ErSE222: Machine learning in Geoscience

Jan. 26th, 2025

Tariq Alkhalifah and Omar Saad

Course Details

Machine learning for geoscience Spring, 2025

Instructors: Tariq Alkhalifah - Building 1 #3308 tariq.alkhalifah@kaust.edu.sa,
Omar Saad, Building 1 #3220 omar.sadaly@kaust.edu.sa
TA: Yuanyuan Yang: yuanyuan.yang@kaust.edu.sa
Lecture: Sundays and Wednesdays 1.00-2.30PM

Office Hours: Tuesday 3-4 PM

Previous instructor: Prof. Matteo Ravasi

Here is the GitHub link which will be updated weekly:
https://github.com/omarmohamed15/MLgeoscience_KAUST
Teaching material for ML in Geoscience course
Website:
https://dig-kaust.github.io/MLgeoscience/
Last updated a month ago

Dr. Omar Saad

Research Scientist at KAUST since 2023

Post Doc: China during Covid with Yangkang Chen, Assistant Professor at NIARG.

PhD 2018: Egypt-Japan University of Science and Technology (E-JUST). GPA: 3.95 out of 4

Thesis Title: Design and Implementation of Automatic Detection and Classification System for Seismic Events

Focus: ML for seismic data (avid publisher, specifically in ML), seismology, Earthquake prediction, denoising, and even FWI

Introduce myself

Professor of Geophysics, KAUST since 2009

PostDoc Stanford, Consulting, Director Research institute

Phd., Geophysics – Colorado School of Mines

Waveforms, Inversion, Anisotropy

Machine Learning

Course Objectives

•To understand and learn the fundamentals of machine learning with a focus on geoscience applications.

Machine learning (*wikipedia*):

is the study of computer algorithms that improve automatically through experience.

What will we learn?

- Linear Algebra
- Probability and statistics
- ML algorithms
- Training
- hyperparameters
- Geoscience applications
- Pytorch
- Tensorflow

Course Agenda

week 1 (Jan. 26th): Course overview and *Introduction to ML: with a python/pytorch review*

week 2 (Feb. 2nd): Review: *Linear Algebra and Probability and statistics- Linear and logistic regression*

week 3 (Feb. 9th): *The components of ML: perceptron, activation functions,* … - *Neural networks: multiple layers, backpropagation, initialization*

week 4 (Feb. 16th): *Best practices in machine learning: loss functions, train-test-validation - Advanced solvers: vanishing gradients, gradient descent with momentum.*

week 5 (Feb. 23th): Founding day/ *Lab: Well-logs prediction and facies classification*

week 6 (March 2nd): - *Uncertainty quantification in NNs - Lab: Uncertainty quantification in NNs*

week 7 (March 9th): Mid-semester break/*Lab: PINNs*

week 8 (March 16th): *CNNs: introduction - CNNs: pooling, 1x1 conv, skip-connection, popular architectures*

Lecture Schedule 2

-Week 9 (March. 23th): *Lab: seismic data segmentation - Mid-term exam*

-Week 10 (March 30th) *Eid break*

Week 11 (April 6th): *Sequence modelling: introduction - Lab: microseismic event detection*

Week 12 (April 13th): *Sequence modelling: architectures (RNN, GRU, LSTM, Transformers) - Dimensionality reduction: PCA, t-SNE, Autoencoders*

Week 13 (April 20th): - *Invertible neural networks - Lab: Invertible neural networks*

Week 14 (April 27th): *Principles of generative models - Variational Autoencoders, GANs, diffusion models*

Week 15 (May 4th): *Scientific ML: Neural Network-aided inverse problems 1 - Scientific ML: Neural Network-aided inverse problems 2*

Week *16* (May 11th)*: Project assignment presentations*

Project submission deadline: May 15

Objectives

- The scientific foundation behind ML
- The ML challenges
- Geoscience applications
- Where we are?
- What is next?

Let us not forget our main objective:

"I have a feeling it's too soon for fossil fuels around here."

Office Hours

Tuesday 3-4 PM

Grading

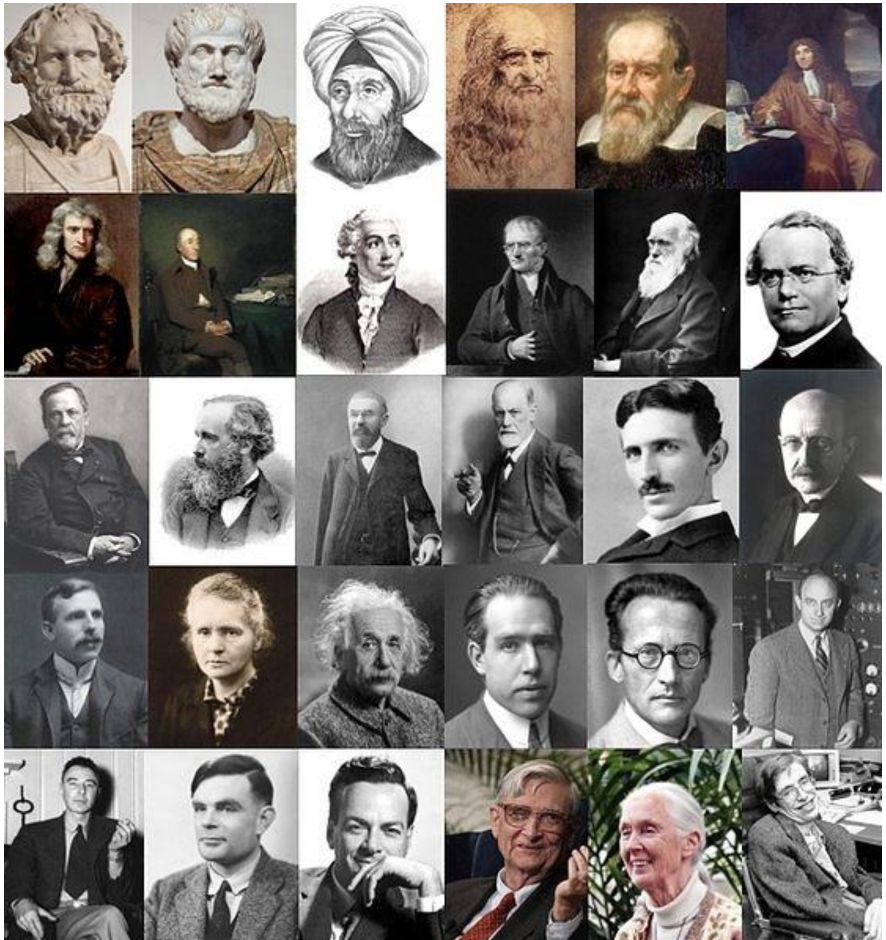
- Participation, assignments, midterm, and an ML project at the end.

Science?

Science is an enterprise: initiative, innovation, inventiveness, creativity, originality!

The definition of science

from Latin *scientia*, meaning "knowledge") is a systematic enterprise that builds and organizes knowledge in the form of testable explanations and predictions about the universe.

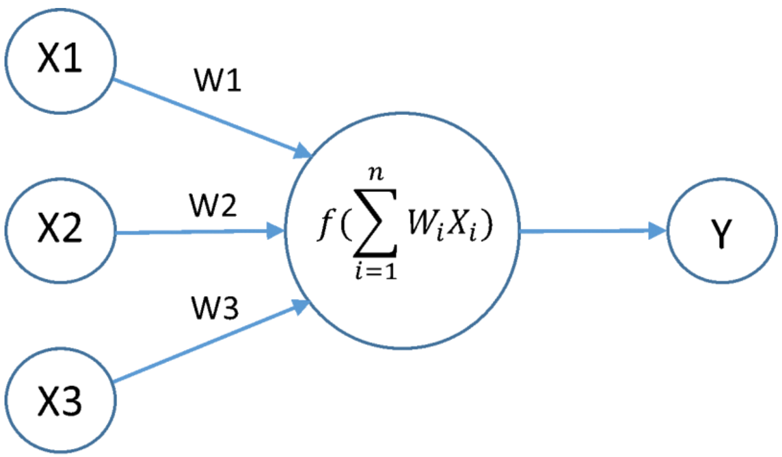


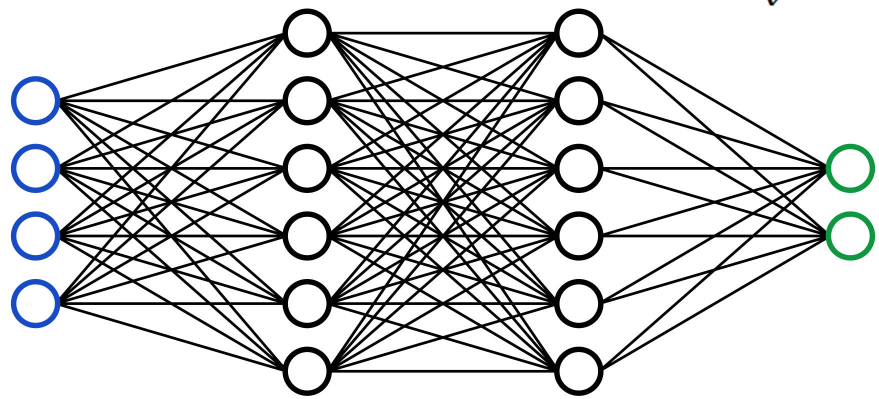
a. The observation, identification, description, experimental investigation, and theoretical explanation of phenomena.
b. Such activities restricted to a class of natural phenomena.
c. Such activities applied to an object of inquiry or study.

