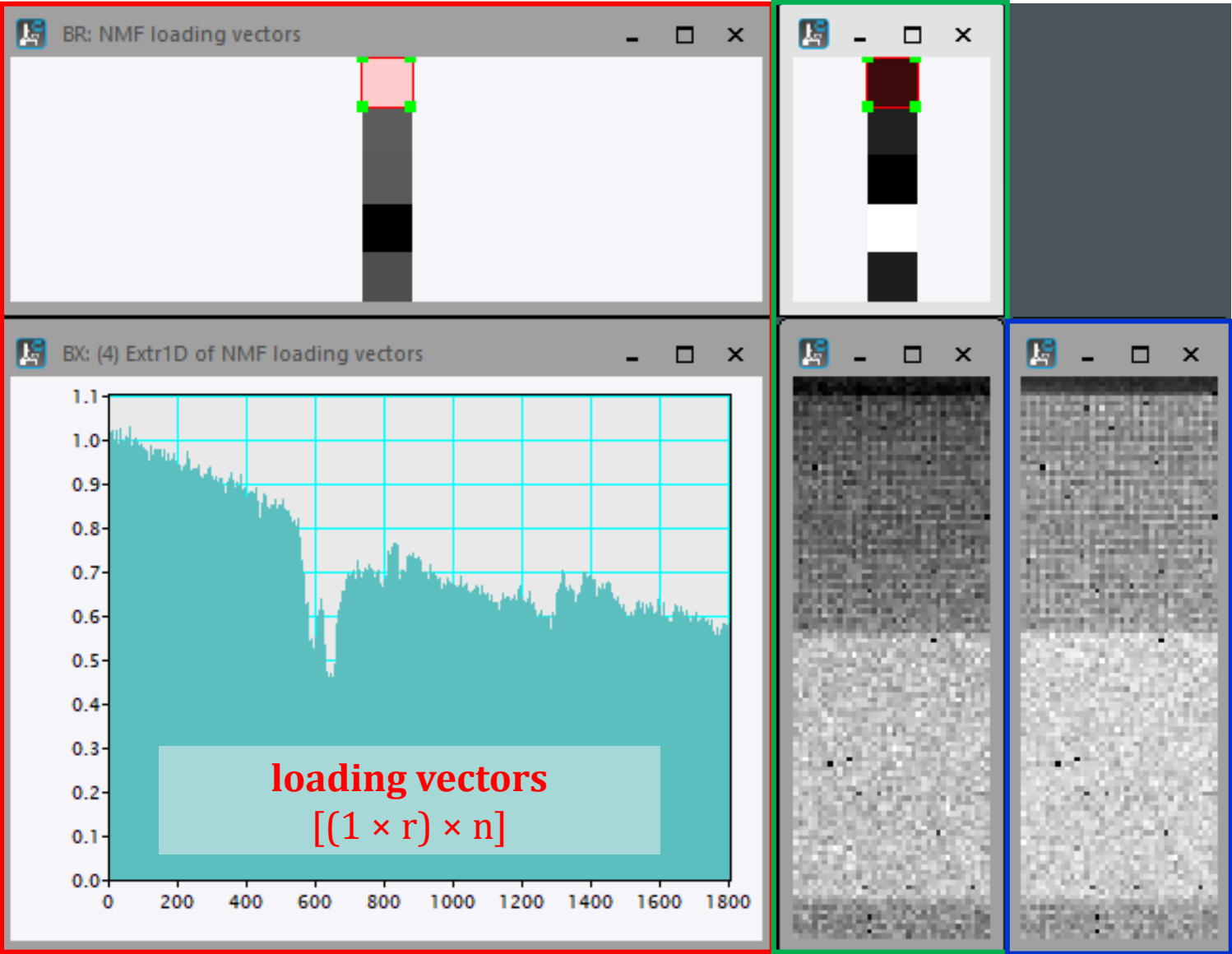


PCA or NMF



select r

Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data



Requirements:
Python-integrated GMS 3, Numpy, Scikit-learn

output example
(EELS-SI)

