Application of machine learning for validation of Geant4 hadronic models

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Outline

1. Motivation, samples and event selection
2. Implementation of Machine Learning technique
3. Preliminary results of ANN-based prediction of secondaries

MC samples and event selection

Main goal: prediction of shower properties using calorimetric observables

MC samples

- CALICE technological prototype geometry and layout
- centrally generated samples of negative pions, 10–80 GeV, 500 kevt / sample
- Geant4 v10.3, physics lists: FTFP_BERT_HP and QGSP_BERT_HP
- official digitisation, no PID

In the current analysis: 40 GeV pions and QGSP_BERT_HP physics list

Reconstruction and event selection

- reconstruction software v04-14
- official reconstruction chain, 0.5 MIP cut for hits, official start finder algorithm
- for analysis: only events with found start at 3–6 AHCAL layers
- no other constraints, no clustering

MVA approach: algorithm, input features and targets

Goal is to predict distributions of parameters of secondaries within a shower

⇒ regression model realised in Artificial Neural Network

⇒ 29 calorimetric observables as input variables

⇒ one of MC-truth variables as a target

Input features and targets

Inputs

- Number of isolated hits in a shower
- Mean shower hit energy
- Shower radius
- Longitudinal shower centre of gravity
- Number of track hits within a shower
- "Ring" observables: 12 energies (MIP) + 12 numbers of isolated hits

Targets

- **Number of neutrons**
  counted per event except for those, which have one parent only that is also neutron (to avoid double counting)
- **Energy of neutral pions**
  sum of energies of all neutral pions in event

Details on observables and MC-truth in the previous talk by Marina

Preprocessing

Sample under study: 40 GeV energy point, about 106k selected events (from full set)

Features

- 29 input features and 1 target (true from mc collection)
- weighting applied with event weights obtained from the inverse target pdf to get more uniform distribution for target in the loss function calculation
- no normalization

Subsets

- 2/3 (64k) of full set for train/validation (t/v set) and about 1/3 (42k) of full set for test
- train subset is 32k events (50% of t/v set)
- validation subset is 32k events (50% of t/v set)
- events are selected randomly without intersections

Results are shown for the test subsample

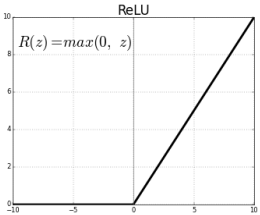
Neural network structure and hyperparameters

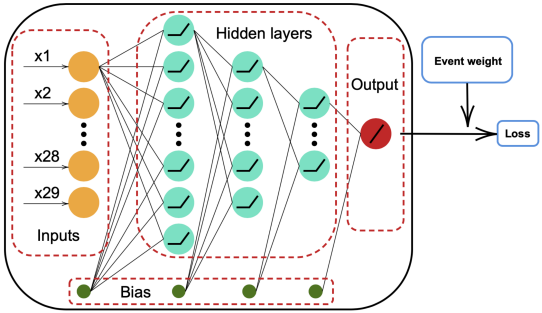
- Keras library
- Architecture:
  - 1 input layer, 3 hidden layers,1 output layer
  - Number of neurons: 29 / 128 / 64 / 32 / 1
  - Activation function: ReLU for hidden layers; linear $(\mathrm{f(y) = y})$ for output layer
- Optimizer: ADAM or NADAM
- Learning rate (lr): from 0.1 to 0.0000001
- Batch size (bs): 1, 2, 4, 8, 16 and 32
  $\Rightarrow$ Events come in batches iteratively
- Number of epochs: 100

Loss function: weighted MSE

$$\mathrm{Loss} = \frac{1}{\mathrm{N}} \cdot \sum_{\mathrm{i}=1}^{\mathrm{N}} \mathrm{W_i} \cdot (\mathrm{Xpred_i} - \mathrm{Xtrue_i})^2, 0 \leq i \leq N,$$

Xpred – prediction, Xtrue – from MC collection and $\mathrm{W_i}$ – weights from pdf of target variable





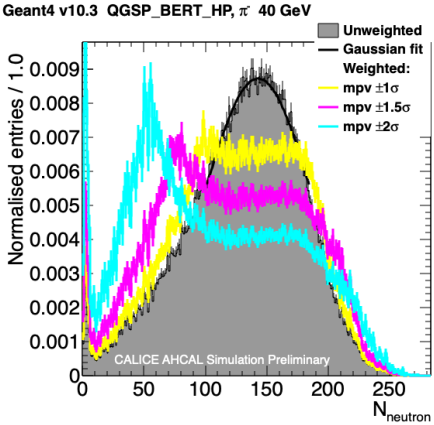
Several launches of the network with different random seed numbers (called *ANN*1... *ANN*5)