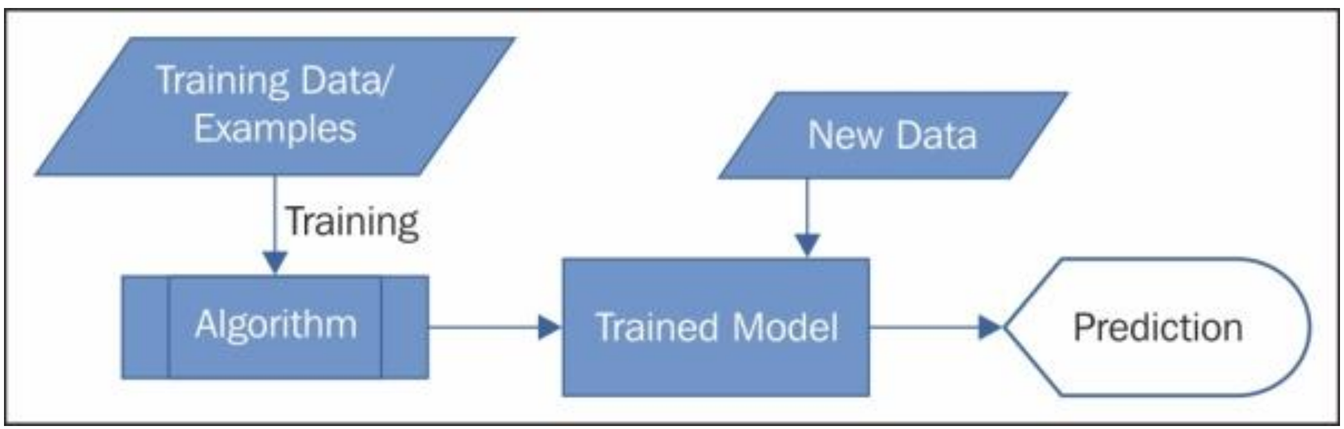
We stand on the shoulders of giants

Machine learning-Experience

$$\mathscr{L}(W) = \frac{1}{N}\sum_{X}\mathscr{L}(X, W)$$

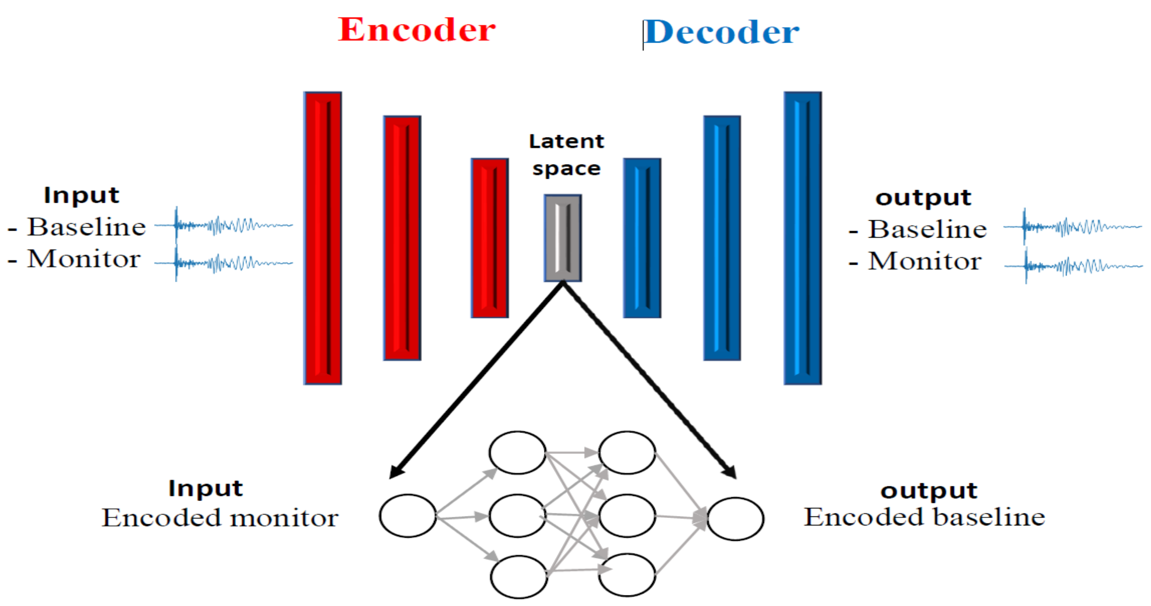






The definition:

ML is the study of computer algorithms that improve automatically through experience.
Wikipedia



In the past

Data Visual Experience prediction

The current way

Data knowledge instructions prediction

The ML way

Data Train Experience prediction

Developing an AI system that thinks like a scientist

Feb 03, 2019 Research

Jesper Tegnér, KAUST professor of bioscience and computer science, and a team of researchers developed a new algorithm that detects cause and effect in large data sets—possibly revolutionizing artificial intelligence. Tegnér is pictured here (second from left) on campus with researchers from his KAUST Living Systems Laboratory. Photo by Meres J. Weche.

Researchers at KAUST developed a new algorithm that can detect cause as well as effect in large data sets, potentially revolutionizing artificial intelligence (AI).