Example

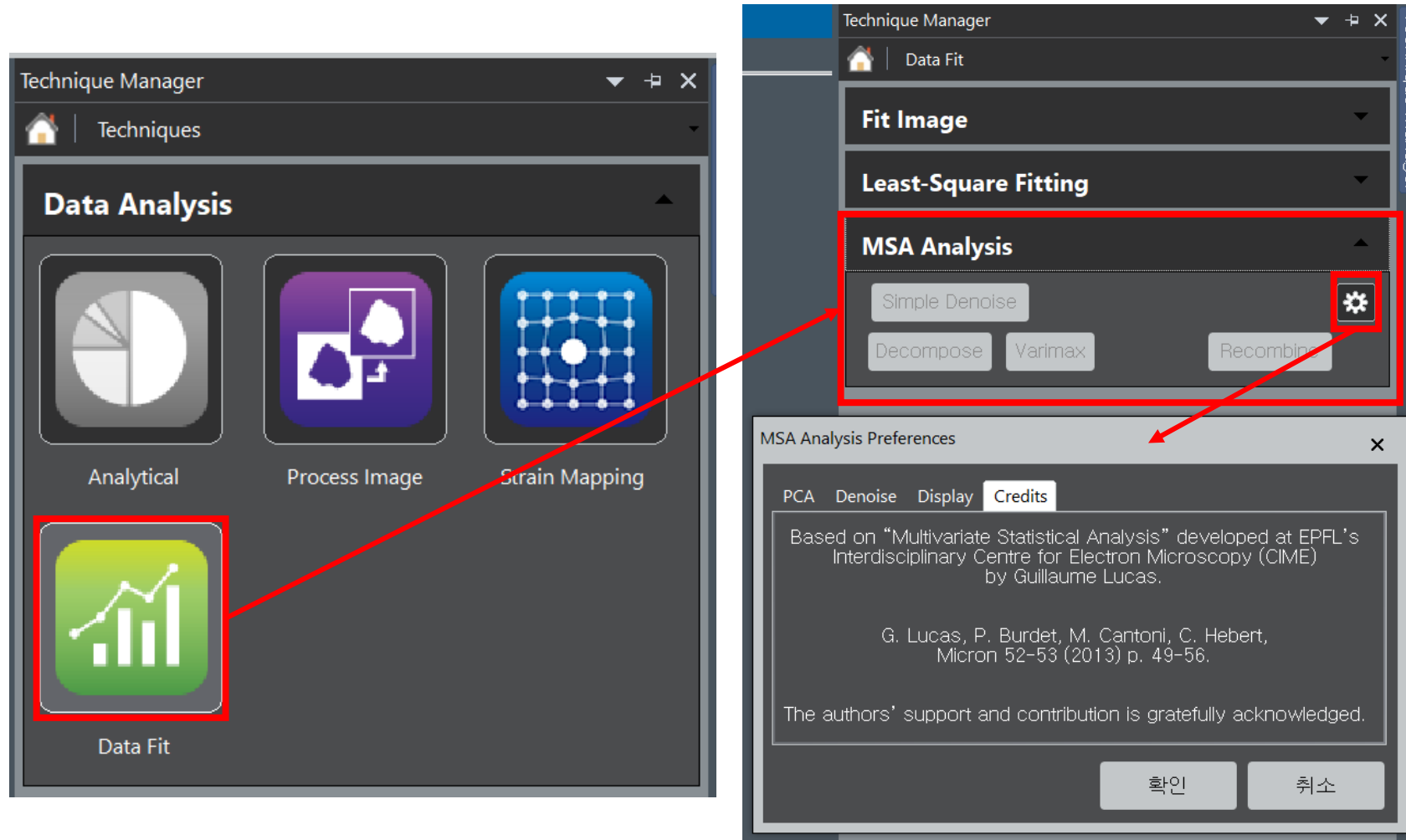
(sx, sy → STEM scanning size)

Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

multivariate statistical analysis in GMS 3

it works only for an EELS-SI

<https://www.youtube.com/watch?v=IgoPApTiN4I>
(official tutorial)



Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

multivariate statistical analysis in GMS 3

<https://www.youtube.com/watch?v=IgoPApTiN4I>
(official tutorial)

