Faculty of Physics
Warsaw University of Technology

# Towards more precise correlation studies with machine learning-based particle identification with missing data


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Toulouse, France
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*Based on:*
EPJ C 84 (2024) 7, 691
JINST 19 (2024) 07, C07013

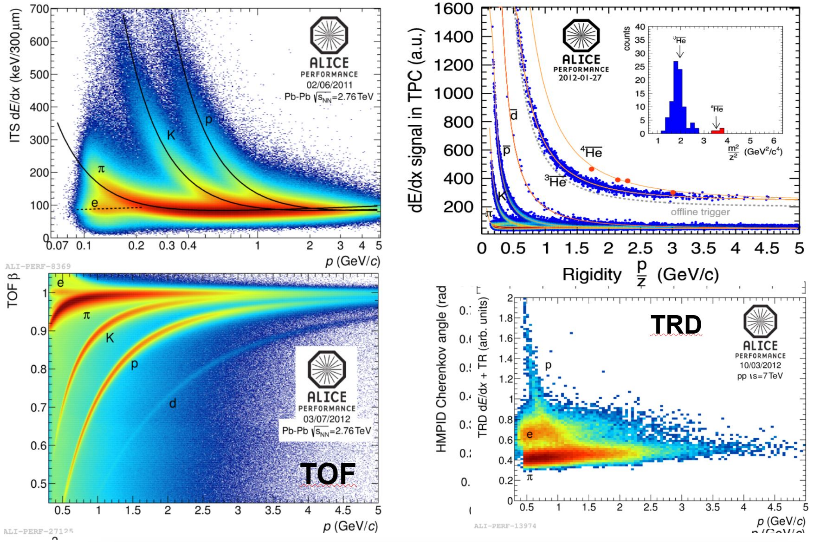
# Goals

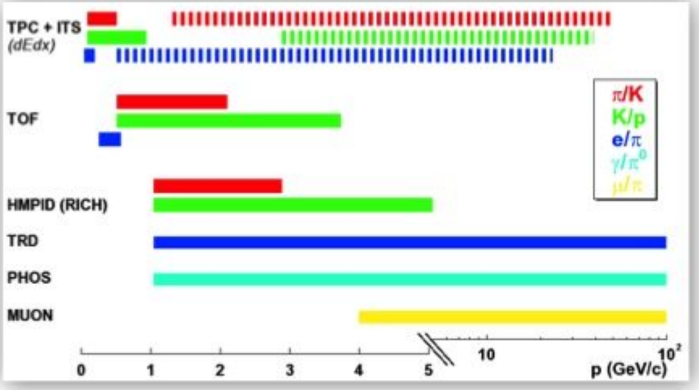
- Use ALICE and its data as a **unique environment** for **Machine Learning (ML) research**
- Identify **areas** where both ALICE (or HEP in general) and ML communities can **mutually benefit** from each other
- Our solutions should be **easily applicable to other experiments** with similar PID capabilities
- **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

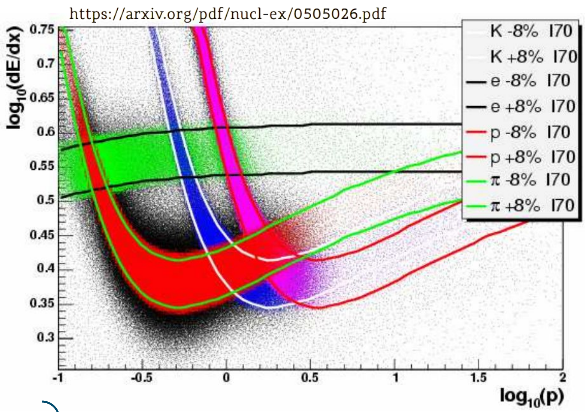



https://arxiv.org/abs/1709.00288

# Present state-of-art

1. **Traditional method:**
   - hand-crafted selections of selected quantities, e.g., nσ
   - problems:
     - overlapping signals
     - high purity at the cost of low efficiency
     - 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

