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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EUROPEAN AI FOR FUNDAMENTAL PHYSICS CONFERENCE
EuCAIFCon 2025

Cagliari, Italy
19 June 2025

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**

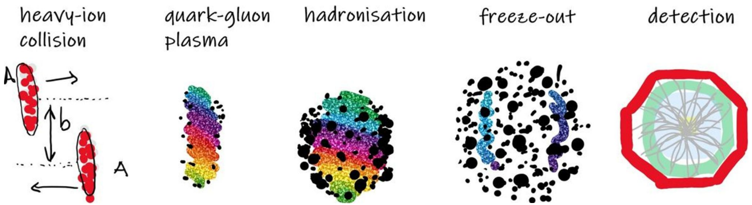
- Identify **areas** where both ALICE (or HEP in general) and ML communities can **mutually benefit** from each other

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

- **Disclaimer:**
    - I'm a **physicist without a big ML background** – few years ago I 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** from a physicist perspective, but the balance is to keep the project interesting for ML itself and be useful for us at the same time!

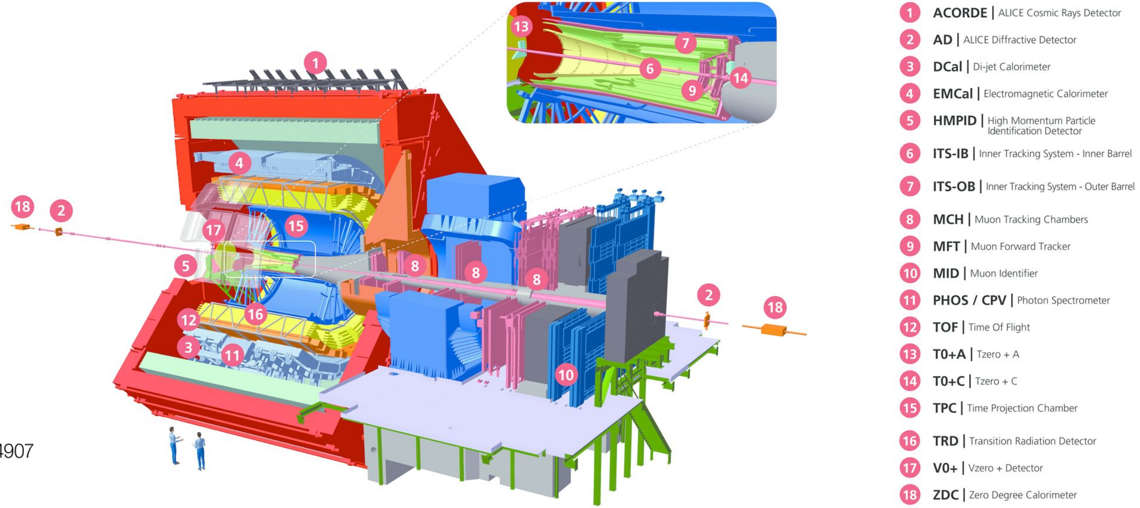
ALICE experiment @ LHC

ALICE (A Large Ion Collider Experiment) is a **heavy-ion collisions optimized** experiment at LHC with primary goal to study the **properties of the Quark-Gluon Plasma**

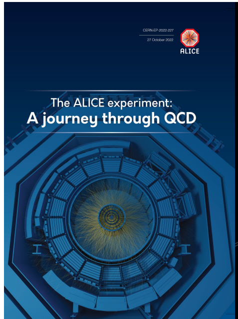


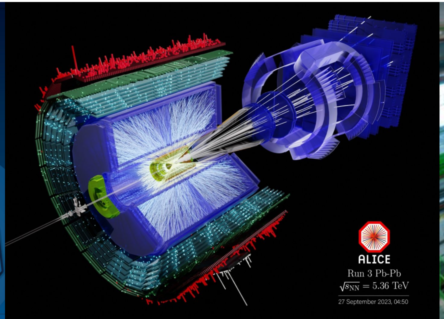
ALICE Collaboration Phys. Rev. C 101, 044907

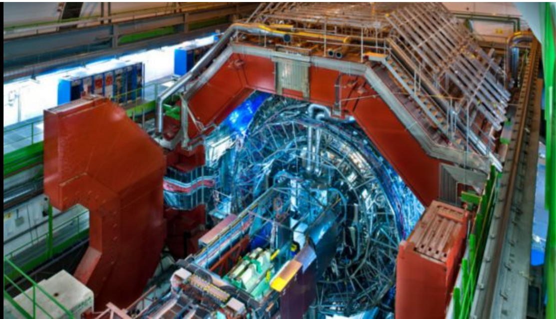
- **Capabilities**:
  - **50 kHz continuous readout** of Pb-Pb collisions with GEM-based TPC in Run 3
  - **particle identification (PID)** and tracking in a **very wide momentum range** down to ~100-150 MeV/c
- **Review paper** of 10 years of operation [Eur. Phys. J. C 84 (2024) 813]



https://cds.cern.ch/



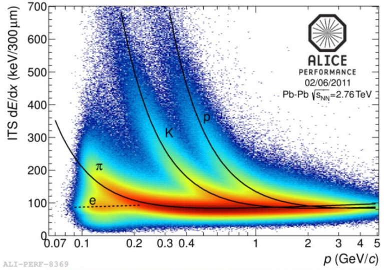


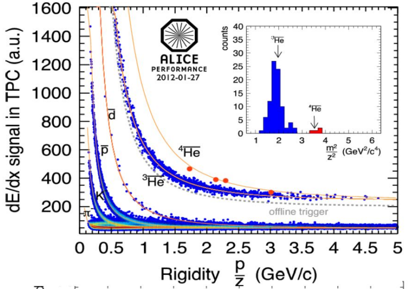


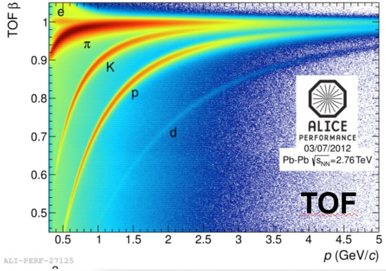
Particle identification (PID)

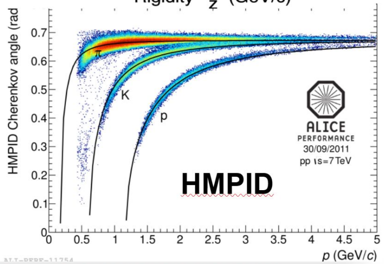
Aim: provide high purity samples of particles of a given type

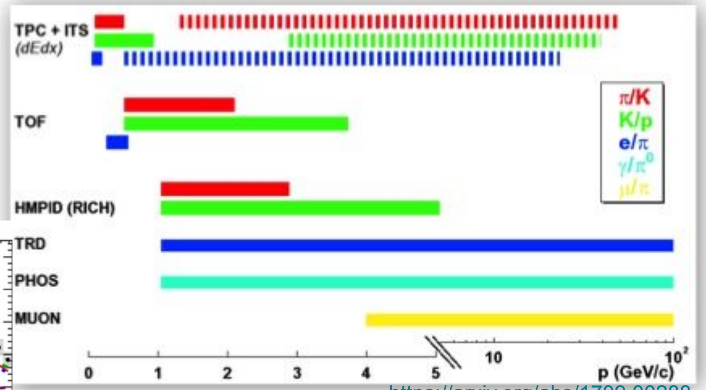
- **an essential step** for many physics analyses, especially **correlations of identified particles**
- we use **ALICE as our R&D environment**
- **PID is a distinguishing feature** of ALICE
    - identification of particles of momenta in a **very wide momentum range**
    - practically **all known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





