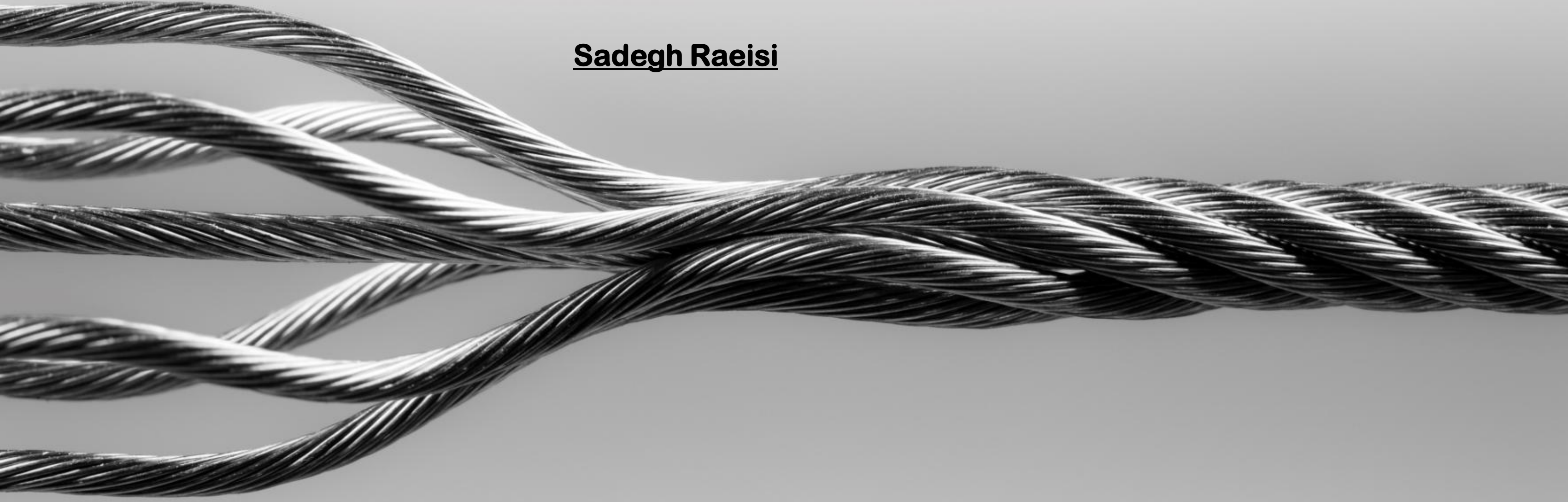
ML in Physics

Sadegh Raeisi

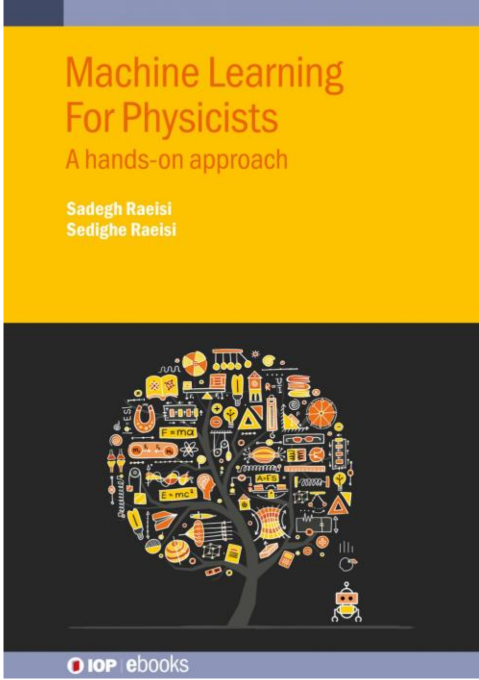


Outline

- ML in science
- ML in Physics
- ML in my research

Some resources

https://github.com/sraeisi/MachineLearning_Physics



https://store.ioppublishing.org/page/detail/Machine-Learning-For-Physicists//?k=9780750349550

ML in Science: Protein Folding

nature

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nature › articles › article

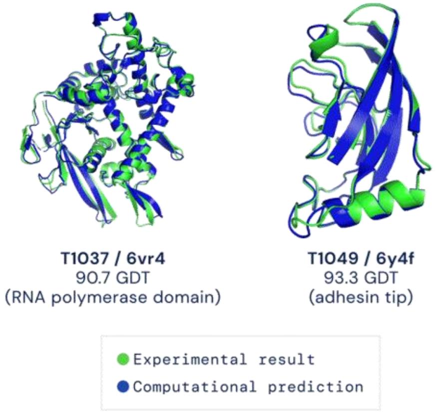
Article | Open Access | Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

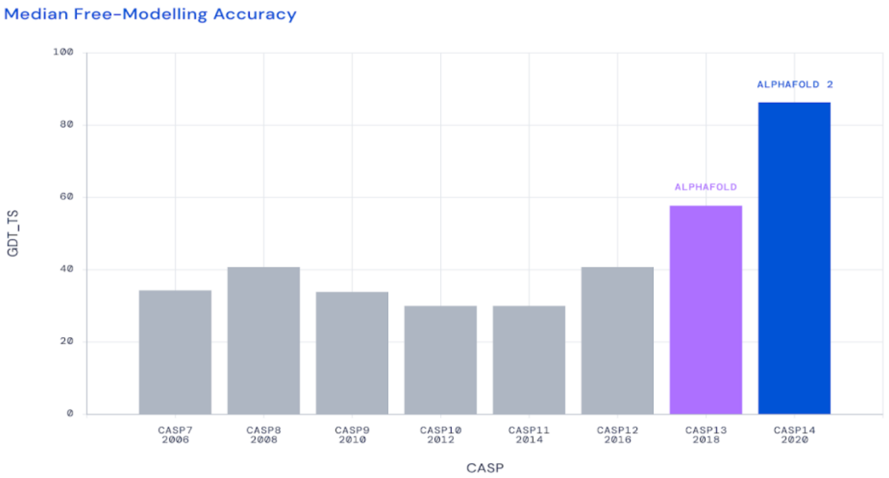
John Jumper, Richard Evans, [...]Demis Hassabis