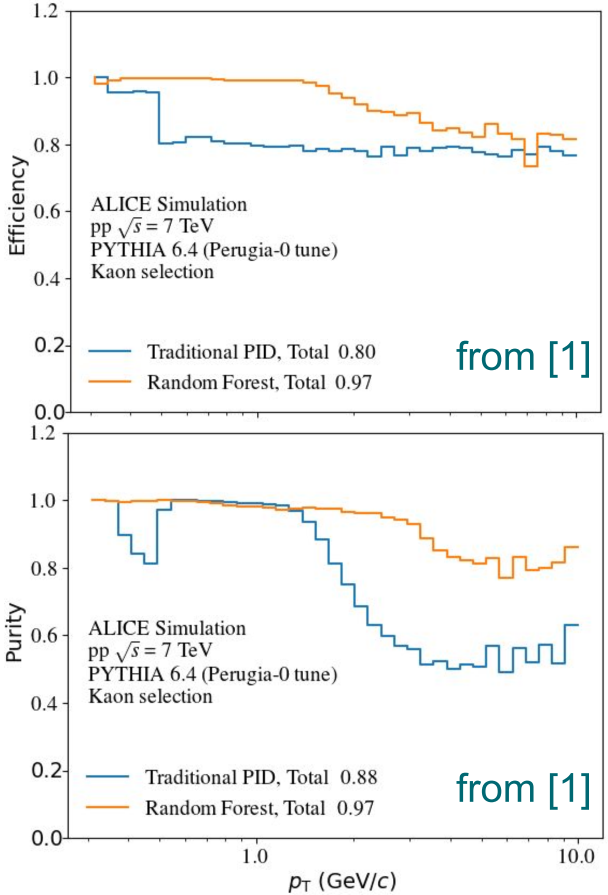
not covered in this talk

**Both methods available in O²** – 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**)

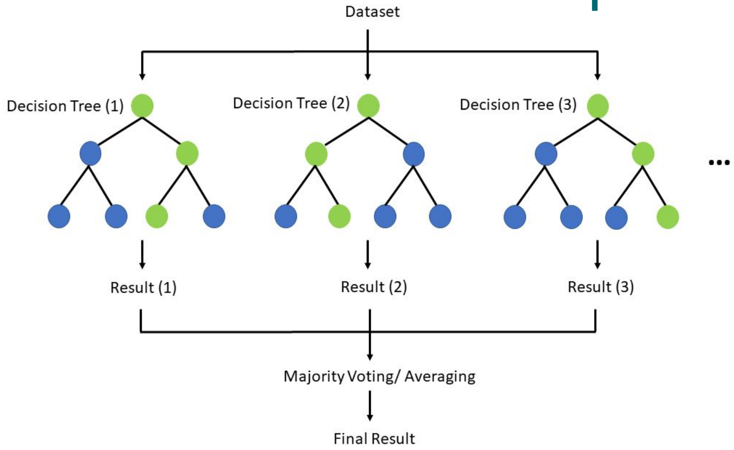
Our **first works** show ML can **greatly improve** purity and efficiency:


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

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

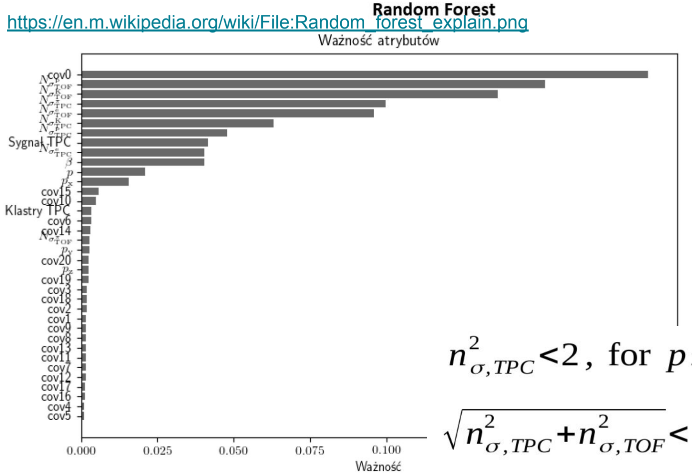
# Proof-of-concept: Random Forest

2018



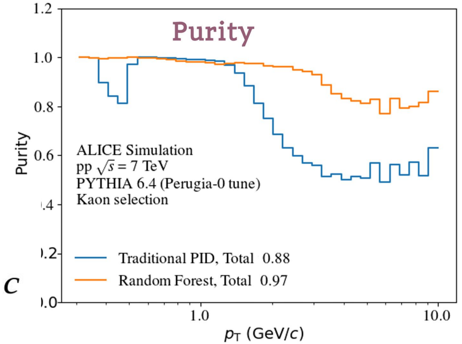

https://en.m.wikipedia.org/wiki/File:Random_forest_explain.png

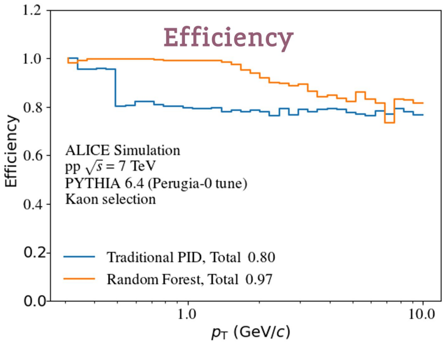
- Preliminary work with ALICE Run 2 data
- First solution - **Random Forest**
- Model works on **high-level track parameters**
- Depends on the **quality of Monte Carlo sample** and **post-processed information** (i.e. nσ calculation)
- Can be used **only for analysis-specific use-case** (concrete dataset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




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

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



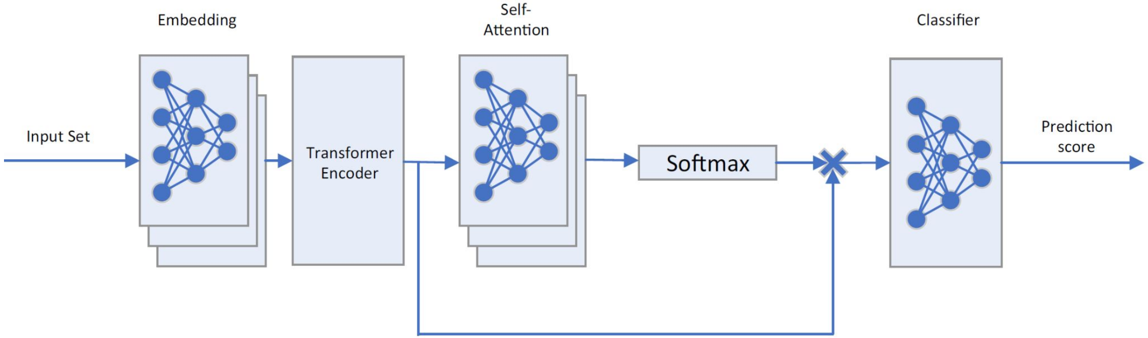



# Current solution - our model

- 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

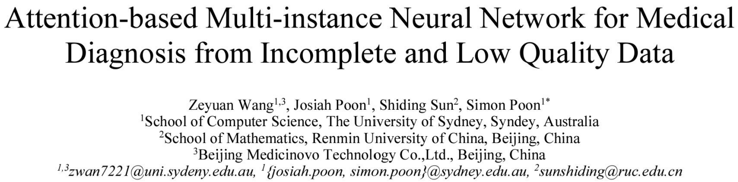
# Current solution - our model

M. Kasak, K. Deja. M. Karwowska, M. Jakubowska, ŁG M. Janik, EPJ C 84 (2024) 7, 691
M. Karwowska, ŁG, K. Deja, M. Kasak, M. Jaik, JINST 19 (2024) 07, C07013




