Philipp Renz

Personal Data

Nationality: Austrian
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web: LinkedIn | Google Scholar

Work Experience

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

- Development of machine learning models for energy demand forecasting.
- Price analysis and forecasting of energy markets.
- Development of backtesting environment.

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

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

Research Assistant, Johannes Kepler University, Linz, Austria — Sep 2018–Sep 2022

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

Education

PhD, Artificial Intelligence, Johannes Kepler University, Linz — Sep 2018–present

- Thesis: Advancing Evaluation of Generative Models for Molecules and Deep Learning for Reaction Prediction
- Advisors: Prof. Günter Klambauer, Prof. Sepp Hochreiter

MSc, Bioinformatics, Johannes Kepler University, Linz — Mar 2015–Sep 2018

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

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

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

Skills

Programming:	Python (advanced); R, C, C++ (familiar); SQL, LaTeX
Frameworks/Tools:	PyTorch, Tensorflow, Keras, NumPy, scikit-learn, SciPy, Pandas rdkit, Git, Unix/Linux
Machine learning:	Deep learning, QSAR, Time series analysis, Generative models, Computer vision
Science	Computer science, Physics, Cheminformatics, Bioinformatics, Mathematics Biology, Chemistry

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

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

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

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

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]
arXiv, 2020

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

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

Teaching

Lecturer - Johannes Kepler University, Linz, Austria

- Machine Learning: Unsupervised Techniques — Summer term 2022
- Artificial Intelligence in Life Sciences — Summer term 2022
- Basic Methods of Data Analysis — Winter term 2021
- Bioinformatics for Biological Chemistry & Molecular Biology — Winter Term 2018 & 2019

Languages

English: Fluent
German: First language

Interests and Activities

Machine Learning:	Generative models, Language Models, Time series forecasting, Uncertainty estimation, Anomaly detection
General:	Physics, Mathematics, Chemistry, Biology, Macroeconomics, Literature, History
Sports:	Kayaking (Secured multiple national championship titles; coaching), Running, Cycling, Hiking, Climbing, Partner acrobatics