Event weights for NN training

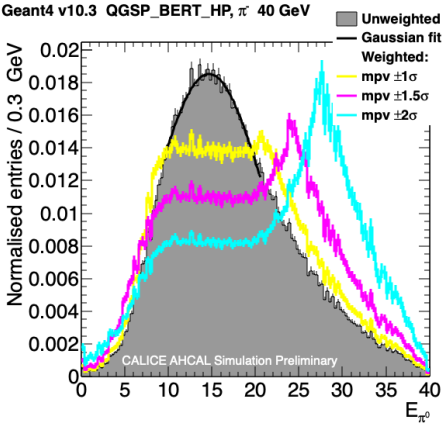
Re-weighting procedure: for i-th event $W_{\mathrm{SR,i}} = 1/\mathrm{pdf}(x_i)$, sigma range (SR) = 1.0, 1.5, 2.0

$$pdf(x) = \begin{cases} Gaus(x, m_{fit}, \sigma_{fit}), & \text{if } m_{fit} - SR \cdot \sigma_{fit} < x < m_{fit} + SR \cdot \sigma_{fit} \\ Gaus(m_{fit} + SR \cdot \sigma_{fit}, m_{fit}, \sigma_{fit}), & \text{otherwise} \end{cases}$$

Number of neutrons



Energy of neutral pions

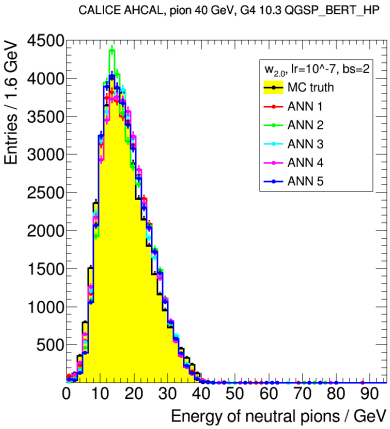


Prediction of neutral pions energy: distributions

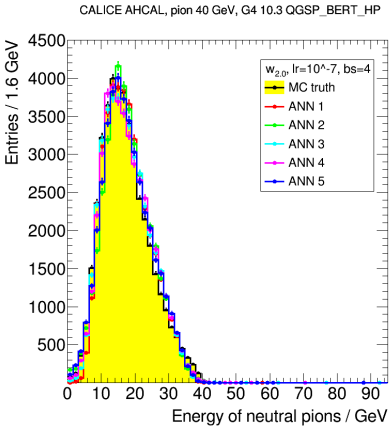
Distribution of true (MC truth) and predicted (ANN) sum of neutral pion energies

Examples of 10 trials with different random seed

$W_{2.0}$, lr $= 10^{-7}$, bs $= 2$, NADAM



$W_{2.0}$, lr $= 10^{-7}$, bs $= 4$, ADAM

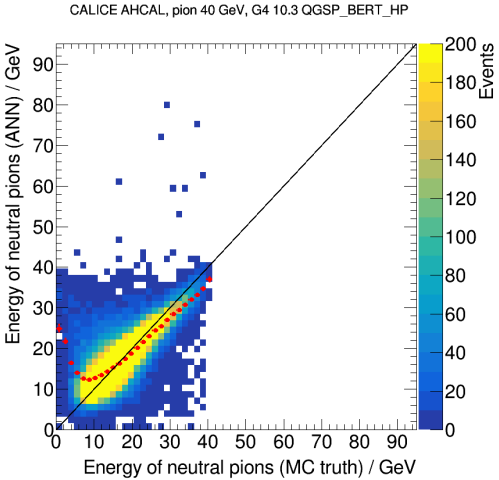


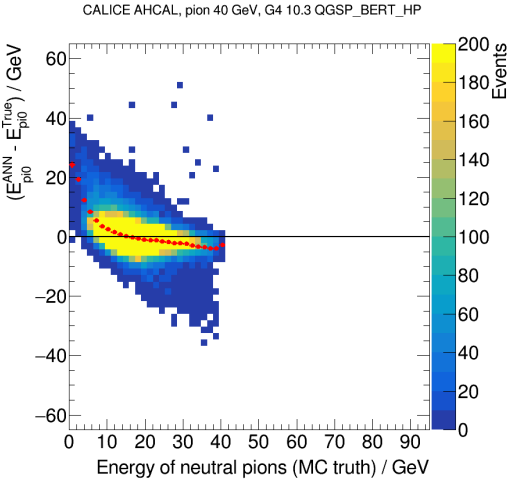
Examples of appropriate performance and well reproduced shape.