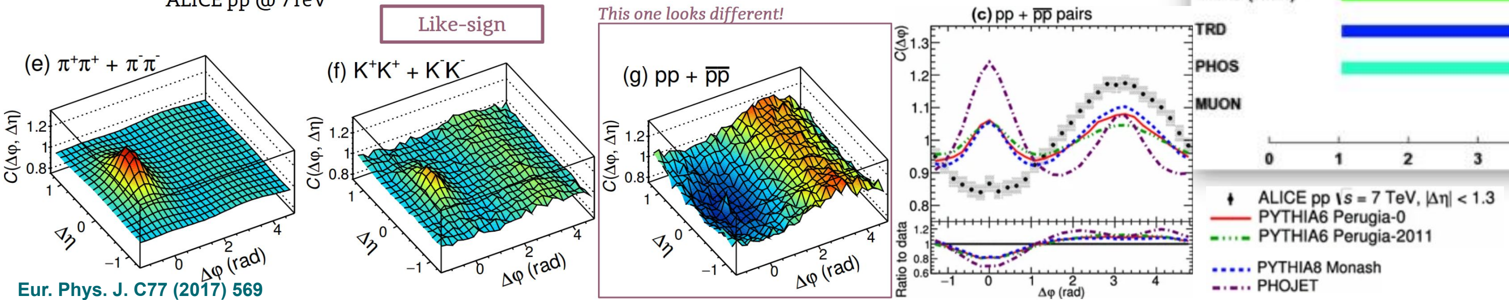






https://arxiv.org/abs/1709.00288

ALICE pp @ 7TeV

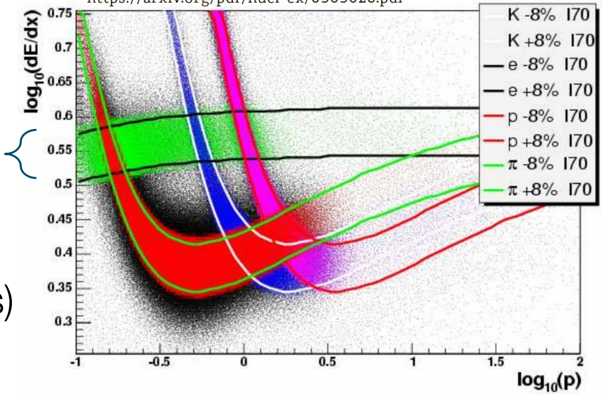


Eur. Phys. J. C77 (2017) 569

Present state-of-art

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

https://arxiv.org/pdf/nucl-ex/0505026.pdf



- **Metrics**
  - **Purity (*precision*)** and **efficiency (*recall*)** calculated from MC simulated data with full detector response (anchored to the specific data collection period = run)
    - normally measured as a function of transverse momentum p_T

$$\text{Efficiency} = \frac{N_{\text{true positives}}}{N_{\text{true particles}}}$$

$$\text{Purity} = \frac{N_{\text{true positives}}}{N_{\text{true positives}} + N_{\text{false positives}}}$$

Present state-of-art

1. **Traditional method:**
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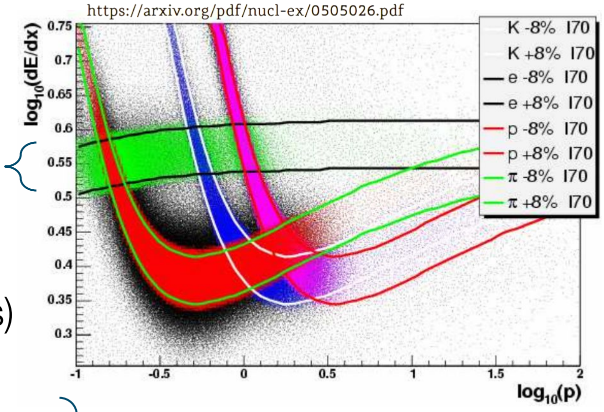
    - problems:
        - overlapping signals
        - high purity at the cost of low efficiency
        - time-consuming optimization (where the signals cross)



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 of a given particle species
    - increased purity, results consistent with the traditional method

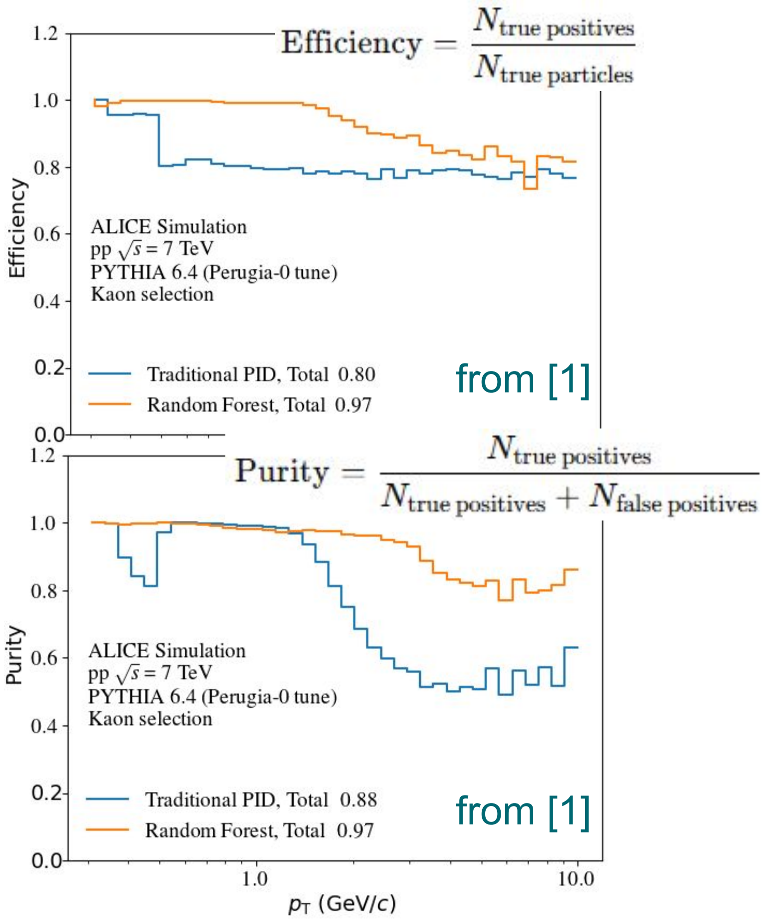
not covered in this talk
yields similar results

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 **quantify uncertainties**
- hard to follow classifier's ''reasoning'' (**black box**)

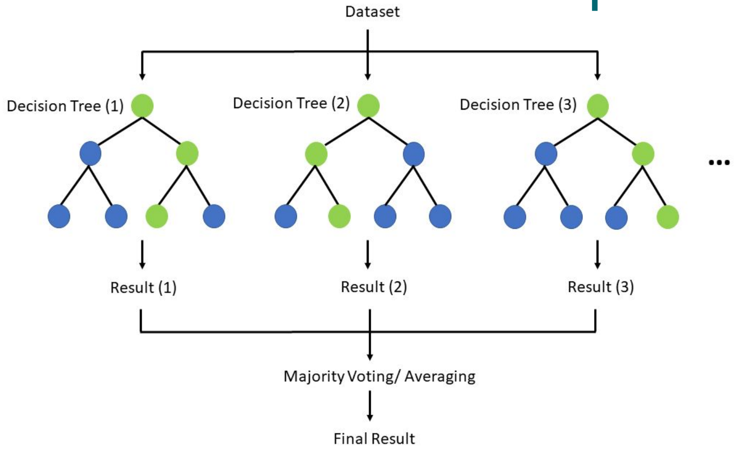
Our **first works** show ML can **greatly improve** purity and efficiency:

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

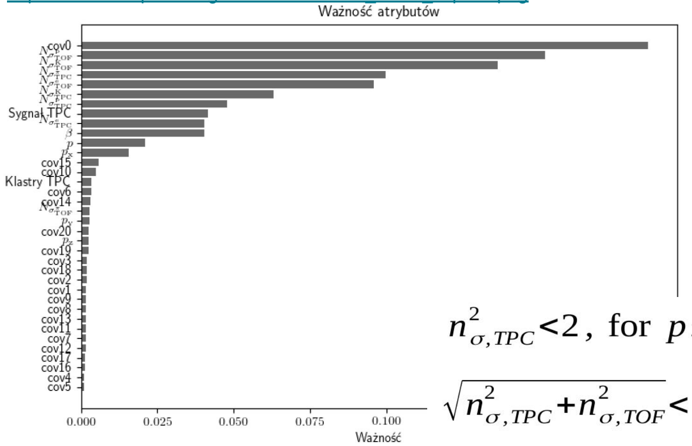
T. Trzciński, Ł. Graczykowski, M. Glinka,
Conference on Information Technology, Systems Research and Computational Physics, 3-17. 2018

2018



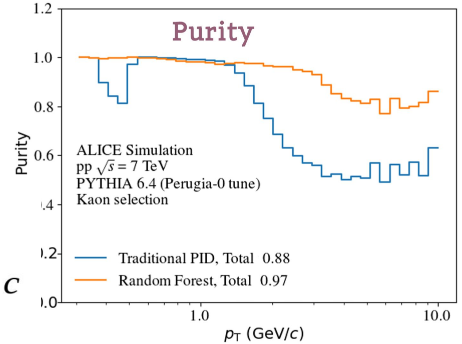
https://en.m.wikipedia.org/wiki/File:Random_forest_explain.png

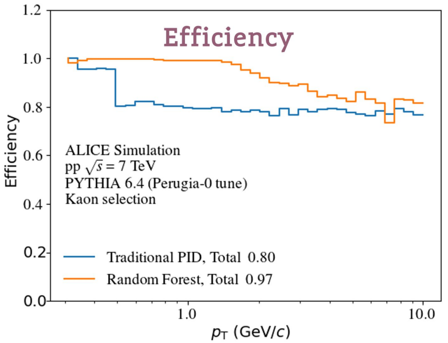
- Preliminary work with ALICE Run 2 data
- First solution - **Random Forest**
- Model works on **high-level track parameters**
- Depends on the **quality of Monte Carlo sample** and **post-processed information** (i.e. nσ calculation)
- Can be used **only for analysis-specific use-case** (concrete dataset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



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

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



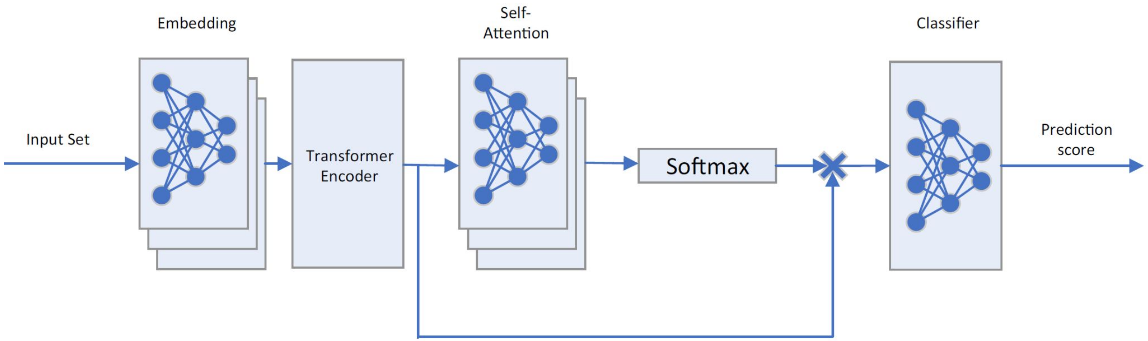


Current solution - our model

- 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}, TPC number of clusters, detector signals (TPC dE/dx, TOF time, TRD signal), etc.
- **Data might be missing** for a given track 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)

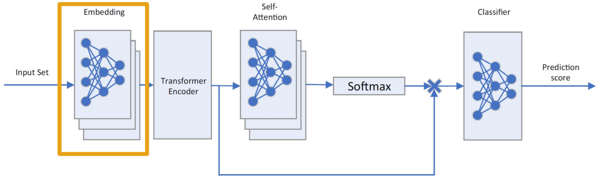
Attention-based Multi-instance Neural Network for Medical Diagnosis from Incomplete and Low Quality Data

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
[3]Beijing Medicinovo Technology Co.,Ltd., Beijing, China
[1,3]zwan7221@uni.sydeny.edu.au, [1]{josiah.poon, simon.poon}@sydney.edu.au, [2]sunshiding@ruc.edu.cn

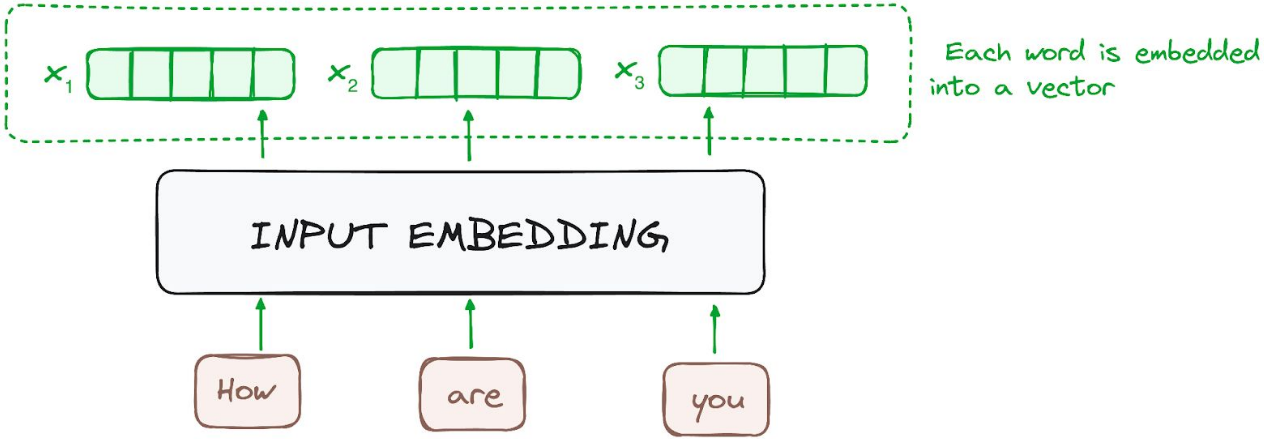
2019 International Joint Conference on Neural Networks (IJCNN)

details on slide 18

Step 1: Embedding

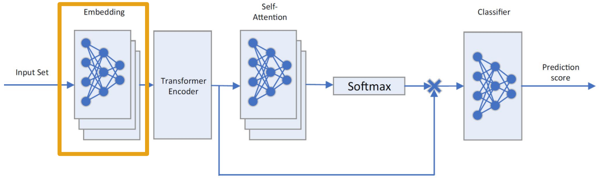


- **Embedding** is a technique to **handle complex data**
- It works by **converting high-dimensional data** (i.e. sequences of words, documents, images, etc.), **into lower-dimensional** and **abstract vector representation (embedding space)**
- It allows for capturing **meaningful relationships between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



