Welcome!

To the MT ARD ST3 pre-meeting
Machine Learning workshop

Andrea Santamaría García[1], Jan Kaiser[2], Stephan Kötter[3], Oliver Stein[2], Chenran Xu[3]

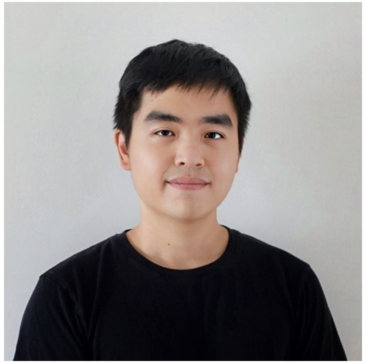
[1]Laboratory for Applications of Synchrotron Radiation (KIT-LAS)
[2] Maschine Strahlkontrollen (DESY-MSK)
[3] Institute for Beam Physics and Technology (KIT-IBPT)

07/09/2022

Workshop schedule

13:30-13:45	8:30 AM → 8:45 AM	**Welcome and introduction to machine learning in accelerator physics** **Speaker**: Andrea Santamaria Garcia (KIT)	15m
13:45-14:05	8:45 AM → 9:05 AM	**Introduction to artificial neural networks** **Speaker**: Andrea Santamaria Garcia (KIT)	20m
14:05-14:45	9:05 AM → 9:45 AM	**Hands-on tutorial: build your own neural network** We will fit non-linear functions with neural networks in PyTorch and understand the role that the different parameters of the model play in the quality of	40m
14:45-15:00	9:45 AM → 10:00 AM	**Special topic: introduction to Bayesian optimization** **Speaker**: Chenran Xu (KIT)	15m
15:00-15:30	10:00 AM → 10:30 AM	**Hands-on tutorial: optimize unknown functions with Bayesian optimization** We will implement all the basic components of Bayesian optimization (BO), and see how to use BO for some sample 1D and 2D functions	30m
15:30-15:45	10:30 AM → 10:45 AM	**Coffee break**	
15:45-16:00	10:45 AM → 11:00 AM	**Application of Bayesian optimization to improve injection efficiency at KARA demo** ¶ **Speaker**: Chenran Xu (KIT)	15m
16:00-17:00	11:00 AM → 12:00 PM	**Special topic: introduction to reinforcement learning & ARES live demo** **Speakers**: Jan Kaiser (DESY), Oliver Stein (MSK (Strahlkontrollen))	1h

Andrea Santamaria Garcia
Researcher



Chenran Xu
Doctoral student

Stephan Robert Kötter
Postdoc

Oliver Stein
Researcher

Jan Kaiser
Doctoral student

"Autonomous Accelerator" project

HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

[TUPAB298, IPAC21]

Code, slides, extras

- Website: https://ansantam.github.io/2022-MT-ARD-ST3-ML-workshop/
- Repository: https://github.com/ansantam/2022-MT-ARD-ST3-ML-workshop

Local installation

Install Anaconda: https://www.anaconda.com/

```
1. git clone https://github.com/ansantam/2022-MT-ARD-ST3-ML-workshop.git
2. cd 2022-MT-ARD-ST3-ML-workshop
3. conda env create -f environment.yaml
4. conda activate mt-ard-st3-ml-workshop
5. jupyter notebook
```

Machine learning in the search for new fundamental physics

Georgia Karagiorgi, Gregor Kasieczka, Scott Kravitz, Benjamin Nachman & David Shih

Nature Reviews Physics 4, 399–412 (2022) | Cite this article

924 Accesses | 11 Altmetric | Metrics

Abstract

Compelling experimental evidence suggests the existence of new physics be
established and tested standard model of particle physics. Various current ar
experiments are searching for signatures of new physics. Despite the variety

Machine Learning Pins Down Cosmological Parameters

August 19, 2022 • *Physics* 15, s111

Cosmological constraints can be improved by applying machine learning to a combination of data from two leading probes of the large-scale structure of the Universe.

Pervasive machine learning in physics

Nature Reviews Physics 4, 353 (2022) | Cite this article

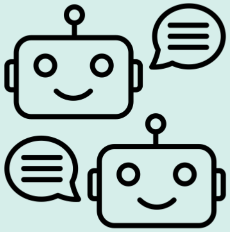
1325 Accesses | 6 Altmetric | Metrics

No longer restricted to data analysis, machine learning is now increasingly being used in theory, experiment and simulation – a sign that data-intensive science is starting to encompass all traditional aspects of research.