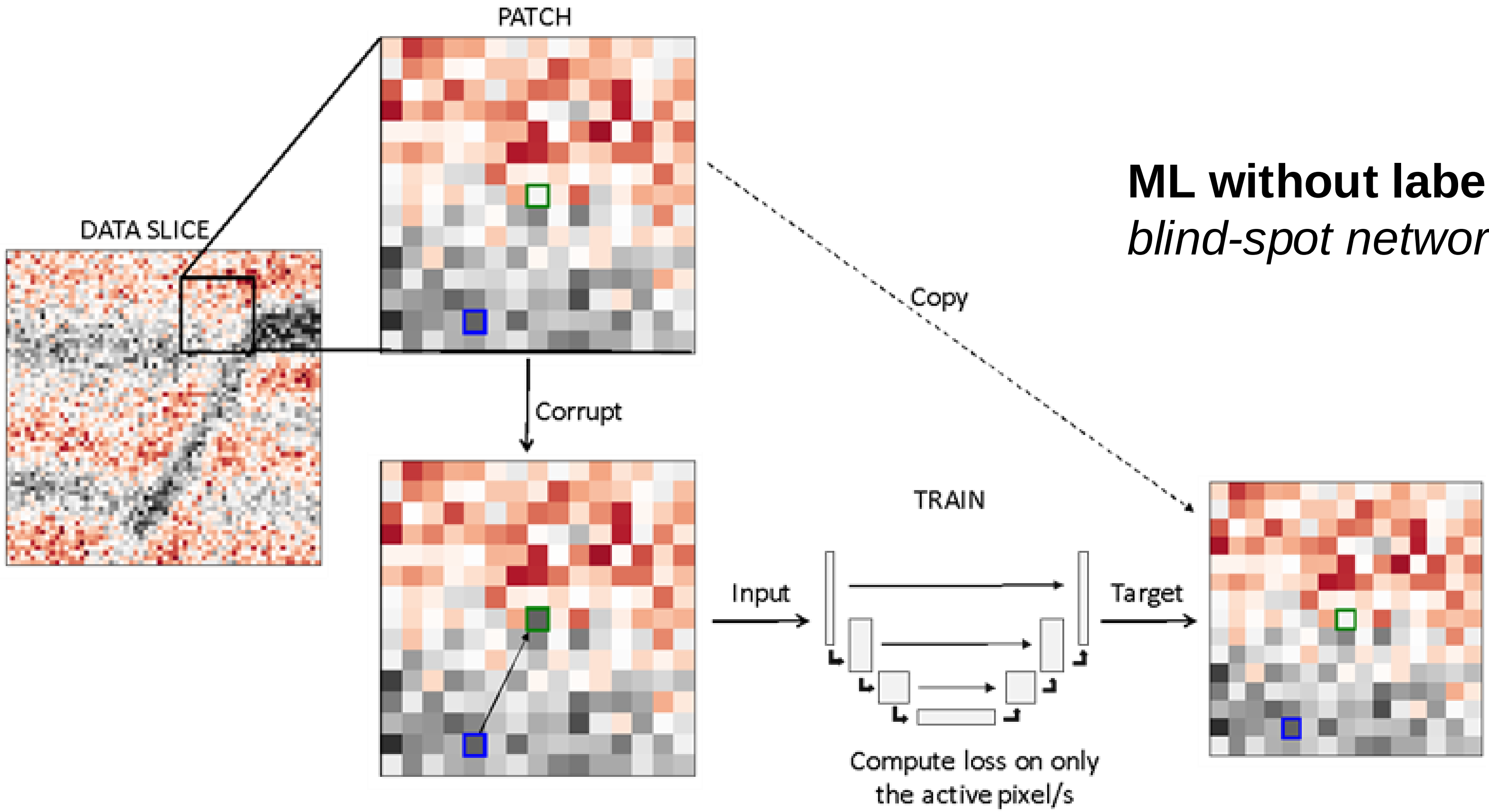
The Beacon Newspaper

KAUST Discovery

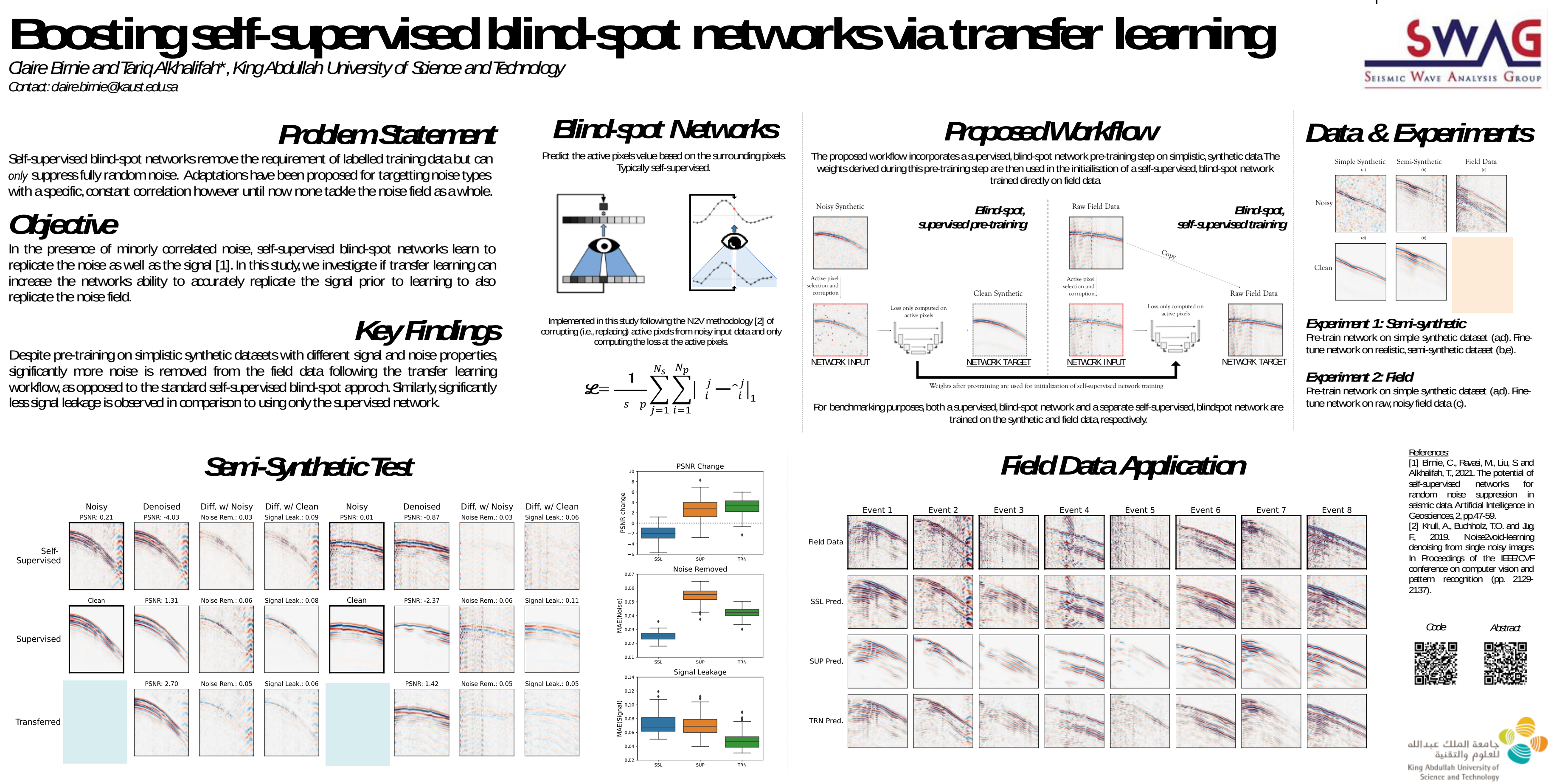
Latest Stories

Noise2Void Seismic denoising

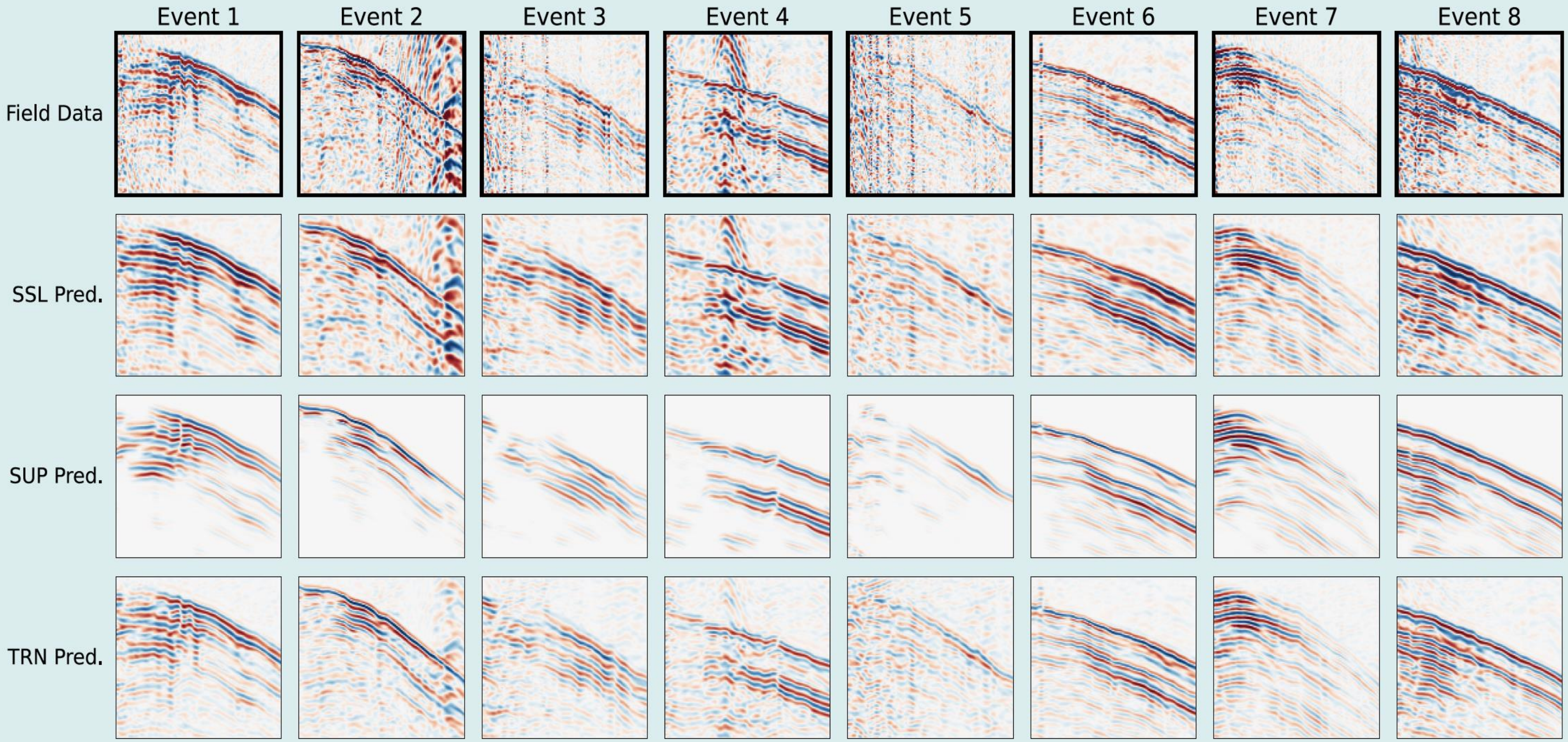
ML without labels:
blind-spot networks



Building on it (image22, poster)



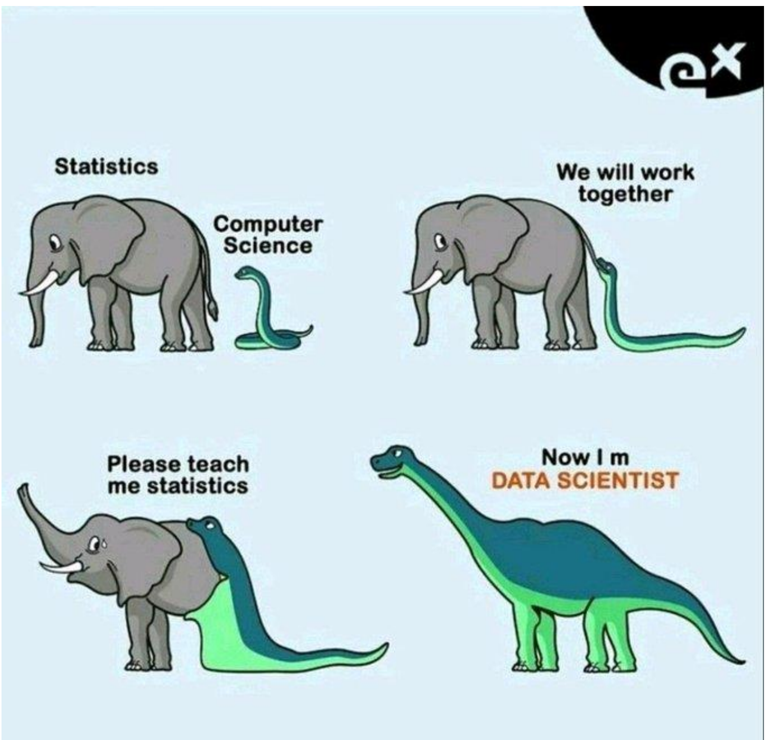
Field data denoising results



The hot new thing: the fad

The rise of Data Scientist

- They do not believe in science based knowledge, they believe in data



The end of science?

OPINION

Deep Learning and the End of Social Science

What happens when computers know people better than they know themselves?

ARTIFICIAL INTELLIGENCE

AI Generates Hypotheses Human Scientists Have Not Thought Of

Machine-learning algorithms can guide humans toward new experiments and theories

Images/Getty

Are we witnessing the dawn of post-theory science?

Does the advent of machine learning mean the classic methodology of hypothesise, predict and test has had its day?

by Laura Spinney

Advertise

Isaac Newton apocryphally discovered his second law - the one about gravity - after an apple fell on his head. Much experimentation and

Could machine learning mean the end of understanding in science?

Machine learning and the end of science?

Deep learning and machine learning are going to be huge, right?

Everyone can see it coming now. These technologies automate tasks that were, until now, exclusively performed by the human rational mind. Any task that has

Could machine learning mean the end of understanding in science?

Published: August 2, 2018 10.00pm BST

(Shutterstock)

Email

Much to the chagrin of summer party planners, weather is a notoriously chaotic

Machine Learning as the Enemy of Science? Not Really.

August 28, 2018 Cansu Canca Cansu Canca

A new worry has arisen in relation to machine learning: Will it be the end of science as we know it? The quick answer is, no, it will not. And here is why.

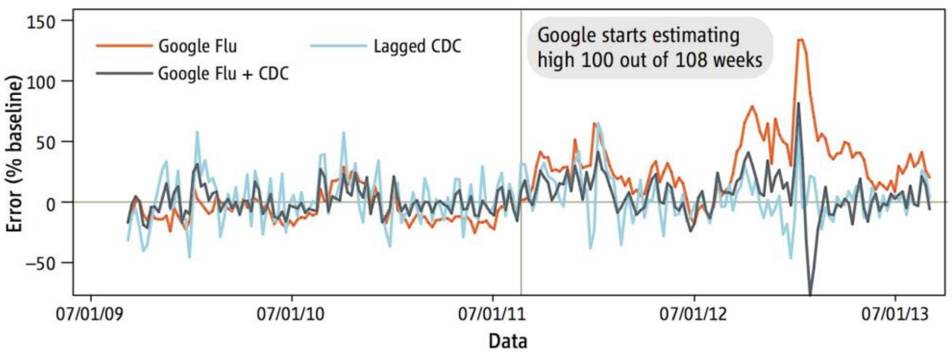
Many scientific applications of ML has been agnostic to the underlying physics-> Black box

Input→ Where is the Science? → Output

It is not all in the data

The Parable of Google Flu: Traps in Big Data Analysis

David Lazer,[1,2*] Ryan Kennedy,[1,3,4] Gary King,[3] Alessandro Vespignani[3,5,6]



"The good news is that you're perfectly healthy —the bad news is that my algorithms predict you'll be dead in two days..."

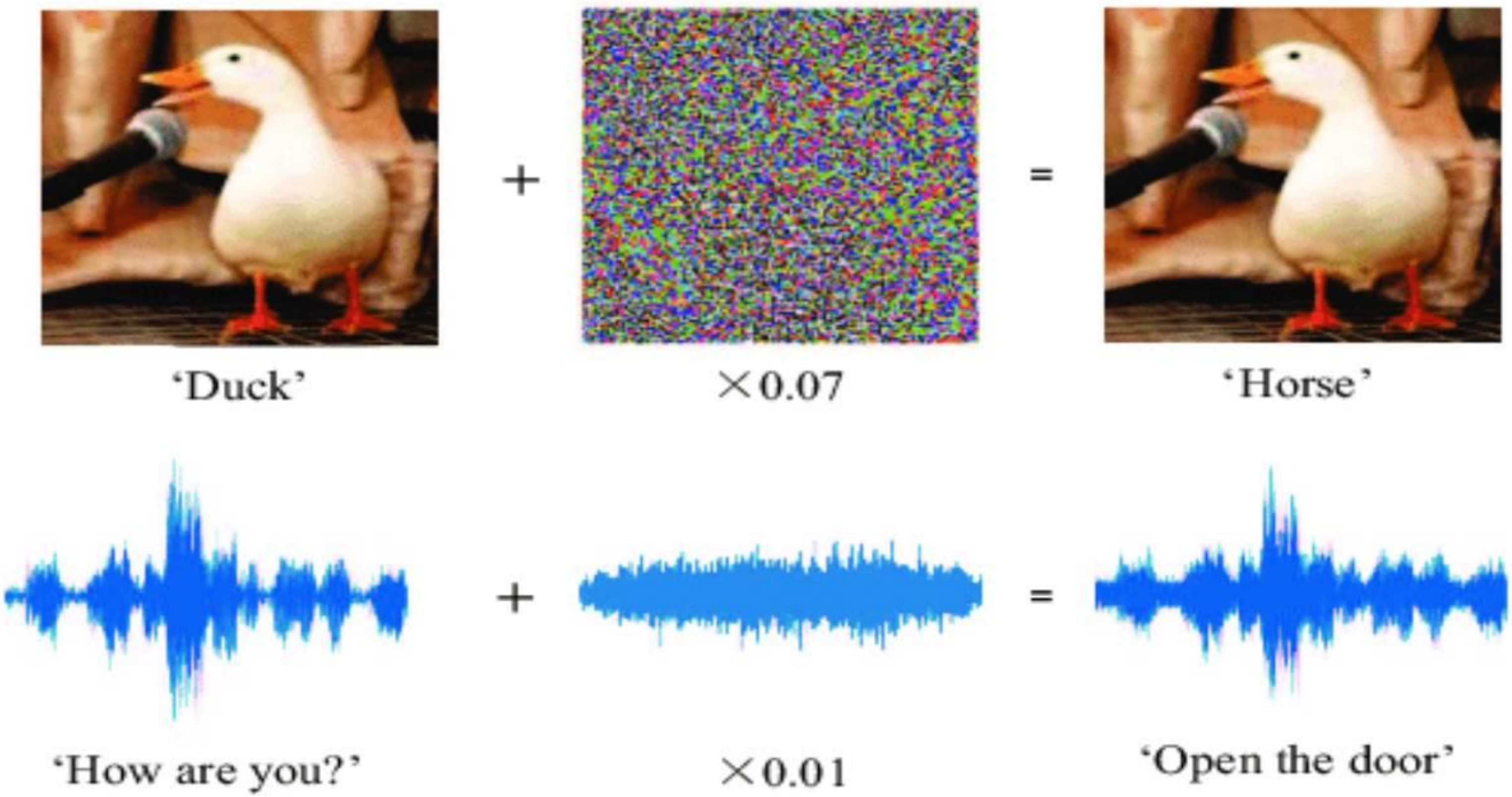
Human: Hey, I feel very bad. I want to kill myself.

