Annotated Bibliography

Raelyn Brooks

September 3, 2025

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.

[4] Pouya Shati, Eldan Cohen, and Sheila McIlraith. Optimal decision trees for interpretable clustering with constraints. In *Proceedings of the Thirty-Second International Joint Conference on Artificial Intelligence*, IJCAI '23, 2023.

This article presents a novel approach to constrained clustering using decision trees, aiming to enhance interpretability while adhering to user-defined constraints. The authors introduce a SAT-based framework that allows for the incorporation of domain-specific knowledge through constraints, improving clustering accuracy. The proposed method addresses the limitations of previous approaches by providing strong theoretical guarantees on solution quality and supporting clustering constraints. Experimental results demonstrate the effectiveness of the framework in producing high-quality and interpretable clustering solutions across various datasets. This work is particularly relevant for applications where interpretability is crucial, such as in healthcare and finance, and contributes to the broader field of explainable artificial intelligence (XAI). Given the focus on decision trees in the current Junior IS project exploring organic chemistry tools, this article offers important insights into creating models that are both effective and understandable. Moreover, the emphasis on constraints aligns with the need to incorporate chemical knowledge into the decision-making process.

[5] Victor F.C. Souza, Ferdinando Cicalese, Eduardo Sany Laber, and Marco Molinaro. Decision trees with short explainable rules. *Theor. Comput. Sci.*, 1047(C), August 2025.

This article investigates the construction of decision trees that produce short and explainable rules for classification tasks. The authors propose a novel approach to building decision trees that prioritize interpretability without significantly compromising predictive accuracy. The paper introduces new metrics for evaluating the explainability of decision tree models and presents algorithms designed to optimize these metrics. Experimental results demonstrate

that the proposed methods can generate decision trees with concise rules while maintaining competitive performance compared to traditional decision tree algorithms. This work is particularly relevant in contexts where model transparency is crucial, such as in healthcare and finance. The article provides valuable insights into balancing the trade-off between model complexity and interpretability in machine learning. Given the focus on decision trees in the current Junior IS project exploring organic chemistry tools, this article offers important perspectives on creating models that are both effective and understandable.