Implementation of Machine Learning Algorithms to Form Di-Muons from Off-Shell Parent Particles

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Introduction

- A Fermionic dark matter model with four muons final state is considered [1, 2]
- Signal events in this model have a topology in which the final state muons come from off-shell parent particles
- Defining a signal region in this analysis requires forming correct di-muons, i.e., paring muons that come from the same parent particle

![Feynman diagram](image)

**Figure 1:** Feynman diagram for the fermionic dark matter model, referred to as the $f_D$ model. The dark $Z$ boson ($Z_D$) provides a vector portal to the dark sector through kinetic mixing. Dark Fermions, $f_{D_1}$'s, then decay to di-muons through off-shell $Z_D$ particles and another stable dark fermion, $f_{D_2}$, that escapes detection.
Introduction

- To pair the muons into di-muons coming from same kind of parent particles, one would reconstruct the invariant mass for all possible permutations.

- Out of all combinations of muons to form di-muons, the arrangement with closest invariant mass is selected.

- This method is not applicable to our case, because the invariant dimuon masses, products of off-shell $Z_D$'s, cover a whole range of values.

- That means one could not rely on requiring two masses to be the same to assign muons correctly to dimuons.

- Alternatively, several Machine Learning (ML) algorithms are employed to achieve this goal.

- The Reconstructed (Reco) data is labeled through matching with Generated (Gen) level muons.

- Having the reco muons labeled enables us to use supervised ML algorithms to solve this problem.

- Observables associated with the di-muons are studied based on the network predictions.

- Signal region for the analysis is defined and the shape of the signal determined.
Data Generation and Processing

- Event data are generated using MadGraph5_aMC@NLO 2.6

- Hadronization and showering are simulated using Pythia8.230

- Event reconstruction is performed under CMSSW_10_2_18

- The Monte-Carlo (MC) samples consist of a scan over the $Z_D$ mass $(125 < m_{Z_D} < 200 \text{ GeV})$, as well a scan over $f_{D_1}$ mass $(5 < m_{f_{D_1}} < 55 \text{ GeV})$, for each given $Z_D$ mass. The $f_{D_2}$ mass for the time being is kept at 2 GeV across all samples

- In total 80 samples are produced, each containing $10^4$ events

- For the purpose of maximizing the number of events to be fed to the network, the selection is kept limited to requiring a pseudo-rapidity of $|\eta| < 2.4$ for each of the muons

- About 4000 events per sample survive selection after cuts are applied
Matching and Labeling

- Data are preprocessed by applying cuts to remove events with failed reconstruction and charge misidentification of final-state muons.

- Algorithm is developed to match the reco muons to their gen muon counterparts as a means to label the reco muons with their parent particles.

- The matching algorithm proceeds as follows:
  1. Angular separation ($\Delta R$) between the reconstructed gen muons and all 4 reco muons is calculated.
  2. First gen muon is sampled randomly and matched with the reco muon with the smallest $\Delta R$.
  3. The other same-charge muon is paired with the remaining reco muon of same charge.
  4. One oppositely charged gen muon is selected and matched via the minimum $\Delta R$ with the 2 remaining reco muons.
  5. Remaining reco muon is paired with gen muon.

- After this matching procedure, the permutation (order of muons) is defined as the correct permutation, and assigned a label 1.
Matching and Labeling

- Requiring that each di-muon comprises 2 oppositely charged muons, we define 2 *wrong permutations* for each event.
- Both incorrectly generated permutations are labeled 0.
- To each permutation (one correct and two wrong), we associate the event features and feed them to the network.

