Using Machine Learning methods for improving data quality in ALICE

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XIII Quark Confinement and the Hadron Spectrum
Maynooth, Ireland
2 August 2018
Goals

- Use ALICE and its data as a unique environment to advance the Machine Learning field of science
- Identify areas where both ALICE (or HEP in general) and ML communities can mutually benefit
- Focus on Machine Learning research rather than using standard ML tools for ALICE use cases
- Disclaimer:
  - I’m a physicist without a 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
Three areas of research

- **Data Quality Assurance** – prediction of detector quality label assignment
  - not covered in this talk

- **Simulation of TPC clusters in Monte Carlo data using generative networks**

- **Development of more precise particle identification (PID)**
Simulation of TPC clusters in Monte Carlo data using generative networks
Time Projection Chamber

- Tracking in ALICE is performed by ITS, TPC, TRD and TOF
- First attempts – focus on the TPC only:
  - main tracking device
  - located from 0.8 m (inner radius) to 2.5 m (outer radius) from the beam and extending ~2.5 m in each direction along the beam axis
  - volume of 95 m³
  - filled with Ne-CO₂ gas mixture (90%-10%)
  - clusters - points in 3D space, together with the energy loss, which were presumably generated by a particle traveling through
  - provides up to 159 clusters per track
Simulation and reconstruction

- Current process relies on 5 independent modules
- The computationally most expensive module is particle propagation through the detector’s matter
Simulation and reconstruction

- Generative solution for cluster simulation:
  - substitute the detector simulation and check for the speed-up
  - full simulation **still needed** to generate training samples
  - immediate **drawback**: quality of such MC data can be either comparable or lower than the full detector simulation – limits potential applications
Generative Adversarial Networks

- Generative Adversarial Network (GAN) is a neural network architecture of two networks competing with each other (playing a min-max game)
  - "Generator" is trained to produce fake data resembling the real data
  - "Discriminator" predicts whether an example data is real or fake
Generative Adversarial Networks

- Typical use cases:
  - mainly generation of photo quality fake images (i.e. of celebrities)

https://arxiv.org/abs/1710.10196

Generative Adversarial Networks

- Extending the GAN architecture – provide a set of initial parameters for the generator and discriminator:
  - generator would not generate a random output, but a customized one
  - in our case: initial momenta of Monte Carlo particles

Initial Parameters

https://giphy.com/gifs/leonardo-dicaprio-catch-me-if-you-can-Sleecharacters-L1h4mnWEWKfn2

https://33milesinnewaygocounty.files.wordpress.com

https://thechive.files.wordpress.com
TPC clusters with GANs

- It is not (yet!) possible to generate the full 3D image of the event at once (especially in the Pb-Pb event)

- Our solution is to:
  - generate clusters for single particles
  - two separate flows for spatial coordinates \((x,y,z)\) and the energy
  - in the beginning focus only on 3D coordinates
  - merge generated samples (individual particles) into full images
  - training of the GAN on original full simulations
Example results

ALICE Simulation
PYTHIA6, Perugia-0, pp @ √s = 7 TeV

TPC Clusters
- GAN Simulation
- Full Simulation

Proton

ALICE Simulation
PYTHIA6, Perugia-0, pp @ √s = 7 TeV

Original event

ALICE Simulation
PYTHIA6, Perugia-0, pp @ √s = 7 TeV

GAN event

Example results

ALICE Simulation
PYTHIA6, Perugia-0, pp @ √s = 7 TeV

TPC Clusters
- GAN Simulation
- Full Simulation

Kaon

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Results

- Mean Squared Error (MSE) from the original helix as a quality measure

- Evaluation conducted on the separate test-set with ~15000 tracks

MSE visualisation:
Red - error
Grey - ideal helix
Orange - original clusters
Blue - generated clusters

<table>
<thead>
<tr>
<th>Method</th>
<th>Mean MSE (mm)</th>
<th>Median MSE (mm)</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>GEANT3</td>
<td>1.20</td>
<td>1.12</td>
<td>1</td>
</tr>
<tr>
<td>Random (estimated)</td>
<td>2500</td>
<td>2500</td>
<td>N/A</td>
</tr>
<tr>
<td>condLSTM GAN</td>
<td>2093.69</td>
<td>2070.32</td>
<td>100</td>
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<tr>
<td>condLSTM GAN+</td>
<td>221.78</td>
<td>190.17</td>
<td>25</td>
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<tr>
<td>condDCGAN</td>
<td>795.08</td>
<td>738.71</td>
<td></td>
</tr>
<tr>
<td>condDCGAN+</td>
<td>136.84</td>
<td>82.72</td>
<td></td>
</tr>
</tbody>
</table>
Computational cost

