

Application of Data Pipelining Technology in Cheminformatics and Bioinformatics

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Application of Data Pipelining Technology in Cheminformatics and Bioinformatics

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Abstract:

Data pipelining is the processing, analysis, and mining of large volumes of data through a branching network of computational steps. A data pipelining system consists of a collection of modular computational components and a network for streaming data between them. By defining a logical path for data through a network of computational components and configuring each component accordingly, a user can create a protocol to perform virtually any desired function with data and extract knowledge from them. A set of data pipelines were constructed to explore the relationship between the biodegradability and structural properties of halogenated aliphatic compounds in a data set in which each compound has one degradation rate and nine structure-derived properties. After training, the data pipeline was able to calculate the degradation rates of new compounds with a relatively accurate rate. A second set of data pipelines was generated to cluster new DNA sequences. The data pipelining technology was applied to identify a core sequence to represent a DNA cluster and construct the 95% confidence distance interval for the cluster. The result shows that 74% of the DNA sequences were correctly clustered and there was no false clustering.

Description:

Submitted to the faculty of the University Graduate School in partial fulfillment of the requirements for the degree Master of Sciences in the School of Informatics Indiana University December 2002

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