

Multivariate indices for experimental data: a comparative evaluation

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Multivariate statistical procedures applied to experiments can allow a better view of a whole set of response variables and allow adequate control of the type I error rates accumulated by experiment. In general, selection indices such as the Mulamba-Mock index and the Desirability index show robustness, simplicity and good discriminative power. Indices based on principal component analysis (PCA), however, may allow evidence of patterns of differences that selection indices cannot. The objective of this work was to empirically validate simple options for multivariate analysis, evaluating the accumulated empirical rates of type I error per experiment, and to compare the power of the multivariate indices based on PCA and the Mulamba-Mock, Desirability and its variations. Additionally, the objective was to validate simple modifications in the indices in order to increase their discriminative power and to evaluate objective criteria for selecting variables for assigning weights. The study was conducted based on the simulation of data from 1600 experiments, which were separated into four scenarios with 400 experiments each: experiments with 4 highly correlated response variables, under total nullity of effects for treatment (i); experiments with 8 response variables with the lowest level of correlation between them, also under total nullity (ii); experiments with 8 response variables with a lower level of correlation between them, but under partial null conditions (iii) and; experiments with 4 uncorrelated response variables, under total nullity of effects for treatments (iv). Six simple multivariate indices were calculated for each experiment: Mulamba-Mock index (MM), Desirability index (Di), Desirability index converted to rank scale (RT-Di), Desirability index without zero (Di-zm) and two proposals for modifying the Di-zm index (Modified Di-zm 1 and Modified Di-zm 2), in addition to two indexes based on PCA. In the simple multivariate indices, the type I error rates were also evaluated considering three criteria for attributing weights to one or two variables. The best results were obtained with the modified Di-zm index 1, where the power of the index reached 46% while the MM reached power of only 31.5% in the evaluated conditions. Attributing a lower weight to a variable, not defined a priori, increased power but resulted in a significant increase in the type I error rates of the simple indices when under zero covariance.

Keywords: Desirability index, principal component analysis, maximum family-wise error.