# Ia Artificial Intelligence all we need?



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# AI vs ML vs DL





## Neural Networks: milestones



Credits: D. Maltoni 3





# A brief history of NNs

First models of artificial neuron (McCulloch, Pitts, 1943)

• Neuron behaviour (i.e. info passing) are determined by "weights": initially randomly set, they are modified during "training"

Towards neural networks: "Perceptron" (Rosenblatt, 1958)

Multi Layer Perceptron (MLP)

• Groups of neurons organized in layers (input layer, output layer, and one or more intermediate "hidden" layers, each with one or more neurons)

Back-propagation algo (Rumelhart, Hinton, Williams, 1986)

• an effective technique to train them (i.e. setting weights' values)

From shallow NN to Deep  $NN \rightarrow$  Deep Learning







# INFN E.g. "supervised learning": ML training vs inference



## AI's past winters and current spring

## Past "winters" of Al

 $\widehat{I^{NFN}}$ 

- '60: shallow NN hard to train
- '90: Support Vector Machines (SVM), Boosted Decision Trees (BDT), ...
- 2000+: advanced deep NN architectures



## Current "spring" explainable by:

- "Big data"
- Technology + ML research
- (cloud and accessibility)





## ML-based publications in science



Extremely large adoption in incredibly short times, towards high level of pervasiveness

# Pervasive ML in HEP [1/3]

## ML in **data acquisition** and **trigger**

- Bkg and trigger rate reduction
- Signal specific trigger paths
- Anomaly detection in data taking
- Unsupervised new physics mining

### E.g. LHC experiments' trigger is a strong "driver" for high-performances ML applications

• Next-gen trigger systems  $\rightarrow$  real-time reconstruction  $\rightarrow$  real time analysis

Challenge is the trade-off between **algorithmic**<br>complexity and the performances achievable under severe time constraints in inference



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# Pervasive ML in HEP [2/3]

### ML in Event Simulation

The production of simulated events (full/fast simulation) is extremely intense from the computation standpoint (up to the point it might impact the physics reach of the experiments). ML can help to reduce such load

- Calorimeter shower surrogate simulator
- Analysis level simulator
- Pile-up overlay generator
- Monte Carlo integration
- ML-enabled fast-simulation
- Invertible full-simulation (probabilistic programming, …)

#### $\bullet$  ……

### ML in Event Reconstruction

Online/offline reconstruction might be partially replaced by surrogate models (approximate  $\rightarrow$ faster) or by new algorithms (that might offer unprecedented performances)

- Charged particle tracking (GraphNN, vertexing, …)
- Calorimeter reconstruction (local, clustering, ...)
- Particle flow (GraphNN, ...)
- Particle identification (boosted jets, isolation, …)
- Pileup mitigation
- Energy regression (end-2-end, …)
- $\bullet$  ...

## Pervasive ML in HEP [3/3]



### ML in Computing Operations

Application of ML to **non-collision (meta-)data** might help to increase efficiency and reduce the need omg personpower in Ops, e.g.<br><u>automating specific tasks</u>, developing intelligent/adaptive systems, ultimately acting<br>on the full chain - from data collection to data analysis - and make it more agile

- Detector control
- Data quality monitoring
- Operational intelligence
- Predictive maintenance
- $\bullet$  ...



ML in HEP started by using domain knowledge to perform **feature extraction/engineering** 

• HEP physicists design high-level features, and send them in punt to traditional ML "shall" algorithms

## Particle id, energy resolution, e oltre..

BDT usati per il learning delle energy corrections usando tutte le info disponibili nei vari sensori calorimetri

**Esempio**

• es. CMS: energy sum, recupero bremsstrahlung con supercluster, inclusione della pre-shower energy, poi energy correction con algo multivariato



*[ 2015 ECAL detector perfor[mance plots, CMS-DP](https://cds.cern.ch/record/2114735)-2015-057. Copyright CERN, reused with permission ]*



LHCb usa delle NN allenate su *O*(30) features da tutti i sottosistemi, ciascuna allenata a identificare uno specifico tipo di particella

•  $\rightarrow$  mis-ID bkg/particle ridotta di ~3x (e oltre..)