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

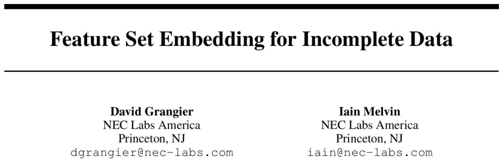
Step 1: Feature Set Embedding



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

Feature Set Embedding (NIPS 2010 article):

- first, create (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 with a single hidden layer) into vectors (embeddings)



Feature Set Embedding for Incomplete Data

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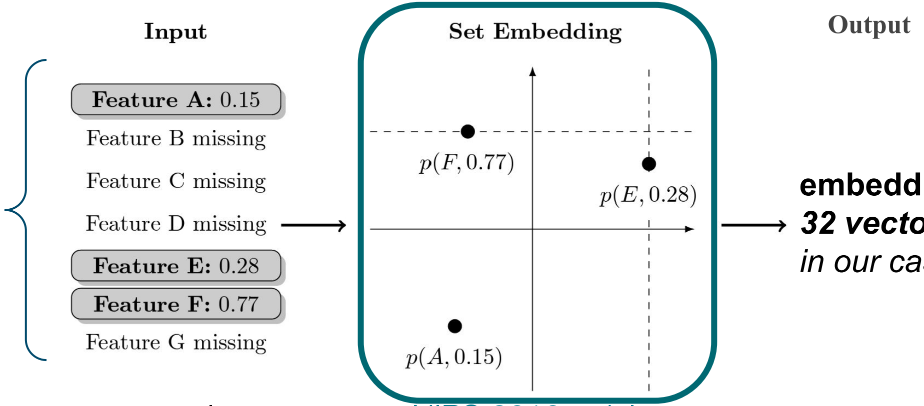
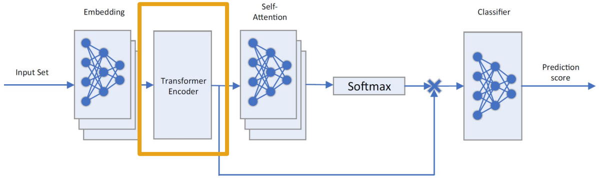
track
19 features
in our case

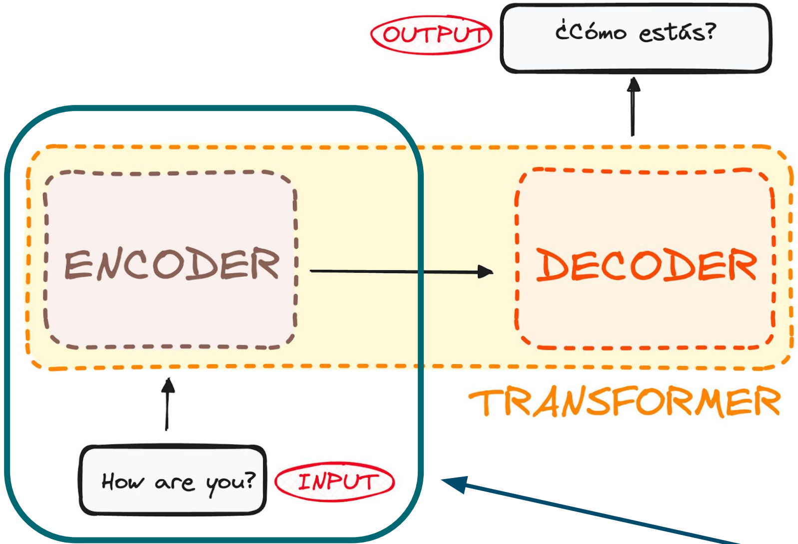


embeddings
32 vectors
in our case

Image source: NIPS 2010 article

Step 2: Transformer Encoder





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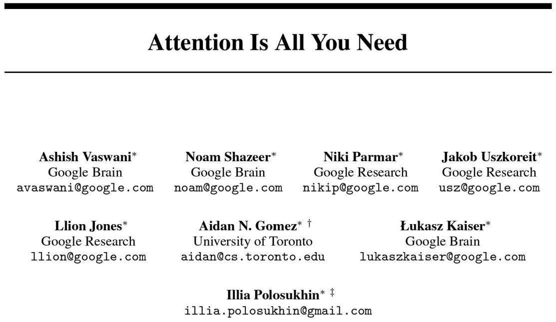

Attention Is All You Need

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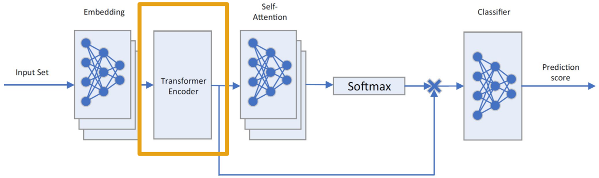
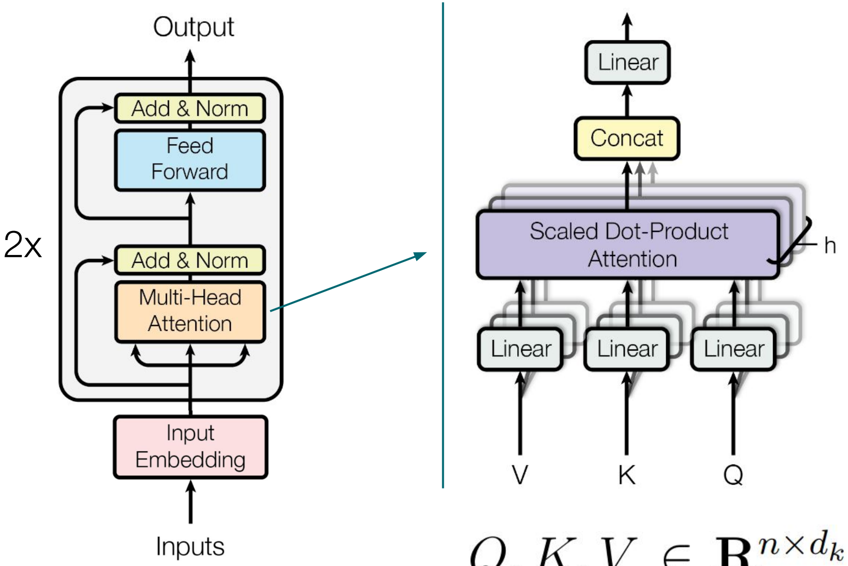
- Idea from original **Transformer** architecture ([NIPS 2017 article](#))

- In our case, **vectors from Embedding are processed by the Encoder only**
  - it finds relations between available features regardless of the amount of missing values

Step 2: Transformer Encoder





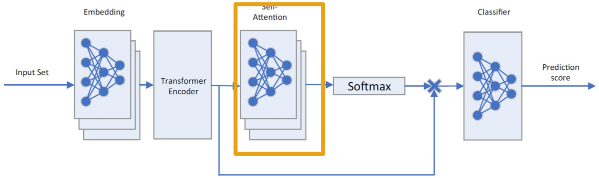
modified diagram from the Transformer article

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

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

- Encoder processes 32 embedding vectors to connect different features each vector represents
  - we use **2-head attention** (to find more complex relationships)
  - each head has **2 layers**: **attention** (for to the whole set of vectors) **+ dense NN** (applied to each vector separately)
  - example: a specific detector signal could be used if and only if the momentum is in a specific range

