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Plenary Session

Invited Talk:

Application of genetic programming in drug lead discovery

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We have shown genetic programming (GP) can fuse given classifiers of diverse types to produce a hybrid classifier. Automatic combinations of neural networks, decision trees and Bayes classifiers have been evolved, which, on a range of real-world and synthetic machine learning benchmarks are better than all of their constituent components.

Machine learning techniques have had mixed success in the drugs industry. Here we investigate machine learning techniques to give predictive models of activity of novel chemicals against specific disease targets.

Initial studies have concentrated upon prediction activity of potential drugs with P450 cell membrane molecules. P450 is important in uptake of drugs within cells.

High throughput screening (HTS) data is being used as training data for supervised learning by artificial neural networks within the Clementine data mining tool. Using just the trained networks, GP automatically evolves a composite classifier. Recent experiments with boosting the networks will be compared with genetic programming.

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