Nature **596**, 583–589 (2021) | Cite this article

336k Accesses | **2765** Altmetric | Metrics



ML in Science: Protein Folding



ML in Science: Drug discovery

nature communication

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nature › nature communications › article

Article | Open Access | Published: 12 July 2

Artificial intelligence protective therapy in i

Debashis Sahoo, Lee Swanson, Ibrahim M, Rama F. Pranadinata, Courtney Tindle, Mac Sandborn, Soumita Das & Pradipta Ghos

Nature Communications **12**, Article numbe

5285 Accesses | **157** Altmetric | Metrics

nature reviews gastroenterology

Explore content ⌄ About the journal ⌄ Publish with

nature › nature reviews gastroenterology & hepatology › r

Review Article | Published: 03 January 2020

Harnessing big 'omics' data and in hepatocellular carcinoma

Bin Chen, Lana Garmire, Diego F. Calvisi, Mei-Sze Chua, Rol

Nature Reviews Gastroenterology & Hepatology **17**, 238–251 (

4354 Accesses | **24** Citations | **48** Altmetric | Metrics

nature biomedical engineering

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nature › nature biomedical engineering › articles › article

Article | Published: 15 April 2021

Optimization of therapeutic antibodies by predicting antigen specificity from antibody sequence via deep learning

Derek M. Mason, Simon Friedensohn, Cédric R. Weber, Christian Jordi, Bastian Wagner, Simon M. Meng, Roy A. Ehling, Lucia Bonati, Jan Dahinden, Pablo Gainza, Bruno E. Correia & Sai T. Reddy

Nature Biomedical Engineering **5**, 600–612 (2021) | Cite this article

4788 Accesses | **2** Citations | **145** Altmetric | Metrics

ML in Science: Mathematics

NewScientist

Volume 242, Issue 3228, 4 May 2019, Page 9

News & Technology

Machine learning

Google's AI mathematician

Leah Crane

HOList: An Environment for Machine Learning of Higher-Order Theorem Proving

Kshitij Bansal, Sarah M. Loos, Markus N. Rabe, Christian Szegedy, Stewart Wilcox

We present an environment, benchmark, and deep learning driven automated theorem prover for higher-order logic. Higher-order interactive theorem provers enable the formalization of arbitrary mathematical theories and thereby present an interesting, open-ended challenge for deep learning. We provide an open-source framework based on the HOL Light theorem prover that can be used as a reinforcement learning environment. HOL Light comes with a broad coverage of basic mathematical theorems on calculus and the formal proof of the Kepler conjecture, from which we derive a challenging benchmark for automated reasoning. We also present a deep reinforcement learning driven automated theorem prover, DeepHOL, with strong initial results on this benchmark.

Comments: Accepted at ICML 2019

Subjects: **Logic in Computer Science (cs.LO)**; Artificial Intelligence (cs.AI); Machine Learning (cs.LG)

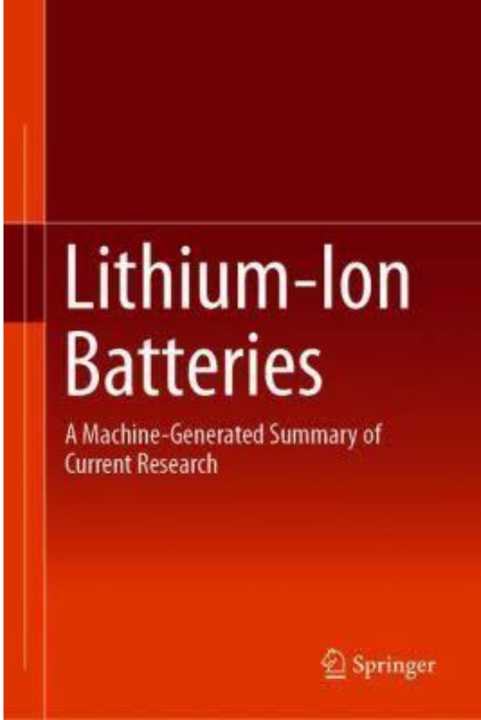
Cite as: arXiv:1904.03241 **[cs.LO]**

(or arXiv:1904.03241v3 **[cs.LO]** for this version)

Artificial intelligence trained by google learns to prove 1200 theorems.

[1904.03241] HOList: An Environment for Machine Learning of Higher-Order Theorem Proving (arxiv.org)