Step 3: self-attention pooling



- The final **classifier** requires a **single output vector**, while we have 32 vectors (processed embeddings) at the output of the Encoder
  - **Solution:** another **self-attention network** (single layer) is used to pool the final vector

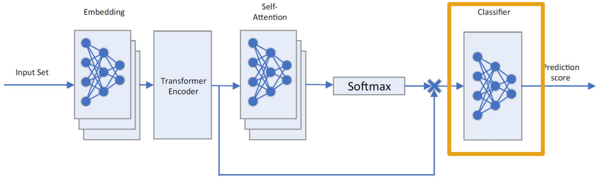
$$\{v_1, v_2, \ldots, v_n\}, \; v_i \in \mathbf{R}^{d_{model}}$$ processed embeddings

$$e_i = NN(v_i) \qquad \forall i \in [1, n]$$ 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** components

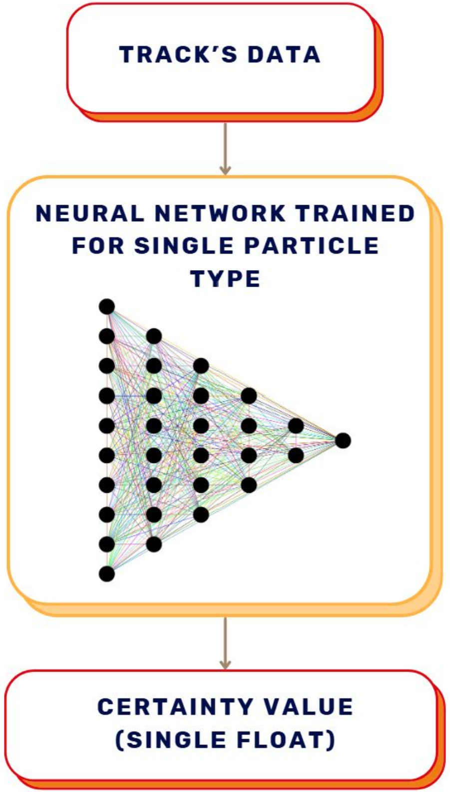
Step 4: classification



- 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** type (**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

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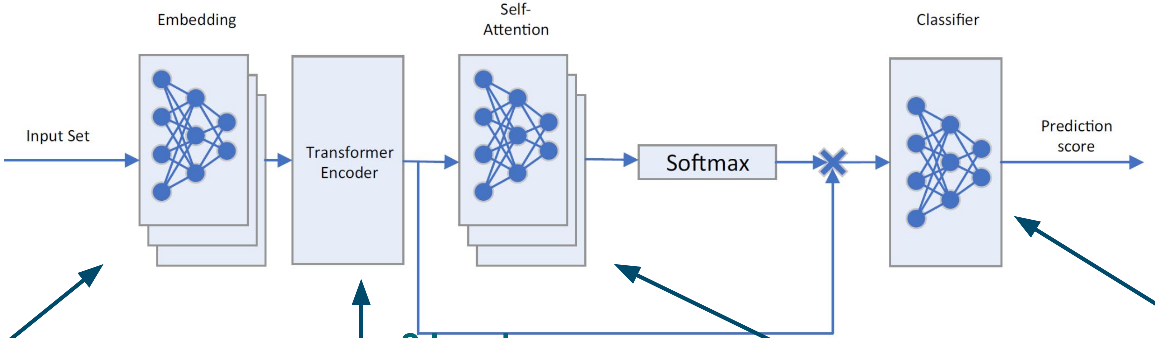

This model is applied **separately** for pions, kaons, protons

“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 Encoder layer (to limit overfitting)
- **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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M. Janik, EPJ C 84 (2024) 7, 691
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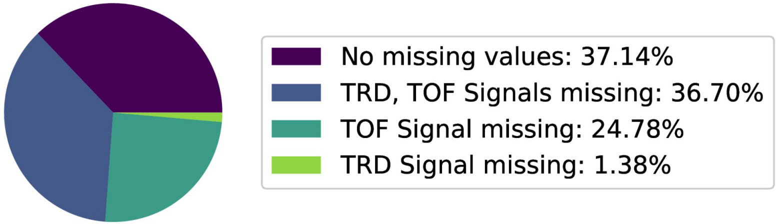
- **Dataset:** Run 2 general-purpose MC (Pythia 8) pp at $\sqrt{s}$ = 13 TeV with full detector simulation with GEANT 4 (both MC truth and reconstructed data are used)
  - TPC signal is always required
- **Standard nσ method:**
  $|n_{\sigma,\,\mathrm{TPC}}| < 3$ for $p_{\mathrm{T}} < 0.5$ GeV/c, $\sqrt{(n_{\sigma,\,\mathrm{TPC}}^2 + n_{\sigma,\,\mathrm{TOF}}^2)} < 3$ 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)**

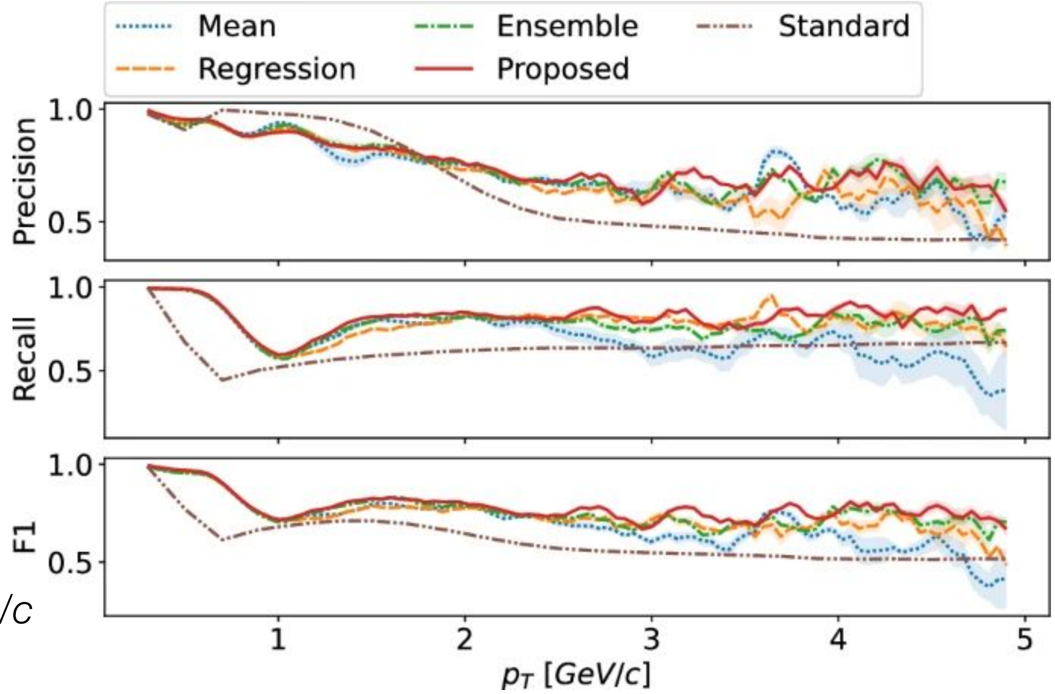
Proposed model (FSE+Attention)
compared to **other approaches:**

