Faculty of Physics
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Towards more precise correlation studies with machine learning-based particle identification with missing data

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in collaboration with
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Warsaw, Poland
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Based on:
EPJ C 84 (2024) 7, 691
JINST 19 (2024) 07, C07013

Goals

- Use ALICE and its data as a **unique environment** for **Machine Learning (ML) research**

- Identify **areas** where both ALICE (or HEP in general) and ML communities can **mutually benefit** from each other

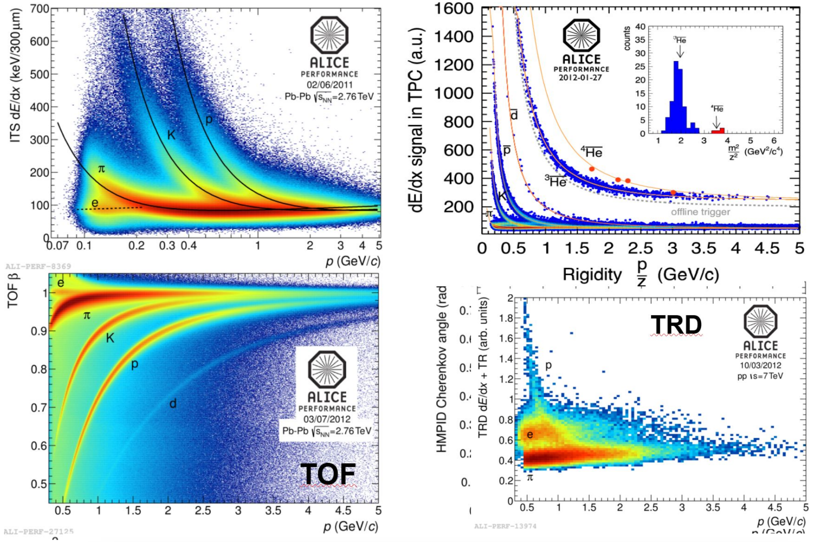
- Our solutions should be **easily applicable to other experiments** with similar PID capabilities

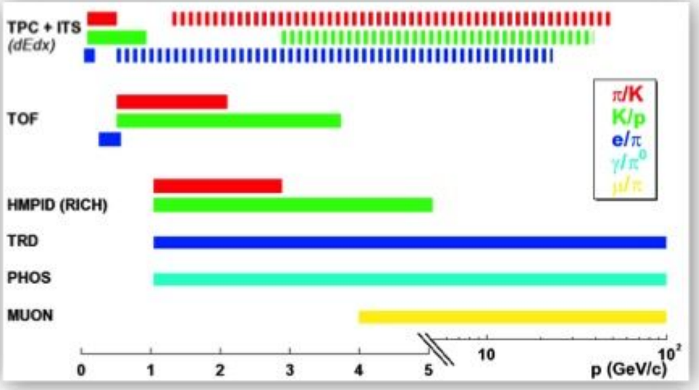
- **Disclaimer:**
    - I'm a **physicist without a big ML expertise** – just started my (human) learning of machine learning :)
    - My task is to **guide and coordinate the work of WUT ML computer scientists** within ALICE
    - The solution may be **complicated** (*shooting a sparrow with a cannon*), but the balance is to keep the project interesting for ML itself and be useful for us at the same time!

Particle identification (PID)

Aim: provide high purity samples of particles of a given type

- **an essential step** for many physics analyses, especially **correlations of identified particles**
- we use **ALICE as our R&D environment**
- **a distinguishing feature** of ALICE among the LHC experiments:
    - identification of particles of momenta in a **very wide momentum range**
    - practically **all known techniques** employed: dE/dx energy loss, time-of-flight, Cherenkov radiation for hadrons and transition radiation for electrons

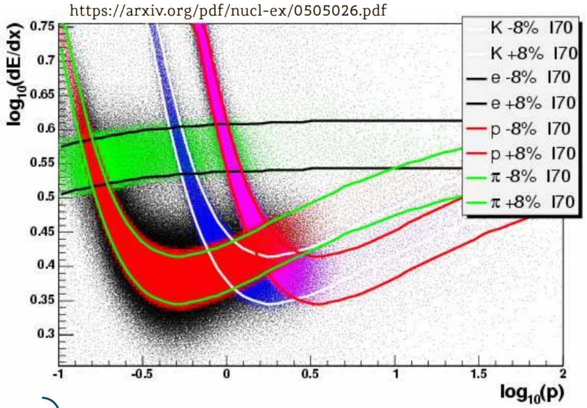




https://arxiv.org/abs/1709.00288

Present state-of-art

1. **Traditional method:**
   - hand-crafted selections of selected quantities, e.g., <u>nσ</u>
   - <u>problems:</u>
     - overlapping signals
     - <u>high purity at the cost of low efficiency</u>
     - time-consuming optimization



2. **Bayesian method** (ALICE, EPJ Plus 131 (2016) 168)**:**
   - updating probability of an hypothesis with each new evidence
   - priors = best guess of true particle yields per events
   - posteriors ~ purity
   - increased purity, results consistent with the traditional method

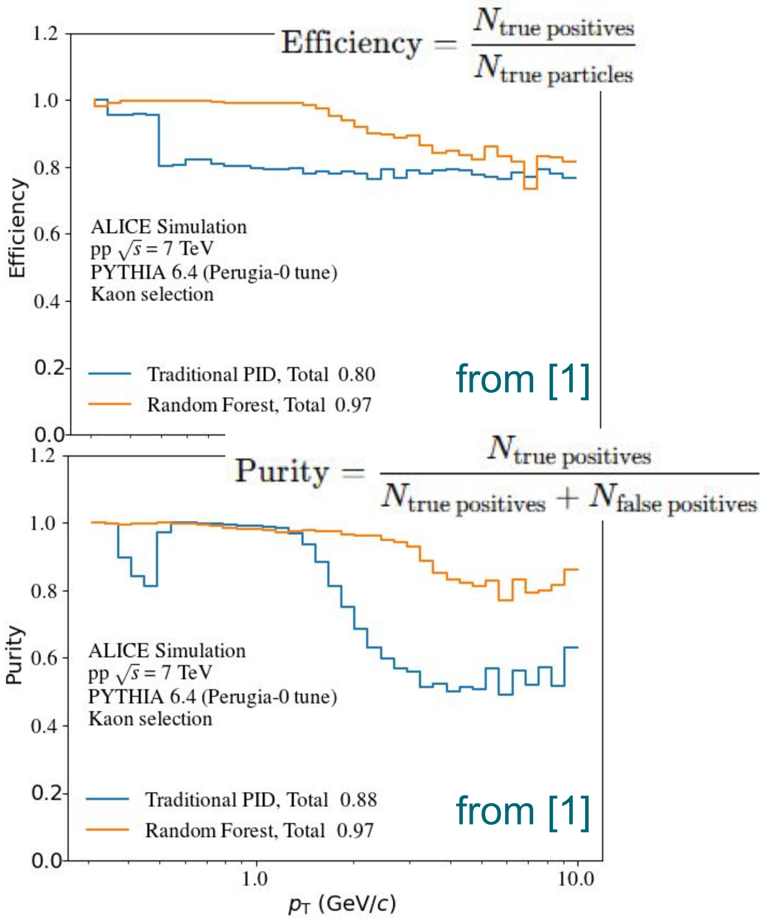
not covered in this talk
yields similar results

Both methods available in O^2 – ALICE Run 3 software

Can we do any better?