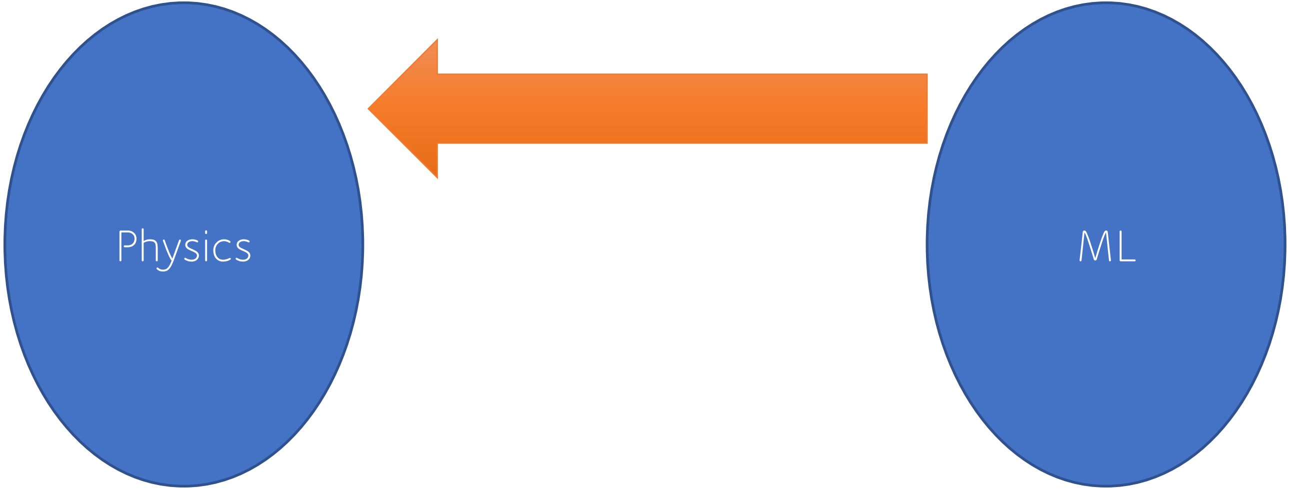
ML in Science: writing books



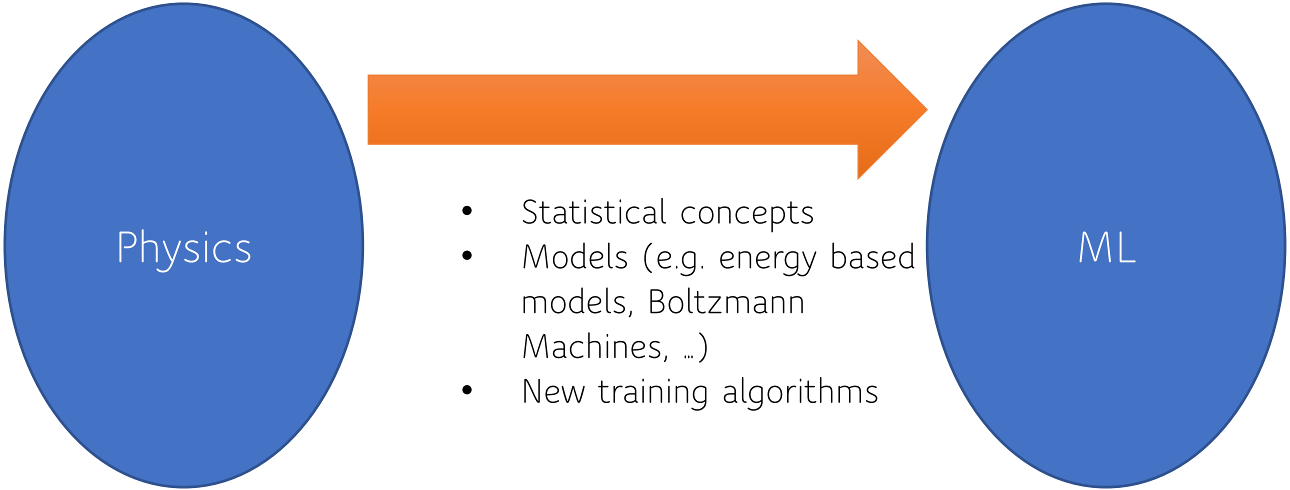
Can machines replace scientists?

What are the key aspects that cannot be replaced?

ML in Physics

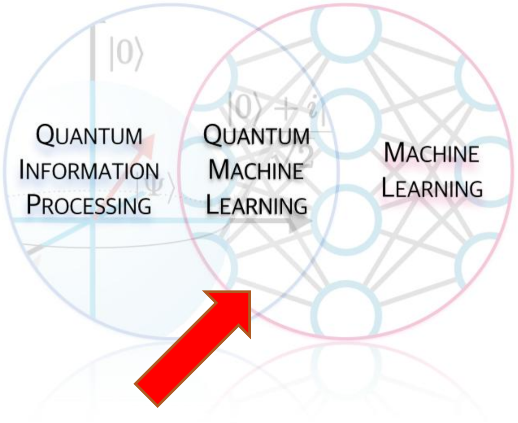


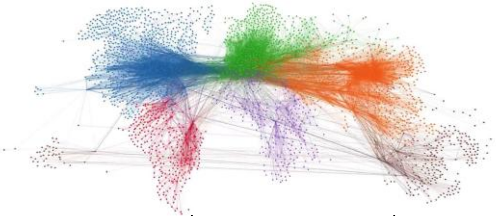
ML in Physics



- Statistical concepts
- Models (e.g. energy based models, Boltzmann Machines, …)
- New training algorithms