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

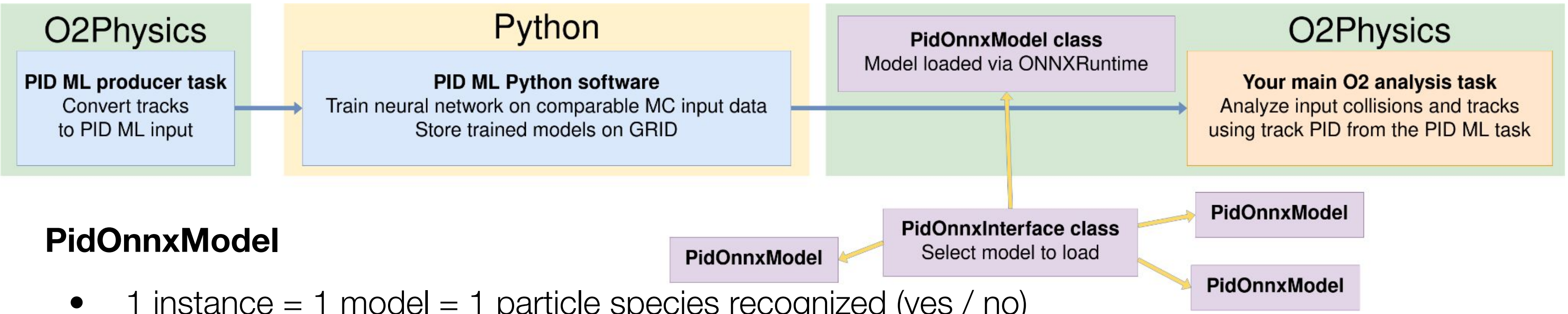
- **NN ensemble** (4 networks)**:**
  potentially large complexity

- **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



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
- models **stored in CCDB** (experiment's database) for each run and available to access in data analysis code by users (via a "helper task")

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/

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*) and outside ALICE

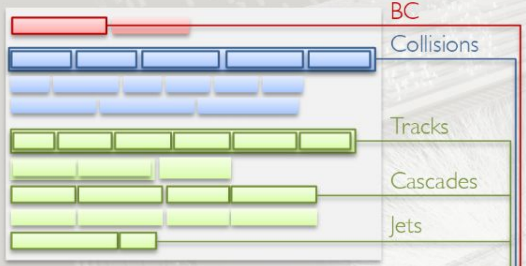
The work has been carried out by an interdisciplinary team from 4 faculties of WUT:

- *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!

In a nutshell: the general analysis task structure

Data Model



Examples:

- loop over tracks in each event
- loop over cascades in each event
- Correlate cascades with jets

  → do **physics**!

Your analysis task!

struct yourAwesomeTask	Basic task definition
produces<something> name;	Declares tables that may be created by this task
Partition declarations	Declares partitions: new tables based on selection criteria
Filter declarations	Declares filters: selection criteria
Output object declarations	Declares output objects: Histograms or HistogramRegistry
Configurable declarations	Declares configurables: values that can be set by user
init()	Set up before processing data
process(●●●●●)	Subscribe (connect to input) and process data
defineDataProcessing()	Information for task -> DPL processor conversion

●●●●● = tells the framework which tables the user is interested in and which to merge / relate to one another

Very theoretical → now we will go practical! Let's run and customize our own task

Crash course: how do you run something?

- Each analysis task is an executable → this means you can run them in the command line!

$\underbrace{\texttt{o2-analysistutorial-histograms}}_{\text{Example task}}\ \underbrace{\texttt{--aod-file AO2D.root}}_{\text{Input file}}\ |\ \underbrace{\texttt{o2-analysis-track-propagation}}_{\text{Helper task, Propagates tracks to PV}}\ |\ \underbrace{\texttt{o2-analysis-timestamp}}_{\text{Helper task, Provides timestamps}}$

- All tasks have to be provided separated with a 'pipe' character ("|")
- `--aod-file` can receive an AO2D file or you can use `--aod-file @listoffiles.txt` with a list of files!
- Typically, many helper tasks are required: we will introduce you to this in the hands-on!
- This is, among other things, a consequence of the AO2D content
    - not all table information is available in the AO2D: minimalistic!
    - Some tables and columns are generated on-the-fly to minimize data storage: a strict necessity in Run 3!

- General event (centrality/multiplicity percentile) and track properties (PID values) have to be calculated!
- And beyond that: tracks are stored at their 'innermost update' in the AO2D (TracksIU)
    - Tracks to be propagated to the primary vertices by the track propagation task
    - We'll also show you this later…

Run 2 results

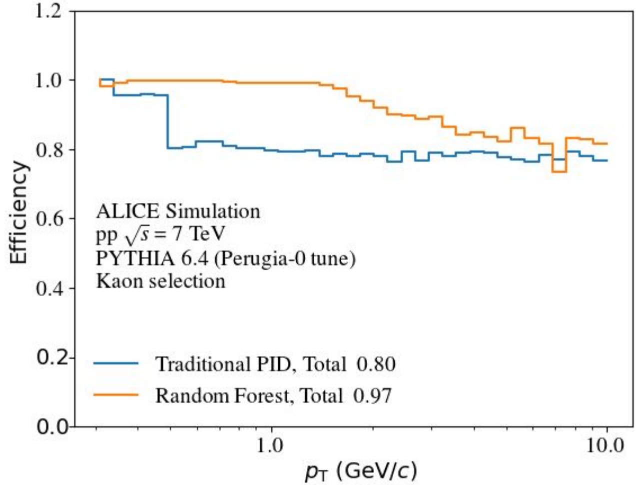
- pp at 7 TeV, Pythia 6 Perugia-0
- kaons vs other particles

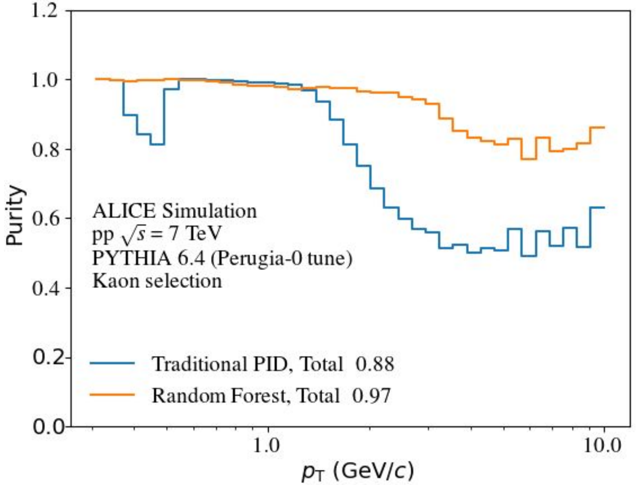
Traditional PID:

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

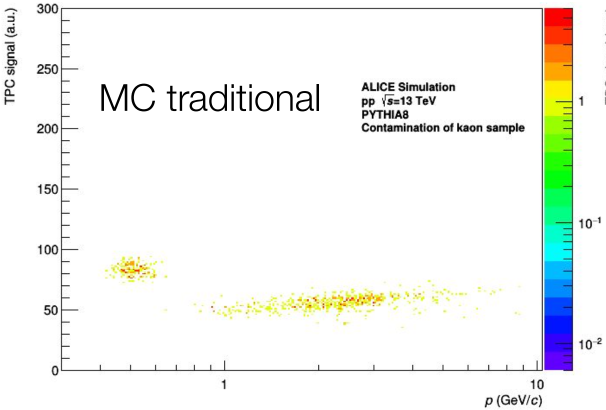
$$\sqrt{n^2_{\sigma,\mathrm{TPC}} + n^2_{\sigma,\mathrm{TOF}}} \qquad p_{\mathrm{T}} > 0.5\mathrm{GeV}/c$$

