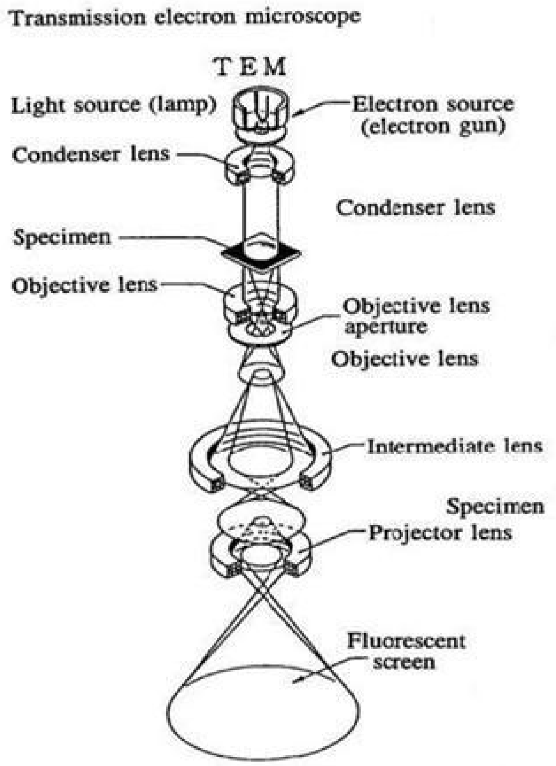
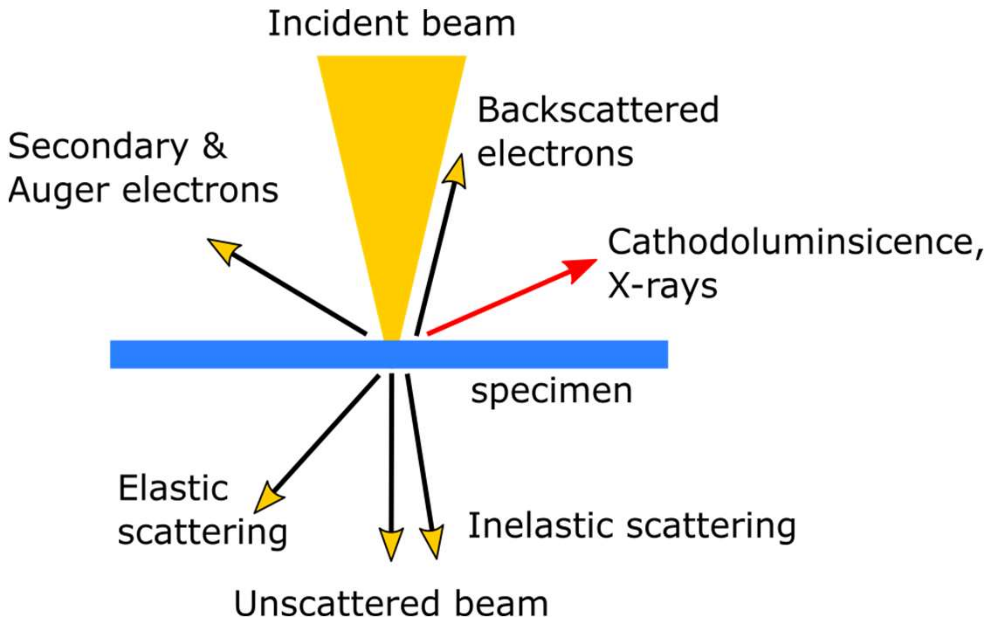
AI for Nanoscale Spectroscopies

Electron Energy Loss Spectroscopy:

It is about measuring the energy lost by electrons (in a TEM).



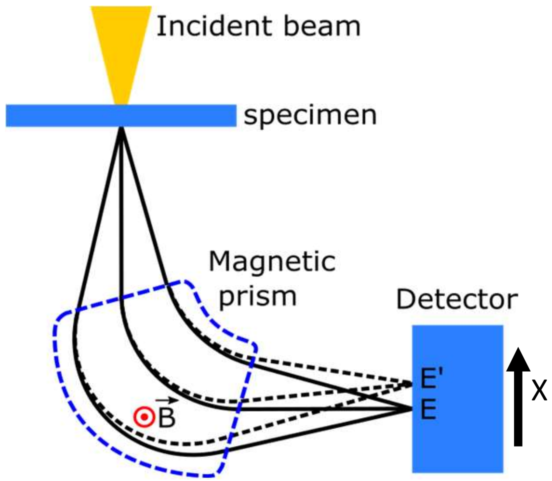


Electron Energy Loss Spectroscopy:

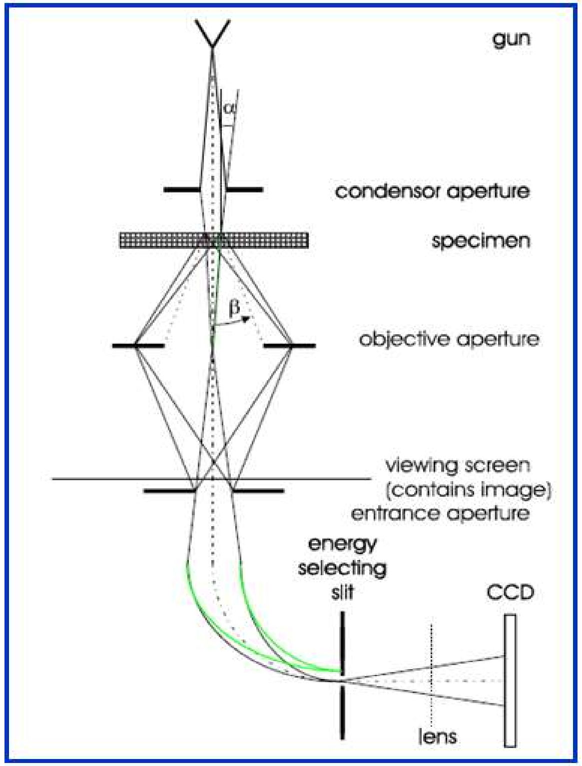
It is about measuring the energy lost by electrons (in a TEM).