Yes!
With ML :)

ML for PID



Advantages of the ML approach to PID:

- **classification** – a ''standard'' ML problem
- can use **more track parameters** as input
- can learn **more complex relationships**
- many software libraries available

Note also **the limitations**:

- depends on **quality of the training data** (MC)
- hard to obtain **systematic uncertainties**
- hard to follow classifier's ''reasoning'' (**black box**)

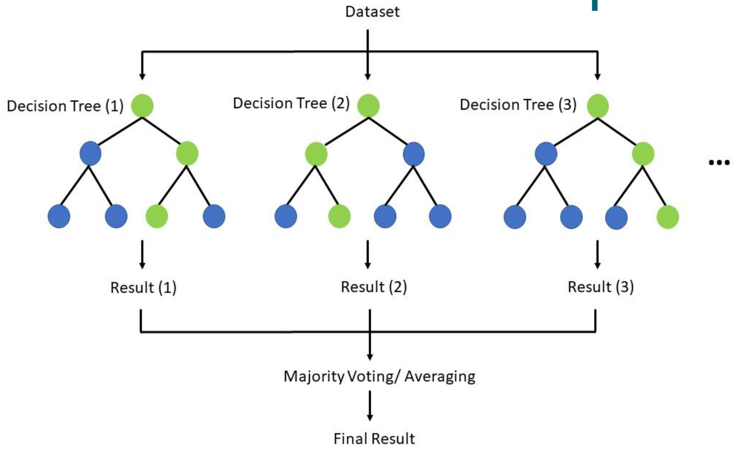
Our **first works** show ML can **greatly improve** purity and efficiency:

1. Random Forest: T. Trzciński, Ł. Graczykowski, M. Glinka, ALICE Collaboration. Using Random Forest classifier for particle identification in the ALICE experiment. Conference on Information Technology, Systems Research and Computational Physics, pp. 3-17. 2018
2. Domain Adaptation: M. Kabus, M. Jakubowska, Ł. Graczykowski, K. Deja, ALICE Collaboration. Using machine learning for particle identification in ALICE. JINST, v. 17, p. C07016. 2022

Proof-of-concept: Random Forest

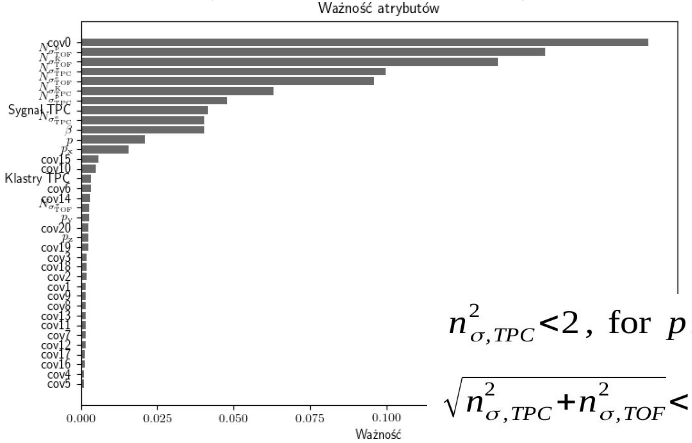
T. Trzciński, Ł. Graczykowski, M. Glinka, Conference on Information Technology, Systems Research and Computational Physics, 3-17. 2018

2018



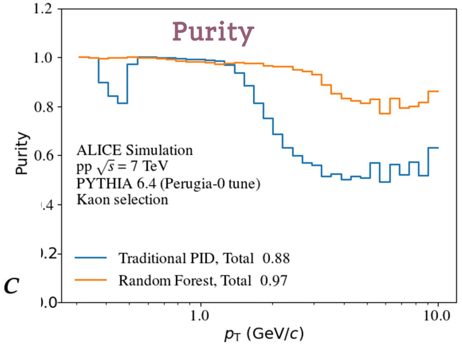
https://en.m.wikipedia.org/wiki/File:Random_forest_explain.png

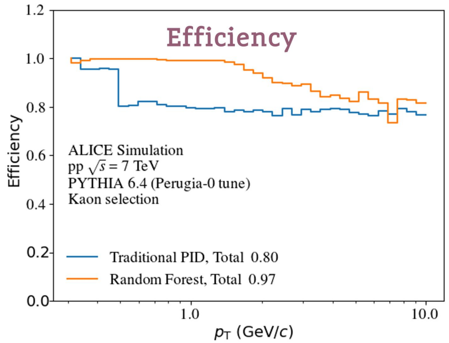
- Preliminary work with ALICE Run 2 data
- First solution - **Random Forest**
- Model works on **high-level track parameters**
- Depends on the **quality of Monte Carlo sample** and **post-processed information** (i.e. nσ calculation)
- Can be used **only for analysis-specific use-case** (concrete dataset and specific particle selection)
  - model has to be **trained by the specific end user**



$$n^2_{\sigma,TPC} < 2, \text{ for } p \leq 0.5 \text{ GeV}/c$$

$$\sqrt{n^2_{\sigma,TPC} + n^2_{\sigma,TOF}} < 2, \text{ for } p > 0.5 \text{ GeV}/c$$





Current solution - our model

- Solution **general enough** to be used for variety of analyses
- **At present our input data has 19 features:** i.e. momentum components, charge sign, DCA_{XY}, DCA_{Z}, detector signals (TPC dE/dx, TOF time, TRD signal), etc.
- **Data might be missing** from one or more detectors due to, e.g., too small p_T
- In **“standard” ML** approaches dealing with such cases, people use **data imputation** or **case deletion** - however artificially altered data may bias the physics results!
  - **Challenge:** classify particles without making any assumptions about the missing values

- The **proposed model** is much more advanced than the proof-of-concept solution and has **4 steps** (see next slides)
- For **details**, see our **two papers**:
  - EPJ C 84 (2024) 7, 691
  - JINST 19 (2024) 07, C07013

Current solution - our model

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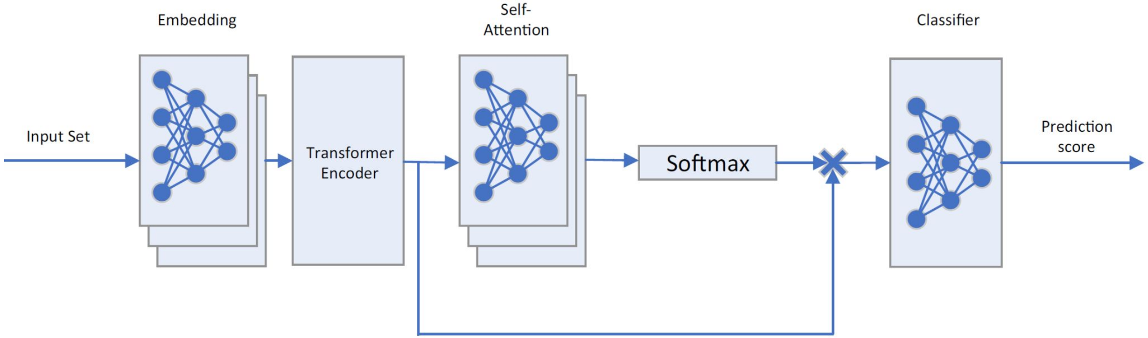