Some of my works



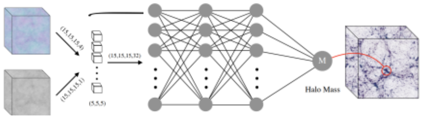


complex networks

Fake news detection

Information spreading

Collaboration with Dr. Ghanbarnejad



Cosmology: Structure formation

Collaboration with Dr. Baghram

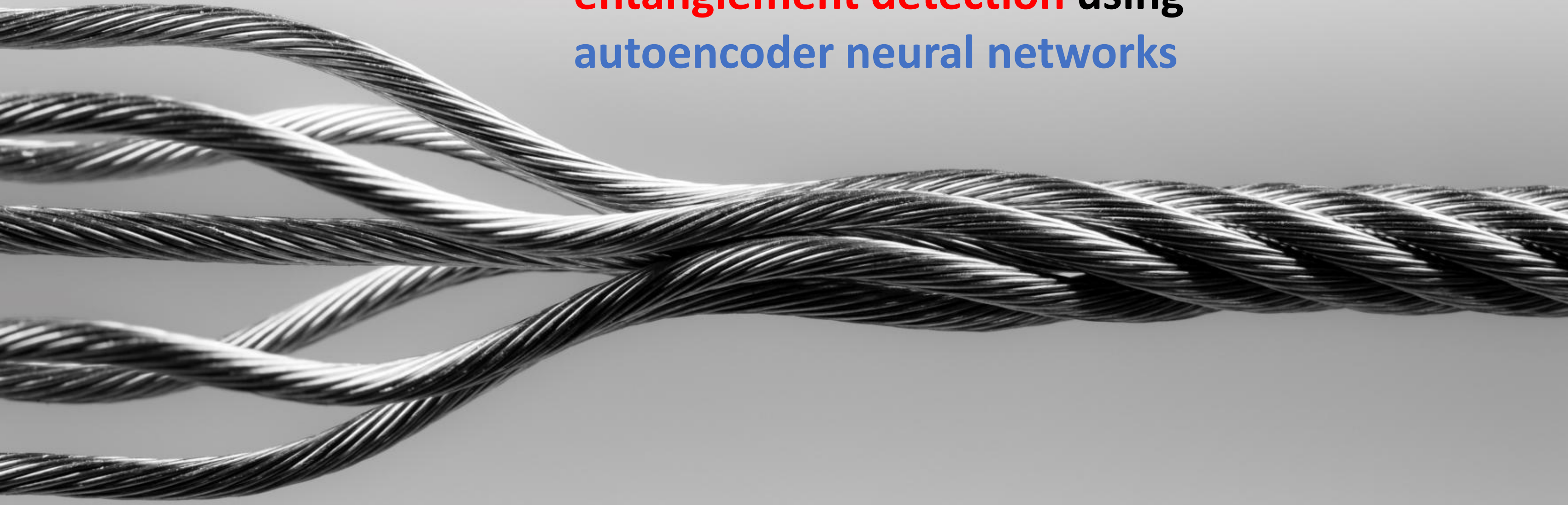
Classification of variable stars

Collaboration with Dr. Rahvar

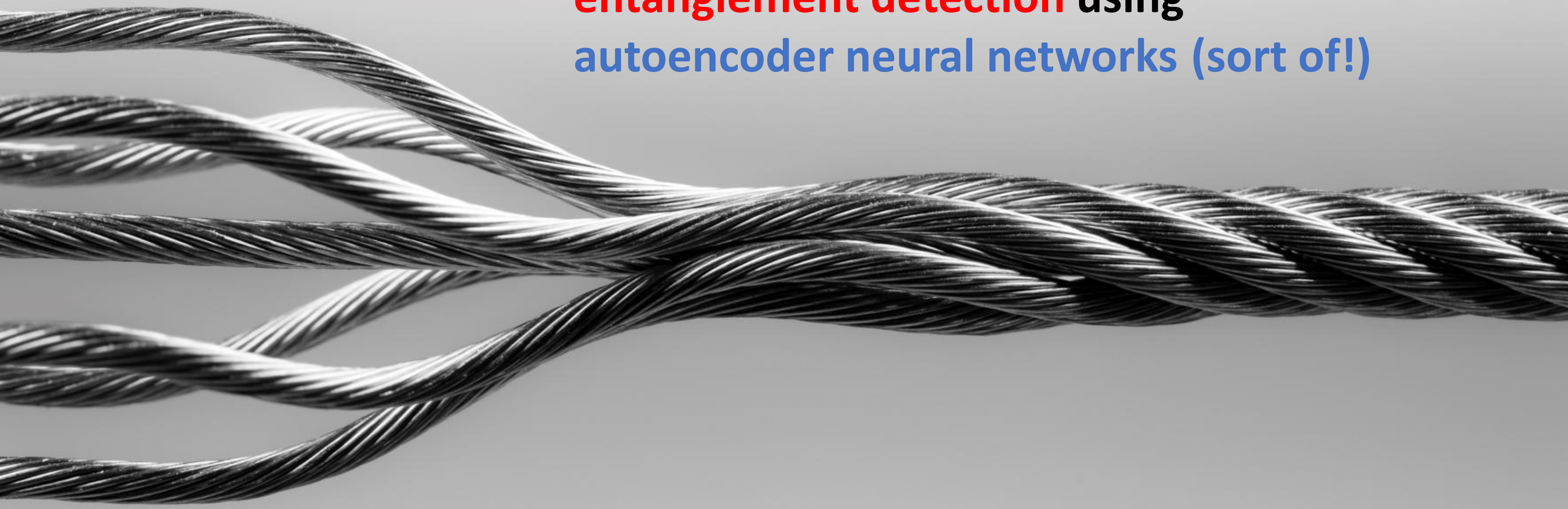
Quantum Machine Learning: Path to a Better Artificial Intelligence? – QML

Silva, F., and L. da F. Costa. "Visualizing Complex Networks (CDT-5)." *Costa's Didactic Texts-CDTs* (2018).

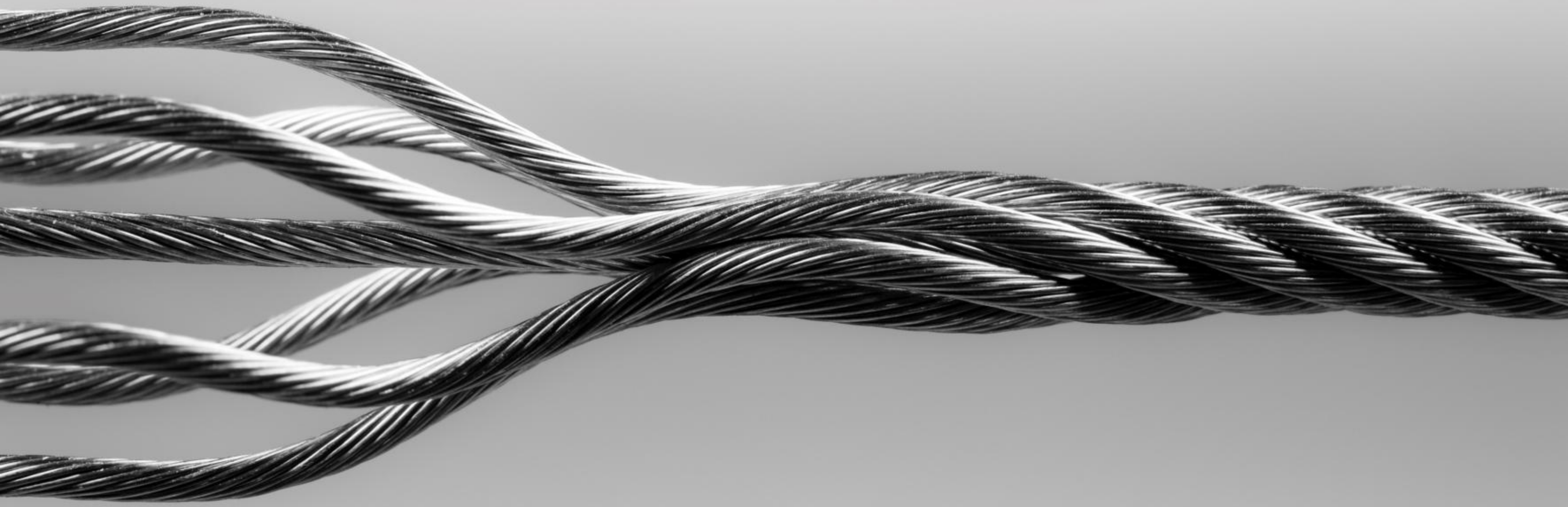
Finding semi-optimal measurements for entanglement detection using autoencoder neural networks



Finding semi-optimal measurements for entanglement detection using autoencoder neural networks (sort of!)

