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EDITORIAL

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Advancements in multivariate analysis of variance

The Journal of Chemometrics is pleased to announce a special issue focused on multivariate analysis of data from designed experiments. ANOVA (Analysis of Variance) is the standard method for analyzing data from experimental designs. The classical ANOVA methods are however univariate and do not handle multiple collinear response variables. Designed experiments with multivariate outputs are prevalent across various scientific disciplines, necessitating methods that appropriately consider both the experimental design and the multivariate nature of the data.

Several multivariate ANOVA techniques have been presented already. The most prevalent approaches involve combining ANOVA with PCA (principal component analysis) or other exploratory component-based techniques in different ways. Some commonly used methods in this context include ASCA, ANOVA-PCA, AComDim, and fifty-fifty MANOVA. These methods integrate ANOVA and PCA in different ways to extract meaningful information from multivariate data. Additionally, there are alternative methods that replace PCA with partial least squares (PLS) regression, which allows for the utilization of PLS-specific validation and variable importance routines. One major advantage of all these methods is that they not only offer interpretation and variable importance metrics from latent variable-based methods but also provide estimates of multivariate effect sizes accompanied by corresponding significance testing.

Despite the progress made in recent years, the field of multivariate analysis of data from designed experiments is still young. Several open questions remain unanswered, and there is a need to make the methodology available to a broader audience. The aim of this special issue was therefore to stimulate and explore advances in methods, applications, and software for multivariate ANOVA.

The collection of papers includes methodical improvements, practical applications, a tutorial, and a software demonstration. Application areas range from spectroscopic control of fermentation processes to metabolomics and gene expressions. Overall, this issue showcases the power and applicability of multivariate ANOVA methods in a wide range of domains.

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