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一种用于计算机辅助产物设计中基于BP-NN优化问题的求解方法

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摘要 Because of the powerful mapping ability, back propagation neural network (BP-NN) has been employed in computer-aided product design (CAPD) to establish the property prediction model. The backward problem in CAPD is to search for the appropriate structure or composition of the product with desired property, which is an optimization problem. In this paper, a global optimization method of using the a BB algorithm to solve the backward problem is presented. In particular, a convex lower bounding function is constructed for the objective function formulated with BP-NN model, and the calculation of the key parameter α is implemented by recurring to the interval Hessian matrix of the objective function. Two case studies involving the design of dopamine β-hydroxylase (DβH) inhibitors and linear low density polyethylene (LLDPE) nano composites are investigated using the proposed method.

关键词 计算机辅助设计； CAPD； 智能； 产品设计； 优化设计； 化工； 制药； 神经网络； PNN；

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**A Method for Solving Computer-Aided Product Design Optimization Problem Based on Back Propagation Neural Network**

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**Abstract** Because of the powerful mapping ability, back propagation neural network (BP-NN) has been employed in computer-aided product design (CAPD) to establish the property prediction model. The backward problem in CAPD is to search for the appropriate structure or composition of the product with desired property, which is an optimization problem. In this paper, a global optimization method of using the a BB algorithm to solve the backward problem is presented. In particular, a convex lower bounding function is constructed for the objective function formulated with BP-NN model, and the calculation of the key parameter α is implemented by recurring to the interval Hessian matrix of the objective function. Two case studies involving the design of dopamine β-hydroxylase (DβH) inhibitors and linear low density polyethylene (LLDPE) nano composites are investigated using the proposed method.

**Key words** computer-aided product design (CAPD); back propagation neural network (BP-NN); a BB algorithm; convex lower bounding function; interval Hessian matrix.

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