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

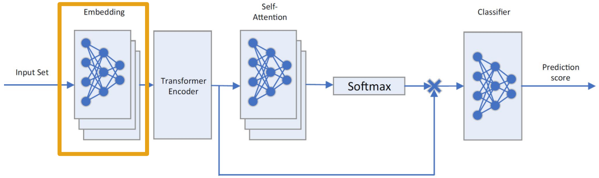
Inspired by AMI-Net proposed for medical diagnosis from incomplete data (medical records)



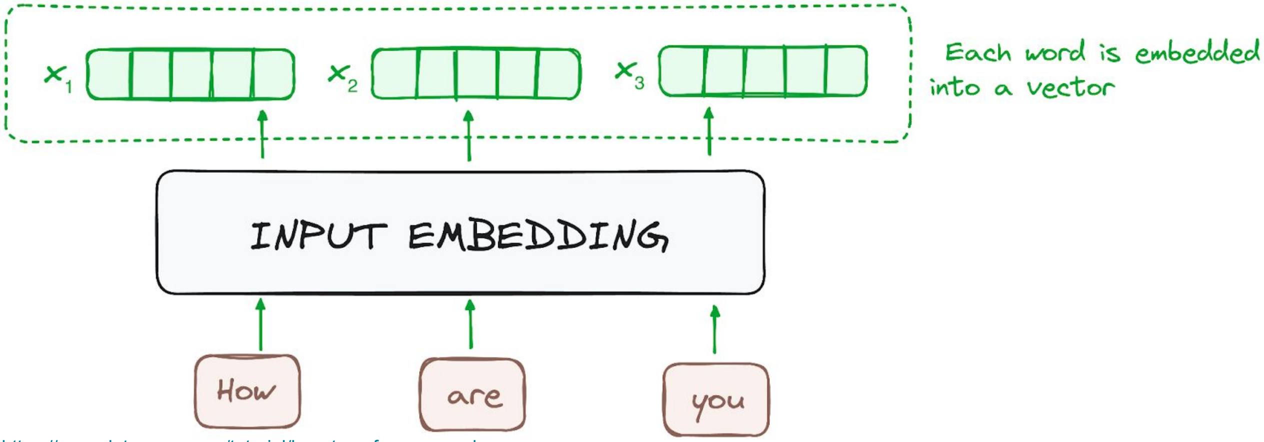

2019 International Joint Conference on Neural Networks (IJCNN)

details on slide 15

# Step 1: Embedding

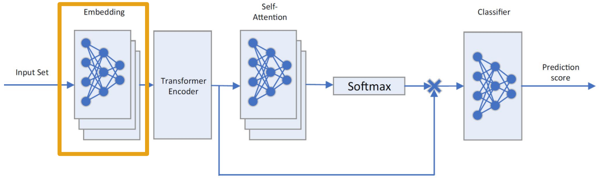



- **Embedding** is a technique to **handle complex data**
- It works by **converting high-dimensional data** (i.e. sequences of words, documents, images, etc.), **into lower-dimensional** and **abstract vector representation (embedding space)**
- It allows for capturing **meaningful relationships between data entities** (words, etc.)