1. **Feature Set Embedding** to encode the inputs

2. **Transformer Encoder** to detect patterns in the input

3. Additional **self-attention** network to pool the encoder output set into a single vector

4. **Classifier** a simple neural network to classify a given particle type

Inspired by AMI-Net proposed for medical diagnosis from incomplete data (medical records)

Attention-based Multi-instance Neural Network for Medical Diagnosis from Incomplete and Low Quality Data

Zeyuan Wang[1,3], Josiah Poon[1], Shiding Sun[2], Simon Poon[1*]
[1]School of Computer Science, The University of Sydney, Syndey, Australia
[2]School of Mathematics, Renmin University of China, Beijing, China
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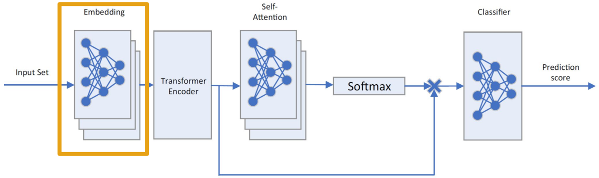
2019 International Joint Conference on Neural Networks (IJCNN)

details on slide 15

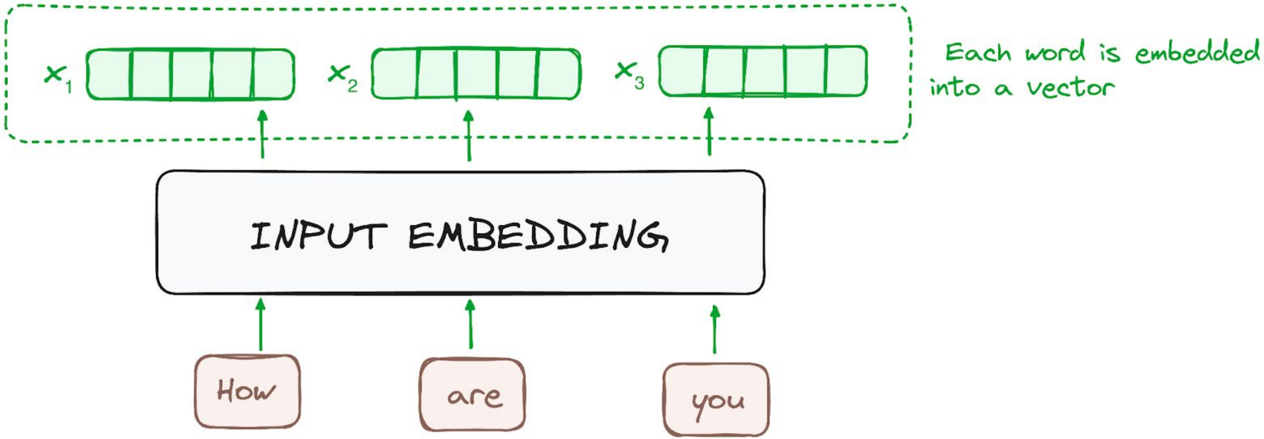
Step 1: Embedding



- **Embedding** is a technique to **handle complex data**

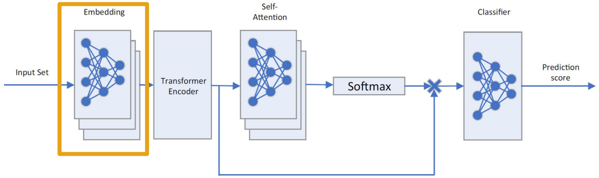
- It works by **converting high-dimensional data** (i.e. sequences of words, documents, images, etc.), **into lower-dimensional** and **abstract vector representation (embedding space)**

- It allows for capturing **meaningful relationships between data entities** (words, etc.)



https://www.datacamp.com/tutorial/how-transformers-work

Step 1: Feature Set Embedding

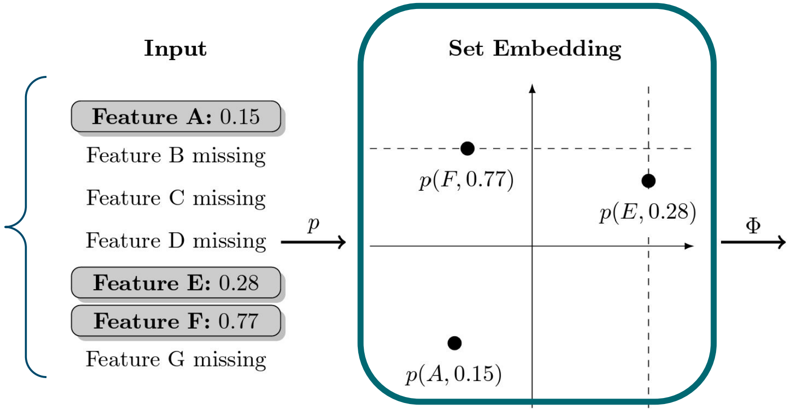


Missing data challenge: classify <u>without making any assumptions</u> about the missing values

Feature Set Embedding (<u>NIPS 2010 article</u>):

- <u>instead of vectors</u>, use <u>(feature,value) pairs</u>; no value → no pair
  - no need to model missing data (i.e. imputation)
- pairs in embedding space: <u>similar features are close to each other</u>
- pairs are then combined (by NN) into vectors (<u>embeddings</u>)

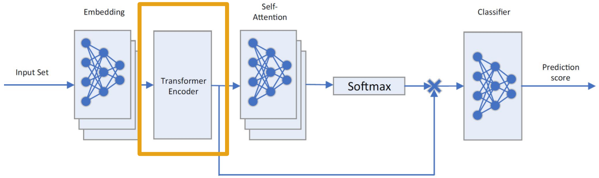
track
19 features in our case



embeddings
32 vectors in our case

Image source: <u>NIPS 2010 article</u>

Step 2: Transformer Encoder



Attention Is All You Need

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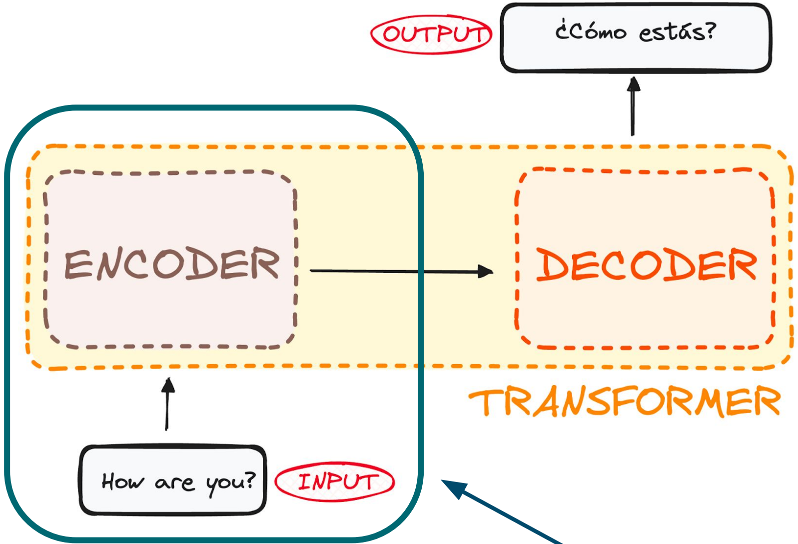


https://www.datacamp.com/tutorial/how-transformers-work

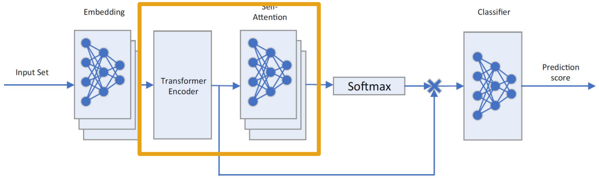
- Idea from original **Transformer** architecture proposed by Google (NIPS 2017 article)
- Developed for **transforming input data** into a **contextualized representation** on the output
- Transformer currently serves as **basis for the Natural Language Processing** tools (such as **ChatGPT**)
- In our case, **vectors from Embedding are processed by the Encoder only**
  - we do not need Decoder in our use-case

