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10 ABSTRACT

Model evaluation plays a central role in chemical modeling. Model population 11 analysis (MPA), a general framework for designing new types of chemometrics 12 algorithms, has shown its advantage in the field of model evaluation. The core idea of 13 MPA is to statistically analyze the outputs of randomly generated sub-models to 14 extract interesting information from the data. One of the most obvious characteristics 15 of MPA-based methods is that they use multiple models instead of a single model for 16 model evaluation. In this review, we first described the concept of MPA, and then 17 discussed the application of MPA in model evaluation, including the relationship 18 between MPA and cross-validation, model comparison, randomization tests, model 19 stability, variable importance and sum of rank differences. Finally, we prospected the 20 potential application of MPA in model evaluation. 21

Keywords: Model population analysis; Model evaluation; Model comparison; Modelselection.

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