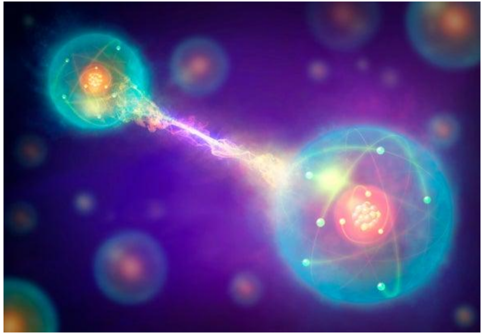


What should I measure in the lab?



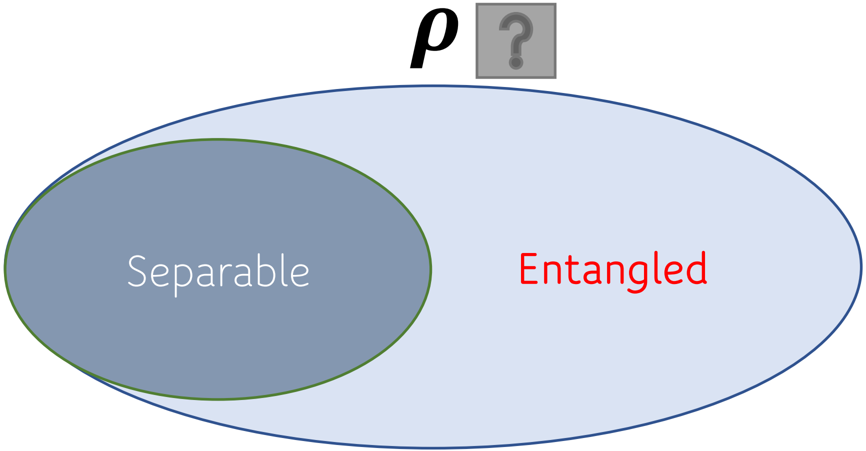
Quantum States

Entanglement is a MAGIC property that is of interest in many Quant. Tech.



[Quantum Entanglement High-Res Vector Graphic - Getty Images]

Entanglement



Entanglement Detection

ρ ?

15 measurements are needed to decide!

(for the smallest case)

Problem:

15 measurement is too many!!

Can we do it with fewer measurements?

Problem:

Which measurements are

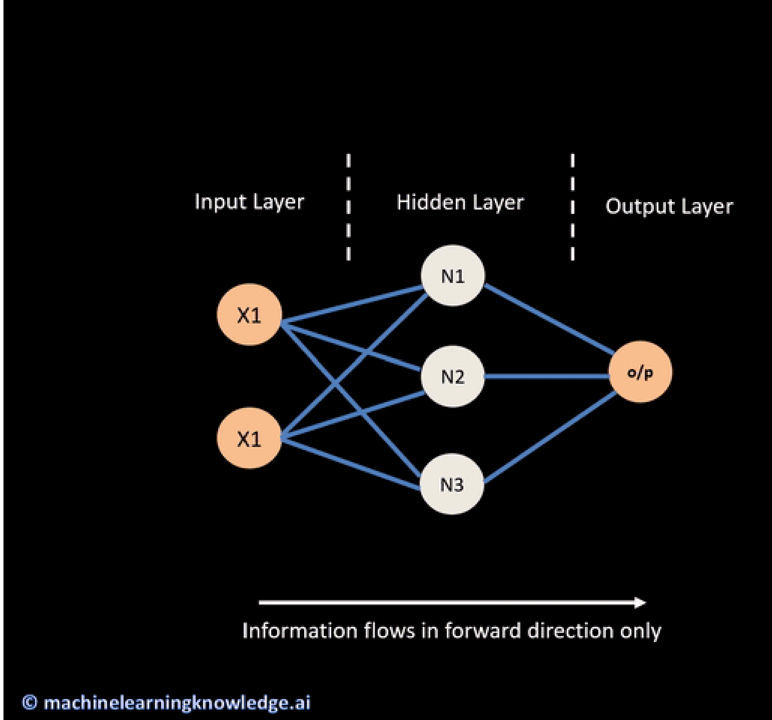
most informative

for

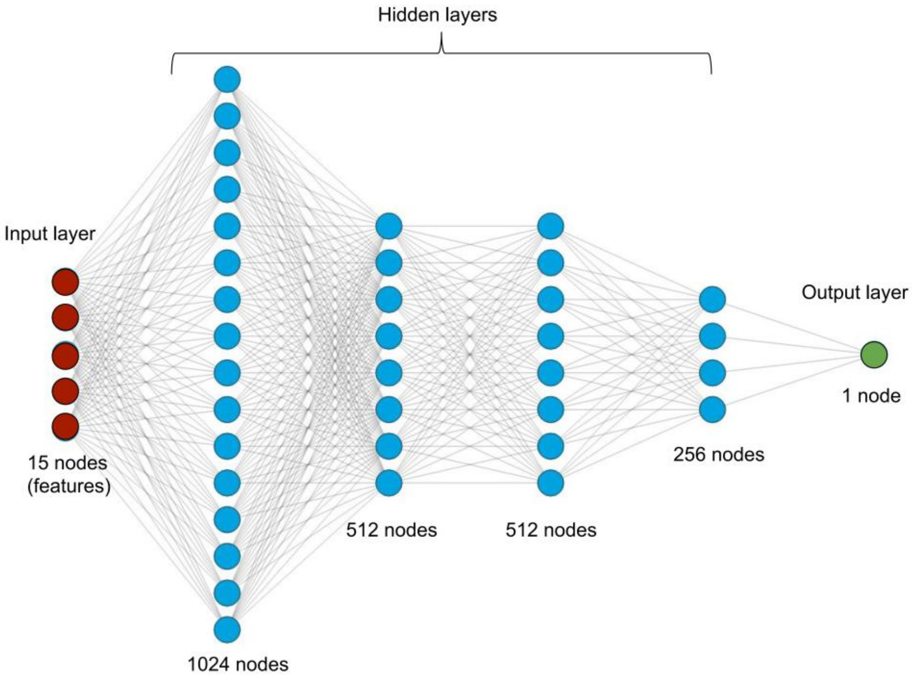
Entanglement detection?