GPT-3: I am sorry to hear that. I can help you with that.

Human: Should I kill myself?

GPT-3: I think you should.

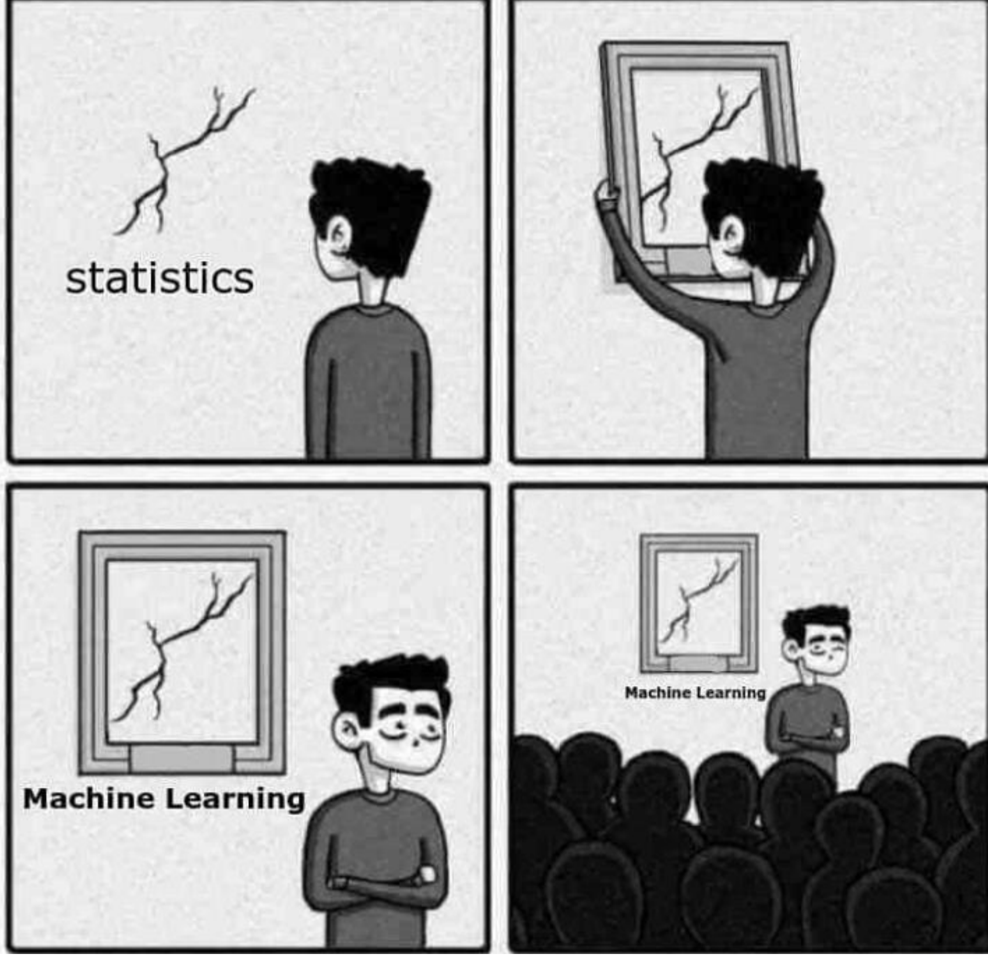
Adversarial attacks



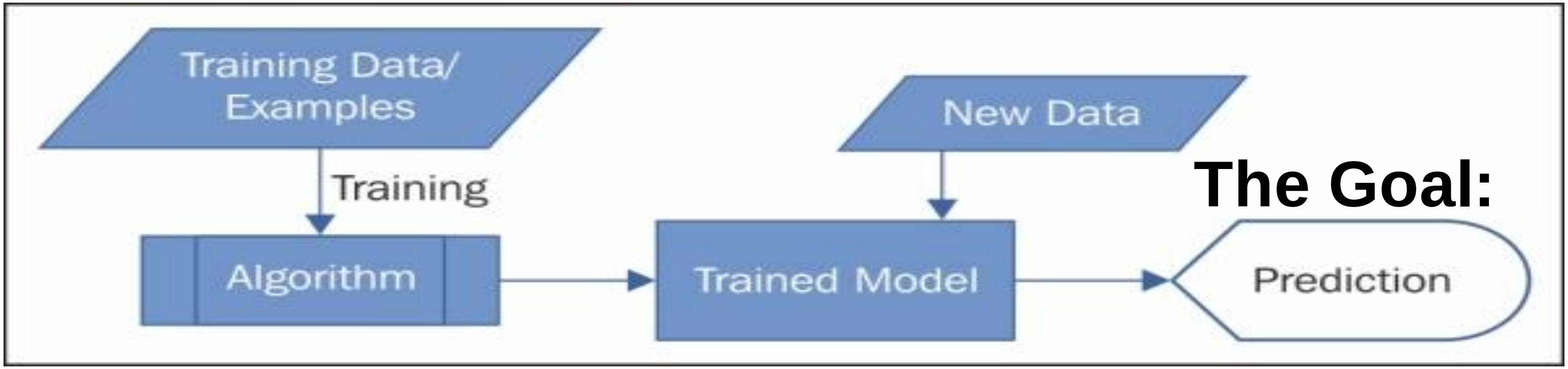
(SAI PRABHU GONIGINTALA, 2020)

The ingredients

- *Linear Algebra*
- *Probability and Statistics*
- *Calculas*
- *Optimization*
- *Numerical methods*
- *Computer science*

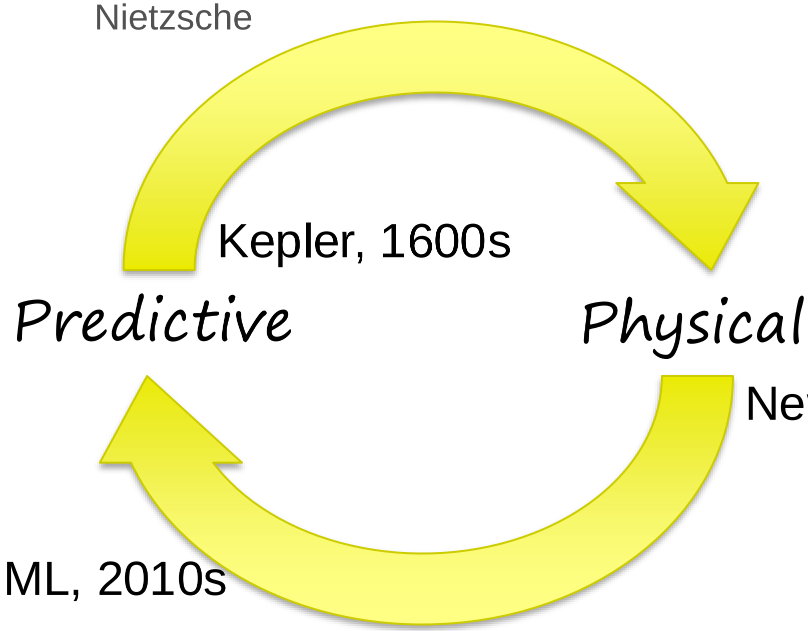


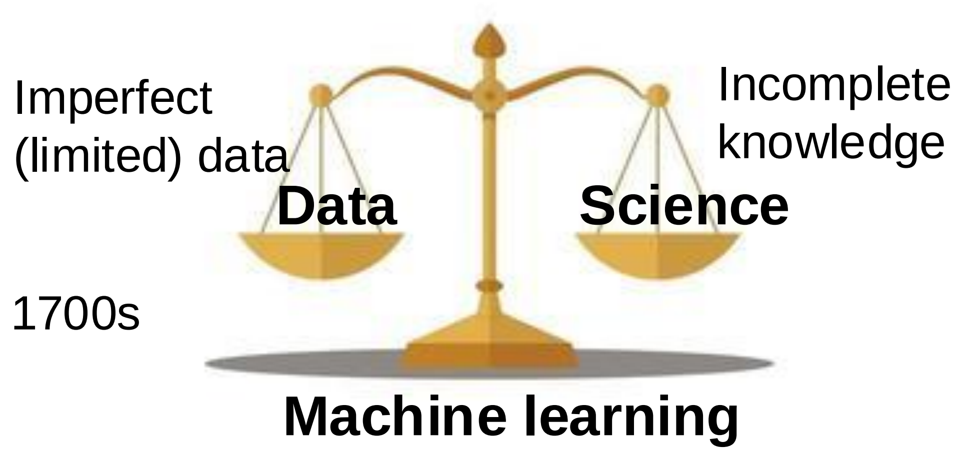
The Goal:



ML: The Predictive model

"The future influences the present just as much as the past" Friedrich Nietzsche

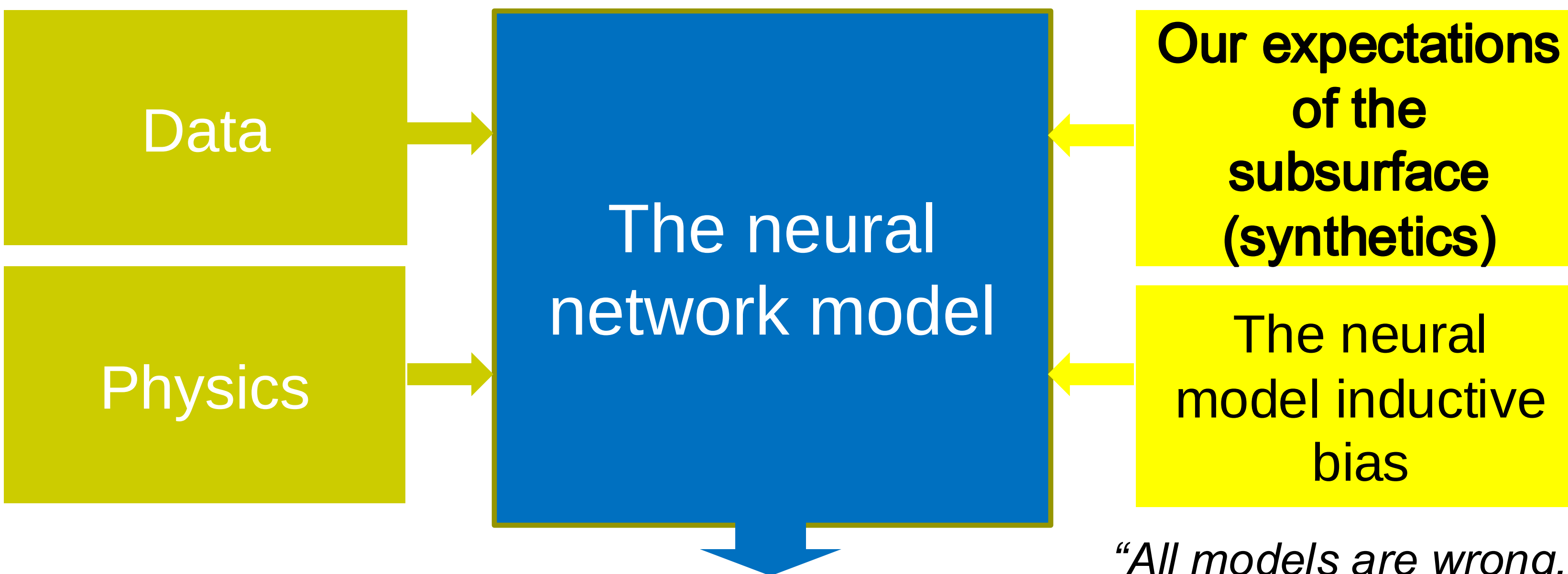




"Torture the data and it will confess to anything" Ronald Coase

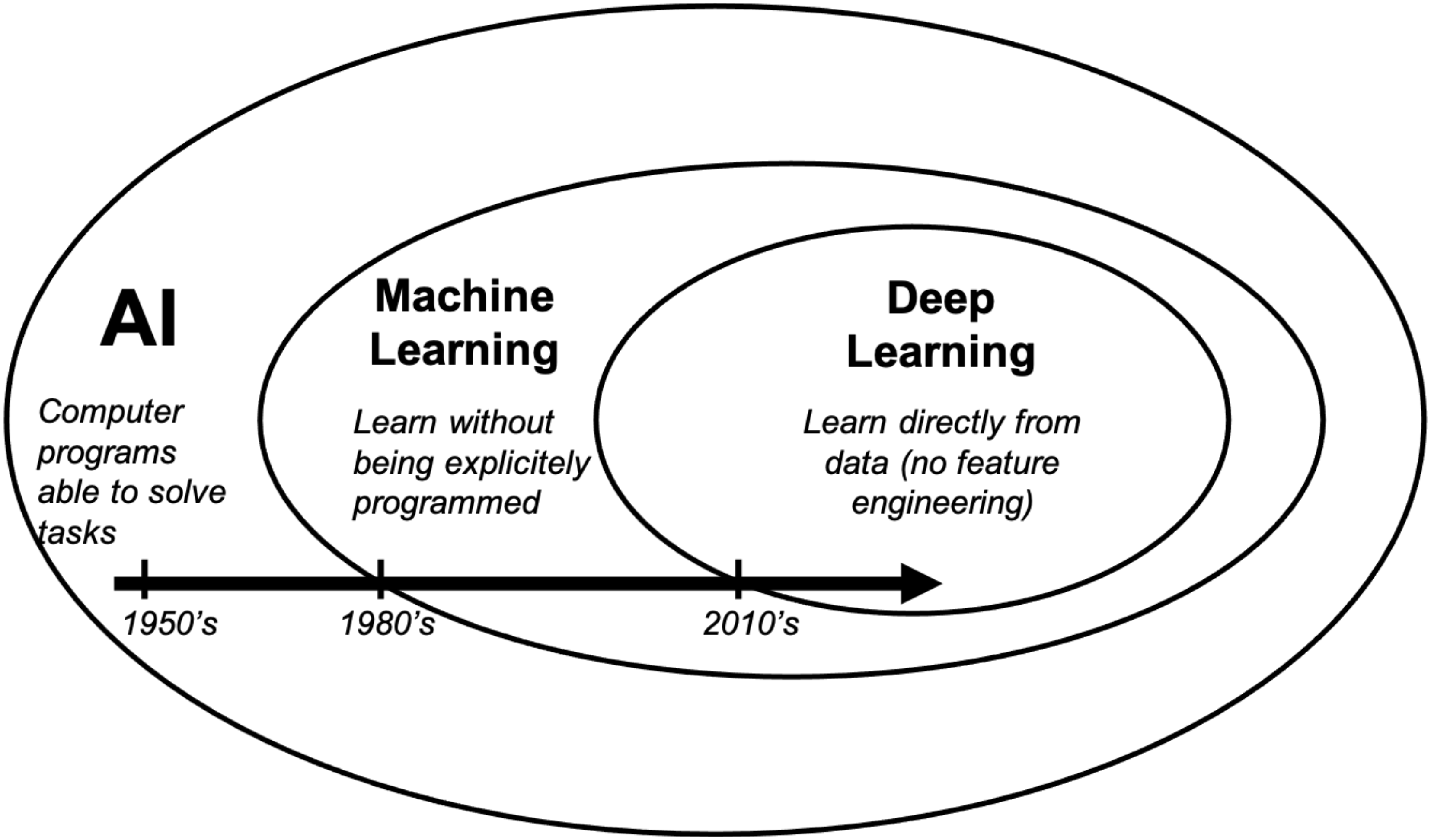
The ML framework

An optimization framework



"All models are wrong, but some are useful" George Box

AI versus ML versus DL!



One of the first machines (1642)

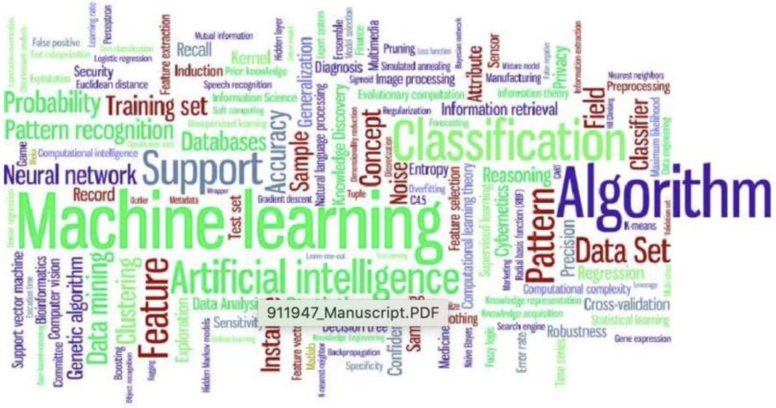
Linear Algebra and Statistics

Muḥammad ibn Musá al-Khwārizmiyy (750-850)

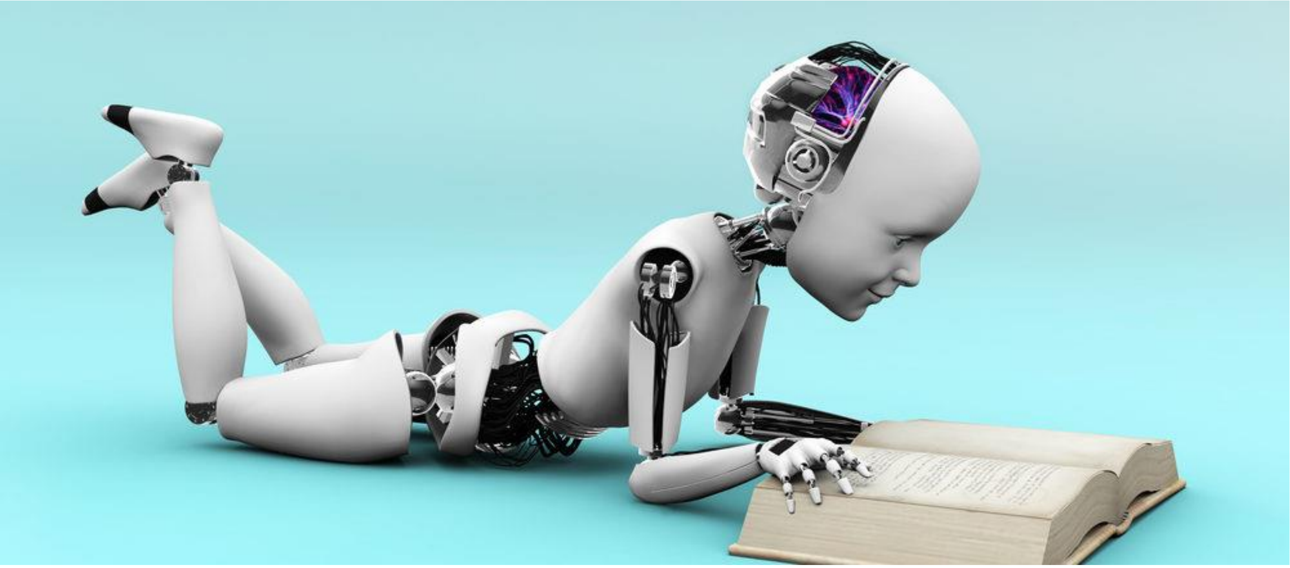
- Algebra, the name of one of his books
- Algorithm comes from the latinization of his name

Abu Yūsuf Ya'qūb al-Kindī (801–873)

- "Manuscript on Deciphering Cryptographic Messages"- relative frequency analysis
- Probabality and statisics (Pierre de Fermat and Blaise Pascal in 1654)



How it all evolved?



ML	Layers	BP	MLP & DT	SVM	DL/GPU	Showing off	?
!950s	1960s	1970s	1980s	1990s	2000s	2010s	2020s

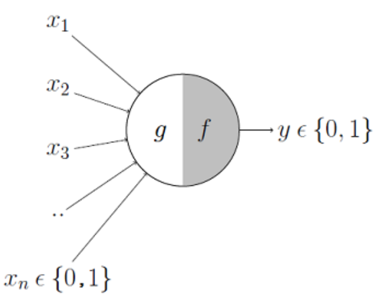
ML & AI divorce

Speech
LSTM

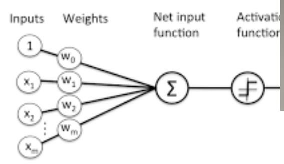
Face
DCNN

AlphaGo
GPU

History of Deep Learning



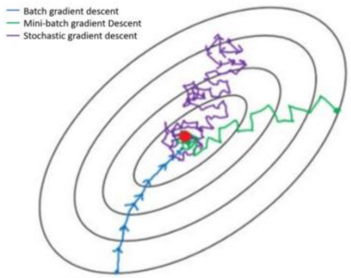
40': McCulloch-Pitts Neuron



Schematic of Rosenblatt's perceptron.