**Correct permutation**

```
Z_{D1}  
1  2

Z_{D2}  
3  4
```

**Incorrect permutation**

```
Z_{D1}  
3  2

Z_{D2}  
1  4
```

**Incorrect permutation**

```
Z_{D1}  
1  4

Z_{D2}  
3  2
```

Figure 2: The correct permutation and the other 2 allowed (but incorrect) permutations.
Figure 3: The $\Delta R$ between the matched reco muons to gen muons based on the developed algorithm. Most matches exhibit very low $\Delta R$ (good match). There are also events where the matches are not near perfect ($\Delta R > 0.005$; bad match). These bad events are cut.
Matched $\Delta R$

Figure 4: The $\Delta R$ between the matched reco muons and gen muons after that events with $\Delta R > 0.005$ are cut out. These events can be trusted to give us the correct parent particles for the reco muons.
Deep Neural Networks

- **Fully connected, deep, feed-Forward Neural Networks** of various topologies created using Keras [6] with a Tensorflow backend
- Data was partitioned and randomly shuffled into a 50/20/30 train/validation/test split
- Hyperparameters were manually tuned
- Final architecture selected had 9 hidden layers:

![Diagram of neural network architecture]

**Figure 5:** Final neural network architecture selected.
After many iterations of hyperparameter tuning, the best classification accuracy was achieved with:

- Features scaled to be in [0, 1]
- Batch size: 32
- Binary Cross-entropy loss function
- Adagrad [7] (Adaptive gradient algorithm) with initial learning rate $\alpha = 10^{-3}$ (with $\alpha$ reduction when validation loss plateaued for more than 10 epochs)
- 9 hidden layers with 64-1024 nodes
- Elastic net regularization (L1 penalty: $10^{-2}$, L2 penalty = $10^{-4}$)
- PReLU activation function
- 30% Dropout
- He [8] normal distribution of node weights
- Biases initialized to 0

- 67.2% test accuracy
Neural Network Results

**Figure 6:** Loss and accuracy as a function of epoch.

Figure 7: Accuracy of correct predictions for the neural network trained on MC simulated samples with $m_{Z_D} = 200$ GeV and $m_{fD_1} = 30$ GeV. Note that the performance is independent of $m_{Z_D}$ and $m_{fD_1}$. 
In an attempt to improve the accuracy of the results, we turn to boosting methods; gradient boosting in particular.

Previously gradient boosting algorithms only focused on improving impurity.

**eXtreme Gradient Boosting (XGBoost)** applies a variety of regularization techniques to avoid over-fitting [9].

Bayesian hyperparameter tuning did not show significant improvement in the scores of XGBoost compared to default hyperparameters.

Default hyperparameters are used for XGBoost here: $\gamma = 0$, $\eta = 0.3$, max depth = 6, ...
(a) XGBoost Classification error

(b) XGBoost Log-Loss scores

Figure 8: XGBoost performance with the network trained with $m_{Z_D} = 200, m_{f_{D_1}} = 30 \text{ GeV}$.
Figure 9: 2D invariant mass distributions for correctly and incorrectly paired di-muons.
Figure 10: 1D invariant mass distributions for correctly and incorrectly paired di-muons.
**Figure 11:** The Network is trained on the MC sample with the highest masses, i.e. \( m_{Z_D} = 200 \text{ [GeV]} \), \( m_{f_{D_1}} = 55 \text{ GeV} \), then the achieved model is saved and tested on the rest of the samples.
Figure 12: Accuracy of correct predictions for the neural network trained on MC simulated data with $m_{Z_D} = 200$ GeV and $m_{f_{D_1}} = 30$ GeV.
Summary and Conclusions

- MC samples generated for a dark fermionic model
- Simulated events used to form di-muons that share the same parent particle for each event
- Supervised ML algorithms, such as XGBoost and deep, feed-forward, fully connected neural networks were examined
- XGBoost shows the highest classification accuracy at $\sim 95\%$
- Neural networks with hyperparameter tuning is the second best performing network with an accuracy of $\sim 67\%$
- These models were tested on samples with different masses to ensure the model is not overfitting on a particular mass
- A model-independent behavior (across samples with different masses) is observed for both network scores
References


[3] MG/ME Development Team, MadGraph5_aMC@NLO (v.2_6_5), http://madgraph.phys.ucl.ac.be/.


[6] The Keras Development Team, Keras (v.2.3.0), https://keras.io/.