Steps 2 and 3: self-attention

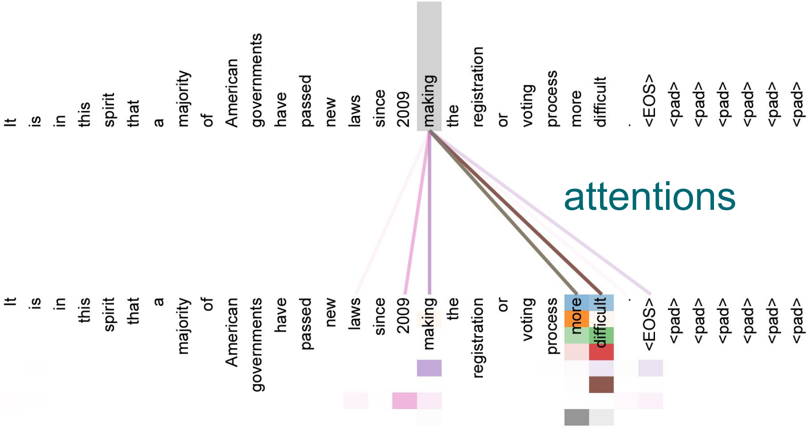
- **Attention** and **self-attention** are mechanisms used to help model focus on relevant parts of the input data
  - **self-attention** focuses on **relationships within the same input sequence**

- ***Example:*** "The cat sat on the mat"
  - when processing the word "cat," it considers other words (i.e. "the" or "mat") to understand their contribution to the meaning of "cat" (<u>in the context of the entire sentence</u>)

- Usage of **self-attention in Transformer architecture:**
  - in **single-head attention**, a <u>single set</u> of attention scores is used to focus on a particular part of the input sequence → limited ability to capture different relationships
  - **multi-headed attention** uses multiple attention heads, where each head focuses on different parts of the input <u>simultaneously</u>



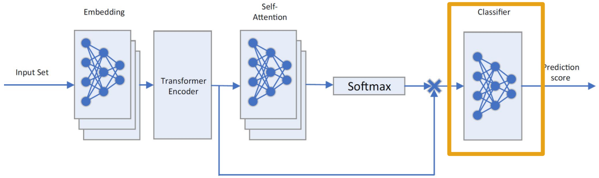
We use **self-attention twice**:
- in **Transformer Encoder**
- before **Classifier**



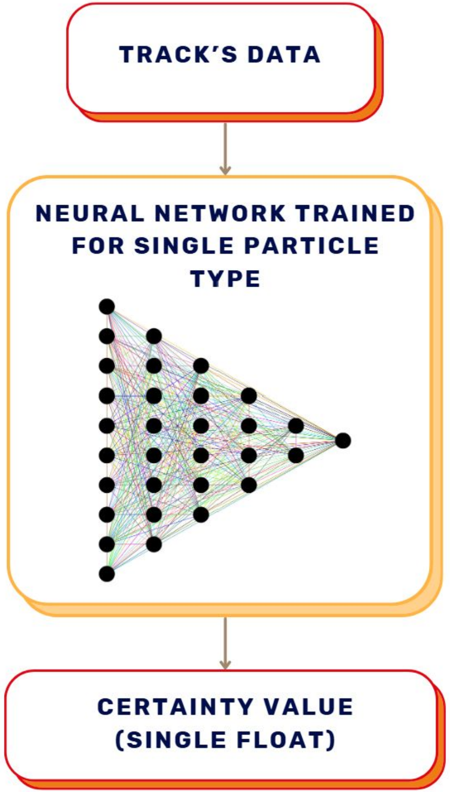
colors = attentions from different heads

NIPS 2017 article

Step 4: classification



- Single **output vector** from the **Self-attention network** is propagated to the **Classifier**
- **Classifier** is represented by **one simple neural network** (one hidden layer) **per particle** (**one vs all** approach)
  - the same architecture is used **separately** for pions, kaons, protons
- **Classifier score:** logistic function $f(x) = \frac{1}{1+e^{-x}}$ in range (0, 1) represents **"certainty"** that a given particle belongs to the given particle type
  - users can still **balance the efficiency and purity** by setting their own **threshold on the "certainty" value**



Details of the architecture

M. Kasak, K. Deja. M. Karwowska,
M. Jakubowska, ŁG
M. Janik, EPJ C 84 (2024) 7, 691
M. Karwowska, ŁG, K. Deja, M. Kasak,
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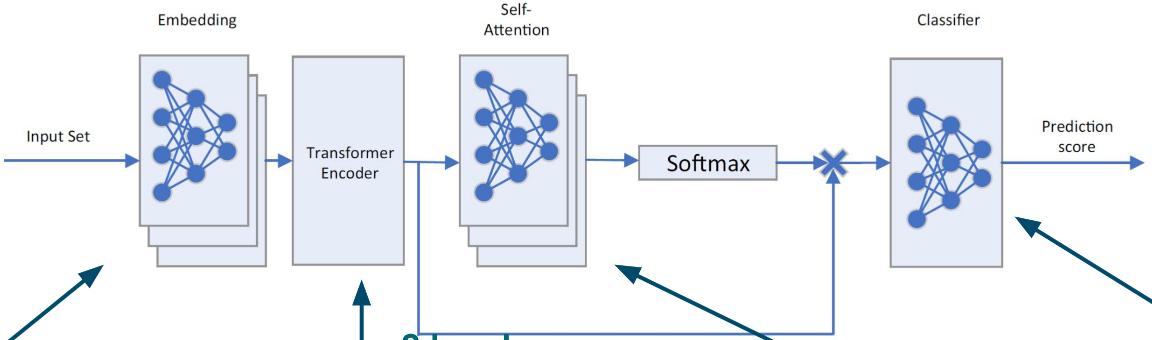

This model is applied **separately** for pions, kaons, protons

“certainty”

2 heads
in each head
2 layers (att.+NN)

Embedding			Transformer encoder					Self-attention			Classifier		
			Encoder layer										
			Multi-head attention		Neural network								
Input	Hidden	Output	Dimension	Heads	Input	Hidden	Output	Input	Hidden	Output	Input	Hidden	Output
19	128	32	32	2	32	128	32	32	64	32	32	64	1

- **dropout** value 0.1 at the output of embedding and each Transformer Encoder layer (to limit overfitting)
- **softmax function** is applied to obtain weights to create a single output (weighted average) vector
- **activation function** (between neural network layers): *ReLU (Rectified Linear Unit)*
- **loss function** that is minimized is *binary cross entropy* (for *one vs all* approach)
  - to minimize differences between *predicted* and *true* values (labels from MC truth data)