The screenshot displays the DigitalMicrograph software interface. On the left, a search bar is highlighted with a red box, showing the search term 'MSA'. Below it, a table lists search results for 'MSA Analysis' and related tools. A red arrow points from the search bar to the 'MSA Analysis' entry in the table. The main window shows the 'MSA Analysis' workflow palette with buttons for 'Simple Denoise', 'Decompose', 'Varimax', and 'Recombine'. Below the palette, text explains the MSA Analysis workflow and provides instructions for 2D, 3D, and 4D data formats. A red box highlights a list of procedures provided by the tool: Simple Denoise, Decompose, Varimax, and Recombine.

| 제목 | 위치 | 순위 |
|----------------|-----------------|----|
| MSA Analysis | DigitalMicro... | 1 |
| Simple Denoise | DigitalMicro... | 2 |
| General Setup | DigitalMicro... | 3 |
| Credits | DigitalMicro... | 4 |
| Decompose | DigitalMicro... | 5 |
| Recombine | DigitalMicro... | 6 |
| Varimax | DigitalMicro... | 7 |

MSA Analysis

The **MSA** Analysis workflow palette provides tools to perform Multivariate Statistical Analysis on data. Buttons of the palette will be shown enabled or disabled depending on the type of data front most on the workspace.

Acceptable source data format is interpreted as follows:

2D Data:
Each row of the image is considered a 1D spectrum. This is the typical format of line-scan type spectrum-images.

3D Data:
X and Y are considered to be spatial dimensions and Z is considered the 1D spectral dimension. This is the typical format of regular spectrum-images for EELS, EDS or CL signals.

4D Data:
X and Y are considered to be spatial dimensions and the remaining two dimensions are considered to be the two dimensions of 2D data. This is the typical format of spectrum images for Diffraction or momentum resolved EELS.

The following procedures are provided by the tool:

- **Simple Denoise:** Reduce data noise by considering only the first few components of a Principal Component Analysis (PCA)
- **Decompose:** Perform a Principal Component Analysis (PCA) and show the most relevant components
- **Varimax:** Perform a Varimax factor rotation on a set of components
- **Recombine:** Recombine a reduced data set from selected components

The gear-shaped icon opens the general [setup dialog](#).

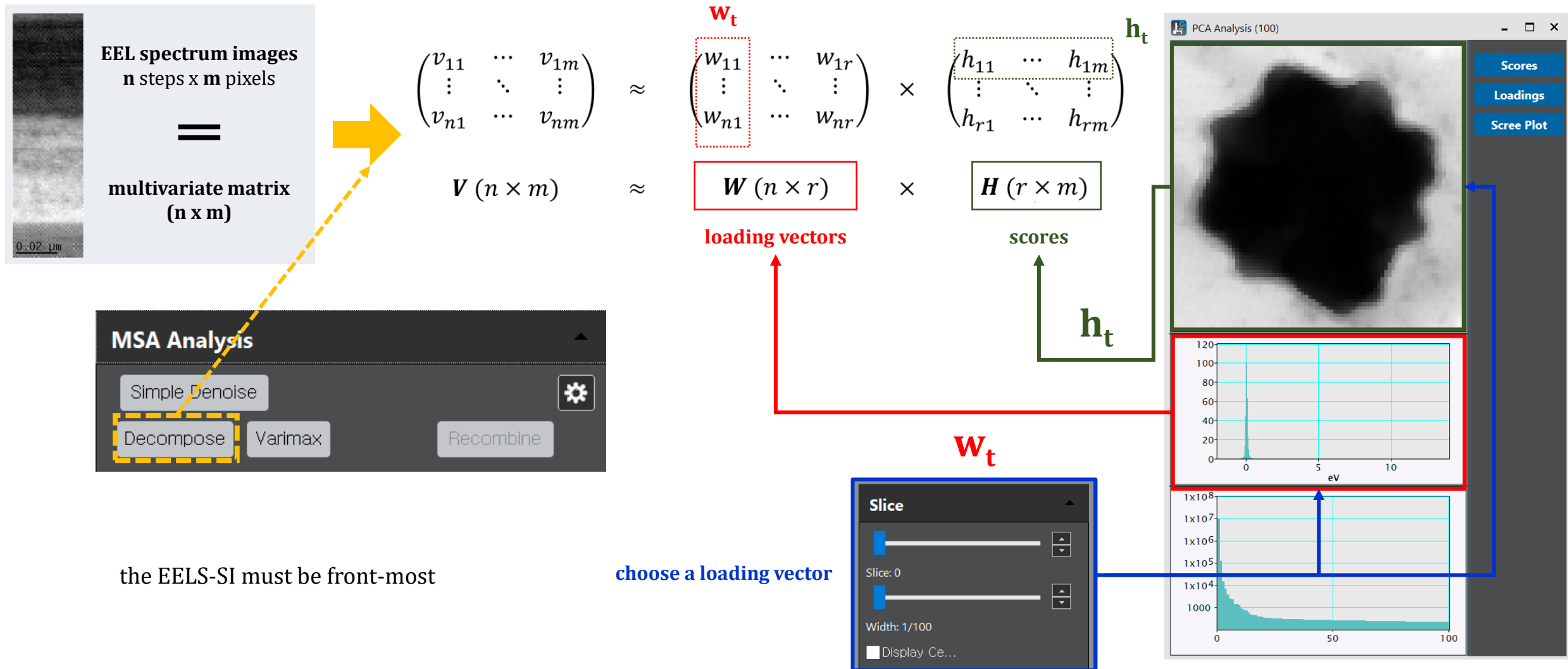
There is also a [script interface](#) to this functionality.

