

Self-organizing neural networks for high-throughput screening system

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For last several years, the great improvement of combinatorial chemistry has enabled synthesis of a huge amount of chemical compounds in a short time. Therefore HTS (High-throughput screening) is required for dealing with the enormous materials. But human intervention (trial & error method) in data mining of experimental results lowers the efficiency of HTS. So self-organizing neural networks that rapidly and accurately transact experimental results are needed for the improvement in HTS performance.

The self-organizing algorithms that were previously developed have randomness which causes unreliability of algorithms which means different trials give quite different performances. However, in the proposed algorithm, randomness of neural networks is effectively eliminated by the optimized construction. So this algorithm always matches the complexity of the model to that of the problem very well. As a result, this algorithm can find a near-optimal network which is compact and shows good generalization performance without human intervention.

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