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

# Step 1: Feature Set Embedding

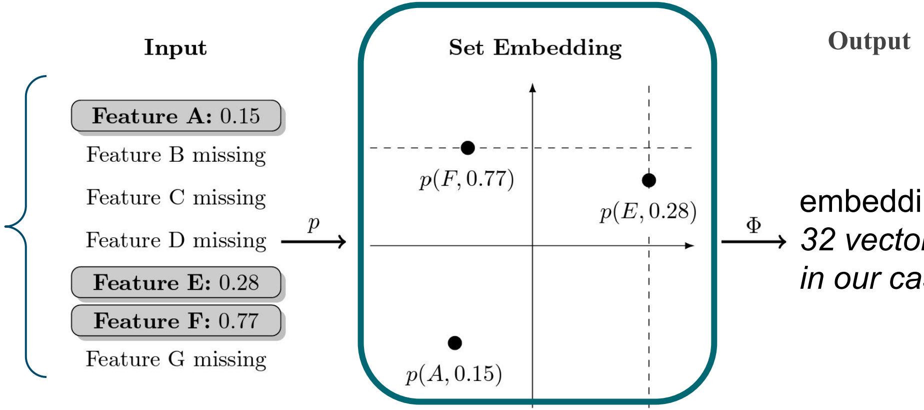



**Missing data challenge:** classify without making any assumptions about the missing values

**Feature Set Embedding** (NIPS 2010 article):

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

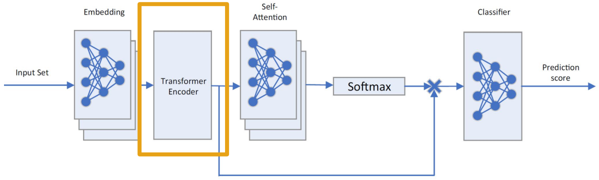
track
*19 features in our case*




embeddings
*32 vectors in our case*

Image source: NIPS 2010 article

# Step 2: Transformer Encoder




**Attention Is All You Need**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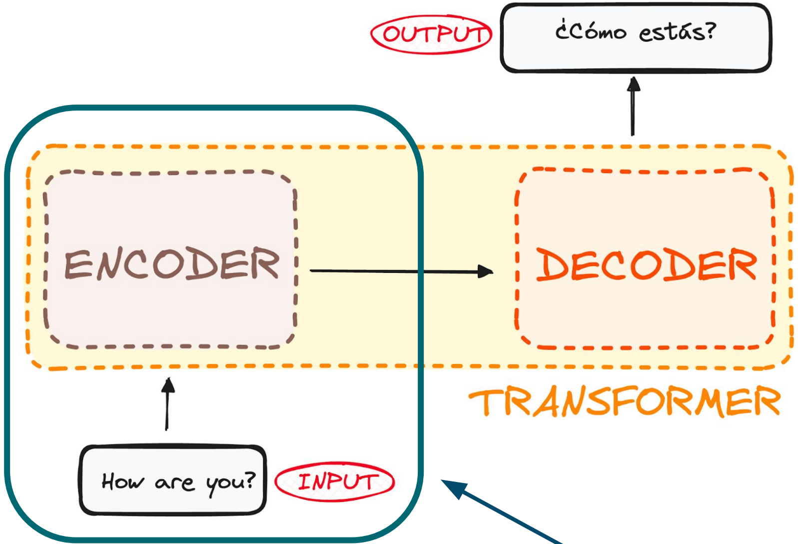
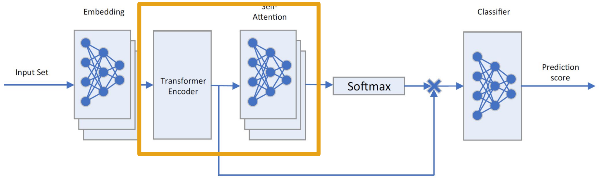



https://www.datacamp.com/tutorial/how-transformers-work

- 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



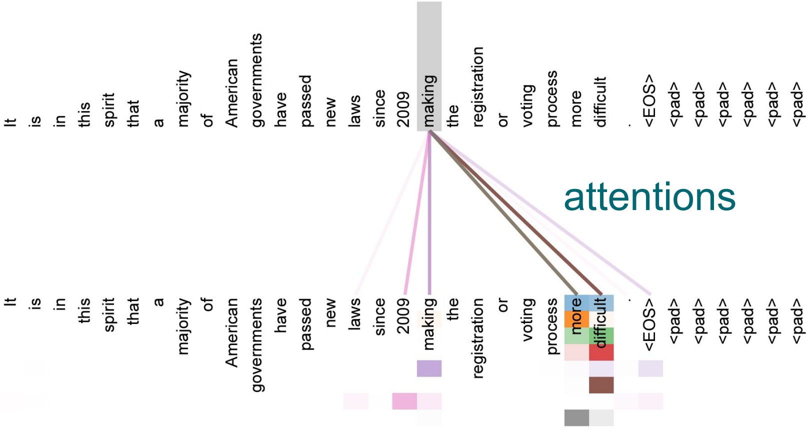

We use **self-attention twice**:

- in **Transformer Encoder**
- before **Classifier**

- **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>)

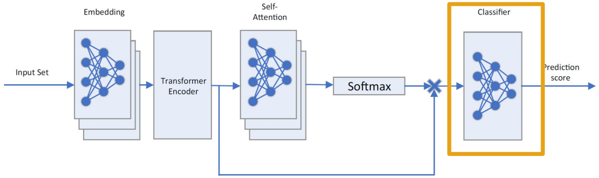
- Usage of **self-attention in Transformer architecture:**
  - in **single-head attention**, a <u>single set</u> of attention scores is used to focus on a particular part of the input sequence → limited ability to capture different relationships
  - **multi-headed attention** uses multiple attention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



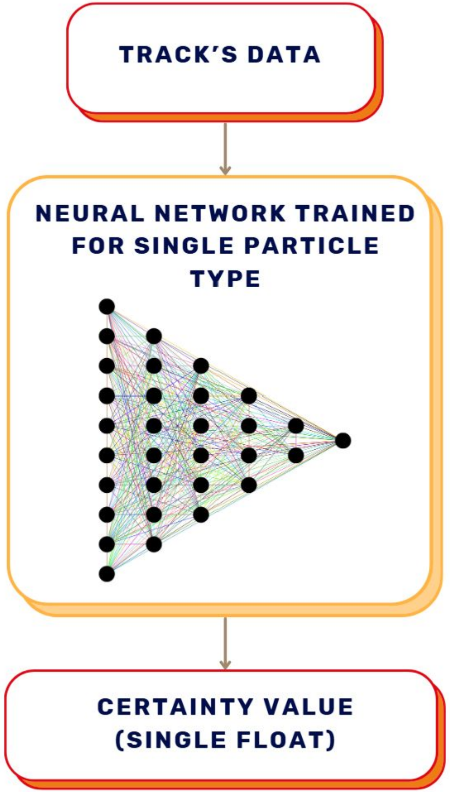

colors = attentions from different heads

[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
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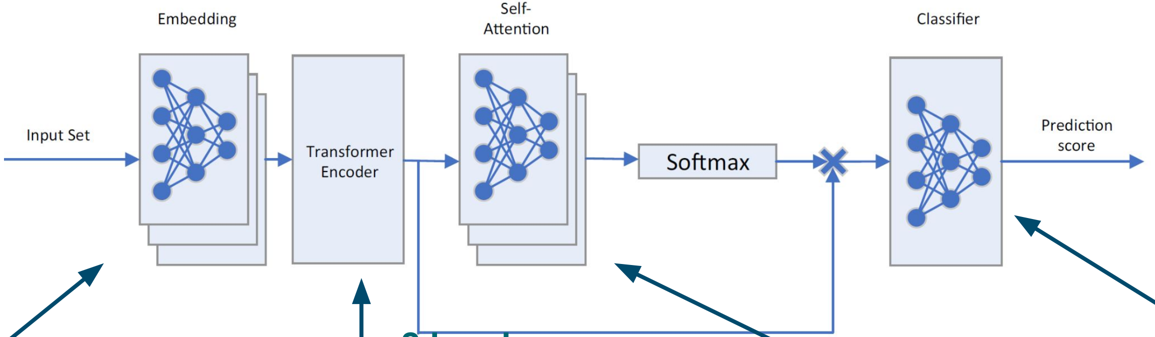