Uso di ML in scoperta e studio delle proprietà Higgs

Ruolo chiave del ML nella scoperta del bosone di<br>Higgs prima delle attese

- es. diphoton analysis di CMS, BDT usati per migliorare la risoluzione e selezionare/categorizzare eventi
- $\bullet \rightarrow$  sensitività aumentata di un ammontare equivalente al ~50% di dati raccolti in più



*[courtesy M.Pierini]*

 $\tau_{\text{lep}}\tau_{\text{had}}$ VBF  $E$ vents / 0.17  $\triangle$  Data  $10<sup>4</sup>$  $H(125)$  ( $\mu=1.4$ )  $\sqrt{s}$  = 8 TeV, 20.3 fb<sup>-1</sup>  $H(125)$  (u=1) **ATLAS**  $Z \rightarrow \tau \tau$  $10^3$ Others Fake τ Uncert.  $10<sup>2</sup>$  $10$ Data / Model  $1.5$  $0.5$  $-1$  $-0.5$  $\Omega$  $0.5$ **BDT** output

Studio delle proprietà H: es.  $\tau$  leptons,<br>**ATLAS** su 6 regioni cinematiche distinte, training di una BDT in ciascuna, con 12 features

→ sensitività migliorata del ~40% rispetto a un approccio non-ML

[1] JHEP 04 (2015) 117

**Esempio**



## Test di alta precisione del MS

 $\mathsf{CMS}\in\mathsf{LHCb}$ : evidenza per il decadimento raro<br>B<sup>0</sup>s→ $\mu^+\mu^-$  con analisi combinata [1]

- es. BDT usati per ridurre la dimensionality dello spazio delle features, poi analisi spettro massa in BDT response bins  $\rightarrow$  decay rate consistente con predizioni SM con precisione ~25%  $\rightarrow$  constraints a estensioni SM
- $\bullet \rightarrow$  es. per avere la stessa sensitività senza ML, LHCb come singolo esperimento avrebbe dovuto raccogliere ~4x più dati



*Mass distribution of the selected B0 → μ<sup>+</sup>μ− candidates with BDT > 0.5 [2]* 

[1] Nature 522 68–72 (2015) [2] *Phys.Rev.Lett.* 118 (2017) 19, 191801



## Since some years, ML (DL) in HEP seeks for more advanced techniques, e.g. deep NNs

### • Use all the features space at its full dimensionality to train deep NN - no more manual feature engineering

→ estract best from data, and do so by exploiting any architecture that might work for a given use-case (e.g. input<br>from CV and NLP solutions..)

## Convolutional Neural Networks (CNN)

CNNs offer translational-invariant feature learning, robustness against noise, versatility in application to a variety of domains

- Extremely vast zoo of architectures! Primary target: computer vision
- are based on sequences of convolutional and pooling layers, and

(e.g., self-driving cars, ..)

Industry: Large adoption in computer vision applications



automation of hist checking (e.g. data quality), …



General tactics: (TPCs, CALOs..): represent your data as 2D/3D images (even 4D w/ timing info)

 $\rightarrow$  problem casting into a computer vision task

## "HEP is so different from other applications..". Are we?



Rivelazione di tracce di neutrini su cosmic background events (metodo: CNN)



Rivelazione di **aeroporti** da immagini satellitari (metodo: CNN)

## Recurrent Neural Networks (RNN)

RNN allow to handle variable-length inputs and process time-series, accumulating and using together info at various times in the sequence

- Based on "recurrent neurons" (backward-pointing connections)
- A variety of application in time-series of all kins, e.g. language translation, ..



Industry: handling "time series" (audio, video, natural language processing)

#### HEP:

Classifiers capable to process variable-length signals of different nature (tracks, particles in jets, etc) - ample application in astro-particle physics



## Autoencoder (AE)

AE is a "data-specific" compression algorithm, able to reduce dimensionality and extract "the juice" of an input

• a feed-forward (un/self-supervised) NN capable to encode the input into a reduced-dimensionally representation ("latent space") and decode it in output



anomaly detection (intestìni events are those whose decoding in output is dtstant from the input, according to a given metric



Potenziale strumento per scoprire nuova fisica in modo "unsupervised"

## (V)AE per "new physics mining" - at LHC and beyond **Esempio**

## A Variational AE has been proposed (CMS) for "new physics mining"

- Traing on known SM processes, build threshold to identity "anomalous" (i.e. interesting: BSM?) events
- Treat them as outliers, save them (no trigger kill!), build a catalog for further inspection
- Model-independence: training not dependent from specific new physics signatures  $\rightarrow$  assumptions-free
- Might be complementary to classical methods, i.e. model-dependent hypothesis testing
- topologie ricorrenti nel catalogo possono ispirare search focalizzate, e anche costruzione di modelli teorici
- Target: up to the trigger level..

