A rigorous methodology is developed that addresses numerical and statistical issues when developing group contribution (GC) based property models such as regression methods, optimization algorithms, performance statistics, outlier treatment, parameter identifiability, and uncertainty of the prediction. The methodology is evaluated through development of a GC method for the prediction of the heat of combustion ($\Delta H_{co}$) for pure components. The results showed that robust regression lead to best performance statistics for parameter estimation. The bootstrap method is found to be a valid alternative to calculate parameter estimation errors when underlying distribution of residuals is unknown. Many parameters (first, second, third order group contributions) are found unidentifiable from the typically available data, with large estimation error bounds and significant correlation. Due to this poor parameter identifiability issues, reporting of the 95% confidence intervals of the predicted property values should be mandatory as opposed to reporting only single value prediction, currently the norm in literature. Moreover, inclusion of higher order groups (additional parameters) does not always lead to improved prediction accuracy for the GC-models; in some cases, it may even increase the prediction error (hence worse prediction accuracy). However, additional parameters do not affect calculated 95% confidence interval. Last but not least, the newly developed GC model of the heat of combustion ($\Delta H_{co}$) shows predictions of great accuracy and quality (the most data falling within the 95% confidence intervals) and provides additional information on the uncertainty of each prediction compared to other $\Delta H_{co}$ models reported in literature.

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