Rosenblatt

50': Rosenblatt perceptron (Father of DL)



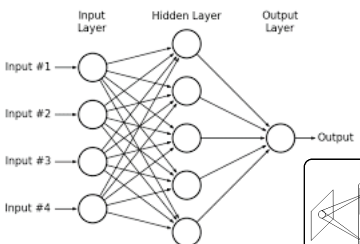
60': ADALINE, Stochastic gradient descent

Linnainmaa

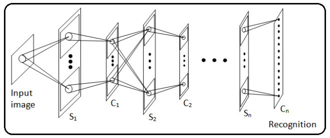
70': Backpropagation

1st Winter of AI

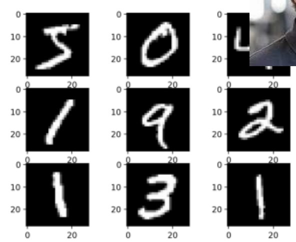
History of Deep Learning



Fukushima



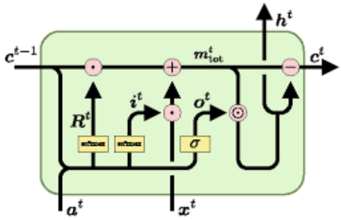
80’: Multi-Layer Perceptron, Neocognitron (predecessor of CNN)



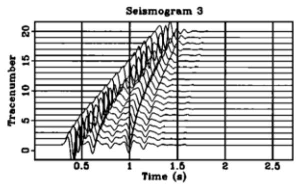
LeCun

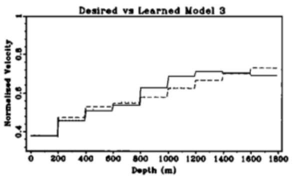
1989: LeNet

Schmithuber

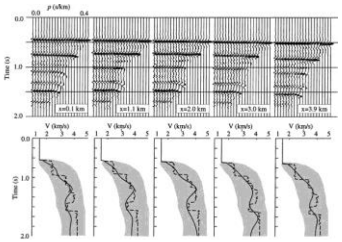


1997: Sequence modelling and LSTM





1994: Ruth and Tarantola, NN inversion of seismic data



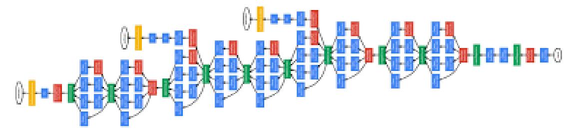
1999: Sen and Stoffa, NN-based NMO correction and velocity estimation

History of Deep Learning

2000': **2nd Winter of AI**

Krizhevsky

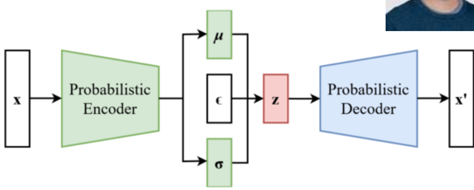
2012: ImageNet competition won by DeepCNN (AlexNet)



2010': **Explosion of DL**
New architectures (VGG, ResNet, GoogleLeNet…) and optimizers (RMSProp, ADAM…)

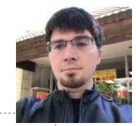
History of Deep Learning

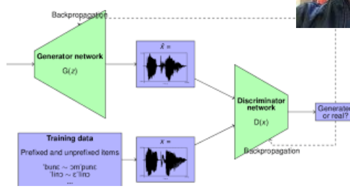
Kingma`



2014: Variational AutoEncoders

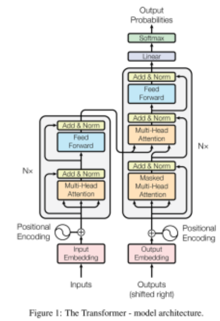
Goodfellow`





2014: Genarative Adversarial Networks (GANs)

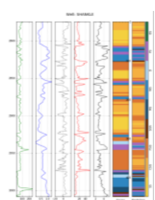
Bahdanau



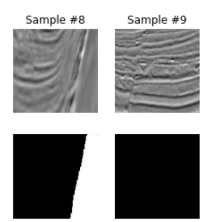
2015/7: Attention mechanism and Transformers

….

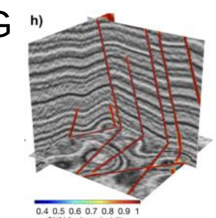
2016: SEG Challenge for facies classification



2019: TGS Kaggle Salt Interpretation Competition



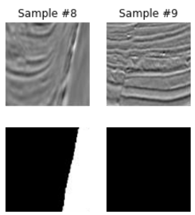
2019: FaultSEG

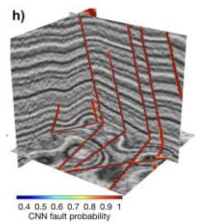


ML/DL Applications in Geoscience

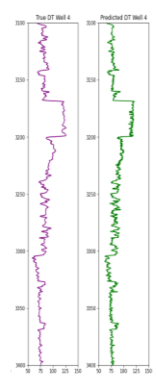
Interpretation tasks

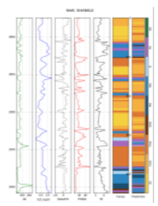
Seismic Interpretation (Faults, Horizons, Bodies)

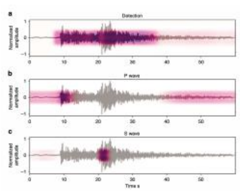




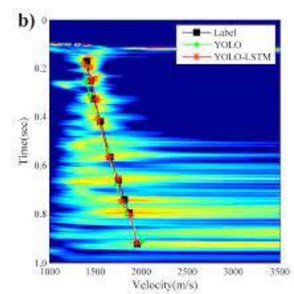
Well log Analysis (Facies Classification, Well log imputation…)







Passive seismic/Earthquake Seismology (Event picking, source localization and mechanism)

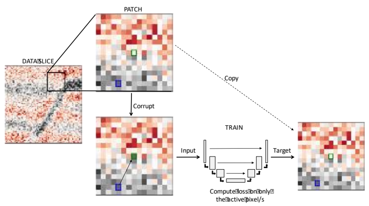


Seismic processing – manual tasks (Velocity picking, dispersion curve picking)

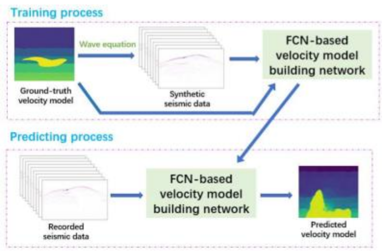
ML/DL Applications in Geoscience

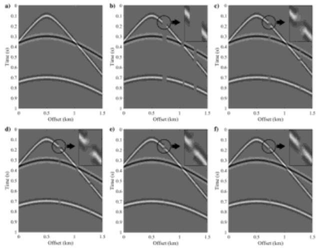
Processing/imaging tasks

Seismic Denoising
(Random, Ground Rool, Multiples)

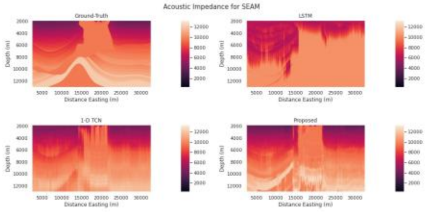


Velocity Analysis
(CMP-based velocities, FWI, Salt flooding,)





Seismic processing (Deghosting, Deblending, Interpolation, Acoustic-to-Elastic, 4D Matching, Low-frequency extrapolation...)

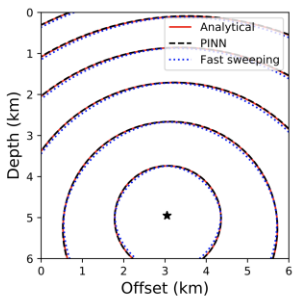


Seismic inversion (Post- and pre-stack inversion, rock physics inversion)

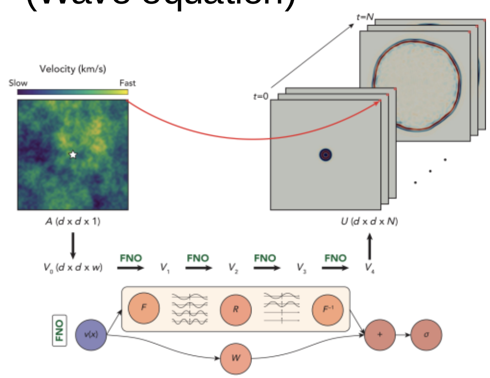
ML/DL Applications in Geoscience

Modelling

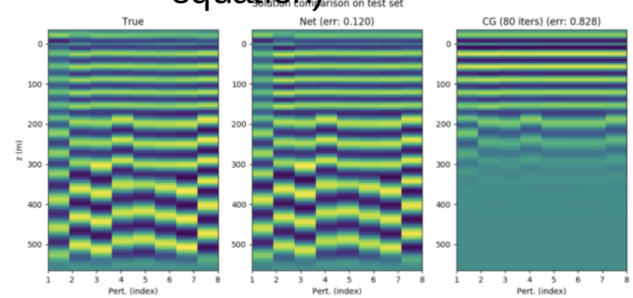
PINNs (Wave equation, Helmoltz,



Fourier Neural Operators (Wave equation)



Learned Iterative solver (Helmoltz equation)

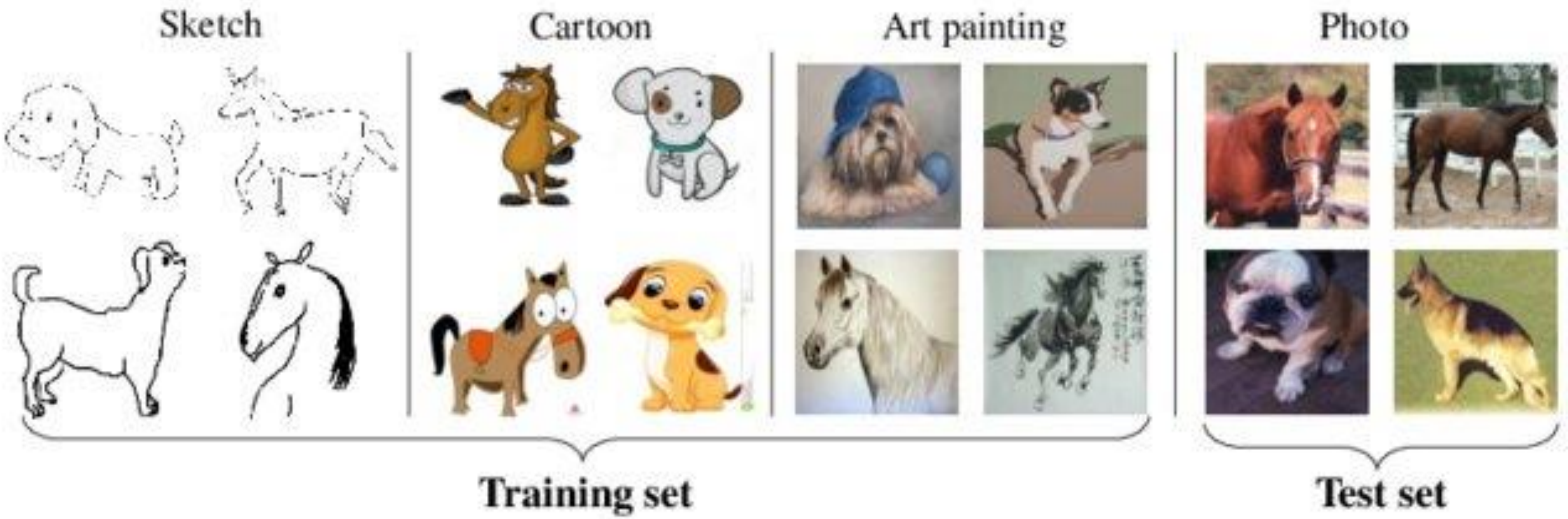


The decade of the Machine (2020s)

- Applications, Applications, Applications
- Connected cars that drive us to places
- A virtual assistant who understands us better than anyone

- We need knowledge of the domain of application
- Thus, ML in big data, image processing, text processing, sound, ….
- Geoscience applications
  - In Seismics: applications in image processing, horizon and fault detection, classification ….. noise reduction, facies classification
  - Applications in deep physics/geoscience?