## Note: going from discriminative AI to generative AI ...

[1] JHEP05 (2019) 036

## Generative Adversarial Networks (GAN)

A generative algorithm, based on an architecture with 2 NNs, a generator G and a discriminator D, which compete

- G creates images from noise, D classifies them real vs fake
- Once trained one against the other, G pursues its goal which is to confuse D, and in the process it learns how to creare fake but very realistic images



Industry: image editing, data generation, security, ..



HEP: Simulate the detector response at reduced computational costs



## Data sparsity and point clouds

HEP handles **high sparsity** datasets: not a HEP-only issue..

- Granularity and occupancy in HEP sensors
- Popolation of stars and galaxies in the cosmos
- Molecular description in computational chemistry

Abstract space with coordinate of sparse elements, each characterized by an array of features, a set of arrays as a function of event/run, …

• e.g. EM shower  $\rightarrow$  E deposited in active volumes of an ECAL

More adequate representation would be a "point cloud", and best approach might be not (HEP-)traditional

- Need to be open-minded towards methods not familiar (co far) to the HEP community
- e.g. problems configurable in extraordinarily similar way to how social media datasets are treated (!)



## Graph Neural Network (GNN)

Think of a CNN acting on its input features (pixels). Its power resides also on a "regular-array dataset" paradigm

• Data represented as sets of dense arrays/tensors, with intrinsic metrics

In a sparse representation, we need a metric that defines proximity in the abstract space of features

How? Migrating from"**datasets**" to "**graphs**"

• Connect elements of a dataset and train a NN to learn which are the relevant connections

GNN  $\rightarrow$  build a data structure, (V,E) with V=vertex and E=edges, choose possible types of vertices (if no prior one builds a fully-connected graph), etc

GNNs start to be part of present/future of DL in HEP









# Natural Language Processing (NLP)

Important advances in the decade 2010-2020, thanks to deepNN ("Deep Learning")

- Machine Translation  $\rightarrow$  e.g. language A Language B translation
- Text/Document Classification  $\rightarrow$  e.g. doc clustering, sentiment analysis, ..
- **Entity Extraction** (a.k.a. Named Entity Recognition)  $\rightarrow$  extracting relevant information from unstructured text (e.g. vital parameters of a patient from her/his medical record)
- Summarisation  $\rightarrow$  e.g. generating concise summaries of docs
- Question-Answering  $\rightarrow$  multi-domain and multi-language factual knowledge
- Digital Assistants  $\rightarrow$  e.g., Amazon Alexa, Google Assistant, Apple Siri, ..

NLP "first generation" (2010 - ~2017):

- RNN, or Long Short-Term Memory (LSTM), trained on text corpus to learn the structure of language
	- $\ast$  Handle text as a sequence of symbola ("token"), mapped to multidimensional vectors ("embedding") and processed through a hierarchy of levels

But then.. a "second generation" came in..



*BTW: is NLP relevant for HFP? → Yes.* 



#### Output Probabilities Softmax Linear Add & Norm Feed Forward Add & Norm Add & Norm Multi-Head Feed Attention Forward  $N \times$ Add & Norm  $N \times$ Add & Norm Masked Multi-Head Multi-Head **Attention** Attention Positional Positional Encoding Encoding Output Input Embedding Embedding Inputs Outputs (shifted right)

# "Attention is all you need"

Google (Brain), 2017: a new deepNN architecture called Transformer

- A native seq-2-seq, with a key element: the "attention" mechanism, that allows to pass the meaning of a token in the context of other tokens in the same text
- Soon became the reference model for language processing (see next)



Residual streams: info channel at high capacity (d=12288 in GPT-3). Attention and MLP modules can read/write from/to subspaces of residual streams w/o interference with message passing.

