Albert-Ludwigs-Universität Freiburg (ALU) Intoduction

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The University & The Faculty

The university was founded in 1457, and is one of the oldest German universities and one of the nation's leading research and teaching institutions. The university is one of the 9 specially awarded research universities in Germany.

The Institute of Computer Sciences (together with the the faculty of Applied Sciences) was founded in 1995, having now 16 Chairs in the covering a wide range of activities like Artificial Intelligence and Robotics to Software Engineering and Image Analysis.

The Chair of Machine Learning & Natural Language Processing

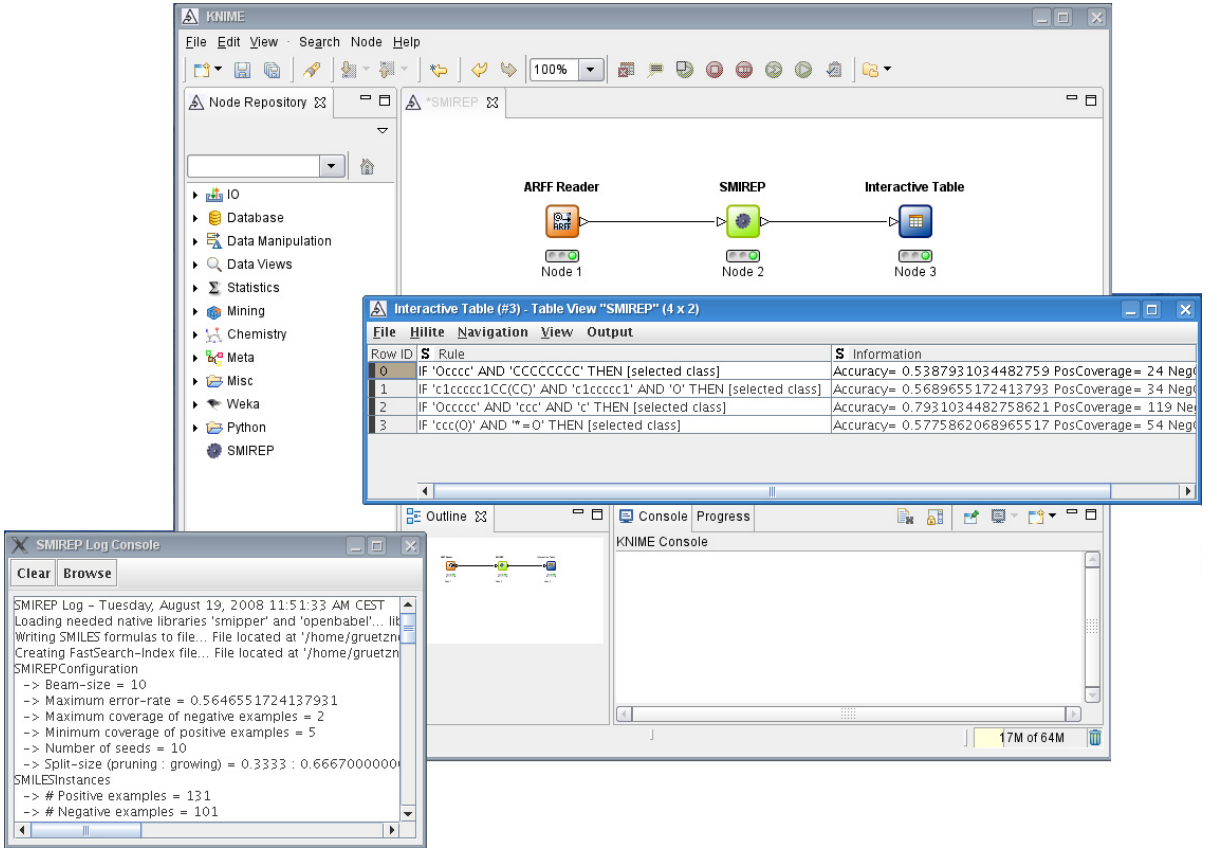
- Former Chair: Prof. Luc De Raedt (now KU Leuven)
- Former Assistant: Prof. Stefan Kramer (now TUM Munich)
- Currently: Acting Head of the group (04. - 08.2008) and Assistant:
  - Andreas Karwath

Relevant Disciplines

- Graph Mining and (Q)SAR:
  - MolFea (by former members: De Readt, Kramer & Helma)
  - SMIREP (Karwath & De Readt)
- Mining and Learning from Complex Objects
  - REAL (Aligning Complex Objects) (Karwath & Kersting)
  - BoostedREAL (Learning Distances of Complex Objects) (Karwath & Kersting)
- Machine Learning & Validation Techniques in General

Ongoing Research I

- SMIREP/SMIPPER
  - Simple, yet powerful and fast heuristic tool to perform (Q)SAR predictions based on SMILES codes
  - Currently, a new version integrating with OpenBabel & KNIME:



Ongoing Research II

- Graph Seritation & BoostedREAL
  - Graph Seritation (Hancock et al 2005) allows to establish distances between graphs, based on semi-definite programming (by converting simple graphs into sequences)
  - BoostedREAL allows to learn distances of atoms within sequences, based on alignments and a learnable cost function.
  - Currently, we are:
    - Upgrading the Hancock approach to be used with more complex graphs, such as molecules
    - This should enable to establish distances for clustering as well to be used in determination of applicability domains

Relevant Publications

- K. Kersting, L. De Raedt, B. Gutmann, A. Karwath and N. Landwehr: *Relational Sequence Learning*. In: L. De Raedt, P. Frasconi, K. Kersting and S. Muggleton (eds.), Probabilistic Inductive Logic Programming. Lecture Notes in Computer Science 4911, Springer-Verlag, pp. 28-55, 2008.

- A. Karwath and K. Kersting. *Relational Sequence Alignments and Logos*. In: S. Muggleton, R. Otero, and Alireza Tamaddoni-Nezhad (Eds.): Proc. 16th International Conference on Inductive Logic Programming (ILP'06). Lecture Notes in Artificial Intelligence 4455, pp.290-303, 2007.

- A. Karwath and L. De Raedt. *SMIREP: Predicting Chemical Activity from SMILES*. In: Journal of Chemical Information and Modeling. 46(6), pp. 2432-2444. 2006.[1]

- A. Karwath and L. De Raedt. *Predictive Graph Mining*. In: E. Suzuki and S. Arikawa (Eds.): Proc. 7th International Conference of Discovery Science, DS 2004. Lecture Notes in Artificial Intelligence 3245. pp. 1-15. Springer-Verlag. 2004. [1]

1 : (Q)SAR specific