Backup
An Introduction to Neural Networks

- Artificial Neural Network (ANN) is a collection of mathematical functions (neurons) that receive $N$ inputs

- Neurons modeled on the neuron of a human brain
  - Take input “signals” along with weights and biases, pass them through an activation function

- Input data called features; in our case, kinematic variables and higher-level, computed observables (e.g., invariant mass)

- Activation function: The mathematical function of the neuron; e.g.,
  - Parametric Rectified Linear Unit (PReLU): $f(x) = \begin{cases} x, & x > 0 \\ \alpha x, & x \leq 0 \end{cases}$

- Data passes through the network (feed-forward), and at the end, the loss function value is computed

- Loss function: the function you are trying to minimize (training a neural network is just one big optimization problem); e.g.,
  - Binary cross-entropy (log-loss):
    $$L(y, \hat{y}) = -N^{-1} \sum_{i=1}^{N} y_i \cdot \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

- The data is back-propagated through the network, and the data are fed forward for another pass

- After each pass, the weights and biases input to the neurons are tuned (this is the learning part)
### An Introduction to Neural Networks

- **Optimizer**: the algorithm used for optimizing the loss function, e.g., Adagrad:

  \[ w_{s+1,i} = w_{s+1,i} - \frac{\alpha}{\sqrt{\Omega_{s,ii} + \epsilon}} \nabla L(\theta) \]

  where \( w \) are the weights, \( \alpha \) is the learning rate, \( \Omega \) is a diagonal matrix with entries representing the summed, squared gradients, and \( \epsilon \) used to prevent division by zero.

- Neural network is run for a predetermined number of **epochs** (iterations).

- Many **trainable parameters** (all of the weights, biases).

- Many **hyperparameters**: learning rate \( \alpha \), number of nodes/hidden layers, regularization methods to reduce overfitting (\( L^1, L^2 \)), dropout, etc.

- Number of nodes in output layer represent the categories (categorization problem) or coefficients (regression problem).

- Generally, data is split into **train/validation/test** datasets so network performance can be evaluated after training (the validation/test sets are data the network hasn’t “seen”).
• Overfitting occurs when the model “learns” the data too well

• Can use regularization techniques, such as the $L^1$ and $L^2$ vector norms, which penalize (constrains) weights that explode, helping network stability
  • Additional terms representing the norm of the weights added to the loss function, i.e.,

$$\hat{L} = L(y, \hat{y}) + \lambda ||w||_p$$

• Norm:

$$||w||_p = \left( \sum_{i}^{N} |w_i|^p \right)^{1/p},$$

where $p = 1, 2, \cdots, \infty$

• Dropout randomly switches a fraction of the nodes in a layer to help “shift” the learning responsibility to other nodes
An Introduction to XGBoost

- **Decision Tree**: a predictive model to go from observations about an item (represented in the branches) to conclusions about the item’s target value (represented in the leaves). Classification trees is our interest.

- A single tree work great with the data used to create them, but they are not flexible when it comes to classifying new data.

- One decision tree is prone to over-fitting.

- To reduce the risk of overfitting, models that combine many decision trees are preferred.

- **Gradient Boosting**: Combining a learning algorithm in series to achieve a strong learner from many sequentially connected weak learners. At each iteration of the gradient boosting procedure, we train a base estimator (single tree) to predict the gradient descent step. Saving these base estimators in memory is what enables us to output predictions for any future sample.

- **Regularization**: Minimum loss reduction required to make a further partition on a leaf node of the tree. The larger gamma is, the more conservative the algorithm will be.

