Philipp Renz

renz.ph@gmail.com | LinkedIn | GitHub | Google Scholar

Experience

Applied Scientist, LinzAG – Linz, Austria — Jan 2024 – present

- Developed machine learning models for energy demand/production forecasting.
- Implementation of backtesting environment for time series forecasting.
- Prediction of commodity prices.

Applied Science Intern, Amazon – London, UK — Oct 2022 – Apr 2023

- Conducted research on anomaly detection in sparse time series data.
- Developed benchmark to capture performance of anomaly detection methods.
- Proposed SOTA algorithm which strongly outperforms baseline methods.
- Published results in peer-reviewed conference paper.

Research assistant, Johannes Kepler University – Linz, Austria — Sept 2018 – Sept 2022

- Conducted research on machine learning applications in drug discovery.
- Developed metrics and benchmarks for generative models for molecules.
- Proposed SOTA deep learning model for retrosynthesis prediction.
- Published multiple peer-reviewed conference and journal papers.
- Held multiple courses (under/post-grad) on machine learning and bioinformatics.

Education

Johannes Kepler University, PhD in Artificial Intelligence — Sept 2018 – exp. Jan 2025

- Thesis: Generative Models in Drug Discovery: Advancing Evaluation and Retrosynthesis Prediction
- Advisors: Prof. Günter Klambauer, Prof. Sepp Hochreiter

Johannes Kepler University, MSc in Bioinformatics — Mar 2015 – Sept 2018

- Thesis: Data Driven Molecule Generation Using Deep Learning
- Advisor: Prof. Sepp Hochreiter, Co-Advisor: Prof. Günter Klambauer
- Graduated with distinction

Technical University Vienna, BSc in Technical Physics — Oct 2011 – Jan 2015

- Thesis: Flat Band Ferromagnetism in Thin Film $SrTiO_3$-(110)-heterostructures
- Advisor: Prof. Karten HELD
- Graduated with distinction

Publications

Diverse Hits in De Novo Molecule Design: Diversity-Based Comparison of Goal-Directed Generators
P. Renz, S. Luukkonen, G. Klambauer
Journal of Chemical Information and Modeling, 2024

On failure modes in molecule generation and optimization
P. Renz, D. Van Rompaey, J. Wegner, S. Hochreiter, G. Klambauer
Drug Discovery Today: Technologies, 2020

Low-count Time Series Anomaly Detection
P. Renz, K. Cutajar, N. Twomey, G. Cheung, H. Xie
IEEE International Workshop on Machine Learning for Signal Processing, 2023

Improving Few-and Zero-Shot Reaction Template Prediction Using Modern Hopfield Networks
P. Seidl, **P. Renz**, N. Dyubankova, P. Neves, J. Verhoeven, J. Wegner, M. Segler, S. Hochreiter, G. Klambauer
Journal of Chemical Information and Modeling, 2022

Fréchet ChemNet distance: A metric for generative models for molecules in drug discovery
K. Preuer, **P. Renz**, T. Unterthiner, S. Hochreiter, G. Klambauer Journal of Chemical Information and Modeling, 2018

Uncertainty Estimation Methods to Support Decision-Making in Early Phases of Drug Discovery
P. Renz, S. Hochreiter, G. Klambauer
Advances in Neural Information Processing Systems (NeurIPS), Workshop on Safety and Robustness in Decision-making, 2019

Understanding the Effects of Dataset Characteristics on Offline Reinforcement Learning
K. Schweighofer, M. Dinu, M. Hofmarcher, A. Bitto, **P. Renz**, V. Patil, S. Hochreiter
Advances in Neural Information Processing Systems (NeurIPS), Workshop on Deep Reinforcement Learning, 2021

Large-scale ligand-based virtual screening for SARS-CoV-2 inhibitors using deep neural networks
M. Hofmarcher, A. Mayr, E. Rumetshofer [and 8 others including **P. Renz**]
SSRN, 2020

Skills

- **Languages:** Python (advanced), R, C (familiar), SQL, LaTeX
- **Frameworks/Tools:** PyTorch, NumPy, scikit-learn, pandas, polars, git, Tensorflow, Keras, SciPy, Unix/Linux, Docker, rdkit
- **Science background:** Computer science, Physics, Cheminformatics, Bioinformatics, Mathematics

Teaching

Johannes Kepler University, Lecturer Sept 2018 – Sept 2022

- **Machine Learning: Unsupervised Techniques:** Clustering, PCA, ICA
- **Artificial Intelligence in Life Sciences:** Molecular property prediction, molecule generation, microscopy image classification
- **Basic Methods of Data Analysis:** Descriptive statistics, Data visualization, SVD, PCA, Multivariate linear regression
- **Bioinformatics for Biological Chemistry & Molecular Biology**: Sequence alignment, phylogenetic trees

Languages

- **English**: Fluent
- **German**: First language

Hobbies

- **Reading:** Popular science, politics, history, novels
- **Sports:** Kayaking (Secured multiple national championship titles; coaching), Running, Cycling, Hiking, Climbing, Partner acrobatics
- **Travelling:** Experiencing the great outdoors and other cultures