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# Language Models: from LM to LLM

"Second generation"  $\rightarrow$  modern Language Models (LM): a class of probabilistic models that learn patterns in NL via more advanced methods

- Architetture change: from RNN to Transformer
- Tokenization  $\rightarrow$  multi-language and multi-domain
- Training on extremely large text corpuses (incl. source code!)

Major players:

- GPT-3 (OpenAI, 2020) from which ChatGPT derived (OpenAI, 2022): trained on 45 TB of text (equiv. 2000x Wikipedia), Estimated training cost: 4.6 M\$. GPT-4 (OpenAI, 2023). Estimate: 1 order of magnitude more params
- Bard/Gemini (Google), Claude (Anthropic), LLaMA (Meta)

Significant efforts into scaling LMs into Large LMs (LLM)

- $\bullet \rightarrow$  training bigger models on more data with greater compute
- $\bullet \rightarrow$  steady+predictable improvements in their ability to learn patterns
- This could be observed in improvements to *quantitative* metrics.. but also *qualitative* (!)

Before getting to this, some examples..

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# LLMs for Multimessenger Astronomy

## Observations in astronomy:



*[ credits: D. Kostunin, A. Alkan, A. Chaikova, V. Sotnikov et al. ]* <sup>33</sup>

## LLMs for Multimessenger Astronomy

Description: Referred to by ATel #: 8706, 8718, 8783, 8789 On Jan 14, 2016, the Large Area Telescope (LAT) observed strong gamma-ray emission from a new source. The best-fit location of this *gamma-ray source* (RA=8.91 deg, Dec=61.52 deg, J2000.0) has a 95% containment radius of 0.08 deg. This source is not in any published LAT atalog and in the past has not been detected by AGILE or EGRET. The closest candidate counterpart is the radio source 87GB 003232.7+611352

An example text based on ATel messages [\(astronomersteleg](https://astronomerstelegram.org/)ram.org)

object name; the type of the object or physical phenomena; event type

Goal is to build an information extraction system, i.e. recognize a list of predefined concepts (celestial objects, astronomical facilities, physical properties, people, organization etc.) from a text and produce LLM-generated event summaries based on the parameters of each event



*[ credits: D. Kostunin, A. Alkan, A. Chaikova, V. Sotnikov et al. ]*

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## A 7B LLM fine-tuned on **Cosmology** papers and textbooks

"*Cosmosage*", a general-purpose AI-assistant specialised in answering questions about cosmology (based on Mistral-7B-v0.1)

• training dataset: arXiv papers, astro textbooks, physics textbooks, wikipedia





## A LLM-based AI-assistant for a CERN experiment

### "ChATLAS" a prototype LLM project in a LHC experiment (ATLAS) at CERN (as of end 2023)

Data gathering part is interesting (data chunking and data retrieval not described here)

- Docs: twiki (>2k), sw docs (>500), e-groups/mails archive (>10k), indico meetings' agendas incl. attached slides and minutes (>440k), Mattermost, Jira tickets, experiment' papers and internal notes (>66k)
- Either HTML or scraped into markdown

Many open challenges:

- highly heterogeneous data
- ensure that collaboration DBs are accessible and exportable; websites should live on a git repo; pubs should be saved as latex, and compiled separately; discussion forums should have anonymisation options... Estimates indicate that this would have saved  $\sim$  1 yr of data wrangling
- Hallucinations are a real problem
- Not many gpu-hrs, but many expert-hrs, needed for any high-quality fine-tuned AI assistant

## Educational Outreach with AI-Assisted CERN Open Data



[https://opendata.ce](https://opendata.cern.ch/)rn.ch/

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## An example: a Higgs analysis guide





## LLM for particle accelerators

A variety of projects..