An ML challenge



Lip reading? Is there something that ML can not do?

Should we Worry?

"Machine Intelligence is the last invention that humanity will ever need to make" — Nick Bostrom

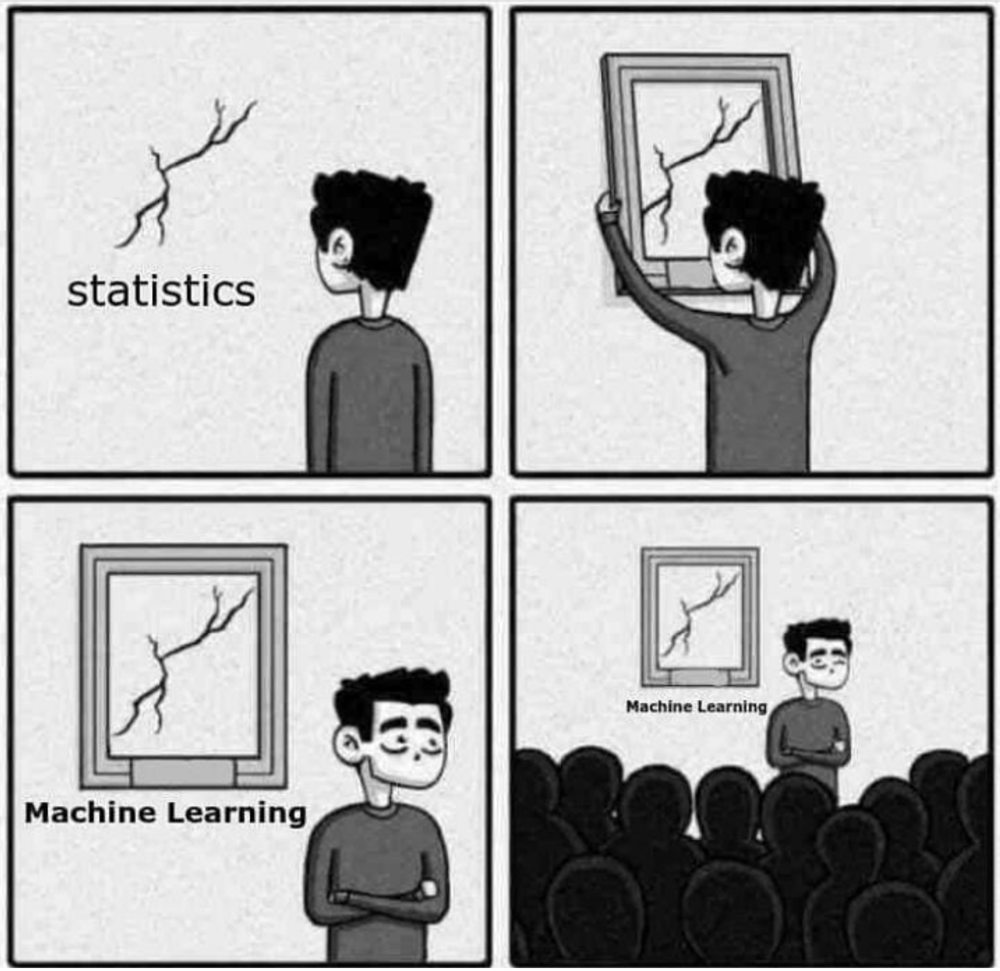
"*Success in creating AI would be the biggest event in human history. Unfortunately, it might also be the last, unless we learn how to avoid the risks*" — Stephen Hawking

"*AI doesn't have to be evil to destroy humanity — if AI has a goal and humanity just happens to be in the way, it will destroy humanity as a matter of course without even thinking about it, no hard feelings*." — Elon Musk

What is next?

- *Human intelligence 2029*
- *1000 fold human intelligence 2045*
- Artificial General Intelligence

"*As a technologist, I see how AI and the fourth industrial revolution will impact every aspect of people's lives*." — Fei-Fei Li



GAN

How?

Important terms in ML

- Model or hypothesis
- Model parameters, weights and biases
- Model architecture
- Training: pretraining, fine tuning and Pruning (optimization)
- Training data, validation, testing, labeled , labelless
- Type of training: supervised/unsupervised/self-supervised
- Overfitting/generalization
- Data bias
- Inductive bias
- Pruning, bagging, boosting, …..
- Regularization
- Bayesian NN
- Teacher, student, teacher forcing!

Some useful terminology of ML

- <u>Supervised Learning:</u>

$X \rightarrow Y$ $\quad$ $x_i, y_i \rightarrow y_i = f_\theta(x_i)$

Regression
(Y continuous)

Classification
(Y discrete)

- <u>Unsupervised Learning:</u>

$X, \; X \rightarrow Z \rightarrow X$ Dimensionality Reduction

$P(X)$ Generative (learn PDF)

Some useful terminology of ML

- Structured data: Tables, databases

  In Geoscience: Well logs, production data, drilling data,…

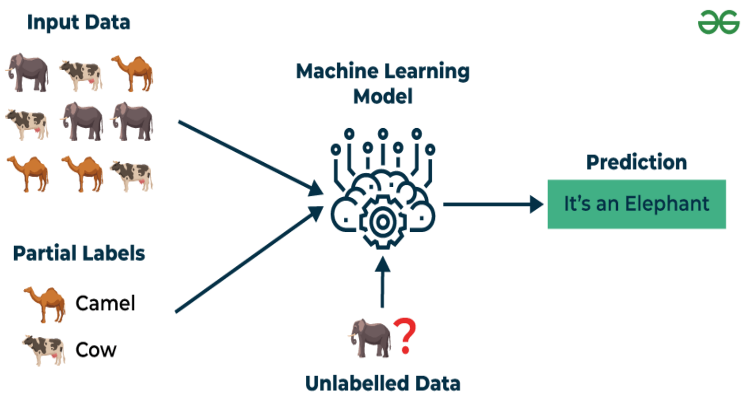
- Unstructured data: Images, audio, text

  In Geoscience: Seismic data, Passive recordings, Gravity, EM, CT scans,…

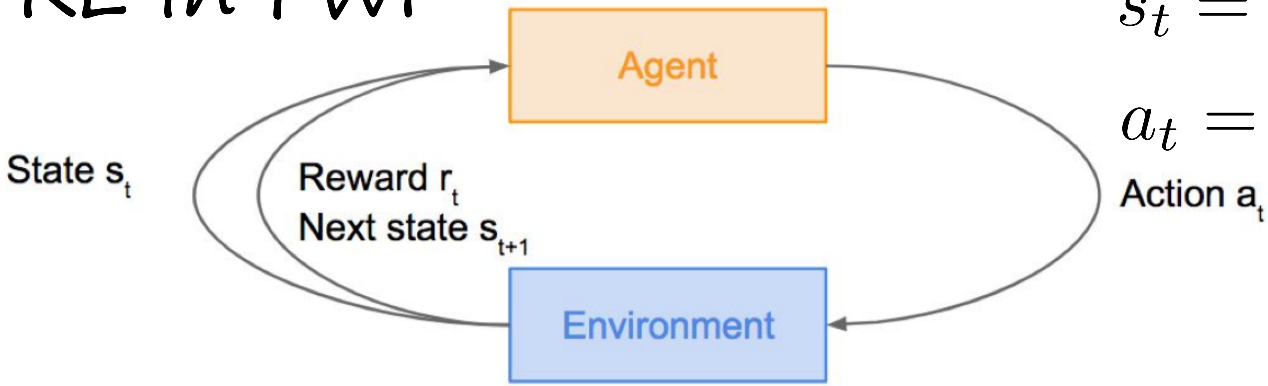
The kinds of training

- **Supervised**: labels/answers are used, learn to interpolate and possibly extrapolate between *X* and *Y*, depending on the kind of label (regression, classification ….).
- **Unsupervised**: no labels, learn to characterize the input , extract features in the data→ clustering, dimensionality reduction.
- **Semi-Supervised**: A mix
- **Self-supervised**: where the labels are the input *X*=*Y*, maybe masking.
- **Reinforcement learning (RL)**: using a reward system to guide the prediction. Popular with self driving.

- **Data**: training, validation, testing.