This model is applied **separately** for pions, kaons, protons

"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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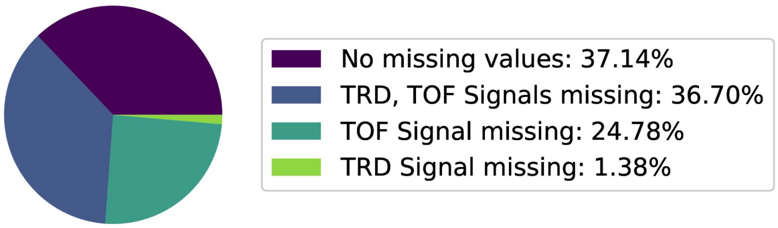
- **Dataset:** Run 2 general-purpose MC (Pythia 8) pp at $\sqrt{s}$ = 13 TeV with full detector simulation with Geant 4 (both MC truth and reconstructed data are used)
- **Standard nσ method:**
  $|n_{\sigma,\ \mathrm{TPC}}| < 3$ for $p_{\mathrm{T}} < 0.5$ GeV/$c$, $\sqrt{(n_{\sigma,\ \mathrm{TPC}}^2 + n_{\sigma,\ \mathrm{TOF}}^2)} < 3$ for $p_{\mathrm{T}} \geq 0.5$ 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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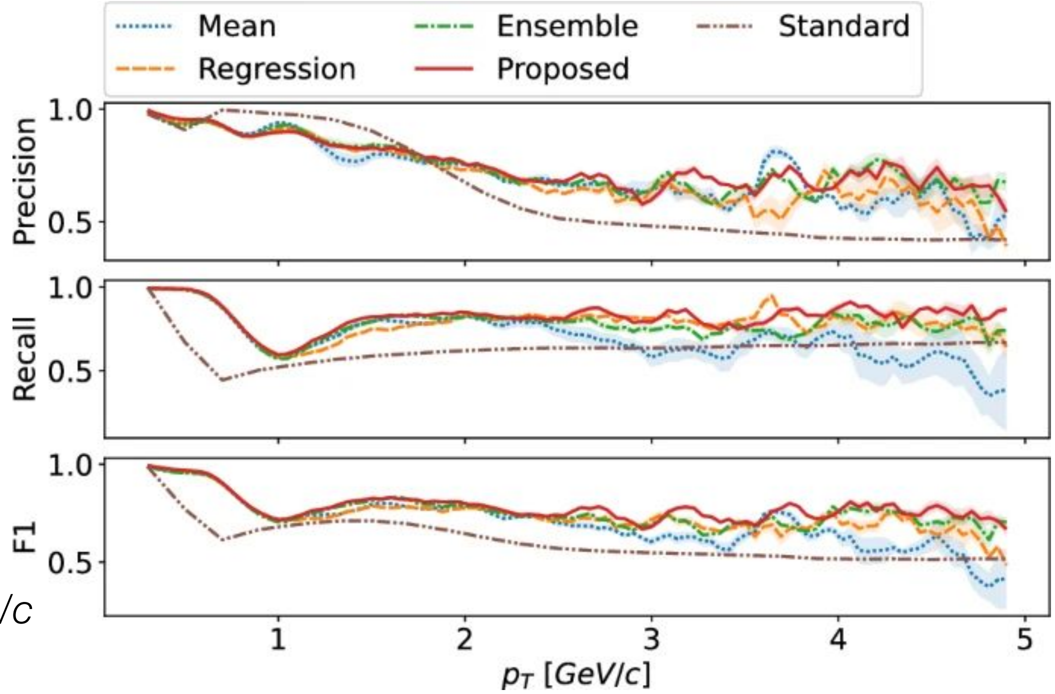
**$F_1$ = (purity x efficiency) / (purity + efficiency)**

**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

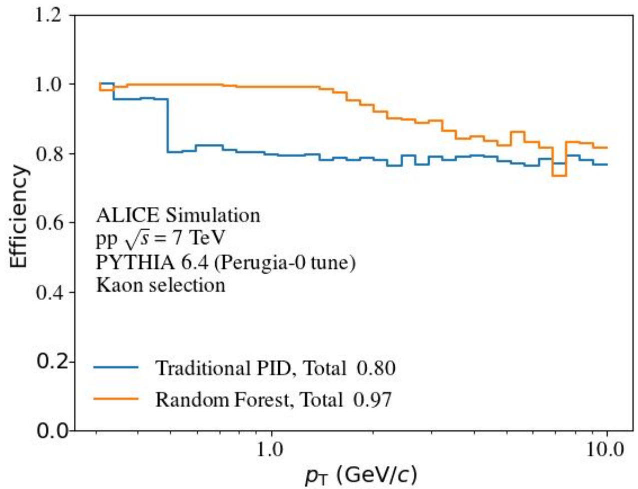
- pp at 7 TeV, Pythia 6 Perugia-0
- kaons vs other particles