Plenty of work in progress on LLMs, showing potential towards natural language driven autonomous particle accelerators

- Attempts with GPT 3.5 Turbo, Megadolphin, Vicuna 7B 16K, Mistral 7B, Mixtral 7x8B, Starling-LM, GPT 4 Turbo, GPT4, Orca 2 7B, Orca 2 13B , Llama 2 70B, Falcon 180B, ..
- Constant seek for (and tests with) better models, better prompting, …



GAIA (@DESY): a General AI-assistant for Intelligent Accelerator Ops

- Experimental "procedures" defined as a collection of high-level "actions" in a Control System e.g. for managing machine pre-sets
- Exploring a LLM (mixtral:8x7b-instruct-v0.1-q8, 0 with 32k context size), agent implemented in Python using the langchain module, prompting based on ReAct (as a combination of chain-of-though prompting and information<br>injection via "actions")



EPA project (@CERN), AccGPT, etc..

- EPA = Efficient Particle Accelerator project
- AccGPT = accelerating science via a chatbot for knowledge retrieval for CERN specific content

*[ credits: F. Mayet, J. Kaiser. F. Rehm et al ]* 39

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# Large Language Models and "emergent abilities"

"*Emergence*": a sudden appearance of a novel behaviour (often referred to as a "phase transition")

- Scaling LLMs  $\rightarrow$  hit a series of critical scales at which new abilities are suddenly "unlocked"
- not directly trained to gain such abilities: they just manifest rapidly and in unpredictable ways

Examples:

• problem solving (math, logic, quantitative reasoning), common sense and social behaviour, (controlled) generation of texts, images, sounds, ..; ability to write, correct, and execute (pseudo)-code



### INFN Large Language Models and "emergent abilities"





## Emergence and prompting

#### LLMs can be prompted:

Zero-shot

One-shot

 $chasea =$ 

no fine-tuning of a model, but give it NL instructions

in-context learning: after training (frozen weights), a model is prompted a set of "gold-standard" examples to illustrate how to complete a task for which it was not trained, and it learns

#### example of the task. No gradient updates are performed. Translate English to French: task description sea otter => loutre de mer example  $cheese$  => prompt Few-shot Few-shot prompting In addition to the task description, the model sees a few examples of the task. No gradient updates are performed. Translate English to French: task description emergence at ~100B params sea otter => loutre de mer examples for a wide range of cases peppermint => menthe poivrée plush girafe => girafe peluche → *prompt engineering, Langchain, ..*  $cheese$  => prompt

The model predicts the answer given only a natural language description of the task. No gradient updates are performed

In addition to the task description, the model sees a single

task description

promp

Translate English to French:

In addition to in-context learning, another set of interesting abilities stem from prompt augmentation

### Chain-of-thought (CoT) reasoning



E.g. it has been demonstrated (in some cases) that just adding "*let's think step by step*" may trigger multi-step reasoning and lead to impressively increased accuracy in arithmetic tasks

45 Chain-of-Thought Prompting Elicits Reasoning in LLMs, Jan 2023, arXiv:2201.11903v6 Emergent Abilities of LLMs, Jun 2022, arXiv:2206.07682

## Biological vs Machine "intelligence"

## Mammalian biological brains LLMs





- Parameters: roughly the same nb  $(10^{14})$  as the human brain
- .. but **more compute**: brain (10<sup>16</sup> FLOPS) over a lifetime (100 years)  $\rightarrow$  10<sup>22</sup> ops, to be compared with LLM training time, around 10<sup>25</sup> ops
	- And it consumes more.. **Red AI** is a serious issue!

## Biological vs Machine "intelligence"

Measuring "intelligence" by number of neurons (or computational units):

- biological  $\rightarrow$  growth by a factor 2x in 1 million years
- machine  $\rightarrow$  growth by a factor 10x in 1 year



# Algorithmic progress in LLMs

The compute required to reach a set performance threshold has **halved approx.** 10<br>every 8 months, with a 95% confidence interval of around 5 to 14 months

• Algorithmic improvements faster than hardware gains per Moore's Law!



## A glance to hardware: the NVIDIA "gravity"

Of the 184 accelerated machines on the TOP500 (June 2023) list, 167 have Nvidia GPUs

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- 11 of them have AMD GPUs
- 6 have other kinds of accelerators like Intel Knights coprocessors.

AMD has 5.9 percent of accelerated system share in GPUs, compared to 90.8 percent for Nvidia (95% in AI)

Nvidia is not slowing down in 2024..