ARTIFICIAL INTELLIGENCE (AI)

Computers mimic human behaviour

- First chatbots
- Robotics
- Expert systems
- Natural language processing
- Fuzzy logic
- Explainable AI



Narrow AI

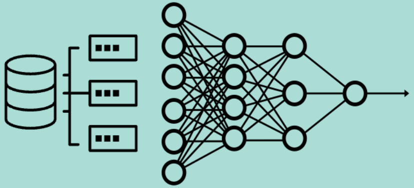
MACHINE LEARNING (ML)

Computers learn without being explicitly programmed to do so and improve with experience

Collection of **data-driven** methods / algorithms

Focused on **prediction** / **optimization / control** based on properties learned from data

Tries to **generalize** to unseen scenarios



Data + Algorithm

DEEP LEARNING (DL)

Multi-layered neural networks perform certain tasks with high accuracy

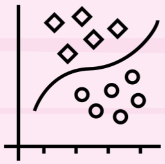
- Speech/handwriting recognition
- Language translation
- Recommendation engines
- Computer vision

MACHINE LEARNING

SUPERVISED LEARNING

Classification, prediction, forecasting

computer learns by example



- Spam detection
- Weather forecasting
- Housing prices prediction
- Stock market prediction

UNSUPERVISED LEARNING

Segmentation of data

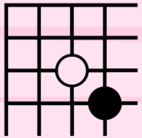
computer learns without prior information about the data

- Medical diagnosis
- Fraud (anomaly) detection
- Market segmentation
- Pattern recognition

REINFORCEMENT LEARNING

Real-time decisions

computer learns through trial and error



- Self-driving cars
- Make financial trades
- Gaming (AlphaGo)
- Robotics manipulation

Machine Learning

Learning style	Task	Popular algorithms
Supervised Learning We know the input & output (labeled data)	**Classification** discrete variables **Regression** continuous variables	▪ Neural networks (e.g. stochastic gradient descent, backpropagation) ▪ Support Vector Machine ▪ K-nearest neighbor ▪ Decision Tree algorithms (e.g. Classification and Regression Tree) ▪ Random Forest (ensemble) ▪ Uni or multivariate, linear or logistic
Unsupervised Learning We only know the input (unlabeled data)	**Clustering**	▪ K-means ▪ K-medians ▪ Expectation Maximization (EM) ▪ Hierarchical clustering
	Association	▪ Apriori algorithm ▪ Eclat algorithm

Reinforcement Learning	**Control**
	
	Prediction
		▪ Model-free
		  ▪ Value based (Q-learning)
		  ▪ Policy based
		    ▪ Deterministic or stochastic
		    ▪ On or off policy
		    ▪ Policy gradient or actor-critic
		▪ Model based
		    ▪ Learn the model
		    ▪ Model given

Deep Learning Networks

- Convolutional Neural Networks
- Recurrent Neural Networks
- Long Short-Term Memory Networks
- Autoencoders
- Deep Boltzmann Machine
- Deep Belief Networks

Bayesian Algorithms

- Naive Bayes
- Gaussian Naive Bayes
- Bayesian Network
- Bayesian Belief Network
- Bayesian optimization

Regularization, dimensionality reduction, ensemble, evolutionary algorithms, computer vision, recommender systems, …

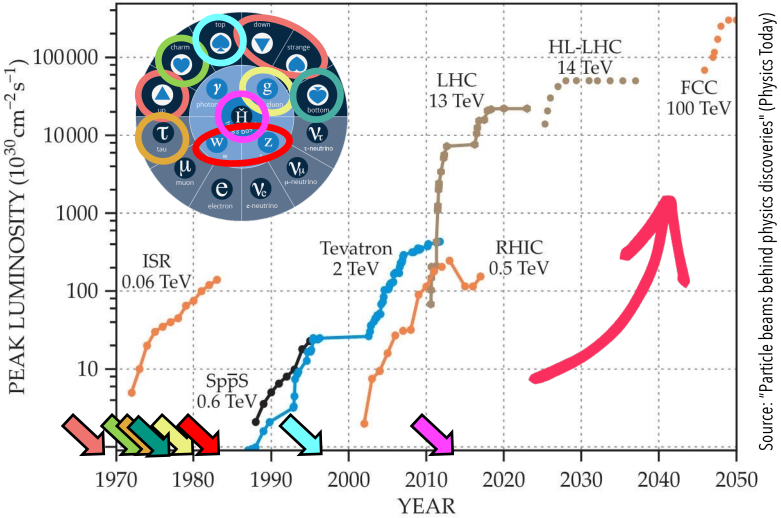
this slide is not exhaustive

PARTICLE ACCELERATORS …

…make fundamental discoveries in particle physics

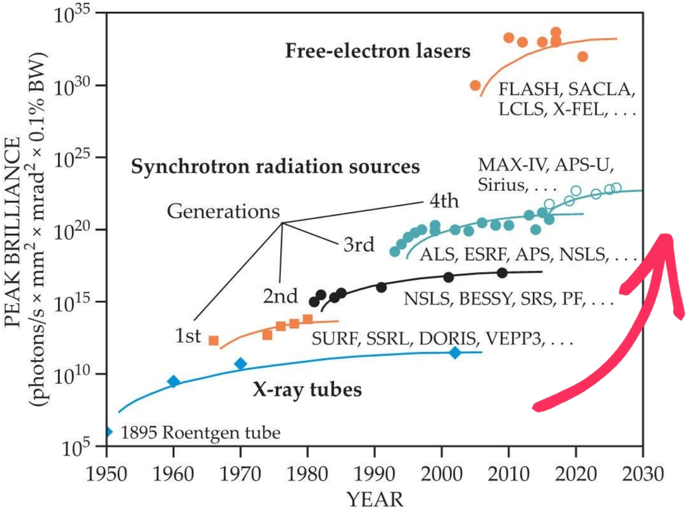
…are major tools for basic and applied research, industry & medicine worldwide