Prediction of neutral pions energy: examples of ANN vs MC truth

Red points show profile (means)

$W_{2.0}$, lr $= 10^{-7}$, bs $= 2$, NADAM, ANN5





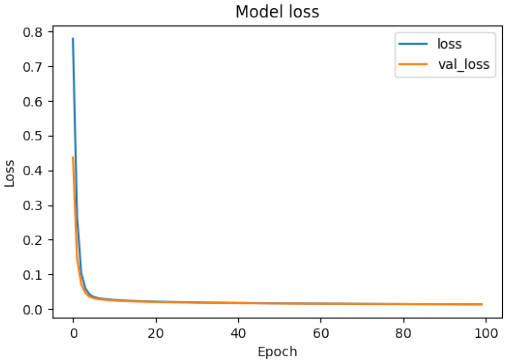
Good agreement above $E_{\pi^0} > 10$ GeV

ANN overestimates small and underestimates large E_{π^0}

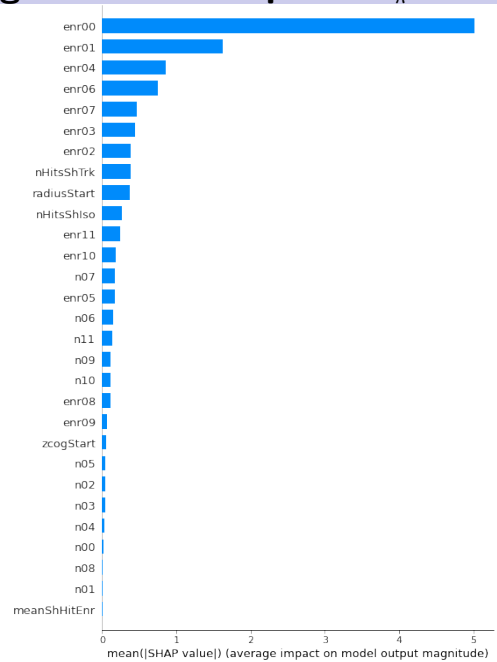
Few outliers

Convergence of loss functions and significance of inputs: E_{π^0}

$W_{2.0}$, lr $= 10^{-7}$, bs $= 2$, NADAM, ANN5



Good convergence of train and validation losses.
The most important features:
energies in central rings.

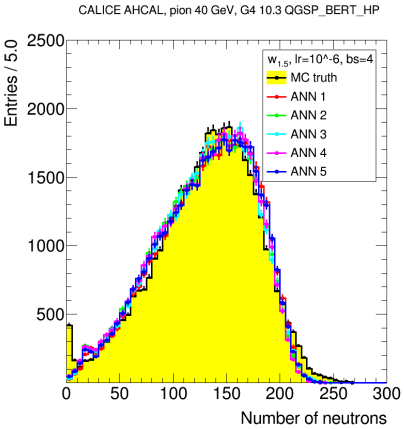


Prediction of number of neutrons: distributions

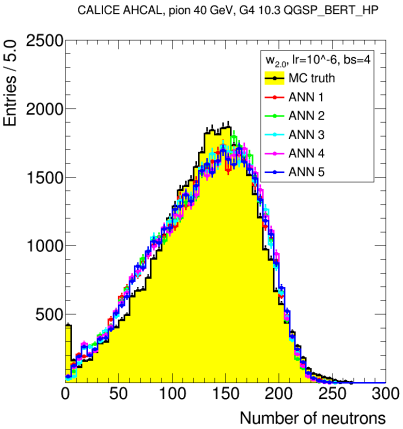
Distribution of true (MC truth) and predicted (ANN) number of neutrons in event

Examples of 10 trials with different random seed

$W_{1.5}$, lr $= 10^{-6}$, bs $= 4$, NADAM



$W_{2.0}$, lr $= 10^{-6}$, bs $= 4$, NADAM



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Prediction of number of neutrons: examples of ANN vs MC truth

