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How to get the most out of my mapping data? A data reduction scheme to analyze all of your mapping data at once

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Due to both new developments in instrument technology and enhanced computing power, elemental mapping of solid samples is performed more and more often. These maps can for example reveal gradients/zonations in crystals or uptake pathways and translocation of potentially toxic elements in plant tissue at a resolution higher than that of optical microscopes and even unravel optically invisible structures.

In many cases, more than one element concentration or absorption spectrum is measured at the same spot, leading to numerous element maps of the exact same sample. While those maps are often regarded separately or only compared visually, this is in fact a 3D "dataspace". This "dataspace" can be analyzed as a whole to get further information on the sample and/or render data analysis and interpretation statistically reliable and repeatable.

We present a chemometric approach analyzing element concentration maps generated with LA-ICP-MS (laser ablation with inductively coupled plasma-mass spectrometry) and the software Iolite that – even for large mappings with around 500,000 data points – can run on a normal desktop PC applying the freely available software R and RStudio®. The workflow is based on a combination of principal component analysis (PCA) and cluster analysis. With this, additional relevant information can be extracted while the amount of data to be critically interpreted is reduced at the same time. In a first example we could not only identify optically invisible generations of growth in calcite crystals but also a) identify which elements altogether indicate the zonation, b) explicitly and mathematically properly assign each point on the xy-mapping space to a growth zone and thus c) allow for a (statistical) interpretation of the whole growth zone instead of regarding only parts in the center [1].

This approach is not limited to either element mapping with LA-ICP-MS or any commercially available software but can be adopted for numerous mapping techniques. Further applications will be shown in the presentation.

[1] Kusturica, van Laaten, Drake & Schäfer (2022), *Environmental Earth Sciences* 81, 371.