Test setup

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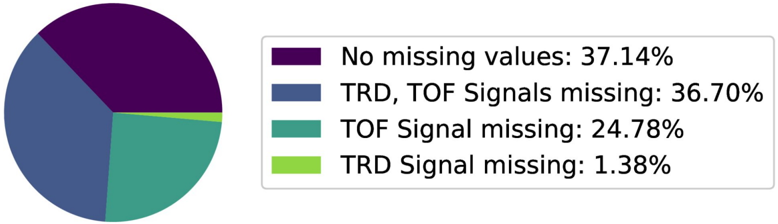
- **Dataset:** Run 2 general-purpose MC (Pythia 8) pp at $\sqrt{s}$ = 13 TeV with full detector simulation with GEANT 4 (both MC truth and reconstructed data are used)
- **Standard nσ method:**
  $|n_{\sigma,\,TPC}| < 3$ for $p_T < 0.5$ GeV/c, $\sqrt{(n_{\sigma,\,TPC}^2 + n_{\sigma,\,TOF}^2)} < 3$ for $p_T \geq 0.5$ GeV/c
- **Dataset details:**
  - no. tracks: ~2.7 million
  - 30% - test dataset
  - from the 70% of the rest:
    - 70% training
    - 30% validation

Missing data distribution



Results – pions, kaons, protons

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F_1 = (purity x efficiency) / (purity + efficiency)

FSE + attention with **very good scores** of **F_1, purity (precision)** and **efficiency (recall)**

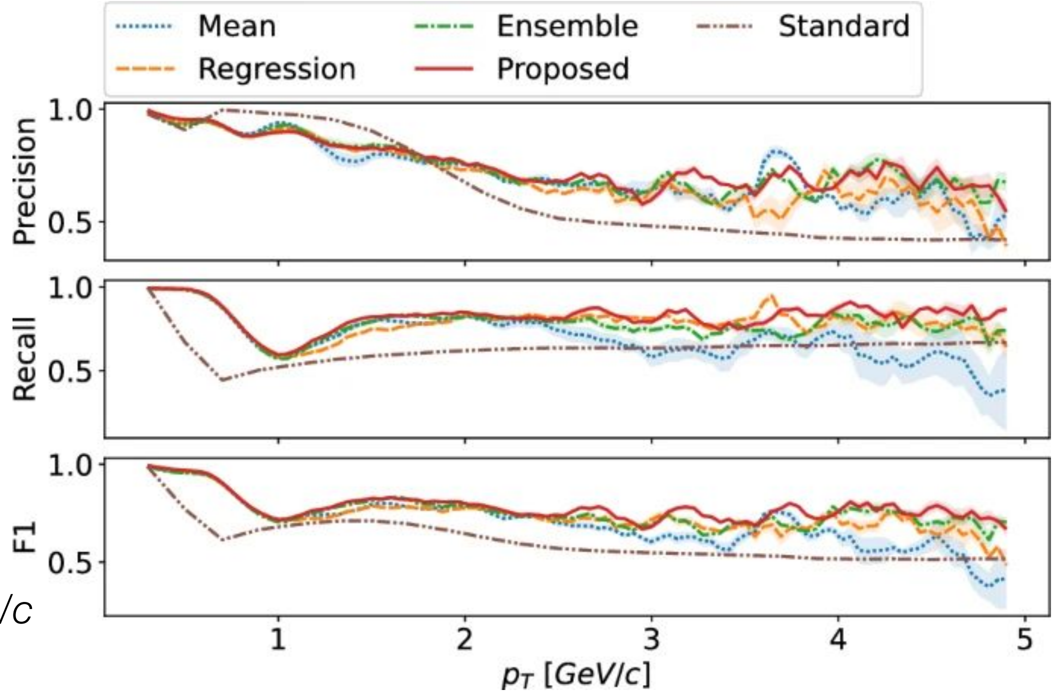
Proposed model (FSE+Attention)
compared to **other approaches:**

- **imputation:**
  artificial bias in data
  - mean
  - regression

- **NN ensemble** (4 networks)**:**
  potentially large complexity

- **standard:**
  nσ method
  $|n_{\sigma,\,TPC}| < 3$ for $p_T < 0.5$ GeV/c
  $\sqrt{(n_{\sigma,\,TPC}^2 + n_{\sigma,\,TOF}^2)} < 3$ for $p_T \geq 0.5$ GeV/c

kaon selection



Conclusions

R&D phase of the ML PID (almost) **finished!**

FSE+Attention model works well for the three basic identified hadron species (pions, kaons, protons)

Lots of work done, but still more ahead!

Plans for future:

- tests with Run 3 data with new O^2 analysis framework (*ongoing*)
- automation of model training and regular training of models for new Run 3 datasets (*implementation*)
- extending the model with domain adaptation (*still to do*)
- advertise PID ML among ALICE analyzers (*to do when fully implemented*)

The work has been carried out by an interdisciplinary team from 4 faculties of WUT:

- *Physics:* Ł. Graczykowski (*general idea, coordination, evaluation*), M. Janik (*evaluation*), M. Karwowska (*implementation*), S. Monira (*tests of implemented model*)
- *Electronics and Information Technology:* Kamil Deja, Miłosz Kasak (*ML R&D*)
- *Electrical Engineering:* Monika Jakubowska (*coordination, evaluation*)
- *Mathematics and Computer Science:* Marek Mytkowski, Mateusz Olędzki (*implementation*)

Thank you!

Run 2 results

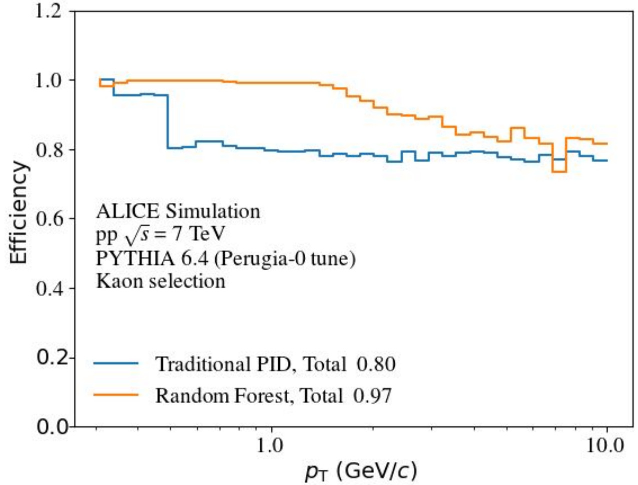
- pp at 7 TeV, Pythia 6 Perugia-0
- kaons vs other particles