Autoencoder Neural Network

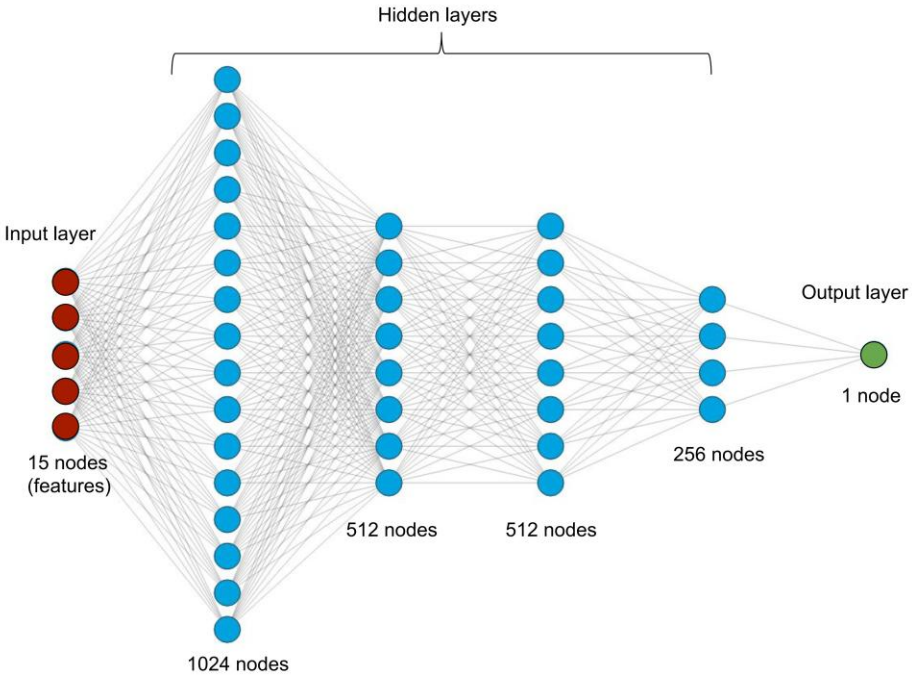
Neural Network



Neural Network for entanglement

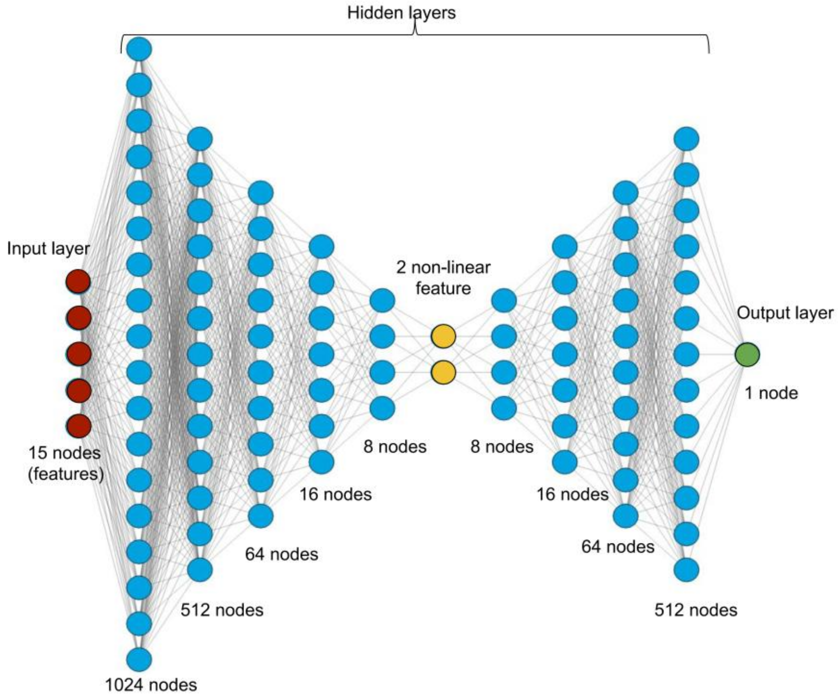


Neural Network for entanglement

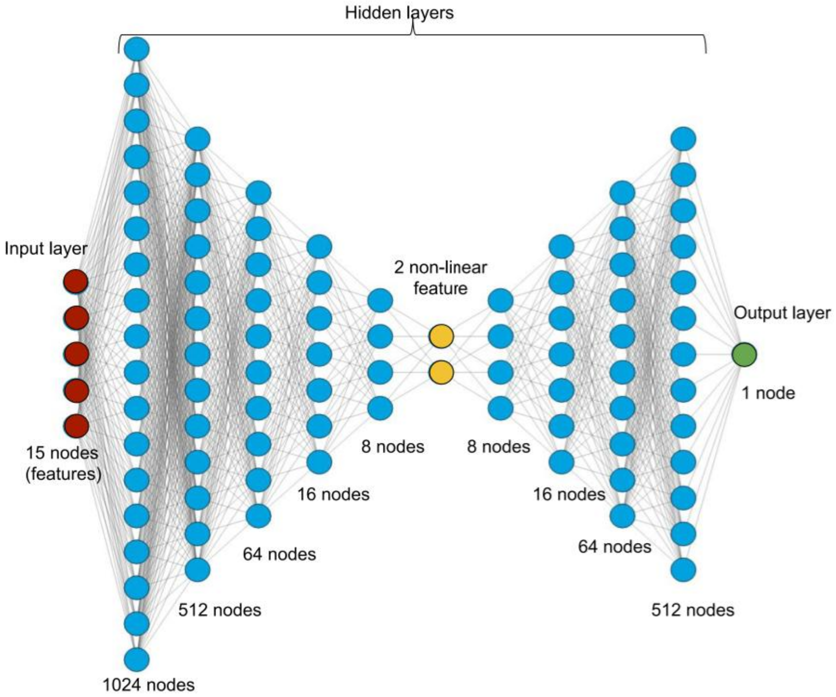


99.7% Accuracy

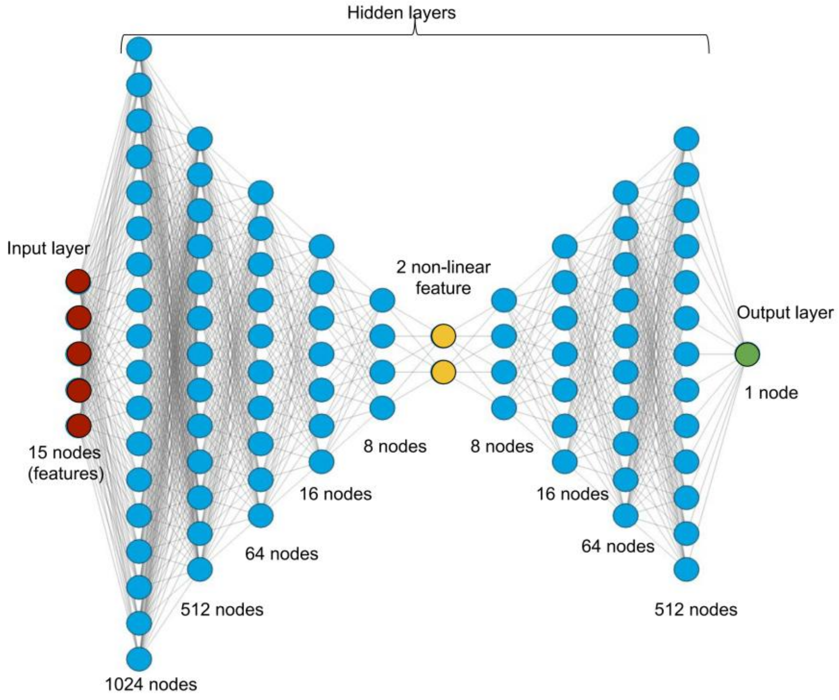
Autoencoder NN



Autoencoder NN

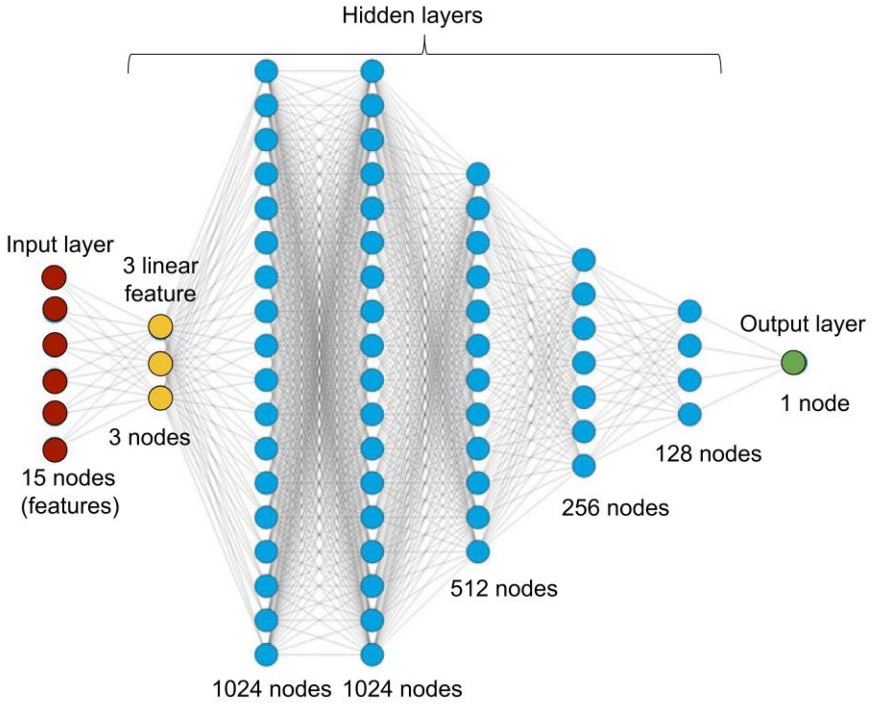


Autoencoder NN



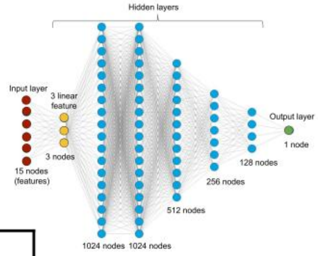
99% Accuracy

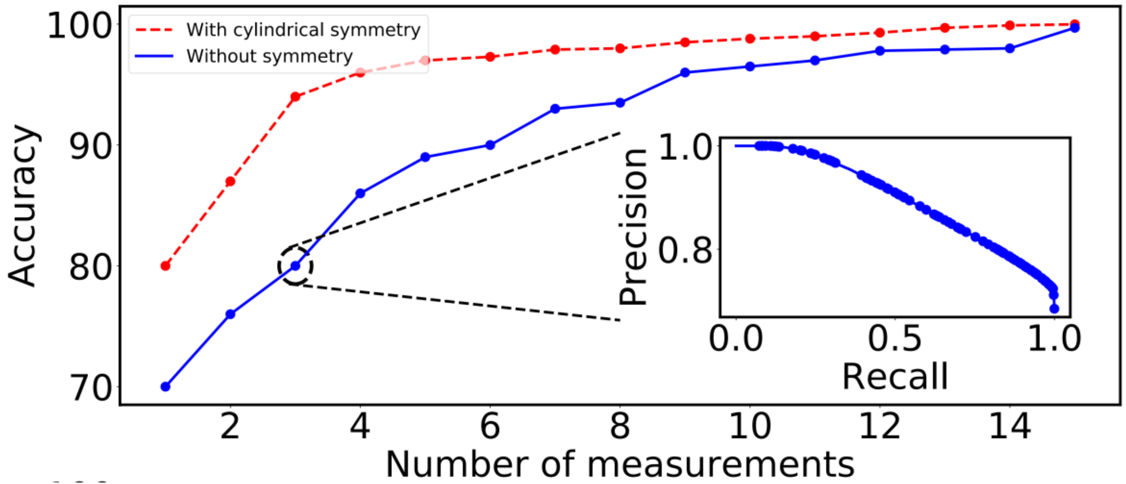
Autoencoder NN: Linear Measurements



80% Accuracy

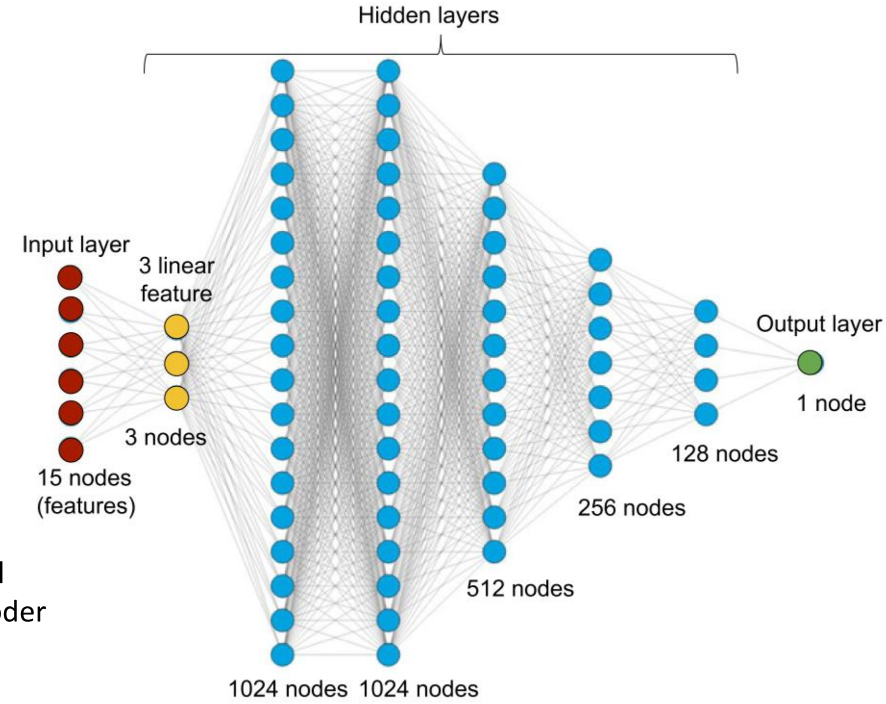
Results


Hidden layers
Input layer