principal component analysis (PCA)

Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

multivariate statistical analysis in GMS 3

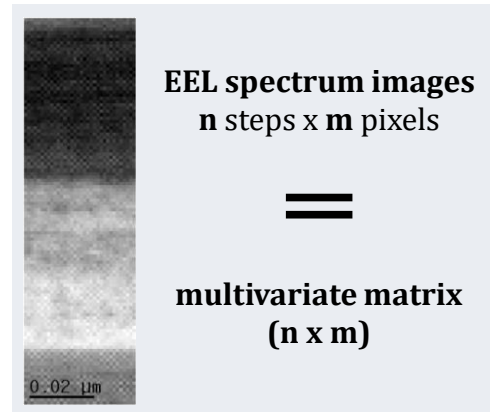
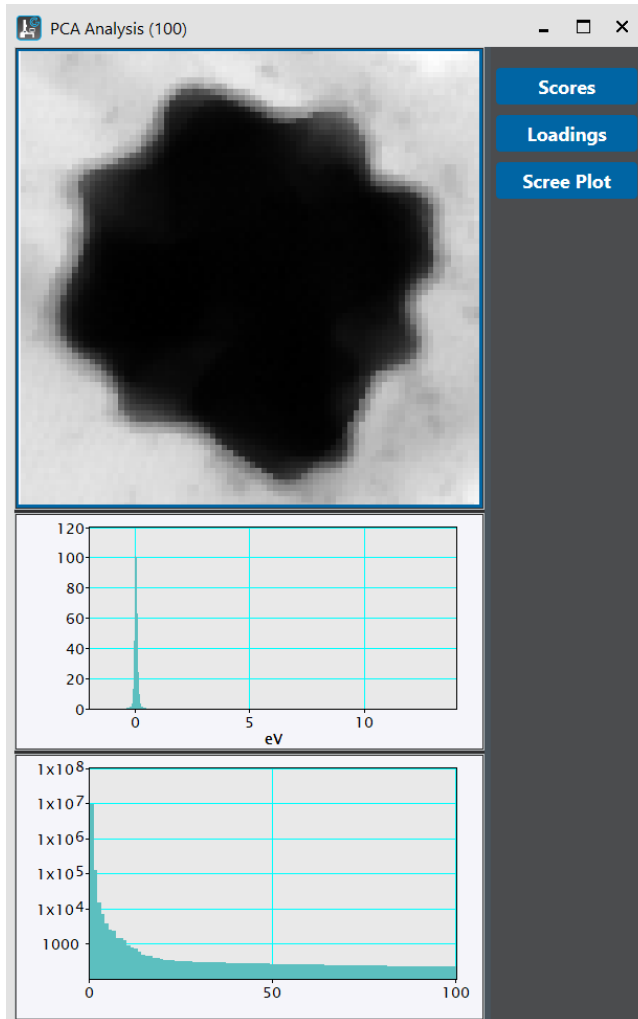
<https://www.youtube.com/watch?v=IgoPAPtiN4I>
(official tutorial)