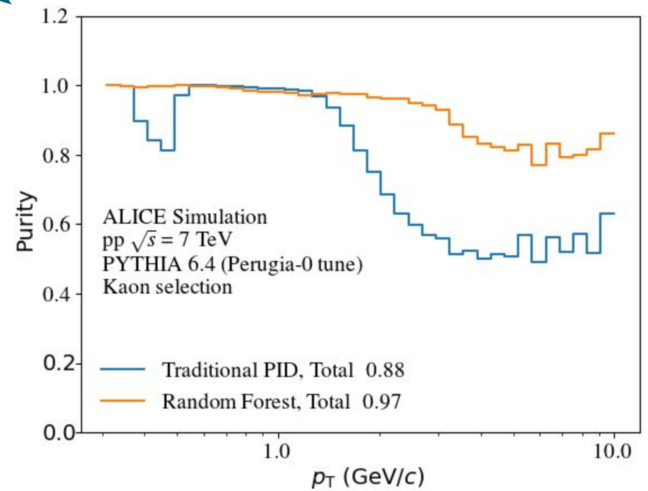
**Traditional PID:**

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

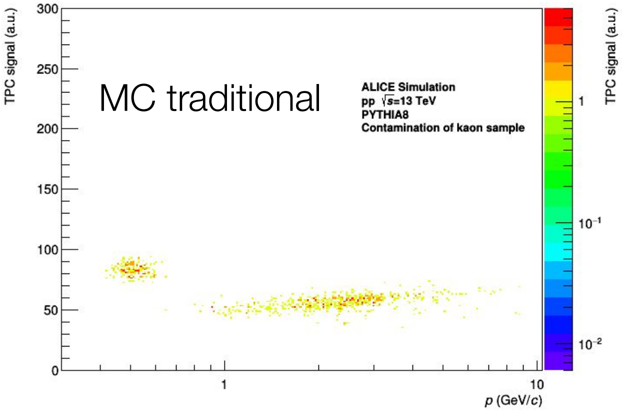
$$\sqrt{n^2_{\sigma,\mathrm{TPC}} + n^2_{\sigma,\mathrm{TOF}}} \qquad p_\mathrm{T} > 0.5\mathrm{GeV}/c$$

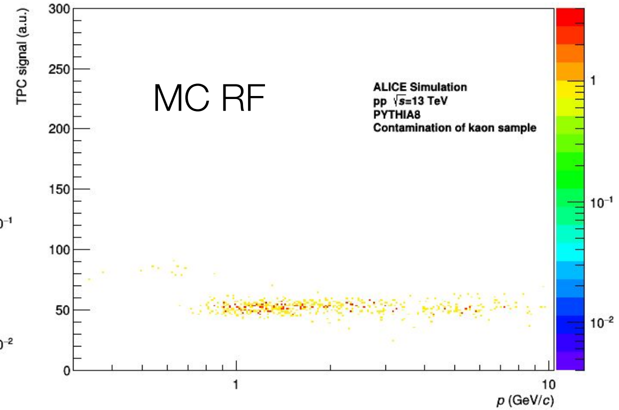
**much higher efficiency** and **purity** with Random Forest




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

| | $\pi$ | $p$ | $K$ | $\bar{\pi}$ | $\bar{p}$ | $\bar{K}$ |
|---|---|---|---|---|---|---|
| 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 |

| | $\pi$, 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.

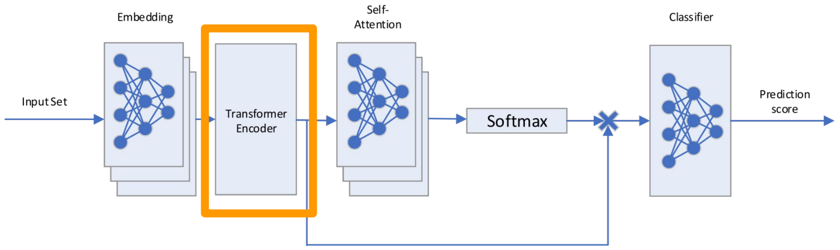
| key | | | | | value |
|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 7 |
| 0 | 1 | 0 | 0 | 0 | 70 |
| 0 | 0 | 1 | 0 | 0 | 24 |
| 0 | 0 | 0 | 1 | 0 | 13 |
| 0 | 0 | 0 | 0 | 1 | 88 |

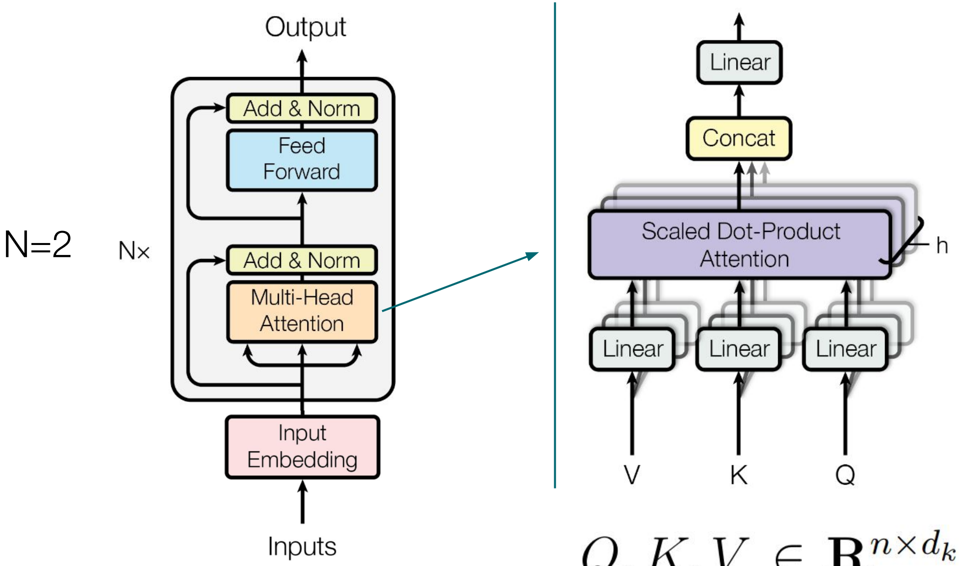
(d) Third particle.

