# Max Horn

Machine Learning in Healthcare  $\cdot$  Deep Learning  $\cdot$  Interpretable ML Time Series  $\cdot$  Probabilistic Modelling

### **EDUCATION**

Mar. 2018 - Nov. 2021<sup>1</sup>

PH.D. IN MACHINE LEARNING AND COMPUTATIONAL BIOLOGY

ETH ZÜRICH, SWITZERLAND

I develop deep learning methods for real world medical time series data where I focus on the property of irregular sampling. Furthermore, I am interested in dimensionality reduction using methods from topology in order to preserve the underlying manifold structure of the data. I also use probabilistic modelling to gain insights into real world biological and chemical problems.

Supervisor: Prof. Dr. Karsten M. Borgwardt

Oct. 2015 - Oct. 2017

M.Sc. IN MOLECULAR BIOSCIENCES: SYSTEMS BIOLOGY HEIDELBERG UNIVERSITY, GERMANY

Thesis title: "Fully Bayesian Modelling of Covariate Effects on the Gut Microbiome Using Horseshoe Priors for

Sparsity Induction"

Supervisors: Prof. Dr. Ursula Kummer, Dr. Frederik Graw & Prof. Eran Elinav

Final grade: 1.0/very good

OCT. 2012 - OCT. 2015

**B.Sc.** Molecular Biotechnology

Heidelberg University, Germany

Thesis title: "Clustering and Scoring the Druggability of Transient Protein Pockets"

Supervisor: Prof. Dr. Rebecca Wade

Final grade: 1.5/very good

Oct. 2004 – Jul. 2012

GENERAL UNIVERSITY ENTRANCE QUALIFICATION (ABITUR) GYMANSIUM GERABRONN, GERMANY

Final grade: 1.5/very good, awards for excellent performance in mathematics and physics

### **PUBLICATIONS**

Authors who equally contributed to a publication are marked with a †.

Conference and Journal Publications

- 1. **Max Horn**, Michael Moor, Christian Bock, Bastian Rieck, and Karsten Borgwardt. Set Functions for Time Series. In *Proceedings of the 37<sup>th</sup> International Conference on Machine Learning (ICML)*, 2020
- 2. Michael Moor<sup>†</sup>, **Max Horn**<sup>†</sup>, Bastian Rieck, and Karsten Borgwardt. Topological Autoencoders. In *Proceedings of the 37<sup>th</sup> International Conference on Machine Learning (ICML)*, 2020
- 3. Caroline Weis<sup>†</sup>, **Max Horn**<sup>†</sup>, Bastian Rieck<sup>†</sup>, Aline Cuénod, Adrian Egli, and Karsten Borgwardt. Topological and kernel-based microbial phenotype prediction from MALDI-TOF mass spectra. In *Bioinformatics* 36, 2020
- 4. Stephanie L. Hyland<sup>†</sup>, Martin Faltys<sup>†</sup>, Matthias Hüser<sup>†</sup>, Xinrui Lyu<sup>†</sup>, Thomas Gumbsch<sup>†</sup>, Cristóbal Esteban, Christian Bock, **Max Horn**, Michael Moor, et al. Machine learning for early prediction of circulatory failure in the intensive care unit. In *Nature Medicine 26* (3), 2019
- Michael Moor, Max Horn, Bastian Rieck, Damian Roqueiro, and Karsten Borgwardt. Early Recognition of Sepsis with Gaussian Process Temporal Convolutional Networks and Dynamic Time Warping. In Proceedings of the 4<sup>th</sup> Machine Learning for Healthcare Conference (MLHC), 2019
- 6. Bastian Rieck<sup>†</sup>, Matteo Togninalli<sup>†</sup>, Christian Bock<sup>†</sup>, Michael Moor, **Max Horn**, Thomas Gumbsch, and Karsten Borgwardt. Neural Persistence: A Complexity Measure for Deep Neural Networks Using Algebraic Topology. In *Proceedings of the 7<sup>th</sup> International Conference on Learning Representations (ICLR)*, 2019

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Expected graduation date

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7. Jotham Suez, Niv Zmora, Gili Zilberman-Schapira, Uria Mor, Mally Dori-Bachash, Stavros Bashiardes, Maya Zur, Dana Regev-Lehavi, Rotem Ben-Zeev Brik, Sara Federici, **Max Horn**, et al. Post-Antibiotic Gut Mucosal Microbiome Reconstitution Is Impaired by Probiotics and Improved by Autologous FMT. In *Cell* 174.6, 2018