Feature extraction using dimensionality reduction methods from a spectrum image or 4D-STEM data

multivariate statistical analysis in GMS 3

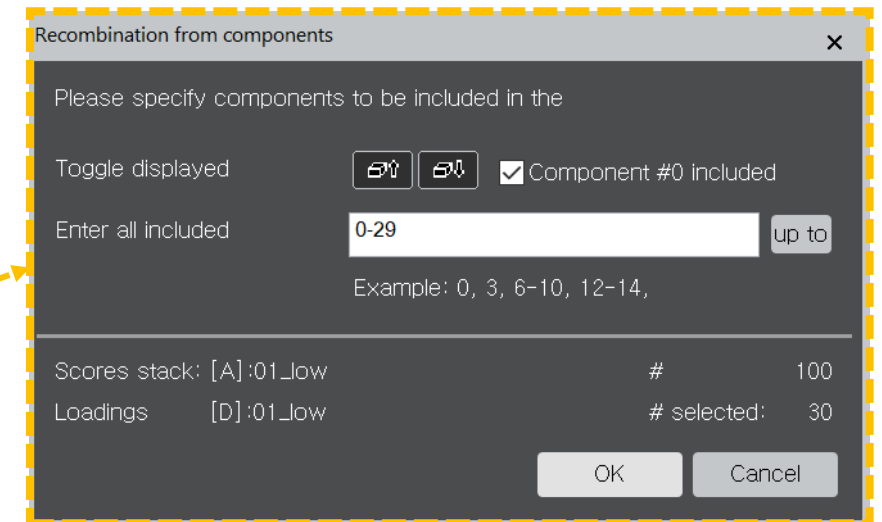
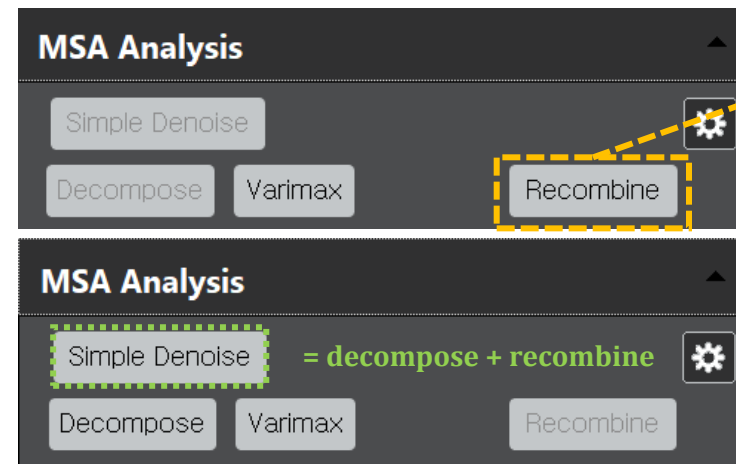
<https://www.youtube.com/watch?v=IgoPAPtiN4I>
(official tutorial)



$$\begin{pmatrix} v_{11} & \cdots & v_{1m} \\ \vdots & \ddots & \vdots \\ v_{n1} & \cdots & v_{nm} \end{pmatrix} \approx \begin{pmatrix} w_{11} & \cdots & w_{1r} \\ \vdots & \ddots & \vdots \\ w_{n1} & \cdots & w_{nr} \end{pmatrix} \times \begin{pmatrix} h_{11} & \cdots & h_{1m} \\ \vdots & \ddots & \vdots \\ h_{r1} & \cdots & h_{rm} \end{pmatrix}$$

$V (n \times m) \approx W (n \times r) \times H (r \times m)$

loading vectors **scores**



choose loading vectors used to
reconstruct the dataset

$$V' = W' \times H'$$

$n \times m \quad n \times r' \quad r' \times m$
($r' \leq r$)