| key | | | | | value |
|---|---|---|---|---|---|
| 0 | 1 | 0 | 0 | 0 | 78 |

# The attention continued

2. [Transformer Encoder]



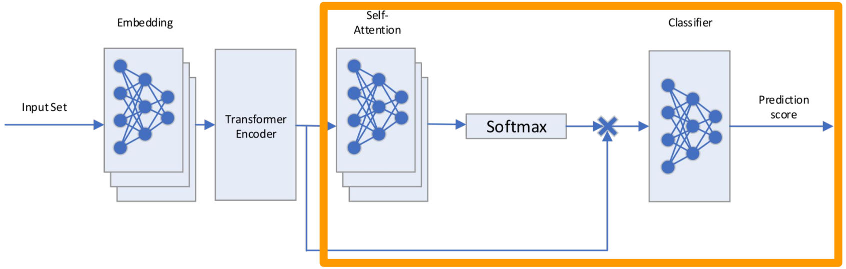

modified diagram from the article

- 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

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

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

# 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

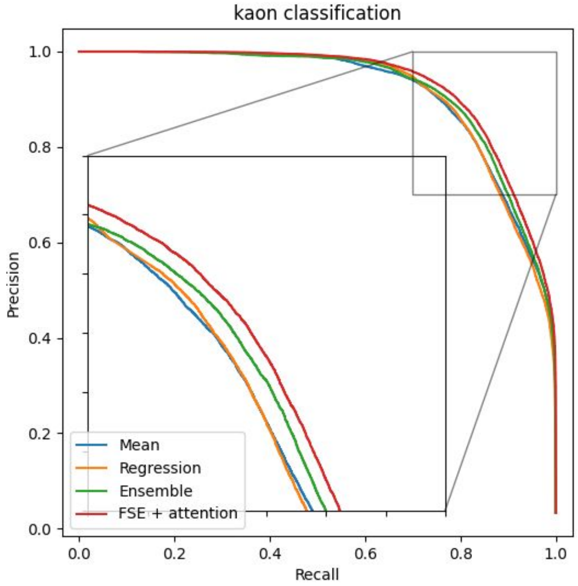
Parameters:

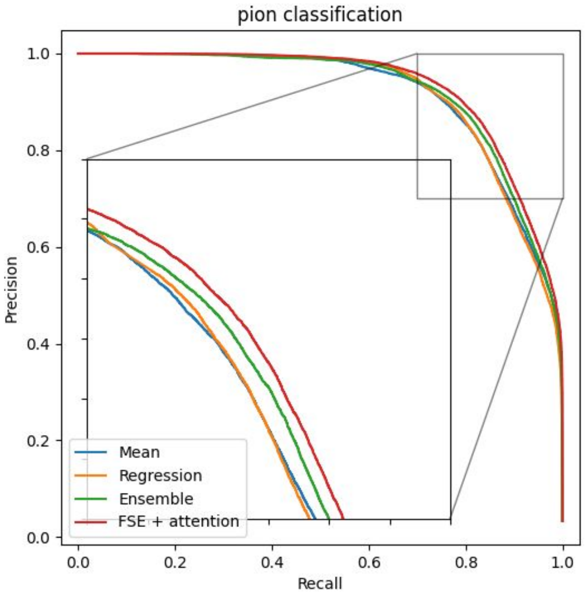
- optimizer: Adam
- output layer: 1 node (yes / no for a given particle)
- loss function: binary cross entropy
- scheduler: exponential with rate 0.98
- learning rate: 0.0005
- batch size: 64
- epochs: 30

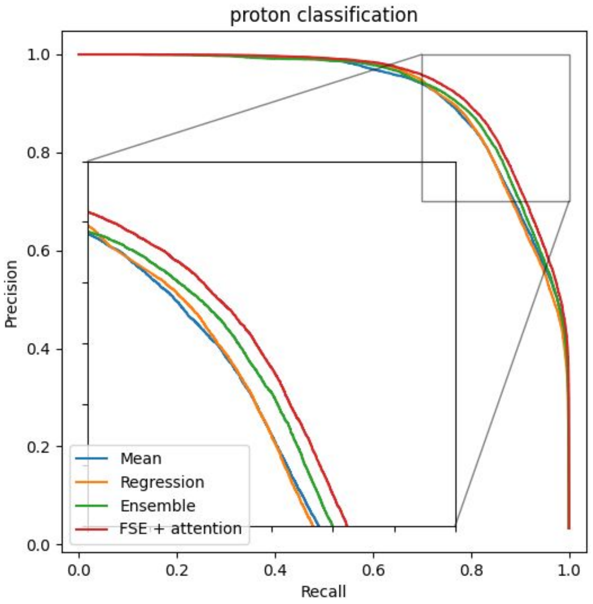
# Sample ROC curves

**FSE+attention** achieves **best results.**

**Little variation** between particle species.



# More to go: domain adaptation

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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

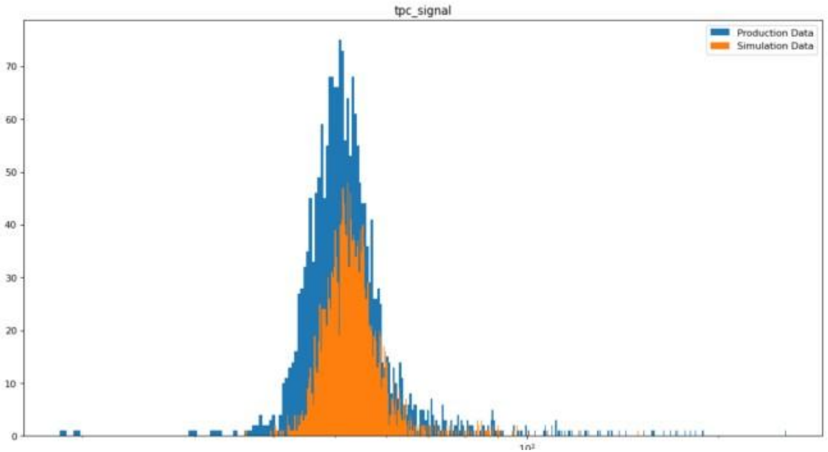
- How can we transfer the knowledge from training to inference?

