doi:10.1017/S1431927613012130
Microsc. Microanal. 19 (Suppl 2), 2013


# Practical Processing of Spectrum Images by Multivariate Statistical Analysis: Advantages and Disadvantages

M. Watanabe
Dept of Materials Science and Engineering, Lehigh University, Bethlehem. PA 18015 USA

Nowadays, it is possible to acquire large scale datasets such as spectrum images, diffraction images, through-focal image series, tomographic image series, etc. Since hardware and acquisition software have already been developed in 64-bit bases, over a few GB data (e.g. one spectrum image with 1024 x 1024 pixels and 2048 channels is ~8 GB) can be obtained in a single acquisition process. Despite that this trend to acquire such large scale datasets is desired for many years, it would be much harder for individual researchers to analyze (or even view) the datasets efficiently, which is the major drawback. The large scale datasets can be efficiently handled by employing advanced statistical approaches such as multivariate statistical analysis (MSA). The several different types of MSA approaches have already been applied to spectrum images obtained in electron microscopy and several software packages to run MSA are available. It is very straightforward to apply MSA but some fundamental knowledge of MSA is essential for appropriate analysis of complex spectrum images. In this tutorial, therefore, principle of the MSA procedure is briefly explained as an author of one of the MSA packages (MSA plugin for Gatan DigitalMicrograph [1]).

Application of MSA exhibits two aspects in analyzing datasets: one is feature identification and other is noise reduction [e.g. 2, 3]. The first aspect is derived from the nature of eigenanalysis of a dataset (Fig.1) [1]. By applying eigenanalysis, information repeated in the dataset can be extracted as significant features (or principal components). This feature extraction process can be performed automatically, which practically assists in data analysis. The frequency of features appear in the dataset is represented as eigenvalues of corresponding features. Therefore, the magnitude of eigenvalues as a scree plot (logarithm of the eigenvalues plotted against the index of component: e.g. Fig. 2) can be used primarily to distinguish between statistically significant (frequently repeated) and sparsely appeared (random) components.

Once the significant components are extracted from the dataset, the dataset can be reconstructed with the limited number of the significant components, which is the second aspect of the MSA application. This reconstruction process is summarized in Fig. 3 [1]. As a result of the data reconstruction, the random-noise parts can be efficiently reduced from the original dataset without degrading the spatial or energy resolution. Figure 4 compares Ti maps extracted from original and MSA-reconstructed EELS spectrum images acquired in a Ni-base superalloy. Although the original map shows distribution of Ti, random noise is clearly reduced in the reconstructed Ti map. It should be mentioned that it is not always straightforward to distinguish significant components from others. Careful evaluation of individual components is always essential to minimize artifacts introduced by the MSA technique.

In addition to the principle of the technique, several MSA applications will be introduced, including the latest atomic-resolution XEDS and EELS mapping. Although the MSA approach is very useful, it may create unexpected artifacts especially in the noise reduction, which may mislead results. Common pitfalls in MSA applications and advantages/disadvantages of the technique will also be discussed in this tutorial.

**References**

[1] M Watanabe et al., *Microscopy and Analysis*, **23**, Issue 7, 5-7., (2009).
[2] I.T. Jolliffe, *Principal Component Analysis*, 2nd ed., Springer, New York, (2002).
[3] E.R. Malinowski, *Factor Analysis in Chemistry*, 3rd ed., Wiley, New York, (2002).
[4] The author wishes to acknowledge financial support from the NSF throu gh grants DMR-0804528 and DMR-1040229.

**Fig. 1**

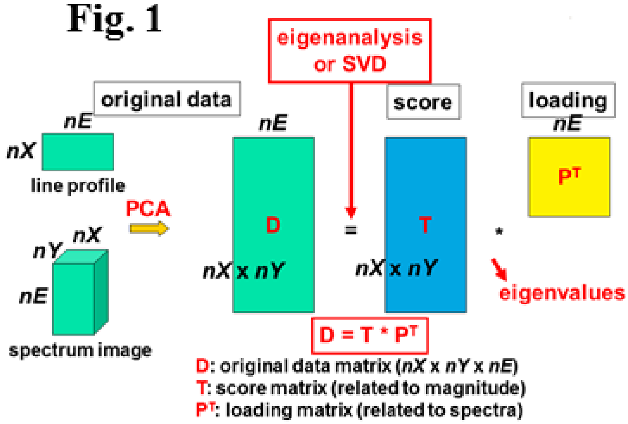


**Fig. 2**

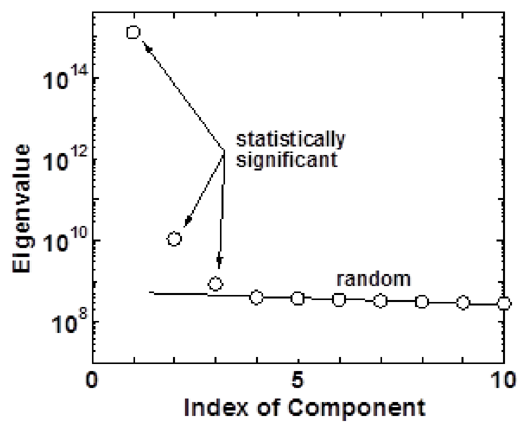


**Fig. 3**

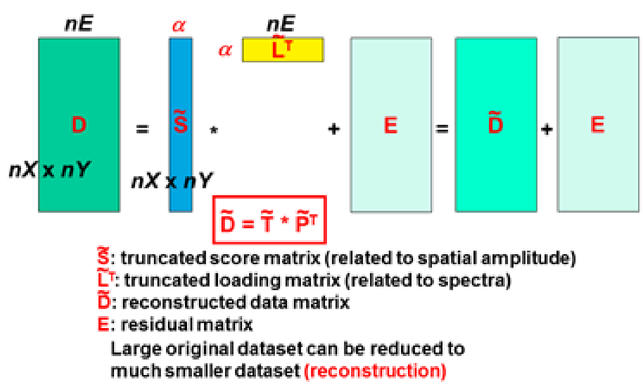


**Fig. 4**

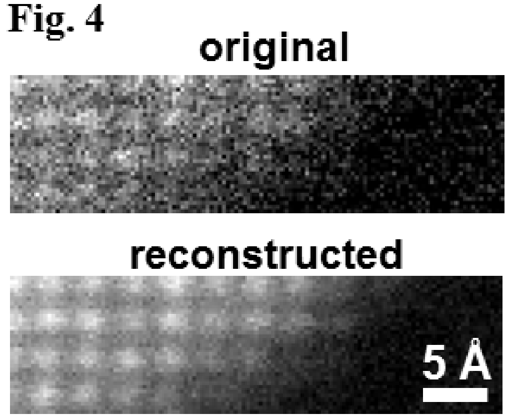


Figure 1: A schematic diagram of data decomposition by eigenanalysis in MSA process.

Figure 2: An example of scree plot.

Figure 3: A schematic diagram of data reconstruction by MSA noise reduction

Figure 4: A comparison of Ti maps extracted from original and MSA-reconstructed EELS spectrum images acquired in a Ni-base superalloy.

https://doi.org/10.1017/S1431927613012130 Published online by Cambridge University Press