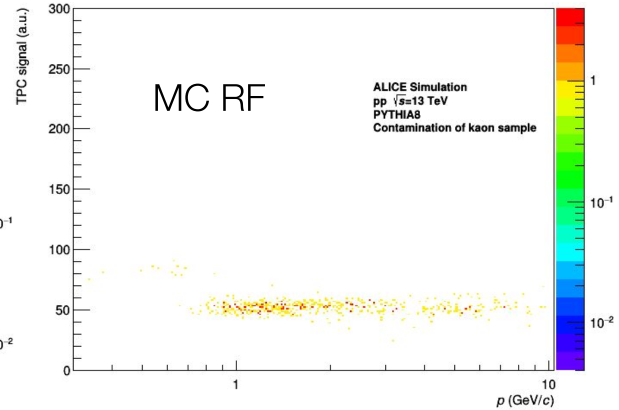
much higher efficiency and **purity** with Random Forest





Contamination of kaon samples





Example: FSE with one-hot encoding

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

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

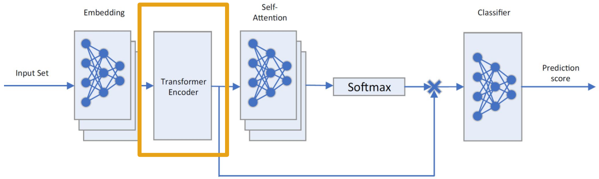
(c) Second particle.

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

Step 2: Transformer Encoder



Attention Is All You Need

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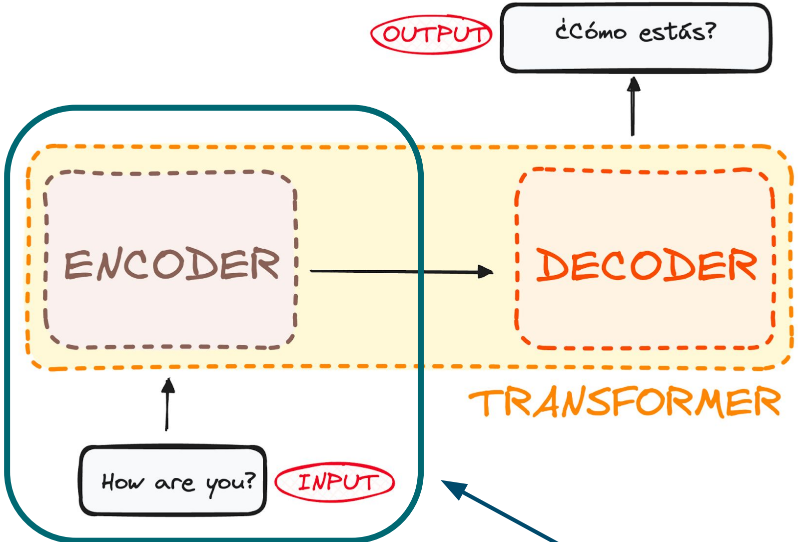


https://www.datacamp.com/tutorial/how-transformers-work

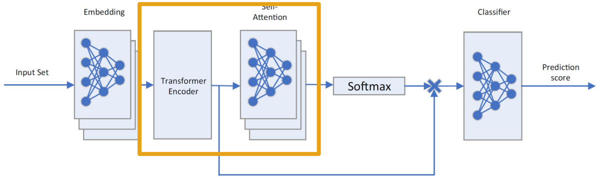
- Idea from original **Transformer** architecture proposed by Google (NIPS 2017 article)
- Developed for **transforming input data** into a **contextualized representation** on the output
- Transformer currently serves as **basis for the Natural Language Processing** tools (such as **ChatGPT**)
- In 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

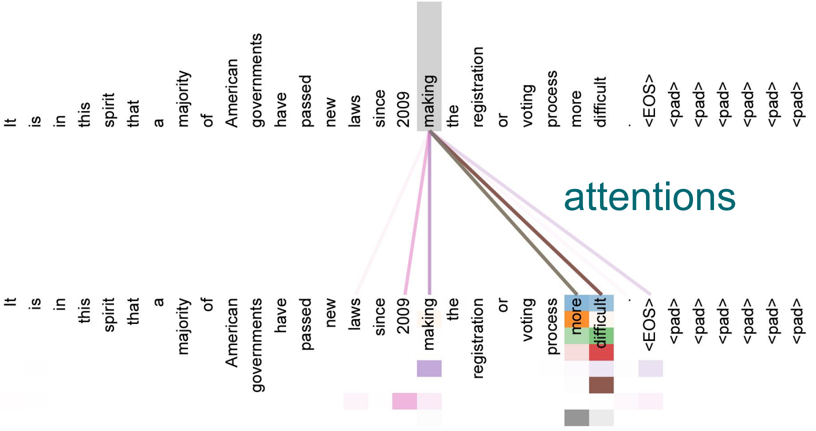
- **Attention** and **self-attention** are mechanisms used to help model focus on relevant parts of the input data
    - **self-attention** focuses on **relationships within the same input sequence**

- ***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]

Results

F_1 = 2 x (purity x efficiency) / (purity + 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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0	0	0	1	0	13
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(d) Third particle.

key					value
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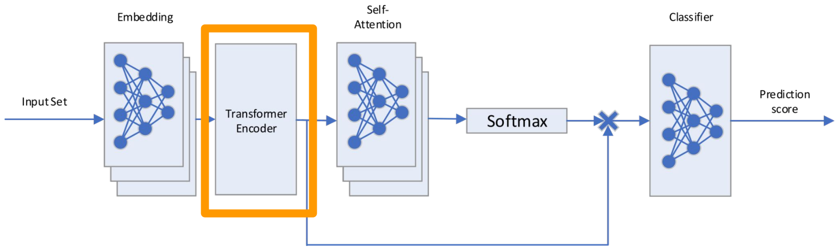
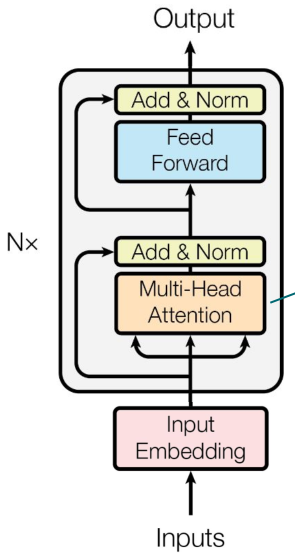
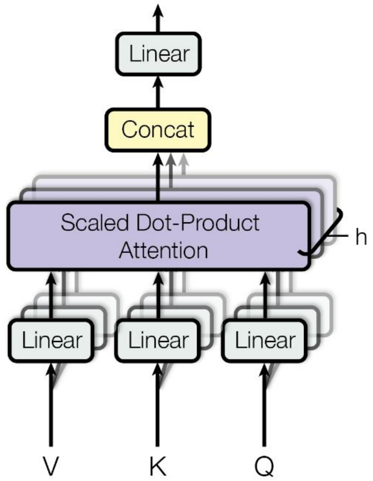
The attention continued

2. Transformer Encoder



N=2





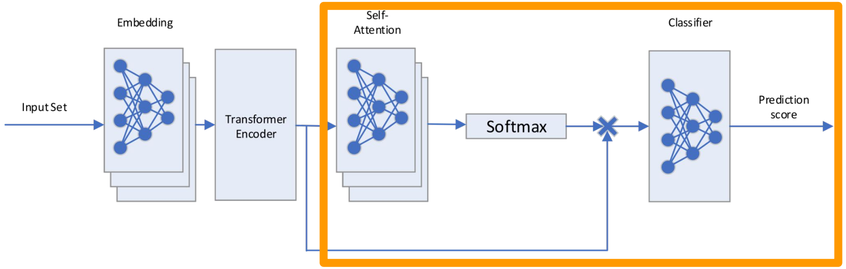
- adjusted original Transformer Encoder
- attention without convolutions and recurrence
- finding self-correlations in an instance set of vectors
- example: a specific detector signal could be used if and only if the momentum is in a specific range