- 8. Antonia Stank, Daria Kokh, **Max Horn**, Elena Sizikova, Rebecca Neil, Joanna Panecka, Stefan Richter, and Rebecca C Wade. TRAPP webserver: predicting protein binding site flexibility and detecting transient binding pockets. In *Nucleic acids research 45.W1*, 2017
- 9. Max C. Waldhauer, Silvan N. Schmitz, Constantin Ahlmann-Eltze, Jan G. Gleixner, Carolin C. Schmelas, Anna G. Huhn, Charlotte Bunne, Magdalena Büscher, **Max Horn**, et al. Backbone circularization of Bacillus subtilis family 11 xylanase increases its thermostability and its resistance against aggregation. In *Molecular BioSystems* 11 (12), 2015

#### Workshops and Preprint Publications

- 10. Michael Moor, **Max Horn**, Christian Bock, Karsten Borgwardt, Bastian Rieck. Path Imputation Strategies for Signature Models. In *Artemiss Workshop, ICML*, 2020
- 11. Caroline Weis<sup>†</sup>, **Max Horn**<sup>†</sup>, Bastian Rieck<sup>†</sup>, Aline Cuenod, Adrian Egli, Karsten Borgwardt. Kernel-based antimicrobial resistance prediction from MALDI-TOF mass spectra. In *Machine Learning for Global Health Workshop, ICML*, 2020
- 12. Stefan Ganscha, Vincent Fortuin, **Max Horn**, Eirini Arvaniti, and Manfred Claassen. Supervised learning on synthetic data for reverse engineering gene regulatory networks from experimental time-series. In *bioRxiv* 356477, 2018

### Honors and Awards

Apr. 2017 – Jun. 2017

## PROMOS SCHOLARSHIP

GERMAN ACADEMIC EXCHANGE SERVICE

for master's thesis project in the group of Prof. Eran Elinav, Weizmann Institute of Science, Israel

Sep. 2016 – Jan. 2017

### PROMOS SCHOLARSHIP

GERMAN ACADEMIC EXCHANGE SERVICE

for research project in the group of Prof. Manfred Claassen, ETH Zürich, Switzerland

Jun. 2016

MINT Excellence Finalist

Wiesloch, Germany

Participated in the assessment center of the MINT Excellence Fellowship and was rated as one of the top 300 applicants

Nov. 2014

GRAD PRIZE WINNER INTERNATIONAL GENETICALLY ENGINEERED MACHINE (IGEM) COMPETITION as participant in the Heidelberg 2014 team we won the Grand Prize and Special Prizes of the categories: Best Foundational Advance Project, Best Supporting Software, iGEMer's prize

### **PRESENTATIONS**

JUL. 2020

SET FUNCTIONS FOR TIME SERIES

 $37^{\text{th}}$  International Conference on Machine Learning

I presented our work on "Set Functions for Time Series" which proposes a novel way to handle irregularly-sampled time series by treating them as sets of observation tuples.

JUL. 2020

Understanding Neurons with Neurons

Machine Learning Summer School 2020

I presented my work on "Understanding Neurons with Neurons – Tackling Spike Sorting with Amortized Variational Inference" where I combine techniques from object recognition and object-centric representations with simulation-based inference to tackle the inverse problem of spike-sorting in neuroscience.

Mar. 2020

Predicting Stability of Fossil-Embedded DNA

MLCB GROUP SEMINAR

In this presentation I showed how probabilistic models can be used to model the stability of DNA in a Fossil-Embedded state. This research is part of an effort to improve long-term data storage in DNA.

Nov. 2019

TOPOLOGICAL AUTOENCODERS

Swiss Machine Learning Day

I presented our work on "Topological Autoencoders" which utilize concepts from topological data analysis in order to derive topology-preserving low-dimensional representations of high dimensional data.

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CLASSIFYING THE IRREGULAR Aug. 2019

BAYER AG, BERLIN

In "Classifying the Irregular - Learning with Sporadically Sampled Medical Time Series" I presented multiple efforts on how to design machine learning methods for irregularly-sampled time series which are omnipresent in the medical domain.

SCALABLE CLASSIFICATION OF IRREGULAR-SAMPLED TIME SERIES

MLCB GROUP SEMINAR

Here I presented preliminary results on our research into the application of set functions as a model for

irregularly-sampled time series.

DENSITY ESTIMATION IN MULTIMODAL TIME SERIES

MLCB GROUP SEMINAR

In "Density Estimation in Multimodal Time Series – A Joint Venture of Neural Processes and Normalizing Flows" I presented research on combining Neural Processes with Normalizing Flows for anomaly detection in time series.

### SKILLS

Excellent knowledge in Python, in the creation of packages and in the utilization of NumPy, pandas, Python Dask and JAX<sup>2</sup>.