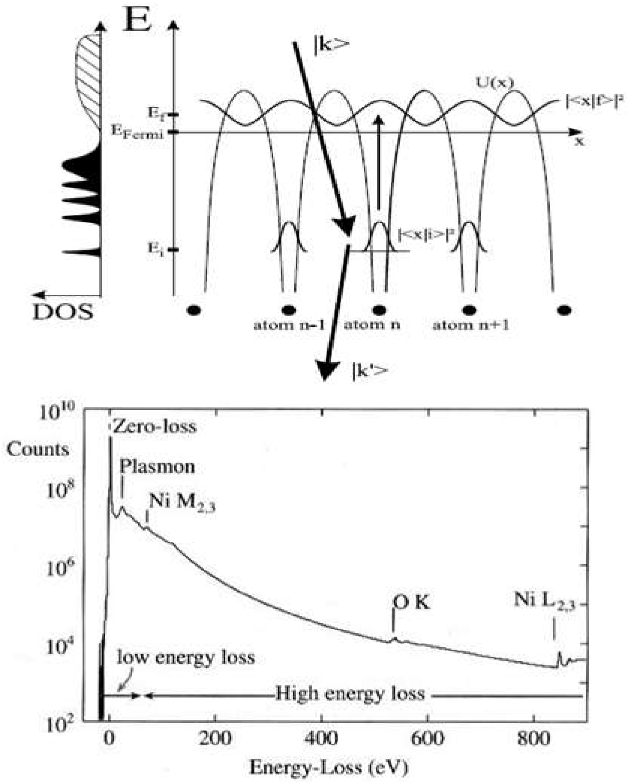
The spectrometer:

Uses a magnetic sector to disperse the transmitted beam by energy.