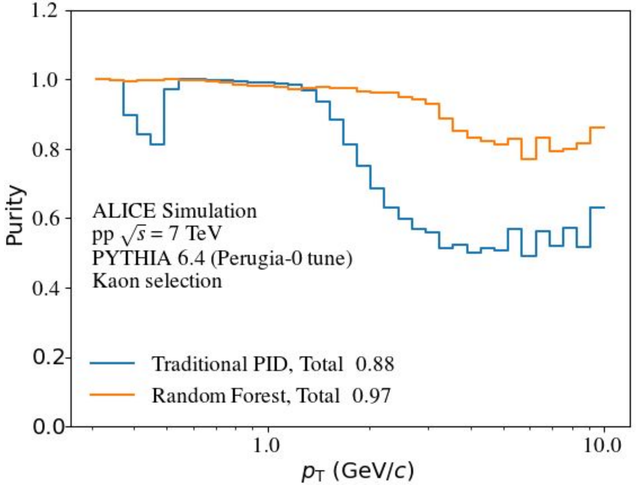
Traditional PID:

$$n^2_{\sigma,\mathrm{TPC}} \qquad p_\mathrm{T} \leq 0.5\mathrm{GeV}/c$$

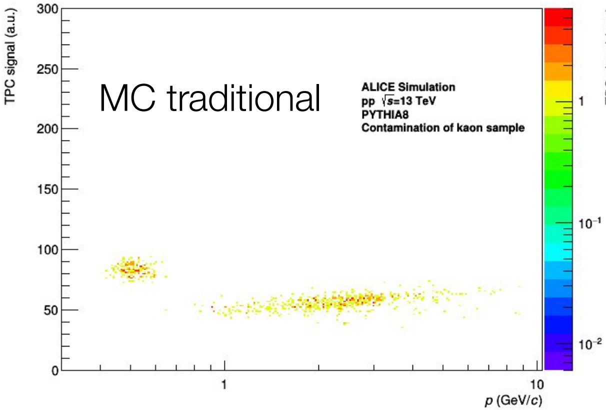
$$\sqrt{n^2_{\sigma,\mathrm{TPC}} + n^2_{\sigma,\mathrm{TOF}}} \qquad p_\mathrm{T} > 0.5\mathrm{GeV}/c$$

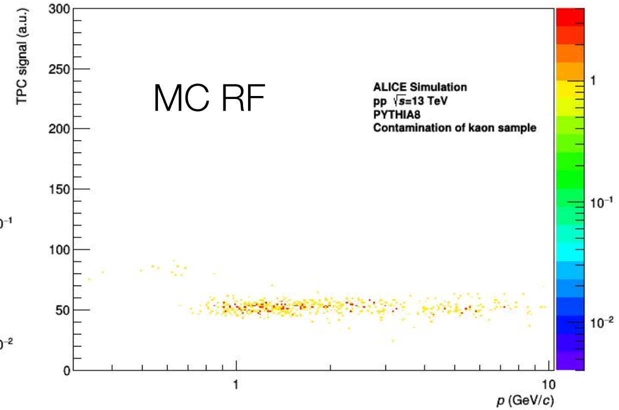
much higher efficiency and **purity** with Random Forest





Contamination of kaon samples





Results

$F_1 = 2 \times (\text{purity} \times \text{efficiency}) / (\text{purity} + \text{efficiency})$

best model, **2nd best model**

ML outperforms the standard way

FSE + attention with **very good scores** of $\mathbf{F_1}$

No flaws of other methods:

- imputation:
  artificial bias in data
- case deletion:
  no ability to analyze samples with missing detector signals
- NN ensemble:
  potentially large complexity

	π	p	K	$\bar{\pi}$	$\bar{p}$	$\bar{K}$
standard	87.87 ± 0.87	74.61 ± 1.88	73.17 ± 1.57	87.66 ± 0.87	69.12 ± 1.93	69.44 ± 1.60
NN ensemble	98.45 ± 0.04	95.42 ± 0.12	86.74 ± 0.16	98.27 ± 0.42	94.60 ± 0.10	84.91 ± 0.48
mean	98.40 ± 0.01	95.54 ± 0.06	86.36 ± 0.34	98.34 ± 0.01	94.75 ± 0.20	84.67 ± 0.38
attention + FSE	98.50 ± 0.02	95.79 ± 0.07	87.44 ± 0.14	98.44 ± 0.02	94.89 ± 0.14	86.00 ± 0.13
regression	98.40 ± 0.04	95.49 ± 0.15	86.22 ± 0.46	98.36 ± 0.03	94.57 ± 0.13	85.01 ± 0.13

	π, only complete data	p, only complete data	K, only complete data	$\bar{\pi}$, only complete data	$\bar{p}$, only complete data	$\bar{K}$, only complete data
case deletion	99.37 ± 0.01	99.43 ± 0.16	96.95 ± 0.06	99.37 ± 0.01	99.13 ± 0.26	96.33 ± 0.11
NN ensemble	99.38 ± 0.01	99.46 ± 0.13	97.23 ± 0.10	99.34 ± 0.18	99.33 ± 0.10	96.87 ± 0.09
mean	99.27 ± 0.04	99.47 ± 0.08	96.08 ± 0.36	99.27 ± 0.04	99.20 ± 0.27	95.45 ± 0.33
attention + FSE	99.36 ± 0.01	99.48 ± 0.02	97.04 ± 0.17	99.37 ± 0.03	99.44 ± 0.08	96.91 ± 0.11
regression	99.25 ± 0.07	99.37 ± 0.07	95.62 ± 0.39	99.28 ± 0.02	99.10 ± 0.13	95.11 ± 0.58

Example: FSE with one-hot encoding

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Table 1: Preprocessing of data samples into feature set values – example.

(a) 3 data samples with 5 attributes with different amount of missing values.

id	momentum	TOF	TPC	TRD	ITS
1	0.1		3		5
2	7	70	24	13	88
3		78			

(b) First particle

key					value
1	0	0	0	0	0.1
0	0	1	0	0	3
0	0	0	0	1	5

(c) Second particle.

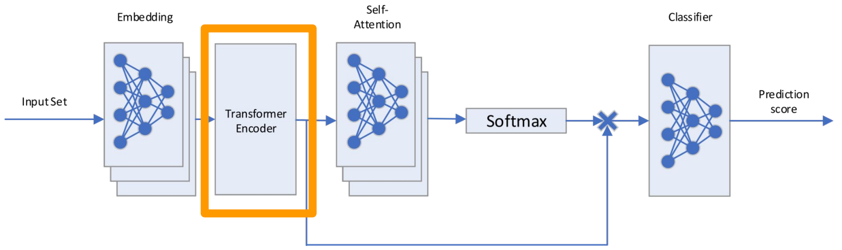
key					value
1	0	0	0	0	7
0	1	0	0	0	70
0	0	1	0	0	24
0	0	0	1	0	13
0	0	0	0	1	88

(d) Third particle.

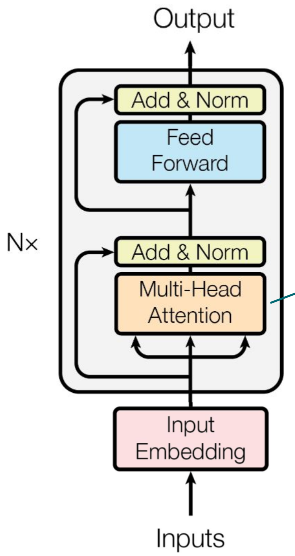
key					value
0	1	0	0	0	78

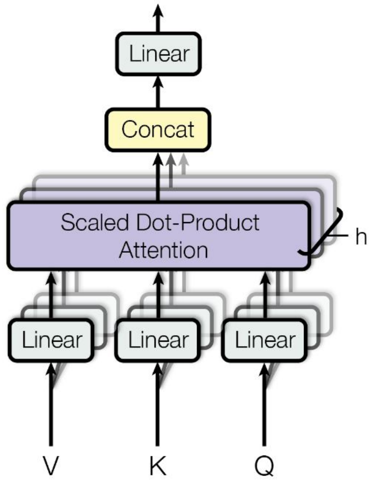
The attention continued

2. [Transformer Encoder]