3 linear feature
3 nodes
15 nodes (features)
1024 nodes
1024 nodes
512 nodes
256 nodes
128 nodes
Output layer
1 node


With cylindrical symmetry
Without symmetry
Accuracy
100
90
80
70
2
4
6
8
10
12
14
Number of measurements
Precision
1.0
0.8
0.0
0.5
1.0
Recall

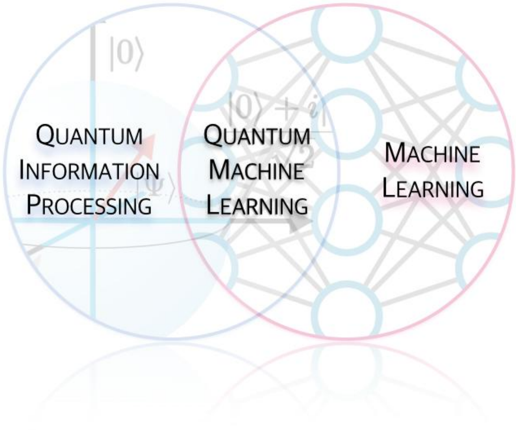
Conclusion

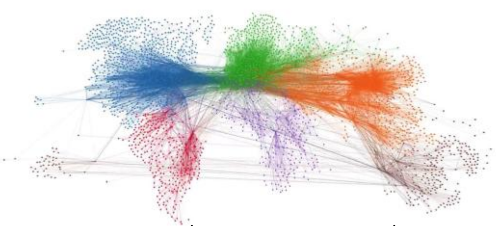
Model	Accuracy
All 15 measurements	99.7%
2 non-linear measurements	99 %
3 linear measurements	80%
4 linear measurements (cyl. symmetry)	99%
3 linear measurements (cyl. symmetry)	96 %
2 linear measurements (cyl. symmetry)	93 %
1 linear measurement (cyl. symmetry)	90 %



