

# Marnix Koops

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## EXPERIENCE

### QuantumBlack, AI by McKinsey

Principal Data Scientist

Sep 2020 – Present

- Leading projects and prototyping, developing, and implementing ML models across industries to solve business problems
- Building AI solutions with cross-functional teams to innovate and accelerate R&D in domains like drug- and materials discovery

### Coolblue

Lead Data Scientist – ML

Aug 2019 – Sep 2020

- Played ping pong, researched and built neural networks for sequence-based embedding recommender systems
- Implemented recommender systems on website and in the app together with multi-disciplinary product teams

Machine Learning Engineer

Apr 2018 – Aug 2019

- Researched, built, and implemented ML models to make customers smile :)

### Blue Field Agency

Research Scientist

Feb 2017 – Jan 2018

## EDUCATION

### Erasmus University Rotterdam

MS in Mathematical Statistics

Sep 2016 – Dec 2017

- Research paper rewarded 9/10 on Gaussian mixture modeling with likelihood penalization

BS in Mathematical Statistics, Econometrics

Sep 2015 – Jul 2016

- Courses include: multivariate stats, prob theory, statistical learning, ML theory, optimization, Bayesian stats, timeseries modeling

### Delft University of Technology

BS in Engineering & Geosciences

Sep 2011 – Jul 2014

- Research paper rewarded 9/10 on oil and gas reservoir simulation modeling to translate lab experiments to field scale
- Courses include: calculus, linear algebra, numerical maths, signal processing, geophysics, thermodynamics, mineralogy, matlab

## PROJECTS

### Molecule discovery

Quantumblack, 2023

- Partnered with one of the biggest US mining companies in worlds first AI-driven metal leaching R&D effort to improve efficacy while reducing environmental impact on a massive scale
- Responsible for building AI system, combining GNN- and Transformer-based molecular foundational models with more traditional chemical representation algorithms to discover, rank, and evaluate molecules
- Built a closed-loop research system together with chemists and other domain experts, including a dedicated testing wet lab

### Compound embedding

QB Labs, 2023

- Generalised Python asset with production-ready models to predict structure, function, or reaction properties of molecules
- Codebase has two main pipelines; embeddings generation, and fine-tuning on biochemical data for downstream modeling
- Framework is used for experimentation, and as starting point in partnerships with major biochemical companies

### mRNA vaccines

QuantumBlack, 2022

- Partnered with new research centre of a leading PharmaCo to design, develop and industrialise AI solutions to research and produce the next generation of mRNA vaccines
- Part of multi-disciplinary team from engineers to computational biologists to researchers and UI designers
- Responsible for in-silico modeling of lipid nanoparticle properties, from representation learning to down-stream target prediction to identify and rank the most promising candidates to sent to the wet lab for in-vitro testing

### Bioluminescence

QuantumBlack, 2021

- Implemented computer-vision algorithms such as Faster R-CNN for object detection and image segmentation applied for in-vivo bioluminescence imaging experiments to develop novel cancer treatments
- Built codebase to enabled rapid model prototyping and experimentation with new ideas while speeding up research timelines

### Lightning-MF

Fun, 2021

- Implemented the classic Matrix Factorization for Recommender Systems algorithm as pytorch lightning module

### Embedding vector search

Fun, 2020

- Built a simple and lightweight Python package for fast vector similarity search using Approximate Nearest Neighbors

### Sequence embedding recommendation

Coolblue, 2019

- Researched, and built sequence-based embedding neural nets like LSTMs and GRUs for personalized item recommendation

## SKILLS

- tensorflow, keras, pytorch, pytorch-lightning, sklearn, xgboost, lightgbm, numpy, pandas, scipy, mlflow