N=2





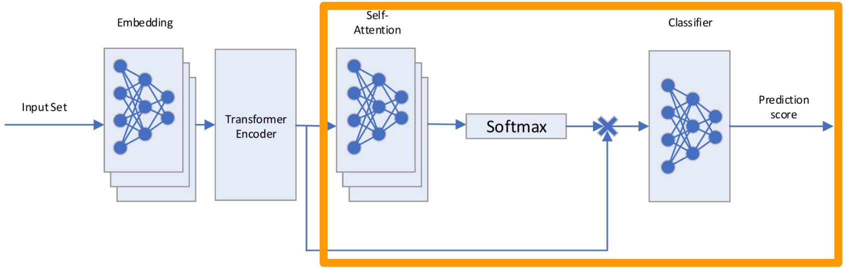
- adjusted original Transformer Encoder
- attention without convolutions and recurrence
- finding self-correlations in an instance set of vectors
- example: a specific detector signal could be used if and only if the momentum is in a specific range

$$Q, K, V \in \mathbf{R}^{n \times d_k}$$

$$Attention(Q, K, V) = softmax\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

modified diagram from the article

Pooling and classification



Classifier: a simple neural network
expects a single vector as an input

Solution: self-attention to pool the variable-size vector set from Transformer Encoder

$$\{v_1, v_2, ..., v_n\},\ v_i \in \mathbf{R}^{d_{model}}$$

$$e_i = NN(v_i) \qquad \forall i \in [1, n]$$ self-attention values

$$\alpha'_j = softmax(e'_j) \qquad \forall j \in [1, d_{model}]$$ self-attention weights

$$o_j = \sum_{k=1}^{n} \alpha_{kj} v_{kj} \qquad \forall j \in [1, d_{model}]$$ pooled output vector

Classifier score: logistic function $f(x) = \frac{1}{1+e^{-x}}$, range (0, 1)
"certainty" that a given particle belongs to the given type

Architecture of tested neural networks

Attention + FSE

- embedding layers: 19 – 128 – 32 neurons
- Transformer Encoder:
    - Multi-Head Attention: dimension 32, 2 heads
    - neural network layers: 32 – 128 – 32 neurons
    - 2 layers of Multi-Head Attention + neural network
- Self-Attention layers: 32 – 64 – 32 neurons
- classifier layers: 32 – 64 – 1 neurons
- dropout 0.1 at the output of embedding and each Transformer Encoder layer
- ReLU activation between neural network layers
- classifier loss function: binary cross entropy

Imputations, case deletion, and NN ensemble

- 3 hidden layers of sizes 64, 32, 16 with Leaky ReLU activation
- dropout 0.1 after each activation layer
- input size:
    - imputations and case deletion: 19 as all missing features are imputed
    - ensemble: 4 networks with input sizes 19, 17, 17, 15

Simple network implementation

PyTorch

- linear layers with ReLU, sigmoid at the end
- simple: dropout after each linear layer

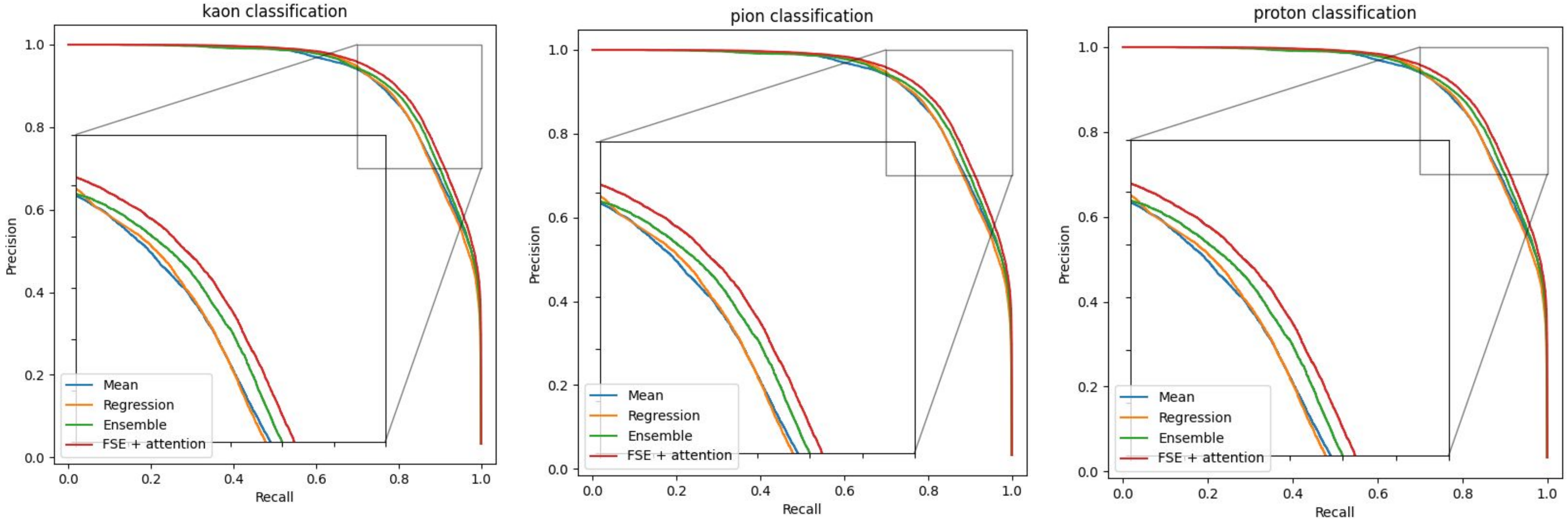
Parameters:

- optimizer: Adam
- output layer: 1 node (yes / no for a given particle)
- loss function: binary cross entropy
- scheduler: exponential with rate 0.98
- learning rate: 0.0005
- batch size: 64
- epochs: 30

Sample ROC curves

FSE+attention achieves **best results.**

Little variation between particle species.



More to go: domain adaptation

M. Kabus, M. Jakubowska,
Ł. Graczykowski, K. Deja
JINST 17, C07016. 2022

- **Monte Carlo never ideally matches the experimental data** (both physics and detector response simulation)

- **Problem:** transferring the knowledge from a **labeled source domain (MC data)** to **unlabeled target domain (experimental data)**, when both domains have different distributions of attributes

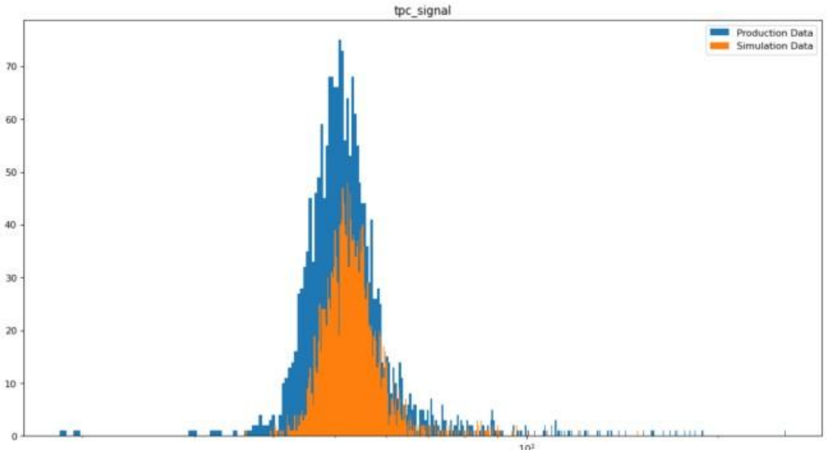
- How can we transfer the knowledge from training to inference?