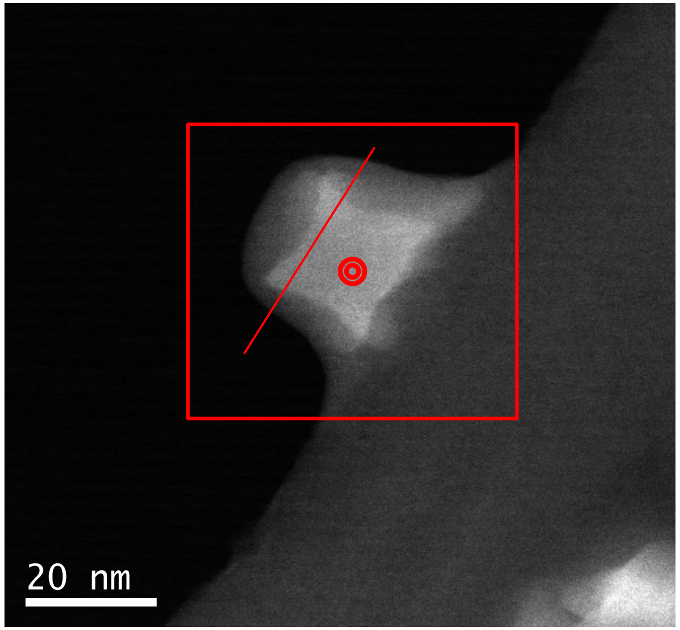
From a physical point of view

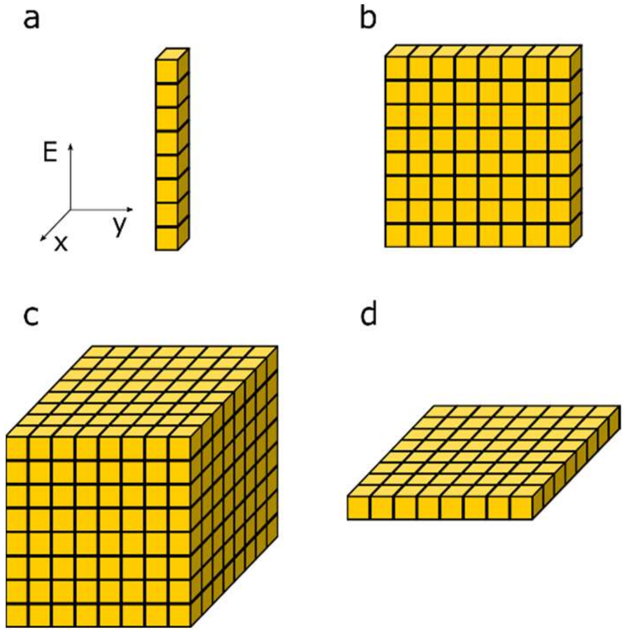


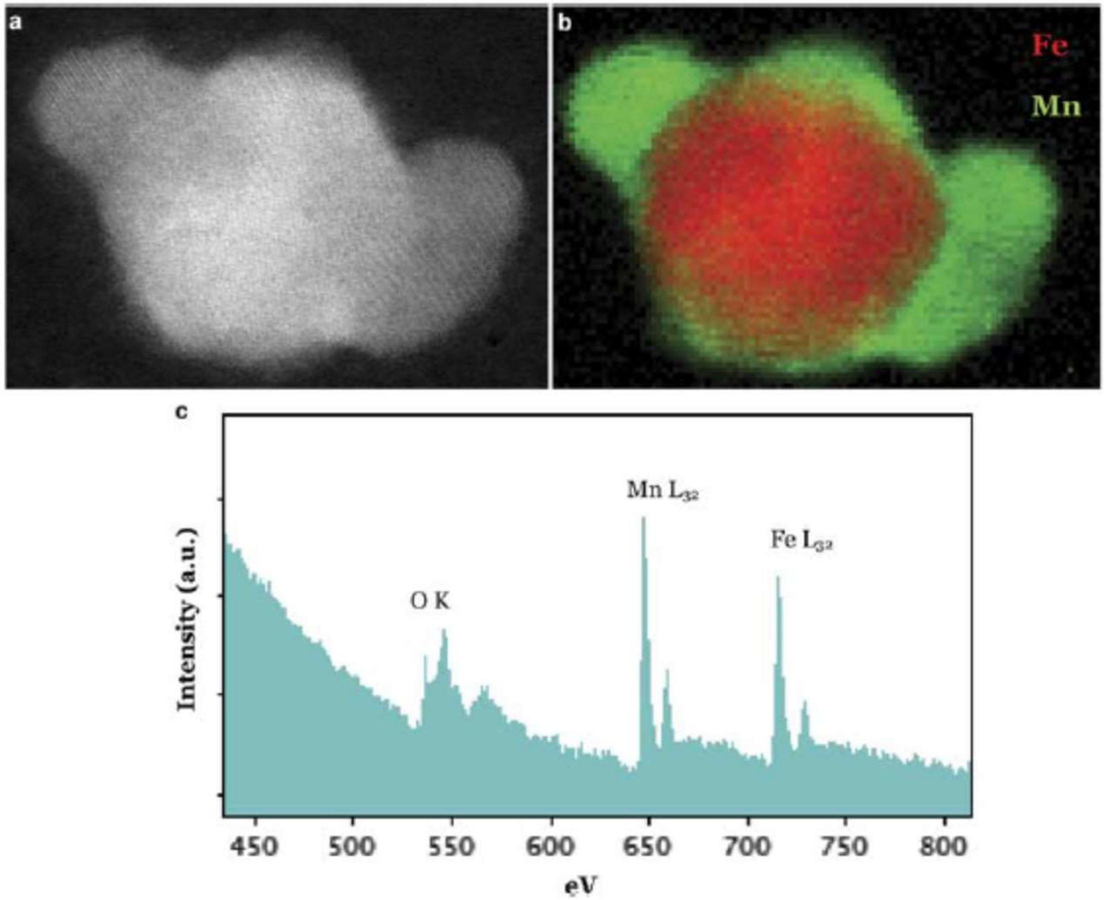


- ionization of specimen e-
- transitions from occup. core states to unocc. states
- interband transitions
- collective vibrations of cond. band electrons
- single scattering / plural scattering / multiple scattering

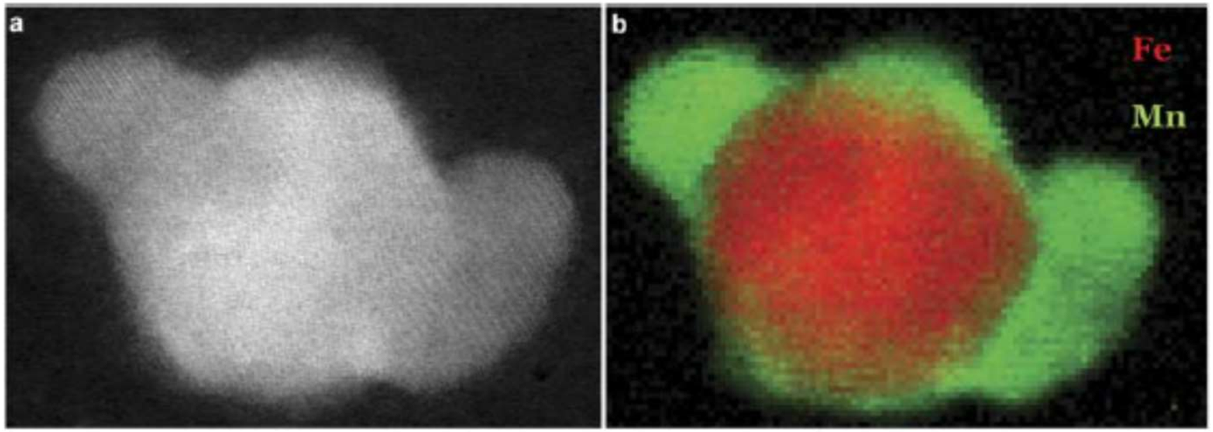
Individual Spectrum, Spectrum Line, Spectrum Image

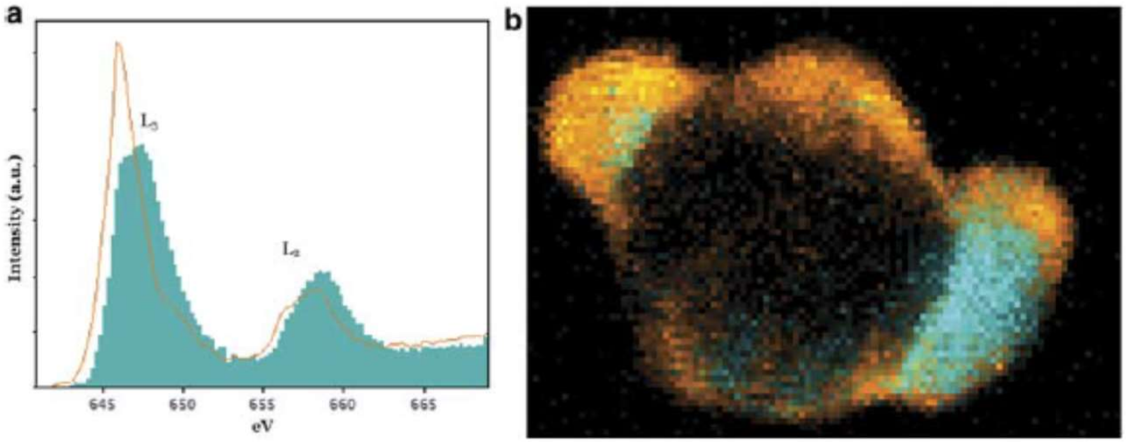






a
b
Fe
Mn
c
Intensity (a.u.)
O K
Mn L_{32}
Fe L_{32}
450 500 550 600 650 700 750 800
eV


