A hybrid genetic programming neural network classifier for use in drug discovery

ABSTRACT

We have shown genetic programming (GP) can automatically fuse given classifiers of diverse types to produce a hybrid classifier. Combinations of neural networks, decision trees and Bayes classifiers have been formed.

On a range of benchmarks the evolved multiple classifier system is better than all of its components. Indeed its Receiver Operating Characteristics (ROC) are better than [Scott et al., 1998]'s "Maximum Realisable Receiver Operating Characteristics" MRROC (convex hull)

An important component in the drug discovery is testing potential drugs for activity with P450 cell membrane molecules. Our technique has been used in a blind trial where artificial neural networks are trained by Clementine on P450 pharmaceutical data. Using just the trained networks, GP automatically evolves a composite classifier. Recent experiments with boosting the networks will be compared with genetic programming.