Standard PID example: **"tune on data"**

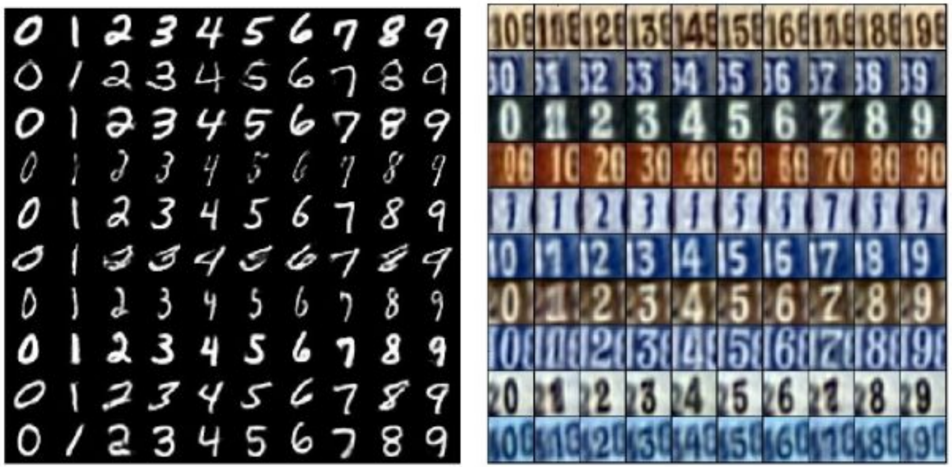
- get parametrization from data → real data
- generate a random detector signal → MC data
- equivalent distributions of real and MC samples – the differences are statistical fluctuations
- does not include correlations between attributes

Machine learning:

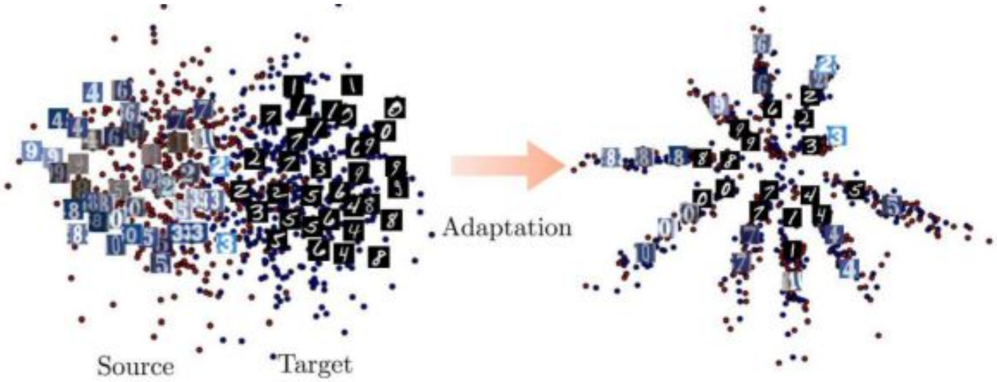
- actually **learn** the difference between data domains
- translate both data to a single common hyperspace



More to go: domain adaptation



(a) MNIST (b) SVHN



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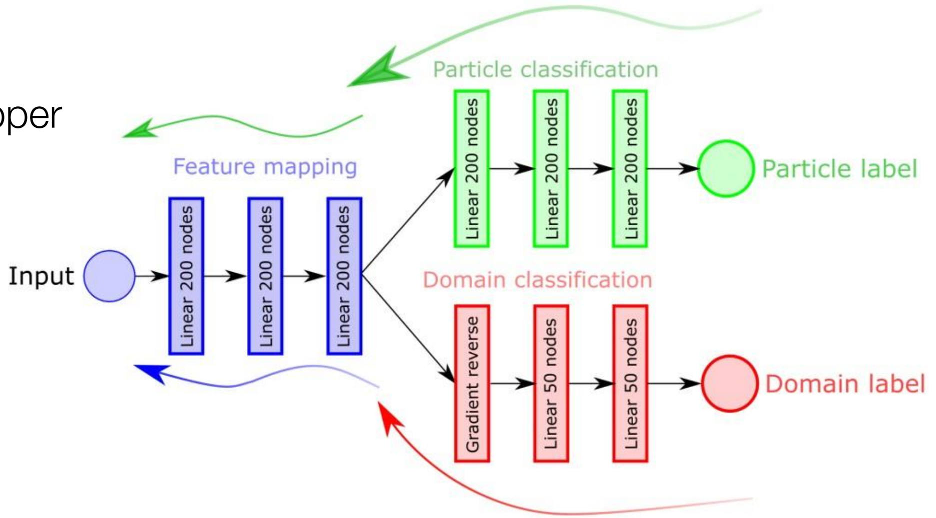
Feature mapping: input → domain invariant features

Particle classifier: recognize particles based on domain invariant latent space

Domain classifier: recognize MC vs real samples

Training more complicated:

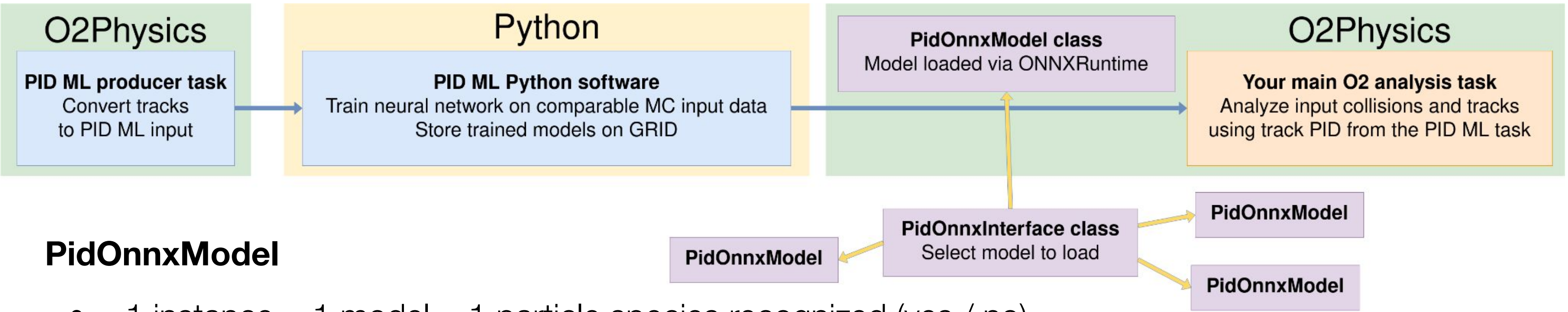
1. Train the domain classifier independently.
2. Freeze the domain classifier.
3. Train jointly particle classifier and feature mapper **adversarially** to the domain classifier.
4. Weights of the feature mapper:
   gradient from particle classifier
   + reversed gradient from domain classifier



Application time similar to a standard classifier

Our current solution still misses this step

Integration with O^2: user interface



PidOnnxModel

- 1 instance = 1 model = 1 particle species recognized (yes / no)
- **convenient interface** clearly separated from the rest of analysis
- using all capabilities of **Python ML libraries** for training
- ONNX file format and **ONNXRuntime** software used for inference in O^2 C++ environment

PidOnnxInterface

- **automatically select most suitable model** for user needs or manual mode
- as **little additional knowledge** from the analyser as possible (*"change 1 line in the code"*)

https://onnx.ai/