M. Yosefpor, M. R. Mostaan, **S. Raeisi** "Finding Semi-optimal Measurements for Entanglement Detection Using Autoencoder Neural Networks", Quantum Sci. Technol. 5 045006 (2020)
https://doi.org/10.1088/2058-9565/aba34c

Some of my works





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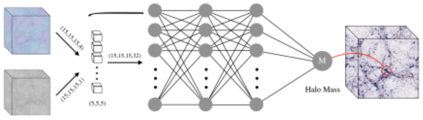
Collaboration with Dr. Ghanbarnejad



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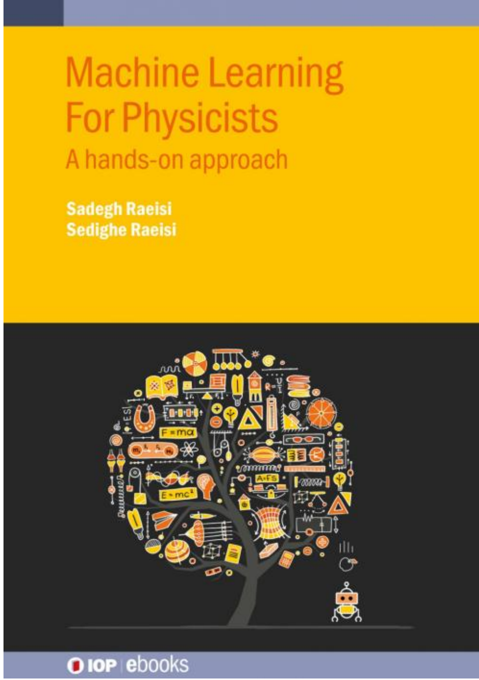
Some resources

https://github.com/sraeisi/MachineLearning_Physics



https://store.ioppublishing.org/page/detail/Machine-Learning-For-Physicists//?k=9780750349550