- Performance test conducted on the standalone machine with Intel Core i7-6850K (3.60 GHz) CPU using single core and no GPU
- Additional order of magnitude speed-up for GAN models with nVidia Titan Xp GPU
PID with Machine Learning
Particle identification

- Particle identification (PID) is one of the most important steps in many physics analyses
- Crucial for Quark-Gluon Plasma measurements
- PID is one of the strongest advantages of ALICE:
  - practically all known techniques used (dE/dx energy loss, time-of-flight, Cherenkov radiation for hadrons and transition radiation for electrons)
  - possibility to identify (anti-)nuclei
  - very good separation of pions, kaons, protons, electrons over a wide momentum range
  - separation of signals of charged hadrons and electrons for very low momenta (down to 0.1 GeV/c)
Particle identification

- ITS
- TOF
- TPC
- TRD
- HMPID

AlICE
Traditional vs ML PID

- **Traditional PID:**
  - a typical analyzer selects particles “manually” by cutting on certain quantities, like the number of standard deviations of a signal from the expected value
  - most limitations come in the regions where signals from different particle species cross
  - “cut” optimization is a time-consuming task

- **Machine learning PID:**
  - perfect task for machine learning
  - can learn non-trivial relations between different track parameters and PID
  - no “trial and error” approach

Results

- **Test data sample:**
  - \( \text{pp @ 7 TeV, Pythia 6 Perugia-0} \)

- **Traditional PID:**
  - \( n_{\sigma,TPC}^2 < 2 \), for \( p \leq 0.5 \text{ GeV/c} \)
  - \( \sqrt{n_{\sigma,TPC}^2 + n_{\sigma,TOF}^2} < 2 \), for \( p > 0.5 \text{ GeV/c} \)

- **Machine Learning PID:**
  - Random Forest classifier
Results

- **Test data sample:**
  - pp @ 7 TeV, Pythia 6 Perugia-0

- **Traditional PID:**
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**Contamination from non kaons**

**Classified as non kaons**

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Summary

- **GANs for TPC cluster simulation**
  - Quality not yet equal to the full simulation
  - Massive speed-up of 25x (CPU) or 250x (GPU) wrt standard simulation
  - First step towards semi-real time anomaly detection tool

- **PID**
  - ML-based PID outperforms traditional PID, especially in the low momentum region
  - Training needed only once for each data set – no need for manual cut optimizations
  - Quality of final classification more vulnerable to discrepancies between MC and real data
Thank you!
Backup
Deep Convolutional GAN

- Class of architectures which use the convolutional tools and deconvolutional layers – mostly used with images
condDCGAN: Conditional DCGAN

- Generator – deconvolutional layers
- Discriminator – convolutional layers
- Network conditioned on particle momenta, mass, and charge
- Output classification – sigmoid function
condDCGAN+: combined loss

- Training on the full MC simulations
- Preparing the noise from initial parameters of MC simulations
- Comparing the generated samples with original ones
- Combining original conditional GAN loss with the results of comparison

\[ \mathcal{L}_G(m, X) = \mathbb{E}_{z \sim p_z(z|m)}[\alpha \log(1 - D(G(z))) + \beta \frac{1}{n} \sum_{i=1}^{n} (X_i - G(\hat{z})_i)^2] \]

- \( m \) - initial parameters (particle momenta),
- \( X \) - original value corresponding to \( m \),
- \( p(z|m) \) - distribution of a noise vector under initial parameters \( m \)
- \( z \) - input into a generator
- \( G \) and \( D \) - generator and discriminator
- \( n \) - the number of produced clusters

Additional parameters \( \alpha \) and \( \beta \) are used to weight the share of individual losses.
Best performing values are \( \alpha = 0.6 \) and \( \beta = 0.8 \)
PID parameter importance

![Bar chart showing the importance of various PID parameters, with the most important parameter on the left and less important ones towards the right.]