Tue J. **Boesen**

Machine learning Researcher

Aarhus, Denmark

(+1) 778-223-3274 Tue.Boesen@protonmail.com tueboesen Tue Boesen

Scientific Focus

My main scientific focus areas are currently: machine learning and protein folding. More specifically, within machine learning, I have worked extensively with equivariant and graph-based networks, as well as transfer and self-supervised learning. The goal of my work in machine learning has always been to fundamentally understand how neural networks work, which I believe is best done by connecting them with well-established areas of mathematics. Parts of this work lead to mimetic neural networks, and constrained neural networks, both of which are novel ideas in machine learning that has given me a deeper understanding of neural networks and allows me to more effectively tailor neural network to specific problems.

Education

Aarhus University *Denmark*

Ph.D. in Geophysics *2015 - 2018*

- Thesis: Numerical methods for electromagnetic geophysics beyond 1D

Aarhus University *Denmark*

M.S. in Theoretical Physics *2010 - 2011*

- Thesis: Foundation for a parallel time-dependent density functional theory simulator in a spherical harmonic basis using the exact exchange energy functional

Aarhus University *Denmark*

B.S. in Physics *2006 - 2010*

- Thesis: Feynmans Pathintegral i 1 dimension med fokus på sinusbaner (Feynman's path integral in 1 dimension with focus on sinusoidal trajectories)

Experience

Proteic Bioscience Inc. *Vancouver, Canada*

Machine Learning Consultant *Jan 2022 - June 2022*

- Developed and trained equivariant and mimetic neural networks for energy and force predictions for biomolecular systems.
- Developed a parallel framework for protein design using PyRosetta.
- Hyperparameter/Model optimization using optuna.
- Used PyRosetta to design protein bindings for KRAS.

University of Bristish Columbia (UBC) *Vancouver, Canada*

Postdoctoral Research Fellow in Machine Learning *May 2019 - Aug 2021*

- Developed methods for applying constraints in high-dimensional space to smoothly constrain/guide a neural network.
- Published reversible mimetic graph neural networks for protein design and folding.
- Developed self-supervised conditional probability neural networks for protein folding inspired by natural language processing models.
- Developed a semi-supervised active learning algorithm.

Computational Geoscience Inc. *Vancouver, Canada*

AI Research Scientist *May 2019 - Aug 2020*

- Published novel graph-based semi-supervised learning methods applied to seismic data.

HydroGeophysics Group at Aarhus University *Aarhus, Denmark*

Research Assistant *Aug 2017 - Nov 2017*

- Open-sourced a sparse iterative parallel linear solver based on my research during my Ph.D.
- Open-sourced an OpenMP parallelization framework developed during my Ph.D.

Danske Bank *Copenhagen, Denmark*

Analyst, Graduate position *Sep 2013 - Apr 2014*

- Worked in customer insight creating forecast models.

HydroGeophysics Group at Aarhus University *Aarhus, Denmark*

Scientific Programming Consultant *Mar 2013 - Sep 2013*

- Created SPIA in Pascal, an application for ground-based electromagnetic measurements.

Publications

In Preparation

A-optimal active learning
Tue Boesen, Eldad Haber
arXiv preprint arXiv:2110.09585 (2022). 2022

Neural DAEs: Constrained neural networks
Tue Boesen, Eldad Haber, Uri M Ascher
arXiv preprint arXiv:2211.14302 (2022). 2022

Journal Articles

Mimetic neural networks: a unified framework for protein design and folding
Moshe Eliasof, Tue Boesen, Eldad Haber, Chen Keasar, Eran Treister
Frontiers in Bioinformatics 2 (2022). 2022

Data-driven semi-supervised clustering for oil prediction
Tue Boesen, Eldad Haber, G Michael Hoversten
Computers & Geosciences 148 (2021) p. 104684. Pergamon, 2021

An efficient 2D inversion scheme for airborne frequency-domain data
Tue Boesen, Esben Auken, Anders Vest Christiansen, Gianluca Fiandaca, Casper Kirkegaard, Andreas Aspmo Pfaffhuber, Malte Vöge
Geophysics 83.4 (2018) E189–E201. Society of Exploration Geophysicists and American Association of Petroleum …, 2018

A parallel computing thin-sheet inversion algorithm for airborne time-domain data utilising a variable overburden
Tue Boesen, Esben Auken, Anders Vest Christiansen, Gianluca Fiandaca, Cyril Schamper
Geophysical Prospecting 66.7 (2018) pp. 1402–1414. European Association of Geoscientists & Engineers, 2018

A review of airborne electromagnetic methods with focus on geotechnical and hydrological applications from 2007 to 2017
Esben Auken, Tue Boesen, Anders V Christiansen
Advances in geophysics 58 (2017) pp. 47–93. Elsevier, 2017

Conference Proceedings

Semi-supervised clustering for oil prospectivity
Tue Boesen, Eldad Haber, G Michael Hoversten
ICLR AI for Earth Sciences workshop, 2020

Efficient 2D hybrid inversion of airborne frequency domain data
E Auken, T Boesen, AVC Christiansen, GF Fiandaca, AA Pfaffhuber, MV Vöge
Second European Airborne Electromagnetics Conference, 2017

2D FEM inversion with a moving footprint and a hybrid 1D and 2D forward and derivative implementation
Tue Boesen, Esben Auken, Malte Vöge, Casper Kirkegaard, Kristoffer Rønne Andersen, Andreas Aspmo Pfaffhuber, Anders Vest Christiansen
AGU Fall Meeting Abstracts, 2016

Rapid inversion of large airborne AEM data datasets utilizing massively parallel co-processors
C Kirkegaard, K Andersen, AV Christiansen, E Auken, T Boesen
First European Airborne Electromagnetics Conference, 2015

Utilizing massively parallel co-processors in the AarhusInv 1D forward and inverse AEM modelling code
Casper Kirkegaard, Kristoffer Andersen, Tue Boesen, Anders V Christiansen, Esben Auken, Gianluca Fiandaca
ASEG Extended Abstracts, 2015

2.5D inversion of sea ice thickness from helicopter EM data
M Vöge, A Pfaffhuber, E Auken, C Kirkegaard, T Boesen, S Hendricks, P Hunkeler
First European Airborne Electromagnetics Conference, 2015

Skills

Platforms	Windows, Linux Ubuntu, AWS
Programming	Python, Pytorch, LaTeX, Git, Matlab, Fortran, Julia, Delphi/Pascal, OpenMp, MPI
Languages	Danish, English

Teaching and supervision

Teaching

Aarhus University, Denmark

Instructor

2009-2017

- Calculus.
- Electric and Electromagnetic methods.
- Data processing and interpretation for groundwater mapping.
- Geophysical methods.
- Hydrogeophysical field course (twice).

Supervision

UBC, Canada

Co-Supervisor

2020

- Jingrong Lin – Ph.D. student in geophysics.