A Correlation and an Artificial Neural Network for the Second Virial Coefficient of Organic and Inorganic Compounds

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The estimation of the second virial coefficient is generally based on the corresponding states principle and takes into account semiempirical correlating methods that are usually valid only for nonpolar gases or small polar molecules. Thus, in this work we present a correlation of the second virial coefficient valid for organic and inorganic compounds. Firstly, we statistically analyzed more than 6000 experimental points collected from literature. The data was deeply investigated with a factor analysis approach in order to identify the most significant parameters that influence the second virial coefficient. The factor analysis, combined with physical considerations, allowed us to find a simple equation that gives lower deviations with respect of those available in literature. Furthermore, we built the architecture of an artificial neural network to improve the prediction capability of the second virial coefficient; in particular, we used a multi-layer perceptron with a single hidden layer. We trained, validated, and tested several configurations of the neural network in order to obtain the number of neurons in the hidden layer that minimizes the deviations between experimental and calculated points. Results show that the artificial neural network is able to predict the second virial coefficient with greater accuracy than that of correlations available in literature.