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

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

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

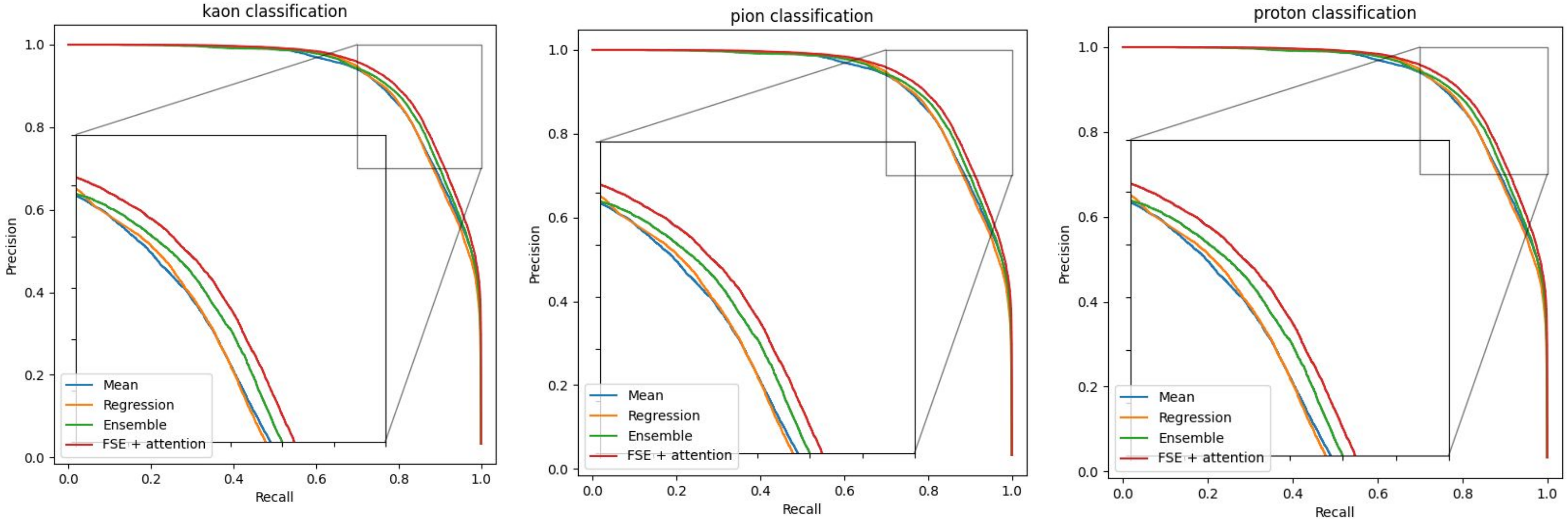
Parameters:

- 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

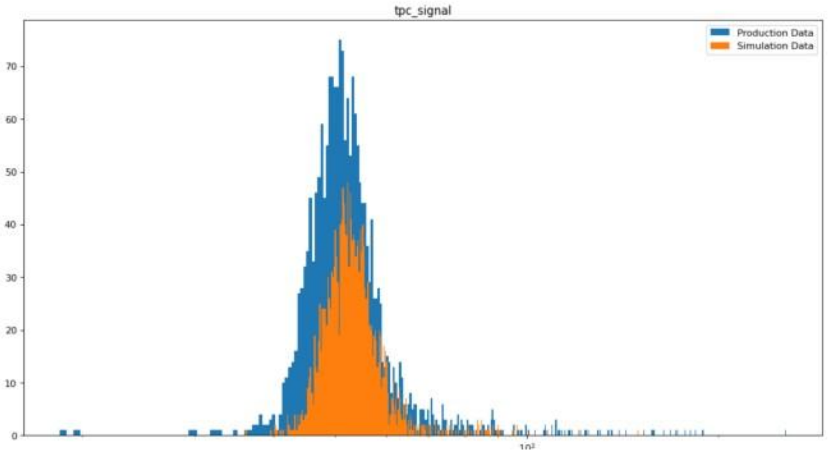
- How can we transfer the knowledge from training to inference?

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:

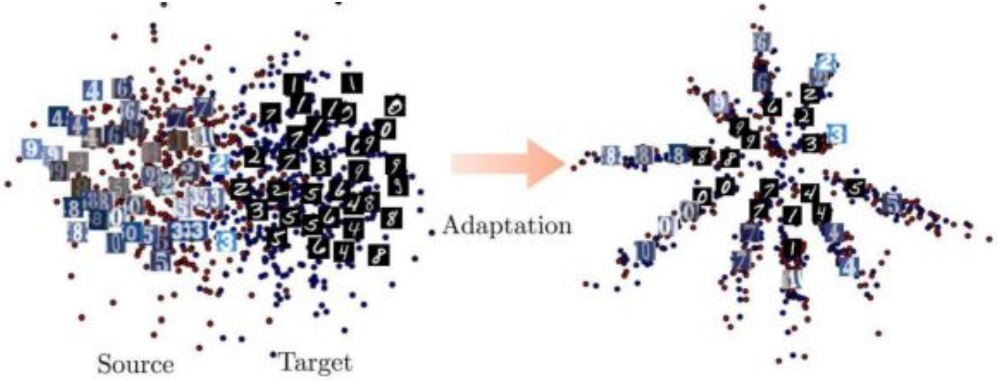
- actually **learn** the difference between data domains
- translate both data to a single common hyperspace



More to go: domain adaptation

(a) MNIST

(b) SVHN



More to go: domain adaptation

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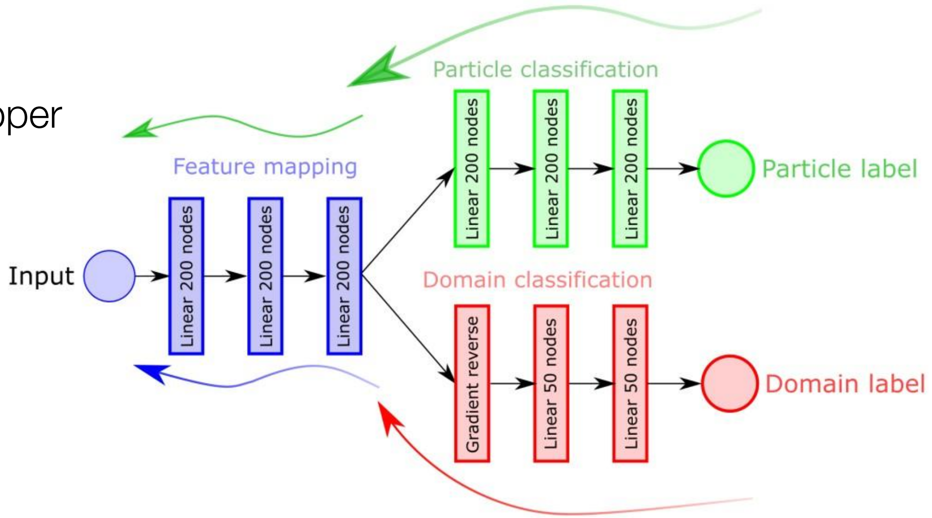
Feature mapping: input → domain invariant features

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