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:**

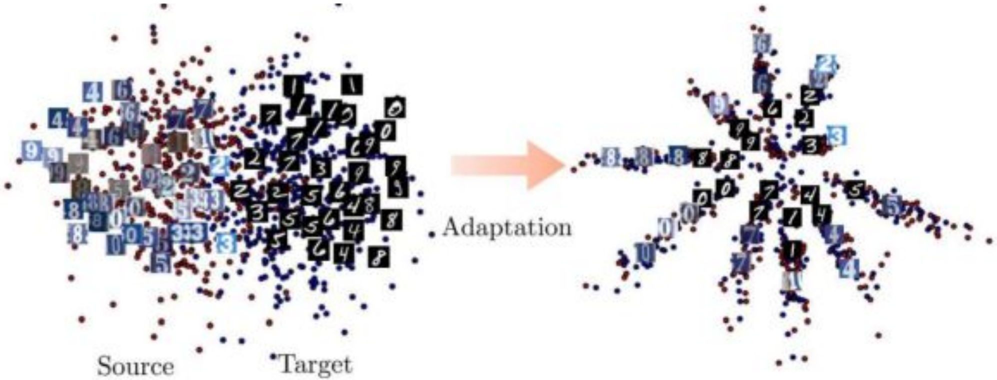
- actually **learn** the difference between data domains
- translate both data to a single common hyperspace



# More to go: domain adaptation

(a) MNIST

(b) SVHN



# More to go: domain adaptation

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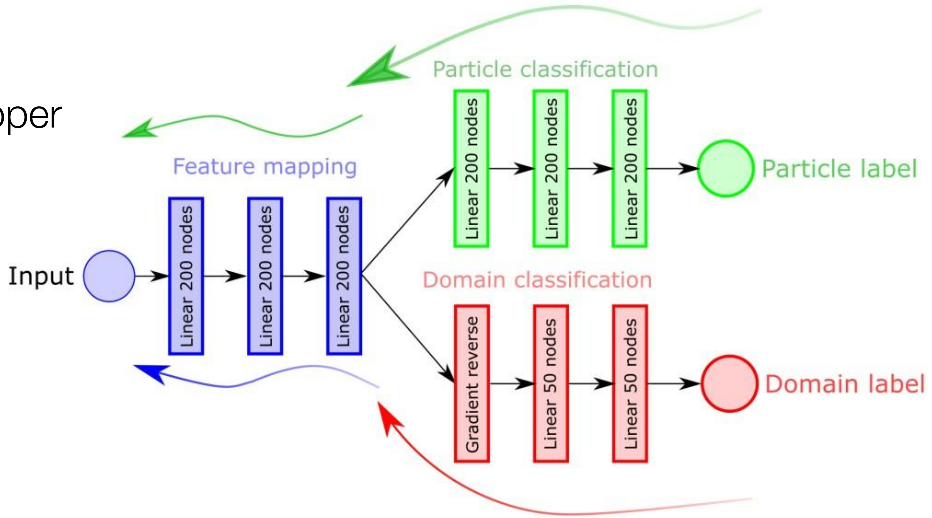
**Feature mapping:** input → domain invariant features

**Particle classifier:** recognize particles based on domain invariant latent space

**Domain classifier:** recognize MC vs real samples

**Training more complicated:**

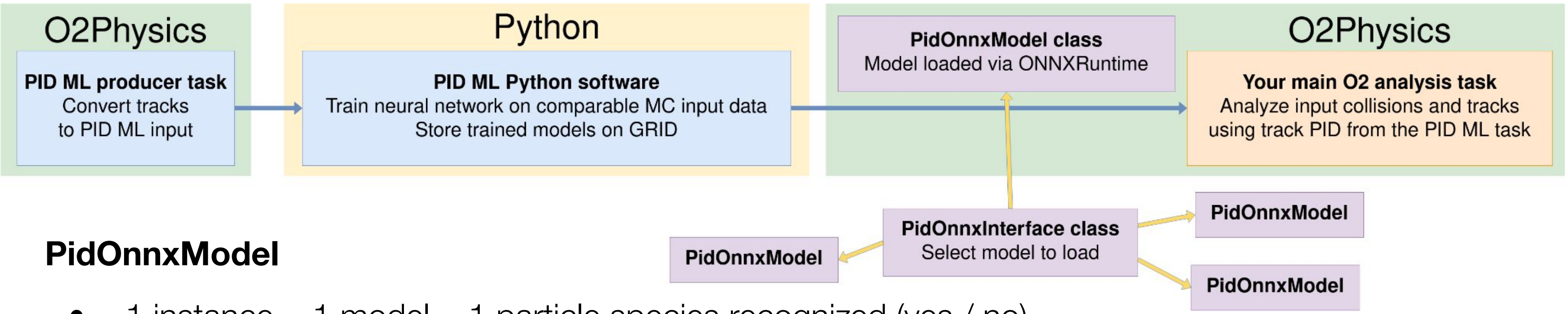
1. Train the domain classifier independently.
2. Freeze the domain classifier.
3. Train jointly particle classifier and feature mapper **adversarially** to the domain classifier.
4. Weights of the feature mapper:
   gradient from particle classifier
   + reversed gradient from domain classifier




**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/