

# Dr. Holger Fröhlich

## Background

1996 - 2002: Studies of Computer Science at University of Marburg  
1999: Exchange Student at Washington State University / USA  
May 2002 - Dec. 2002: Diploma thesis on "Feature Selection for Support Vector Machines by Means of Genetic Algorithms" at the Max-Planck-Institute for Biological Cybernetics, Tübingen, in the group of Prof. Dr. B. Schölkopf  
Since March 2003: Research assistant / PhD student at the Centre for Bioinformatics Tübingen (ZBIT) in the group of Prof. Dr. A. Zell  
Since June 2006: Postdoctoral researcher at the German Cancer Research Center (DKFZ) in the group of Prof. Dr. A. Poustka>



## Research Interests

Statistical data analysis and Kernel Methods in Bio- and Chemoinformatics, Support Vector Machines

## Publications

### Journal Articles

*Kernel Functions for Attributed Molecular Graphs - A New Similarity Based Approach To ADME Prediction in Classification and Regression*

H. Fröhlich, J. Wegner, F. Sieker, A. Zell, *QSAR & Combinatorial Science*, 25(4):317 - 326, 2006

*Data and Graph Mining in Chemical Space for ADME and Activity Data Sets*

J. Wegner, H. Fröhlich, H. Mielenz, A. Zell, *QSAR & Combinatorial Science*, 25(3):205 - 220, 2006

*Towards Optimal Descriptor Subset Selection with Support Vector Machines in Classification and Regression*

H. Fröhlich, J. Wegner, A. Zell, *QSAR & Combinatorial Science*, 23:311 - 318, 2004

*Feature Selection for Descriptor based Classification Models: Part I - Theory and GA-SEC Algorithm*

J. Wegner, H. Fröhlich, A. Zell, *Journal of Chemical Information and Computer Science*, 44:921 - 930, 2004

*Feature Selection for Descriptor based Classification Models: Part II - Human Intestinal Absorption (HIA)*

J. Wegner, H. Fröhlich, A. Zell, *Journal of Chemical Information and Computer Science*, 44:931 - 939, 2004

*Feature Selection for Support Vector Machines using Genetic Algorithms*

H. Fröhlich, O. Chapelle, B. Schölkopf, *International Journal on Artificial Intelligence: Special Issue on Selected Papers from the 15th IEEE International Conference on Tools with Artificial Intelligence 2003*, 13(4):791 - 800, 2004

## Conference Papers (peer reviewed)

*Gene Regulatory Network Inference via Regression Based Topological Refinement*

Jochen Supper, Holger Fröhlich and Andreas Zell, *Asia-Pacific Bioinformatics Conference (APBC 2007)*, Hong Kong, accepted

*Inferring Gene Regulatory Networks by Machine Learning Methods*

Jochen Supper, Holger Fröhlich, Christian Spieth, Andreas Dräger and Andreas Zell, *Asia-*

Pacific Bioinformatics Conference (APBC 2007), Hong Kong, accepted

*Vibration-based Terrain Classification Using Support Vector Machines*

C. Weiss, H. Fröhlich and A. Zell, Proc. IEEE/RSJ Int. Conf. Intel. Robots and Systems (IROS 2006), 2006, accepted

*Kernel Based Functional Gene Grouping*

H. Fröhlich, N. Speer, C. Spieth, and A. Zell, Proc. Int. Joint Conf. on Neural Networks (IJCNN), pp. 6886 - 6891, 2006

*Functional Distances for Genes Based on GO Feature Maps and their Application to Clustering*

N. Speer, H. Fröhlich, C. Spieth, and A. Zell, Proc. Symp. on Comp. Int. in Bioinformatics and Comp. Biology (CIBCB), pp. 142-149, 2005

*Optimal Assignment Kernels for Attributed Molecular Graphs*

H. Fröhlich, J. Wegner, F. Sieker, A. Zell, Proc. Int. Conf. on Machine Learning (ICML), pp. 225 - 232, 2005

*Which Features Trigger Action Potentials in Cortical Neurons in Vivo?*

H. Fröhlich, B. Naundorf, M. Volgushev, F. Wolf, Proc. Int. Joint Conf. on Neural Networks (IJCNN), pp. 250 - 255, 2005

*Functional Grouping of Genes Using Spectral Clustering and Gene Ontology*

N. Speer, H. Fröhlich, A. Zell, Proc. Int. Joint Conf. on Neural Networks (IJCNN), pp. 298 - 303, 2005

*Assignment Kernels For Chemical Compounds*

H. Fröhlich, J. Wegner, A. Zell, Proc. Int. Joint Conf. on Neural Networks (IJCNN), pp. 913 - 918, 2005

*Efficient Parameter Selection for Support Vector Machines in Classification and Regression via Model-Based Global Optimization*

H. Fröhlich, A. Zell, Proc. Int. Joint Conf. on Neural Networks (IJCNN), pp. 1431 - 1438, 2005

*Learning to Detect Proximity to a Gas Source with a Mobile Robot*

A. Lilienthal, H. Ulmer, H. Fröhlich, A. Stützle, F. Werner, A. Zell, IEEE/RSJ Int. Conf. on Intelligent Robots and Systems (IROS 2004), pp. 1444 - 1449, 2004

*Feature Subset Selection for Support Vector Machines by Incremental Regularized Risk Minimization*

H. Fröhlich, A. Zell, Proc. Int. Joint Conf. on Neural Networks (IJCNN) 2004, 3:2041 - 2046, 2004

*Gas Source Declaration with a Mobile Robot*

A. Lilienthal, H. Ulmer, H. Fröhlich, A. Stützle, F. Werner, A. Zell, Proceedings of the IEEE International Conference on Robotics and Automation (ICRA 2004), pp. 1430 - 1435, 2004

*Feature Selection for Support Vector Machines by Means of Genetic Algorithms*

H. Fröhlich, O. Chapelle, B. Schölkopf, Proc. Int. Conf. on Tools with Artificial Intelligence, pp. 142 - 148, 2003

## **Thesis**

*Feature Selection for Support Vector Machines by Means of Genetic Algorithms, Master's thesis, University of Marburg, 2002>*

## **Software**

*Feature Selection for SVMs via Genetic Algorithms, RFE, Fisher Score, Relief-F (C++)*

*NEW VERSION 3.1: Optimal Assignment Kernels, Optimal Assignment Kernels for reduced graphs, Marginalized Graph Kernels, Hungarian method (JAVA)*

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