a
b
Fe
Mn


a
L_3
L_2
Intensity (a.u.)
645
650
655
660
665
eV
b

Multivariate analysis (PCA, ICA) and model fitting: Hyperspy

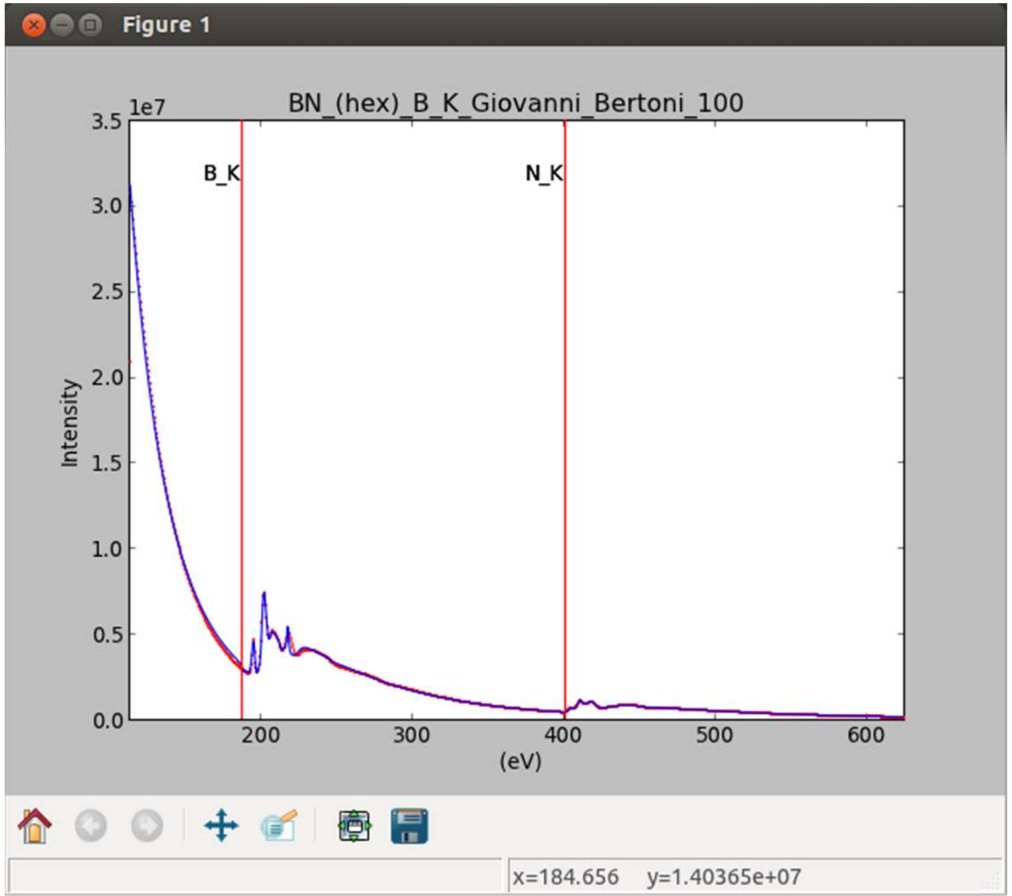
Developed by de La Peña and coworkers

Decomposition algorithms, such as principal component analysis (PCA), or blind source separation (BSS) algorithms, such as independent component analysis (ICA), are available.

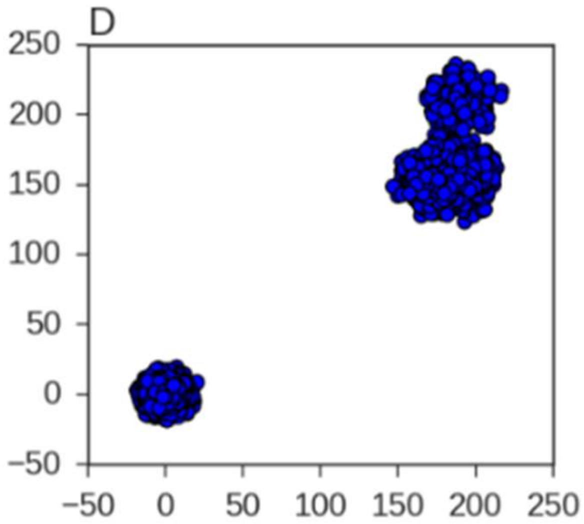
$$D_{(x,y,E),\theta} = \sum_{i=1}^{n} S_{(x,y),i,\theta} L_{E,i}^{T}$$

Typically used for denoising

Multivariate analysis (PCA, ICA) and model fitting: Hyperspy



Adapting clustering analysis to EELS

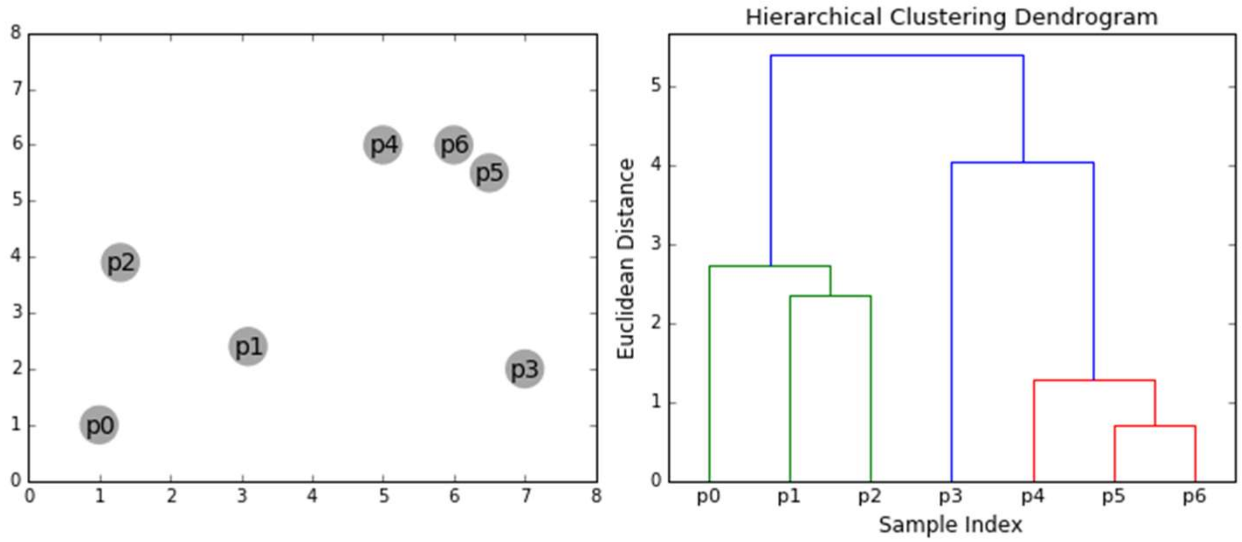


The goal of EEL spectrum imaging is mapping the spatial distribution of properties reflected in the shape of individual EEL spectra.

