Data mining software development for high-throughput screening of heterogeneous catalysts

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Large amounts of experimental data are simultaneously accumulated in a relatively short period of time by High-Throughput Experimentation (HTE). The large number of variables in play and the applications of complex optimization algorithms for the experimental design make the direct human interpretation of data derived from HTE very difficult. Artificial neural networks using multi-layer perceptrons have been successfully applied to modeling for new catalyst development. But the complexity of the network significantly affects its learning capability and generalization. So we propose a new self-organizing algorithm of artificial neural networks that always matches the complexity of the model to that of the problem. Then the algorithm is applied to the data mining software for high-throughput screening of heterogeneous catalysts.
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