Ability to generate new particles via high-energy collisions



Source: "Particle beams behind physics discoveries" (Physics Today)

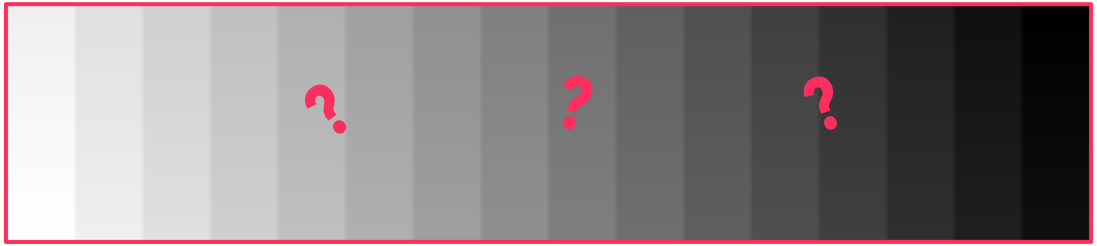
Ability to probe atomic structures



Technological innovation is needed to keep up with the challenging goals!

WHEN TO APPLY MACHINE LEARNING?

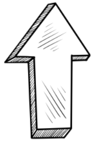
Classical control theory



Machine Learning

there are some clear cases

Optimization and control tasks in accelerators



Both perform equally

Cost of implementation and maintenance should then be considered

FUTURE ACCELERATORS TRENDS AND CHALLENGES

and this is not considering user's needs!

Denser beams for higher luminosity & brilliance

- complex beam dynamics & instabilities
- complex design & operation

Larger circular colliders for higher energies

- orders of magnitude more signals
- machine protection limits

Compact plasma accelerators with higher gradients

- very tight tolerances
- very high-quality beams required

WHAT CAN MACHINE LEARNING DO FOR US?

Very fast predictions by evaluating an already trained model

Classification task

Detect outliers and anomalies in accelerator data

- Fault detection
- Predictive maintenance
- Data cleaning

Optimization task

Achieve desired beam properties or states by tuning machine parameters

- Bayesian algorithms
- Optimizers

Prediction task

Predict the beam properties based on current accelerator parameters

- Surrogate models
- Virtual diagnostics

Control task

Control the state of the beam in real time in a dynamically changing environment

- Reinforcement learning

Check out the references we provide here!

https://github.com/ansantam/2022-MT-ARD-ST3-ML-workshop/blob/main/references/references.pdf

Recorded seminars:

https://sites.google.com/view/owle/past-ml-seminars

WHAT CAN MACHINE LEARNING DO FOR US?

Very fast predictions by evaluating an already trained model

Classification task

Detect outliers and anomalies in accelerator data

- Cavity fault classification
- Detection of faulty BPMs

Optimization task

Achieve desired beam properties or states by tuning machine parameters

- Injection efficiency
- Orbit correction
- Collimator alignment

Prediction task

Predict the beam properties based on current accelerator parameters

- Virtual diagnostics: beam energy

Control task

Control the state of the beam in real time in a dynamically changing environment

- Microbunching instability
- Trajectory control

Check out the references we provide here!

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WHY MACHINE LEARNING NOW?

1943 Perceptron
W. McCulloch, W. Pitts

1951 "A Stochastic Approximation Method"
H. Robbins, S. Monro

1958 Perceptron implementation
F. Rosenblatt

1959 "Machine Learning"
A. Samuel

1969 Perceptron (book)
M. Minsky, S. Papert

1973 The Lighthill report
J. Lighthill

Pessimistic reviews & abandonment of connectionism

1974 AI winter
Collapse of the billion-dollar AI industry

1993 Handwritten digit recognition
Y. LeCun et al

2000's AI Spring
Google translate
Google image search
AlphaZero
AlphaGo
Watson

Big Data
Large datasets
Easy collection
Easy storage

Software
New libraries, models, techniques

Hardware
GPUs
Generally better computers

THERE IS NOT ONE LIBRARY TO RULE THEM ALL

python

Neural networks/ Deep learning

TensorFlow
Google

PyTorch
facebook
(Meta-AI)

Keras
Tensorflow backend

mxnet
Caffe2
Microsoft Cognitive Toolkit

ML algorithms / optimization

scikit learn → SciPy NumPy

Apache Spark
theano

REINFORCEMENT LEARNING

Frameworks

OpenAI Baselines

Dopamine

rllib

Chainer RL

DeepMind TRFL

Tensorforce

Stable baselines

TF-Agents

Environments

OpenAI Gym

Google DeepMind

DeepMind Control Suite

MuJoCo

Advanced physics simulation

https://neptune.ai/blog/the-best-tools-for-reinforcement-learning-in-python

Thank you for being here today!

Ask away

Let's connect! andrea.santamaria@kit.edu / @ansantam

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