# "but physics requires creativity.." (?!)

Article | Open access | Published: 10 February 2024

## The current state of artificial intelligence generative language models is more creative than humans on divergent thinking tasks

#### Kent F. Hubert <sup>⊠</sup>, Kim N. Awa & Darya L. Zabelina

The emergence of publicly accessible artificial intelligence (AI) large language models such as ChatGPT has given rise to global conversations on the implications of AI capabilities. Emergent research on AI has challenged the assumption that creative potential is a uniquely human trait thus, there seems to be a disconnect between human perception versus what AI is objectively capable of creating. Here, we aimed to assess the creative potential of humans in comparison to AI. In the present study, human participants (N = 151) and GPT-4 provided responses for the Alternative Uses Task, Consequences Task, and Divergent Associations Task. We found that AI was robustly more creative along each divergent thinking measurement in comparison to the human counterparts. Specifically, when controlling for fluency of responses, AI was more original and elaborate. The present findings suggest that the current state of AI language models demonstrate higher creative potential than human respondents.



GPT4 more creative than 99% of humans..

Nature *Sci Rep* 14, 3440 (2024) 50

## Is this "augmented" intelligence?

## Can LLM help "consultants"?

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## AI-assistants as skill-levellers



Average consultants using AI perform as good as best consultants



## Machines not limited by biology

## Can AI be a skill-leveller (or more) for e.g. HEP theory?



Credits: M. Schwartz, Harvard and NSF IAIFI, elaborating on hard theoretical physics problems and AI, at EuCAIFCon (Amsterdam, 2024)

In the past, we made progress depsite many dead ends



Are we even making forward progress anymore?



Maybe the problems are just too difficult (for us)?

• E.g. could a cat ever learn to play chess? Humans have limits too.. i.e. biology



For a machine, 2D is not special: it can easily visualise in d dimensions

Humans hold few concepts in  $i\partial_t \psi = H\psi$ <br>  $G_{\mu\nu} = \kappa T_{\mu\nu}$ working memory at once, and like "simple and elegant" equations

A computer memory can handle much more concepts at once, and can understand systems not governed by simple equations

Credits: M. Schwartz

# We are a training set for machines

Current state-of-the-art AI can answer questions / (~) solve textbook problems How?  $\rightarrow$  via training on huge datasets of answered questions / solved problems By whom?  $\rightarrow$  Us! we answered and solved all that, we actually generated its training set

• (and we do the same for ourselves)

### E.g. LLMs:

 $\widehat{I^{NFN}}$ 

- learn from our training set
- Human feedback helps refine the models
- Machines generates data and refines its models

Humans and machines seem very close to be not so different..





# (Beyond) augmented intelligence

Suppose a machine understands the theory of everything but we don't

- e.g. can calculate the fine-structure constant from scratch
- e.g. can preduct the endpoint of black-hole evaporation

## Is this enough or do we need to understand it too?



The authors of Popular science books  $\bullet$ understand the details; we just get the general idea

I don't understand the proof of Fermat's last theorem

- I'm glad that somebody does  $\bullet$
- Does it matter that the person is human?  $\bullet$

If a machine understands fundamental physics it can

- 1. Dumb it down so we can get the general idea
- 2. Find practical applications

Is this what we want? I quess not.

But..

What if this is the best we will get? What if AI makes us optimistic for substantive progress in HEP theory in our lifetime?

Credits: M. Schwartz

## So, in a nutshell: is AI all we need?

AI is not "all" we need, but "something" that we need for sure, at some level.

- Software/Computing challenges to keep up with HEP goals are tough: AI as "part of the solution" Nevertheless, we had better start envisioning ML/DL not as mere "tools"
- Think of this as a **discipline** that showed up to be impressively useful, but whose theory is "under construction" Our best:
	- Early career researchers
	- Domain knowledge and scientific rigour, ability to explore what's solid and ignore the hype, direct efforts.

Our risk:

- Hard to keep the pace, but reluctant (time-wise, funding-wise, ..) to admit that this is not a part-time job
- R&D vs production: need more efforts to bring approaches to **production quality** (e.g. DL pipelines on AI infrastructures)

Given the AI recent past, in a 5-years timescale something radically new may probably come up.

If we fail to prepare for it, let's prepare to fail in exploiting its value