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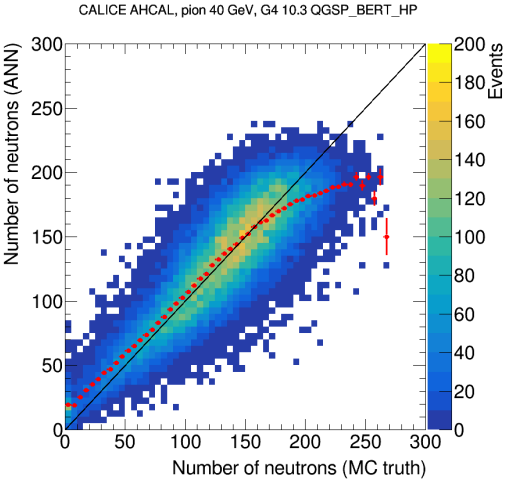
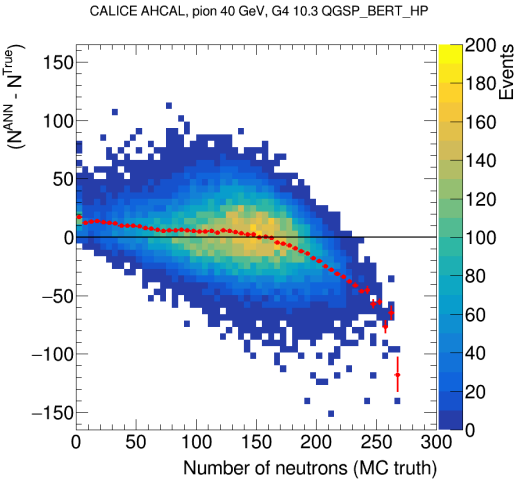


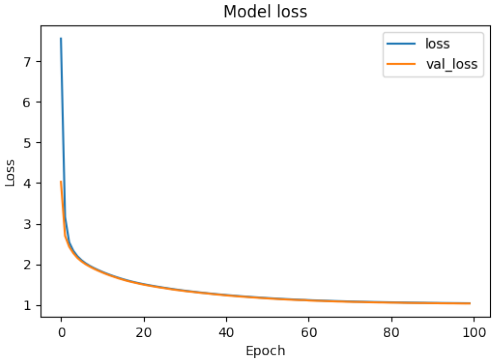
Good prediction of N_n by ANN except for tail



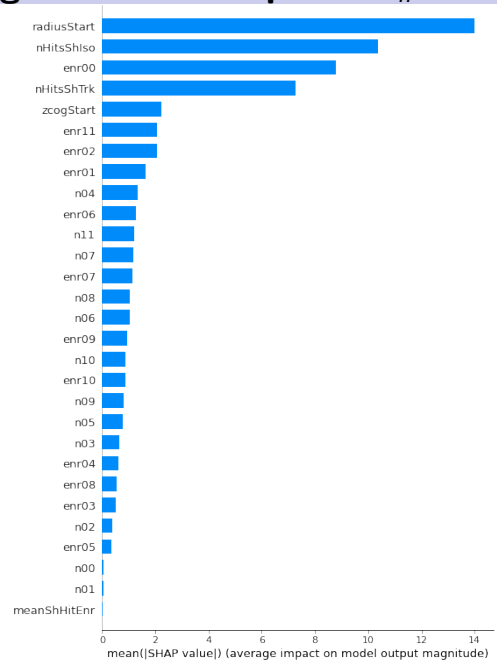
Underestimation of N_n for tail

Convergence of loss functions and significance of inputs: N_n

$W_{1.5}$, lr $= 10^{-6}$, bs $= 4$, NADAM, ANN5



Good convergence of train and validation losses.
The most important features: shower radius and number of isolated hits in a shower.



Summary

Highly granular calorimeters provide unique information about hadronic shower development.

Preliminary results

- An artificial neural network from Keras package was trained to **predict, for the first time, energy of neutral pions and number of neutrons in a hadronic shower using calorimetric observables**.
- Showers induced by simulated pions of 40 GeV in the CALICE AHCAL were studied (G4 v10.3, QGSP_BERT_HP).
- Good predictions of distributions have been achieved of energy sum of neutral pions and number of neutrons within a shower.

Plans

- Define algorithm performance
- Train models for pions with several energies in the range 10–80 GeV
- Prepare conference talk at ILCX2021 event and publication (MC only)
- Apply trained NN to data
- Prepare CALICE Analysis Note involving data