Title: Automatic Selection of Optimal Configuration of Artificial Neural Networks

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Objectives: A novel mixed-integer nonlinear programming (MINLP) based mathematical formulation for artificial neural network (ANN) analysis which minimises the complexity of the configuration of the network is presented.

Methods: Traditionally, the configuration of the artificial neural network (ANN), which comprises of the number of hidden layers, number of nodes in the hidden layers and the interconnections between the nodes, is fixed and then an optimisation problem is solved to minimise the error between the observed data and model predictions. In case the error is too large, the configuration is changed and another optimisation problem is solved, this procedure is repeated until an acceptable error is obtained. A reduction in the number of hidden layers and nodes can result in an increase in the error whereas increasing the number of hidden layers and nodes can lead to over-fitting or over-learning [3]. A reduction in the number of interconnections can reduce the degeneracy in the input-output relationships and may also provide some insight into the behaviour of the model. Selection of the optimal number of layers, nodes and interconnections can be formulated as a combinatorial problem by introducing 0-1 binary variables to represent existence or not of a layer, node or interconnection. This results in a mixed integer nonlinear program (MINLP) where the objective is to minimise the complexity of the network subject to equality constraints, representing the transformations across the network, and an inequality constraint on the upper bound on the error [1]. This generic mathematical formulation also allows incorporation of any logical constraints and other constraints, such as, that the drug concentration is always positive. The solution of this problem is given by an optimal network configuration which meets the error criteria as well as any other constraints included in the formulation.

Results: This methodology was applied to a kinetic and dynamic dataset available in open literature for a CNS compound [2]. A comparison of the observed and predicted data is shown in figures 1 and 2.

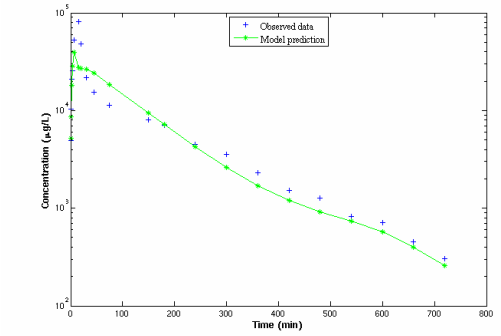

Figure 1: Observed and predicted concentration versus time

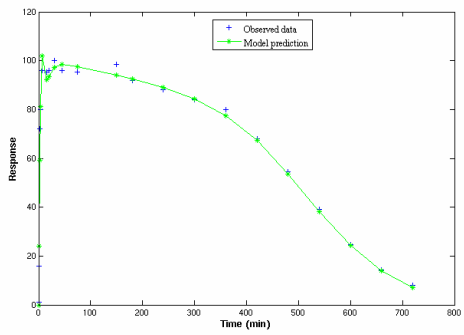

Figure 2: Observed and predicted response versus time

Conclusions: A new mathematical formulation for automatic selection of the configuration of the network with minimum complexity has been presented and tested on an example. The main advantage of this approach is that redundant nodes, layers and interconnections are eliminated and a compact representation of the input-output correlations is obtained.

References:

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[2] Gabrielsson, J. and Weiner, D. (2000) Pharmacokinetic and pharmacodynamic data analysis: concepts & applications, 3rd ed., Taylor and Francis, p829.

[3] Gobburu, J.V.S. and Chen, E.P. (1996) Artificial neural networks as a novel approach to integrated pharmacokinetic-pharmacodynamic analysis, J. Pharmaceutical Sciences, 85, 505-510.