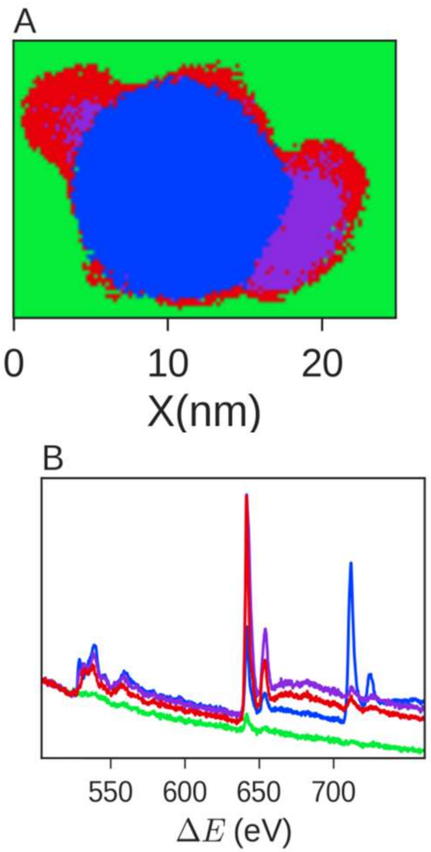
In many cases, this implies finding a way to segment a given SI into different regions.

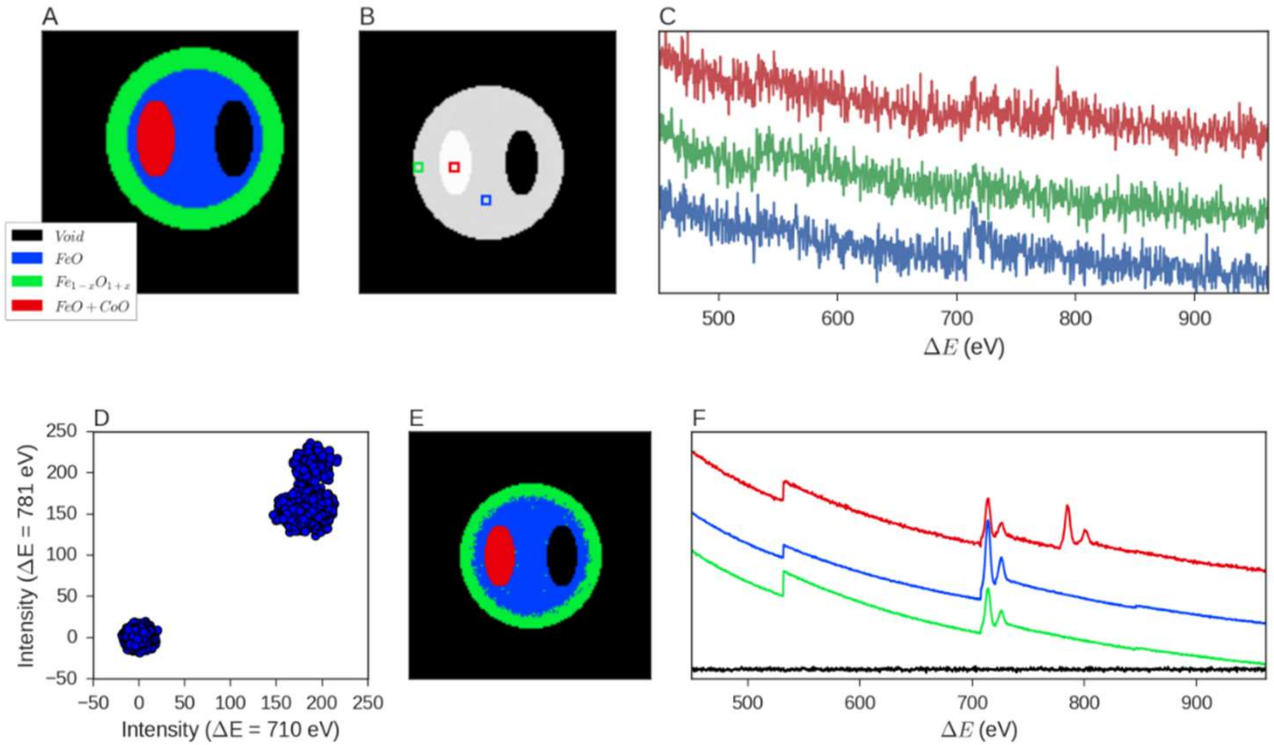
= Classifying spectra into groups with similar characteristics.

Interestingly, this corresponds to **clustering**.



