Dr. Lars Rosenbaum

Background

- Since January 2010: Research assistant at the Center for Bioinformatics (ZBIT), Department of Cognitive Systems, University of Tübingen
- August 2006 - July 2007: Exchange student at Uppsala University, Sweden
- October 2003 - December 2009: Studies of Bioinformatics at the University of Tübingen

Research Interests

My research focuses on machine learning, feature selection and statistical analysis in various application fields, such as multiomics, cheminformatics, and automotive applications. Particularly, I am interested in the following topics:

- Interpretable machine learning models for cheminformatic problems
- Visualization techniques for interpretable machine learning models
- Large scale learning in Chem-/Bioinformatics
- Statistical methods for the analysis of multiomics data
- Machine learning in automotive applications
- Machine learning in computer vision

Projects

Current:

- Machine learning algorithms/Proteochemometric models for multi-target drug development
- Development of interpretable models for mining chemical databases
- Implementation of a (parallelized) machine learning library for large scale learning in cheminformatics
- Improvement of optimal assignment methods for cheminformatic problems
- Kompetenznetz Diabetes mellitus: Statistical analysis of multiomics and development of a central data management platform based on Plone

Finished:

- Simulation and prediction of engine parameters in coorperation with the Daimler AG

Software

• InCroMAP: Integrated analysis of Cross-platform MicroArray, Metabolomics and Pathway data.
• OA Edge Optimization: Optimization and visualization of the edge weights in optimal assignment methods for virtual screening
• jCompoundMapper: An open source Java library and command-line tool for chemical fingerprints
• HeatmapColoring: Rudimentary tool for the visualization of chemical information contained in models trained with LIBLINEAR

Awards and honors

- 2003: Award for outstanding work in mathematics by Otto-Hahn-Gymnasium Landau (Secondary school).

Publications

[1] Alexander Dörr, Lars Rosenbaum, and Andreas Zell. A ranking method for the concurrent learning of compounds with various activity profiles. *J. Cheminf.*, 7(1), January 2015.

[2] Johannes Eichner, Lars Rosenbaum, Clemens Wrzodek, Hans-Ulrich Häring, Andreas Zell, and Rainer Lehmann. Integrated enrichment analysis and pathway-centered visualization of metabolomics, proteomics, transcriptomics, and genomics data by using the InCroMAP software. *Journal of Chromatography B*, May 2014. [DOI | link]

[3] Peiyuan Yin, Andreas Peter, Holger Franken, Xinjie Zhao, Sabine Sarah Neukamm, Lars Rosenbaum, Marianna Lucio, Andreas Zell, Hans-Ulrich Häring, Guowang Xu, and Rainer Lehmann. Pre-analytical aspects and sample quality assessment in metabolomics studies of human blood. *Clinical Chemistry*, 59(5):833--845, May 2013.

[4] R. Lehmann, H. Franken, S. Dammeier, L. Rosenbaum, K. Kantartzis, A. Peter, A. Zell, P. Adam, J. Li, G. Xu, A. Königsrainer, J. Machann, F. Schick, M. Hrabe de Angelis, M. Schwab, H. Staiger, E. Schleicher, A. Gastaldelli, A. Fritsche, H.-U. Häring, and N. Stefan. Circulating lyso-phosphatidylcholines are markers of ametabolically benign nonalcoholic fatty liver. *Diabetes Care*, 36(8):2331--2338, 2013.

[5] Lars Rosenbaum, Alexander Dörr, Matthias R. Bauer, Frank M. Boeckler, and Andreas Zell. Inferring multi-target QSAR models with taxonomy-based multi-task learning. *J. Cheminf.*, 5:33, 2013.

[6] Lars Rosenbaum, Andreas Jahn, Alexander Dörr, and Andreas Zell. Optimization and visualization of the edge weights in optimal assignment methods for virtual screening. *BioData Mining*, 6:7, 2013.

[7] E. Kenar, H. Franken, L. Rosenbaum, R. Lehmann, S. Forcisi, K. Wörmann, M. Lucio, A. König, J. Rahnenführer, P. Schmidt-Kopplin, H.-U. Häring, A. Zell, and O. Kohlbacher. Mit bioinformatik zu biomarkern. *Medizinische Welt*, 63(5):245--250, 2012.

[8] Lars Rosenbaum, Andreas Jahn, and Andreas Zell. Optimizing the edge weights in optimal assignment methods for virtual screening with particle swarm optimization. In Mario Giacobini, Leonardo Vanneschi, and William Bush, editors, *Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics*, volume 7246 of *Lecture Notes in Computer Science*, pages 26--37. Springer Berlin / Heidelberg, 2012. [link]

[9] K. Wörmann, M. Lucio, S. Forcisi, S.S. Heinzmann, E. Kenar, H. Franken, L. Rosenbaum, P. Schmitt-Kopplin, O. Kohlbacher, A. Zell, H.-U. Häring, and R. Lehmann. Metabolomics in der Diabetesforschung. *Der Diabetologe*, pages 1--5, 2012. 10.1007/s11428-011-0778-9. [link]

[10] Georg Hinselmann, Andreas Jahn, Nikolas Fechner, Lars Rosenbaum, and Andreas Zell. Approximation of graph kernel similarities for chemical graphs by kernel principal component analysis. In Clara Pizzuti, Marylyn D. Ritchie, and Mario Giacobini, editors, *Evolutionary Computation, Machine Learning and Data Mining in Bioinformatics*, volume 6623 of *Lecture Notes in Computer Science*, pages 123--134. Springer Berlin Heidelberg, 2011.

[11] Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, and Andreas Zell. Fast data mining with sparse chemical graph fingerprints by estimating the probability of unique patterns. In Michel Verleysen, editor, *Proceedings of 19th European Symposium on Artificial Neural Networks (ESANN 2011)*, pages 417--422, Bruges, Belgium, 2011.

[12] Georg Hinselmann, Lars Rosenbaum, Andreas Jahn, Nikolas Fechner, Claude Ostermann, and Andreas Zell. Large-scale learning of structure-activity relationships using a linear support vector machine and problem-specific metrics. *Journal of Chemical Information and Modeling*, 52:203--213, 2011.

[13] Georg Hinselmann, Lars Rosenbaum, Andreas Jahn, Nikolas Fechner, and Andreas Zell. jcompoundmapper: An open source java library and command-line tool for chemical fingerprints. *Journal of Cheminformatics*, 3(3), 2011.

[14] Andreas Jahn, Georg Hinselmann, Lars Rosenbaum, Nikolas Fechner, and Andreas Zell. Boltzmann-enhanced flexible atom-pair kernel with dynamic dimension reduction. *Molecular Informatics*, 30(4):307--315, 2011.

[15] Andreas Jahn, Lars Rosenbaum, Georg Hinselmann, and Andreas Zell. 4D Flexible Atom-Pairs: An efficient probabilistic conformational space comparison for ligand-based virtual screening. *Journal of Cheminformatics*, 3(23), 2011.

[16] Lars Rosenbaum, Georg Hinselmann, Andreas Jahn, and Andreas Zell. Interpreting linear support vector machine models with heat map atom and bond coloring. *Journal of Cheminformatics*, 3:11, 2011.

[17] Nikolas Fechner, Georg Hinselmann, Andreas Jahn, Lars Rosenbaum, and Andreas Zell. A Free-Wilson-like approach to analyze QSAR models based on graph decomposition kernels. *Molecular Informatics*, 29:491--497, 2010. [DOI | link]

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