> Good knowledge of C++ and experienced in the implementation of CUDA kernels for accelerating computations using GPUs<sup>3</sup>.

Excellent experience in the development and application of Deep Learning models in both TensorFlow and PyTorch<sup>4</sup>.

Excellent experience in probabilistic modelling, in particular in the utilization of probabilistic programming frameworks such as PyMC35.

Excellent technical skills in the maintenance of network infrastructures and Linux server environments and in setting up computation clusters using the SLURM scheduler.

Good knowledge of LaTex and experienced in the design of figures using TikZ.

## SOFTWARE

Command line tool for handling and distributing a queue of jobs among GPUs. simple-gpu-scheduler

☐ ExpectationMax/simple\_gpu\_scheduler ≈ 300 downloads/month

Implementation of Set Function for Time Series model in TensorFlow and Keras.

BorgwardtLab/Set Functions for Time Series ≈ 30 users

Implementation of **Topo**logical **A**uto**e**ncoders model in PyTorch.

 $\bigcirc$  BorgwardtLab/topological-autoencoders  $\approx$  25 users

Composable kernels for scikit-learn classes implemented in JAX. sklearn-jax-kernels

 $\square$  ExpectationMax/sklearn-jax-kernels  $\approx$  100 downloads/month

Medical time series datasets for deep learning implemented using TensorFlow Datasets. medical-ts-datasets

ExpectationMax/medical\_ts\_datasets

Models for analysing microbiome-covariate effects using hierarchical Dirichlet-Multinomial regression models with sparsity inducing Horseshoe priors.

S ExpectationMax/HorseshoeDMRegression

Time series datasets of the UEA and UCR repository for deep learning frameworks.

□ BorgwardtLab/uea\_ucr\_datasets

C++ Library for large-scale simulations of interacting bacterial populations using GPUs.

♠ ExpectationMax/bactSim

3/4

JUL. 2019

DEC. 2018

C++

Deep Learning

Probabilistic Modelling

Linux, HPC

LaTeX

SeFT

TopoAE

HorseshoeDMRegression

uea-ucr-datasets

bastSim

See projects simple-gpu-scheduler, sklearn-jax-kernels, and uea-ucr-datasets.

See project bactSim.

See projects SeFT, medical-ts-datasets and topological-autoencoders.

See project HorseshoeDMRegression.

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### SERVICE TO THE SCIENTIFIC COMMUNITY

### REVIEWING

TDA and Beyond NeurIPS Workshop (2020), NeurIPS (2020), AAAI (2021), MLHC (2020, 2019), ISMB (2020), Swiss Machine Learning Day (2019), ECML-PKDD (2019), Springer Machine Learning (2019)

#### **TEACHING**

Teaching assistant in Data Mining I – ETH Zürich (2019)

### Contributions to Open source software

- 🗘 tensorflow/tensorflow, 🗘 tensorflow/datasets, 🗘 hyperopt/hyperopt,
- $oldsymbol{\Omega}$  palantir/python-language-server,  $oldsymbol{\Omega}$  PyTorchLightning/pytorch-lightning,
- IDSIA/sacred

### EXTRACURRICULAR ACTIVITIES

### Machine Learning Summer School 2020

Online

Accepted as a full participant after competitive selection process (acceptance rate of  $\approx 13\%$ ). Presented work on "Understanding Neurons with Neurons – Tackling Spike Sorting with Amortized Variational Inference". Participated in two weeks of lectures and discussion rounds with many core players in the field of Machine Learning.

### MLFPN SUMMER SCHOOL 2019

MUTTENZ, SWITZERLAND

Accepted as participant of the Machine Learning Frontiers in Precision Medicine summer school which consisted of one week of lectures and discussions with experts at the intersection of machine learning and precision medicine.

## PERSONAL

Blogging

2020

2019

One of the most important aspects of this internet is that it allows us to share experiences and information with people of similar interests. I use my blog to help others who need to deal with similar issues and to share thoughts and summaries about research I am interested in.

NeoVim

As a passionate programmer, I optimized my editor to fit my needs and be compatible with the projects I am working on. NeoVim has become an essential tool of my day-to-day life. I write my lab book, papers, presentations and code in NeoVim and occasionally blog about how to extend it into a full-fledged IDE using modern approaches such as language servers.

Reverse Engineering

In my free time I enjoy working on small electronics projects, often involving reverse engineering old devices and making them function again or adapting their use case. In my most recent project I obtained an old Flip-dot display built in the 1970's, reverse engineered it in order to understand how to display digits and repurposed it as a minimal clock.

Recreational

As recreational activities I enjoy reading popular science and science fiction books and bouldering.