

Tue J. Boesen

MACHINE LEARNING RESEARCHER

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🎓 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.
- 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 mimetic graph neural networks for protein design and folding.
- Developed self-supervised conditional probability neural networks for protein folding.
- 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 Aspömo 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, 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 Aspömo 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

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