

Annotated Bibliography

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References

- [1] Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, and Clifford Stein. *Introduction to Algorithms, Third Edition*. The MIT Press, 3rd edition, 2009.

This is a popular algorithms textbook which is well-cited. In particular, Part VI on graph algorithms will be of interest. Chapter 26 discusses flow networks and introduces commonly used notation. It formally describes the problem of obtaining a maximum flow and its equivalence to obtaining a minimum cut. The classical method of Ford and Fulkerson’s algorithm for finding a maximum flow is described, and it includes several examples. Additional methods for obtaining a maximum flow, including the push-relabel method, are also described. The chapter notes include additional references to specific articles which may be helpful, such as those of historical interest (the article in which an algorithm was originally proposed) as well as state-of-the-art improvements (more recent articles to improve the approach).

- [2] Ella Gale, Leo Lobski, and Fabio Zanasi. A categorical model for organic chemistry. *Theor. Comput. Sci.*, 1032(C), April 2025.

This article presents a novel approach to modeling organic chemistry using category theory. The authors introduce a categorical framework that captures the structure and behavior of organic molecules and their reactions. The model allows for the representation of chemical reactions as morphisms between objects, providing a new perspective on retrosynthesis and disconnection rules. The paper includes several examples to illustrate the application of the categorical model to various organic chemistry problems. This work has potential implications for computational chemistry and the development of new algorithms for chemical synthesis planning. With a goal of this Junior IS project being to explore the intersection of computer science and chemistry, this article provides a foundational understanding of how advanced mathematical concepts can be applied to chemical problems.

- [3] Barry O’Sullivan, Alex Ferguson, and Eugene C. Freuder. Boosting constraint satisfaction using decision trees. In *Proceedings of the 16th IEEE International Conference on Tools with Artificial Intelligence*, ICTAI ’04, page 646–651, USA, 2004. IEEE Computer Society.

This article explores the use of decision trees to enhance the efficiency of constraint satisfaction problems (CSPs). The authors propose a hybrid approach that combines decision tree learning with traditional backtrack search methods. By leveraging knowledge from previously solved instances of CSPs, the method aims to reduce the search space and improve solution times. The paper presents experimental results demonstrating significant performance improvements, often achieving nearly an order-of-magnitude reduction in search effort. This approach is particularly relevant for applications such as product configuration and interactive constraint solving, where problems are solved repeatedly over time. The article provides valuable insights into how machine learning techniques can be integrated with constraint satisfaction to optimize problem-solving processes. More within current proposals for Junior IS project that is exploring building an organic chemistry tool using decision trees there is a need to understand constraint satisfaction, making this article a useful resource.