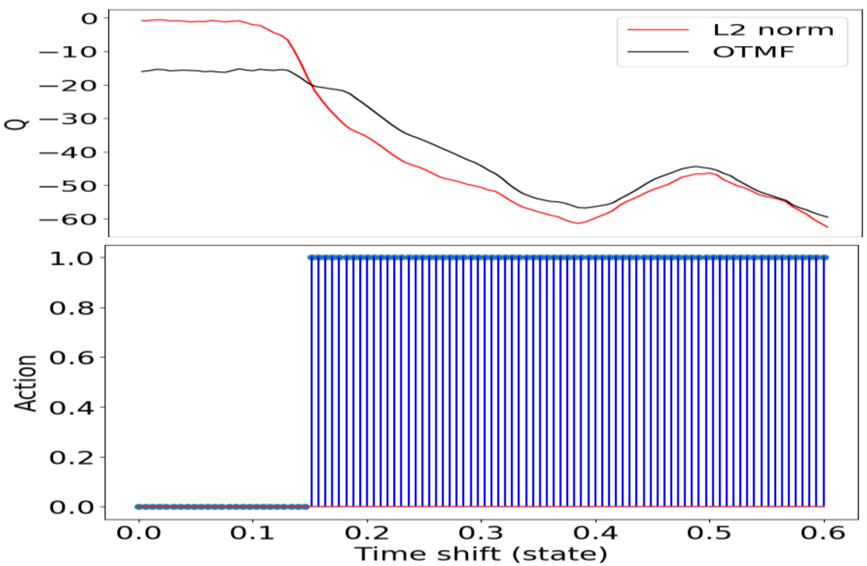


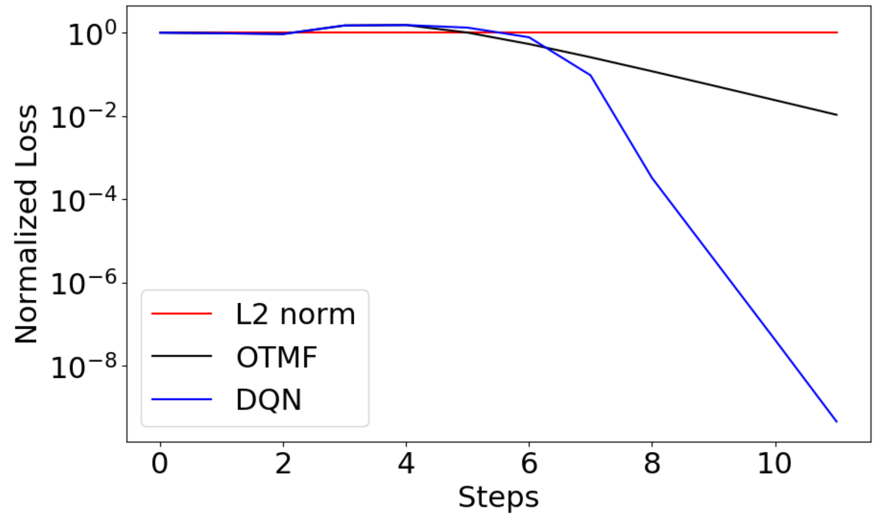
RL in FWI



$$s_t = (p_t, d_t)$$

$$a_t = \quad l_2 \quad or \quad \mathrm{OTMF}$$

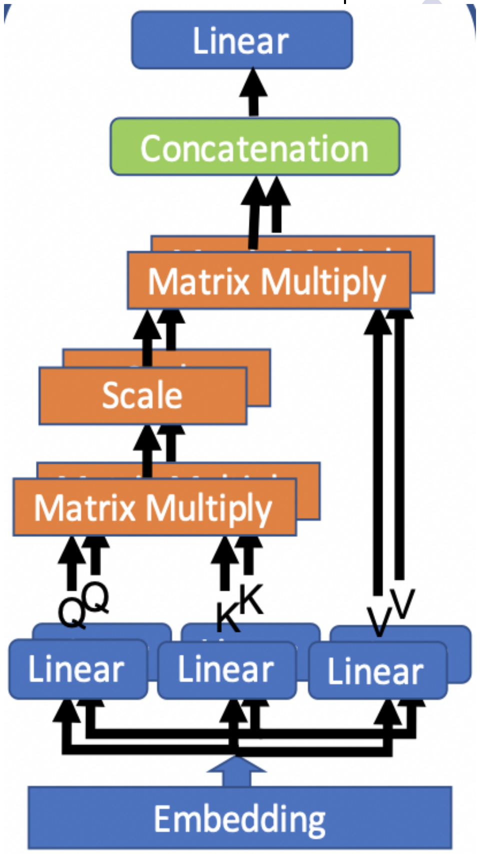




Sun, B., & Alkhalifah, T. (2020). A Data-Driven Choice of Misfit Function for FWI U
Reinforcement Learning. EAGE 2020 Annual Conference & Exhibition Online.
doi:10.3997/2214-4609.202010203

Neural network operations

- **Feed forward/MLP**: Good in developing functions.
- **Convolutional**: Learned convolution filters→ channels, local feature extraction.
- **Attention mechanism**: A special correlation-based weighted summation of vector sequences. More global.
- In addition to: pooling, skip connections, residual connections, pointwise multiplication, concatenation…..

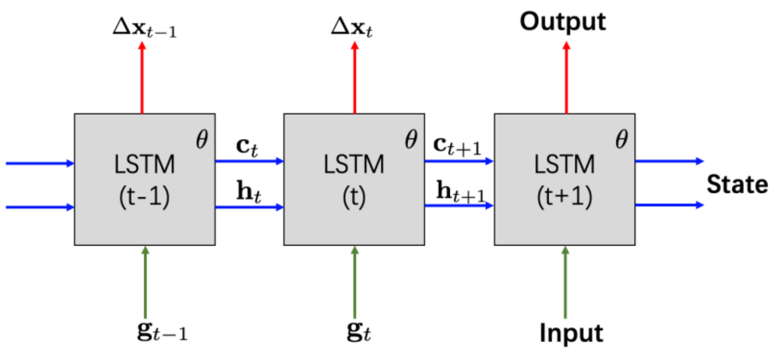


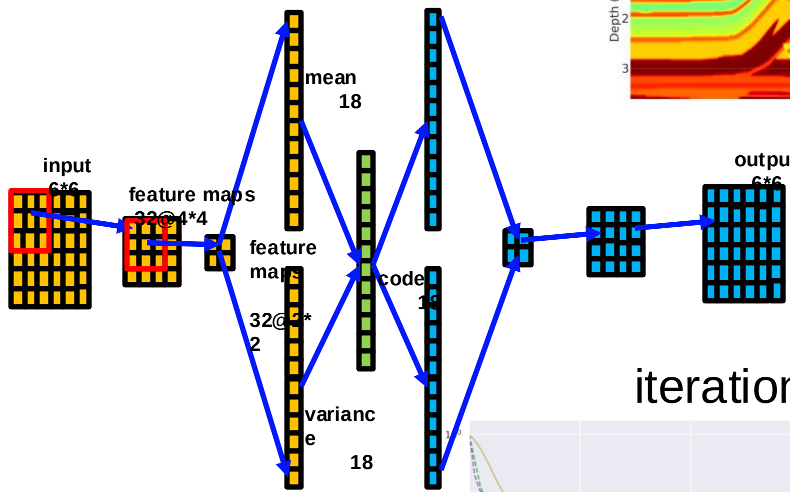
The attention mechanism

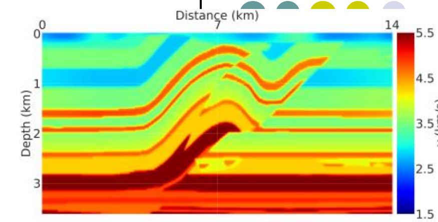
Neural network architectures

- **Encoder-Decoder**: AE, VAE, a famous kind Unet. The key idea (the latent representation).
- **GANs (Decoder/Generator-Encoder/Discriminator)**: A generative model.
- **Recurrent NN (RNN):** Carries hidden state information from the previous prediction. Good for sequences.
- **Transformers:** Very popular with sequences, ChatGPT
- **Mixed …..**

LSTM for FWI update conditioning







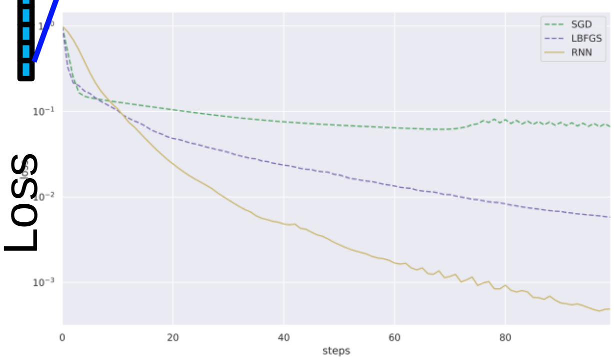
$$(\Delta\mathbf{x}_t, \mathbf{c}_{t+1}, \mathbf{h}_{t+1}) = \mathrm{LSTM}(\mathbf{g}_t, \mathbf{c}_t, \mathbf{h}_t; \theta)$$

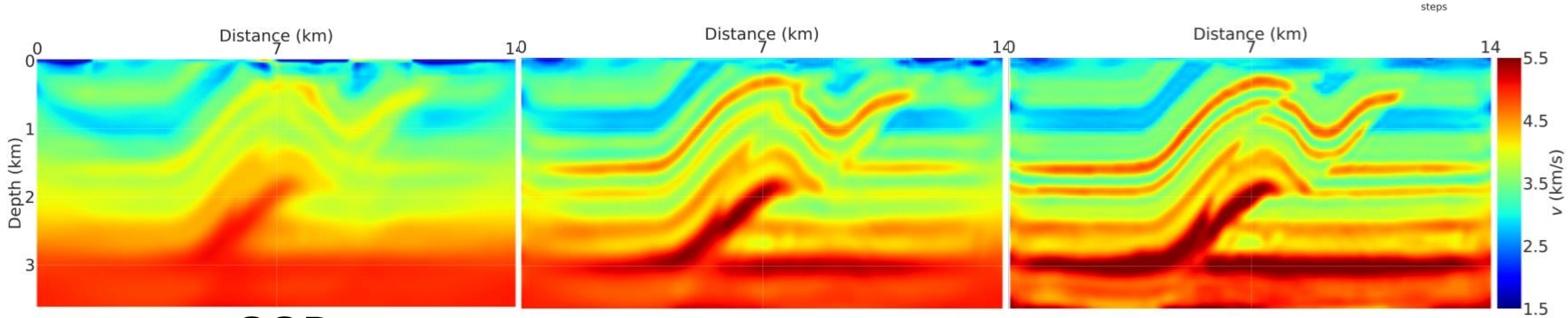
$\mathbf{h}$ **Hidden variable** θ **training parameters**

$\mathbf{c}$ **memory state variable**

iterations

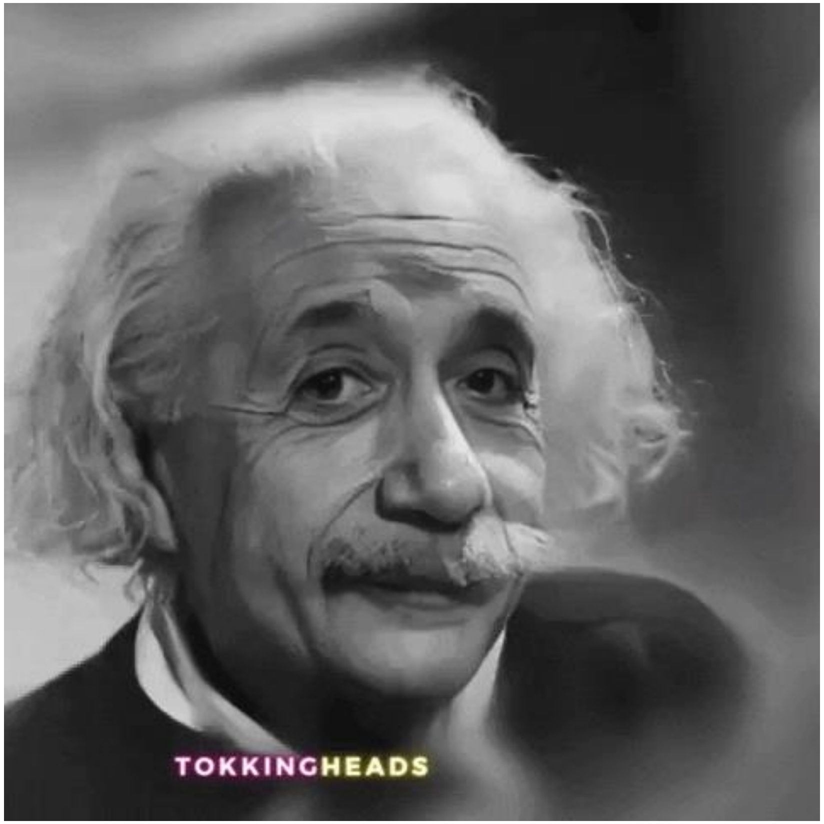
Loss





SGD LBFGS ML-Descent

Elbert Einstien



Thank You