

# Tue J. Boesen

MACHINE LEARNING RESEARCHER

Aarhus, Denmark

☎ (+45) 2991 3001

✉ 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

PH.D. IN GEOPHYSICS

[Denmark](#)

2015 - 2018

- Thesis: Numerical methods for electromagnetic geophysics beyond 1D

### Aarhus University

M.S. IN THEORETICAL PHYSICS

[Denmark](#)

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

B.S. IN PHYSICS

[Denmark](#)

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.

MACHINE LEARNING CONSULTANT

[Vancouver, Canada](#)

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 British Columbia (UBC)

POSTDOCTORAL RESEARCH FELLOW IN MACHINE LEARNING

[Vancouver, Canada](#)

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.

AI RESEARCH SCIENTIST

[Vancouver, Canada](#)

May 2019 - Aug 2020

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

### HydroGeophysics Group at Aarhus University

RESEARCH ASSISTANT

[Aarhus, Denmark](#)

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

ANALYST, GRADUATE POSITION

[Copenhagen, Denmark](#)

Sep 2013 - Apr 2014

- Worked in customer insight creating forecast models.

### HydroGeophysics Group at Aarhus University

SCIENTIFIC PROGRAMMING CONSULTANT

[Aarhus, Denmark](#)

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 Aspömpfhuber, 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, AV 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 Aspömpfhuber, 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

### INSTRUCTOR

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

*Aarhus University, Denmark*

2009-2017

## Supervision

CO-SUPERVISOR

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

UBC, Canada

2020