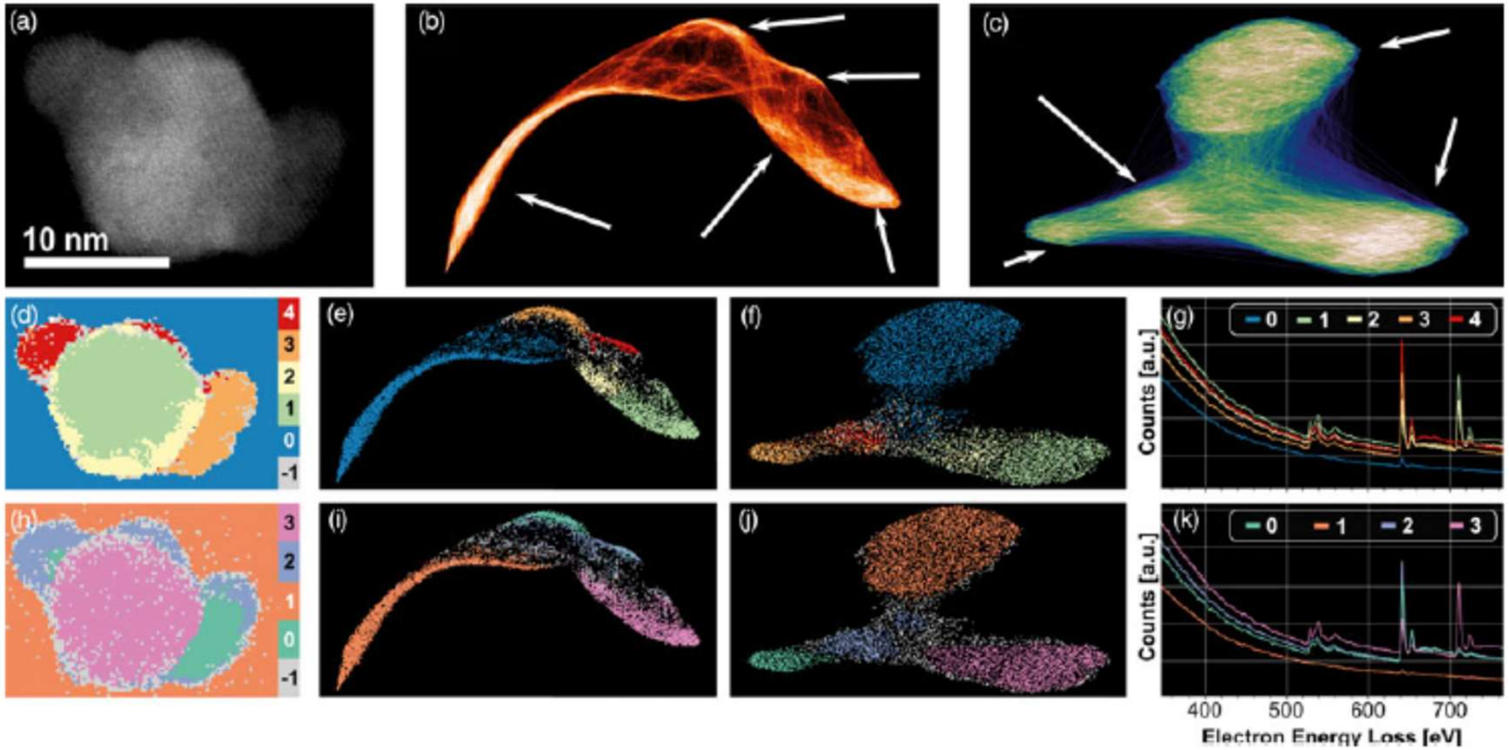
Good results obtained for phantoms and experimental data using the more typical clustering algorithms, agglomerative clustering and K-means.





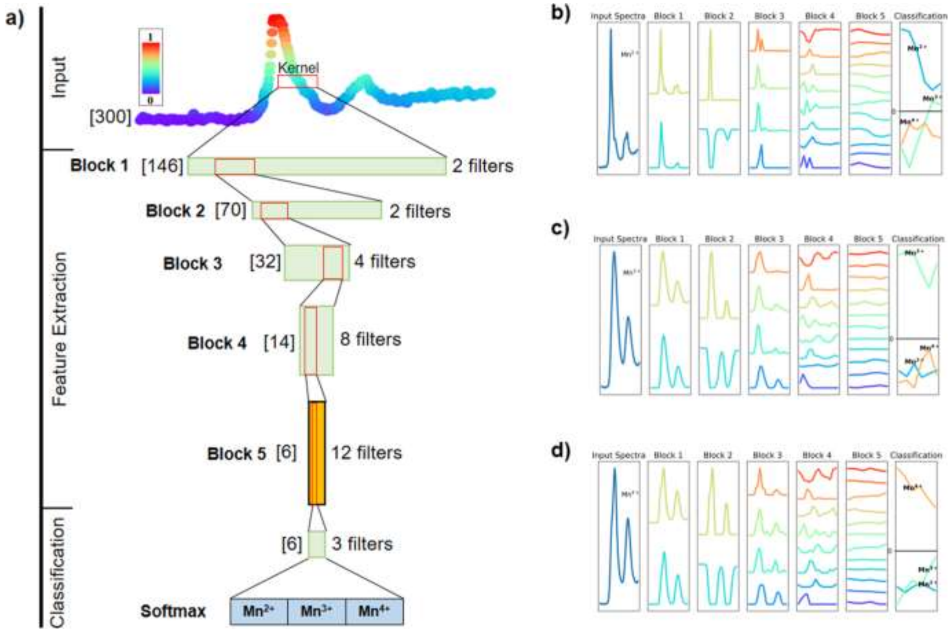
P. Torruella et al., Ultramicroscopy (2018)

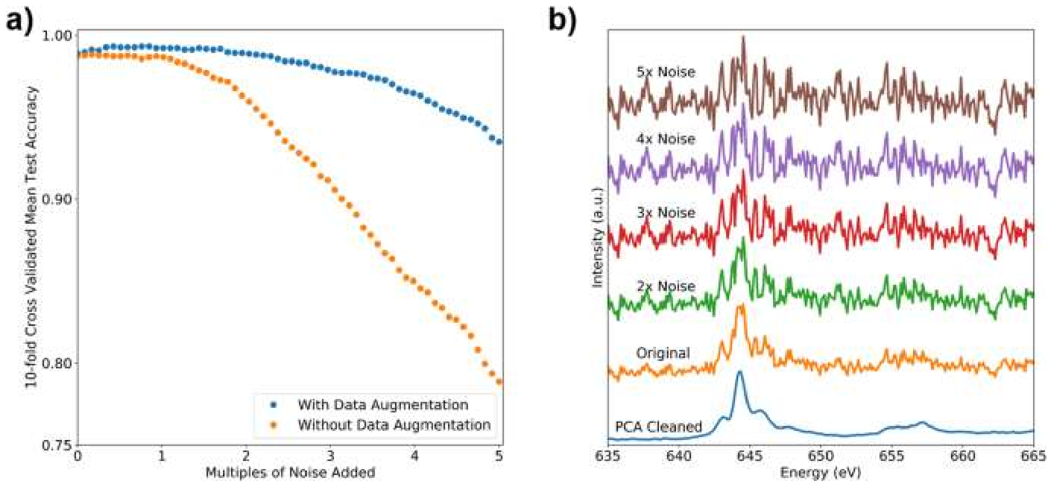
Hierarchical density-based spatial clustering of applications with noise (HDBSCAN) and uniform manifold approximation and projection (UMAP), state-of-the-art algorithms for clustering analysis, and dimensionality reduction, respectively, can also be used for the segmentation of core-loss electron energy loss spectroscopy (EELS) spectrum images.



Blanco-Portals, J., Peiró, F., & Estradé,S. Microscopy and Microanalysis (2021)

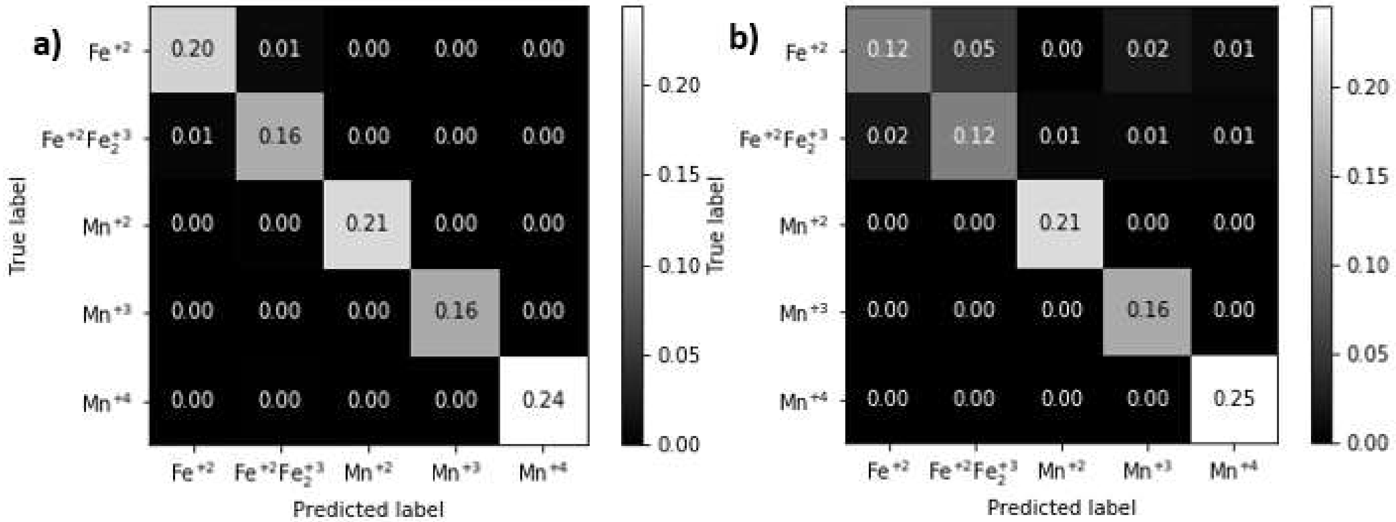
Other Big Data Strategies: Neural Networks for Mn oxidation state determination





M. Chatzidakis & G. A. Botton, Scientific Reports(2019)

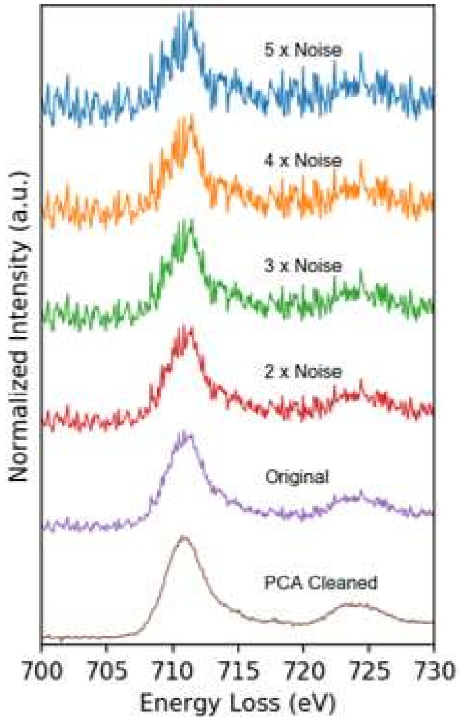
Other Big Data Strategies: Support Vector Machines for Mn and Fe oxidation state determination

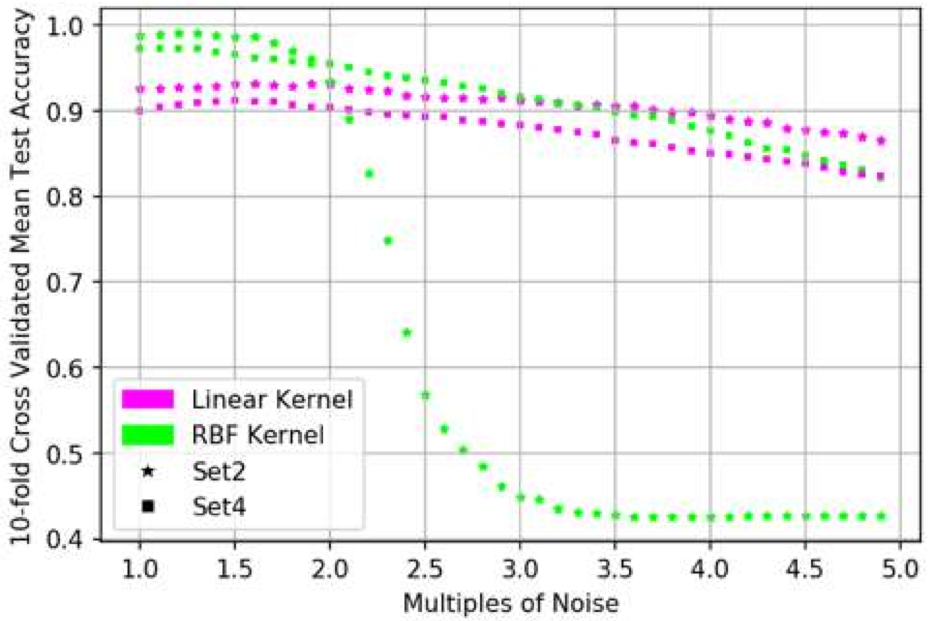


*Normalized confusion matrices of the test set 4 for the model 12 (**a** matrix), and the model 7 (**b** matrix).*

Del Pozo Bueno, D., Peiró, F., & Estradé, S. Ultramicroscopy (2021)

Other Big Data Strategies: Support Vector Machines for Mn and Fe oxidation state determination



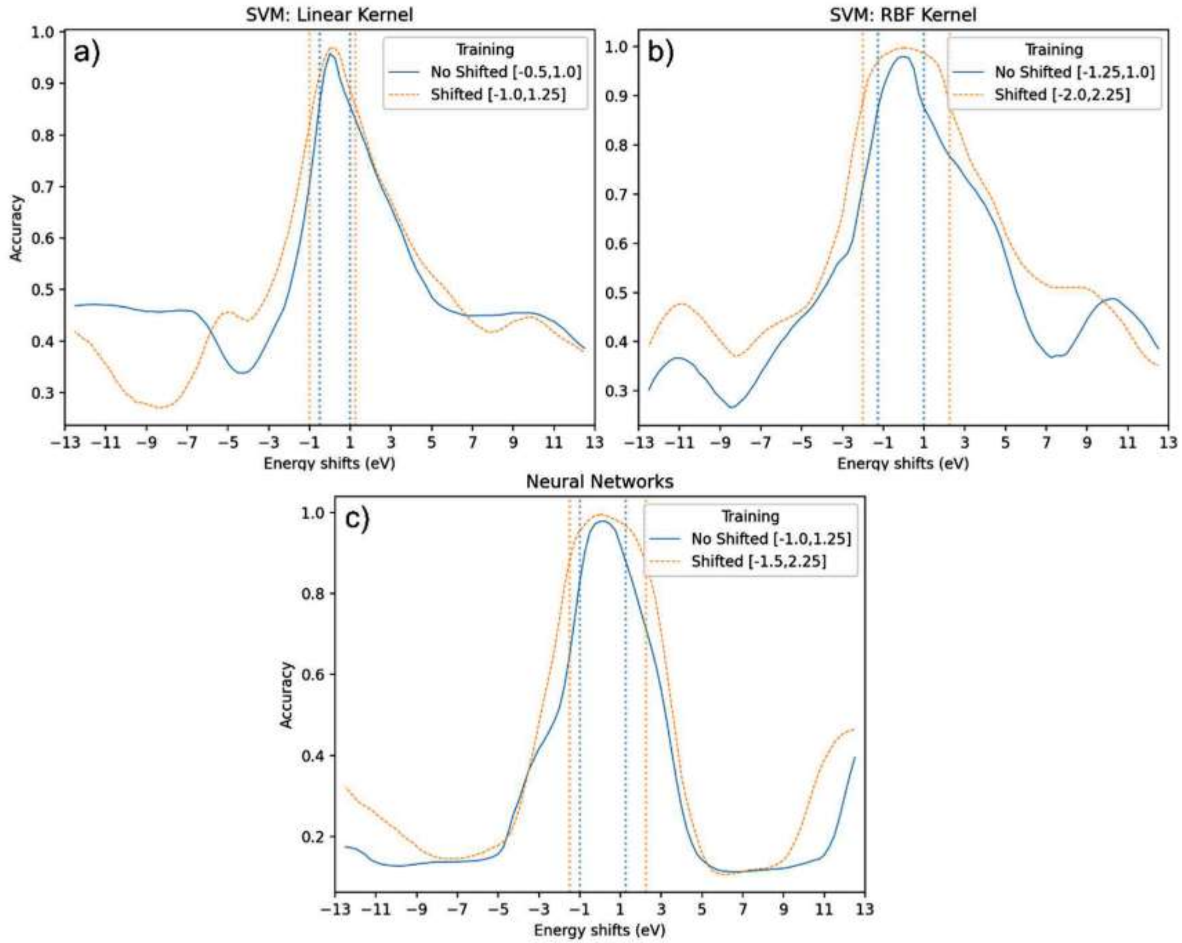


Del Pozo Bueno, D., Peiró, F., & Estradé,S. Ultramicroscopy (2021)

Comparison of SVM and NN

Success ratio of the models per structure. The table includes the results for dense and convolutional structures. The first and last columns indicate the structure's number and the central columns the success ratio for each structure and epochs used in the training. Then, the rows show the different structures, the ones marked in purple correspond with most successful structures.

	Success ratio per structure (%)				
Dense Structures	10 epochs	30 epochs	10 epochs	30 epochs	Conv. Structures
0	47	54	48	45	0
1	42	65	57	74	1
2	50	74	48	64	2
3	55	78	52	62	3
4	61	72	44	49	4
5	42	51	69	85	**5**
6	54	59	75	78	**6**
7	29	40	88	80	**7**
8	33	62			
9	19	38			
10	50	65			
11	36	30			
12	67	78			
13	50	63			



Del Pozo Bueno, D., Kepaptsoglou, D., Peiró, F., & Estradé, S. Ultramicroscopy (2023)