- **eXtreme Gradient Boosting**: Previously gradient boosting models only focused on improving impurity (a measure of how often a randomly chosen element from the set would be incorrectly labeled if it was randomly labeled according to the distribution of labels in the subset.). “XGBoost” applies a variety of regularization techniques to avoid over-fitting.
Data frame

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</tr>
</tbody>
</table>

---

**Figure 13:** The data frame structure. All features do a 3 way permutations.
Feynman Diagrams

Correct permutation

Wrong permutation - scenario one

Wrong permutation - scenario two
**XGBoost Classification Report**

Table 1: Classification report

<table>
<thead>
<tr>
<th>Training classification</th>
<th>precision</th>
<th>recall</th>
<th>f1-score</th>
<th>support</th>
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</thead>
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<td>accuracy</td>
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<td></td>
<td>1.00</td>
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</tr>
<tr>
<td>macro ave</td>
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<td>7197</td>
</tr>
<tr>
<td>weighted ave</td>
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<td>1.00</td>
<td>1.00</td>
<td>7197</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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<th>precision</th>
<th>recall</th>
<th>f1-score</th>
<th>support</th>
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<td>macro ave</td>
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<tr>
<td>weighted ave</td>
<td>0.98</td>
<td>0.98</td>
<td>0.98</td>
<td>2400</td>
</tr>
</tbody>
</table>
Figure 14: XGBoost Receiver operating characteristic, ROC plot. No Skill: ROC AUC=0.500, Logistic: ROC AUC=0.999
XGBoost Hyper Parameters

- $\eta$ [default=0.3, alias: learning_rate]: Step size shrinkage used in update to prevent over-fitting. After each boosting step, we can directly get the weights of new features, and eta shrinks the feature weights to make the boosting process more conservative. Range: [0,1]

- $\gamma$ [default=0, alias: min_split_loss]: Minimum loss reduction required to make a further partition on a leaf node of the tree. The larger gamma is, the more conservative the algorithm will be. range: [0,\infty]
• **max_depth [default=6]**: Maximum depth of a tree. Increasing this value will make the model more complex and more likely to overfit. 0 is only accepted in loss guided growing policy when tree_method is set as hist or gpu_hist and it indicates no limit on depth. Beware that XGBoost aggressively consumes memory when training a deep tree. Range: \([0, \infty]\) (0 is only accepted in loss guided growing policy when tree_method is set as hist or gpu_hist)

• **min_child_weight [default=1]**: Minimum sum of instance weight (hessian) needed in a child. If the tree partition step results in a leaf node with the sum of instance weight less than min_child_weight, then the building process will give up further partitioning. In linear regression task, this simply corresponds to minimum number of instances needed to be in each node. The larger min_child_weight is, the more conservative the algorithm will be. Range: \([0, \infty]\)
**XGBoost Hyper Parameters**

- **`max_delta_step` [default=0]:** Maximum delta step we allow each leaf output to be. If the value is set to 0, it means there is no constraint. If it is set to a positive value, it can help making the update step more conservative. Usually this parameter is not needed, but it might help in logistic regression when class is extremely imbalanced. Set it to value of 1-10 might help control the update. Range: \([0, \infty)\]

- **`subsample` [default=1]:** Subsample ratio of the training instances. Setting it to 0.5 means that XGBoost would randomly sample half of the training data prior to growing trees. and this will prevent overfitting. Subsampling will occur once in every boosting iteration. Range: \((0,1]\)

- **`sampling_method` [default= uniform]:** The method to use to sample the training instances. uniform: each training instance has an equal probability of being selected. Typically set subsample \(\approx 0.5\) for good results.
**XGBoost Hyper Parameters**

- **gradient_based**: the selection probability for each training instance is proportional to the regularized absolute value of gradients. Subsample may be set to as low as 0.1 without loss of model accuracy. Note that this sampling method is only supported when tree_method is set to gpu_hist; other tree methods only support uniform sampling.

- **colsample_bytree, colsample_bylevel, colsample_bynode**
  
  [default=1]: This is a family of parameters for subsampling of columns. All colsample_by* parameters have a range of (0, 1], the default value of 1, and specify the fraction of columns to be subsampled.

  - **colsample_bytree** is the subsample ratio of columns when constructing each tree. Subsampling occurs once for every tree constructed.

  - **colsample_bylevel** is the subsample ratio of columns for each level. Subsampling occurs once for every new depth level reached in a tree. Columns are subsampled from the set of columns chosen for the current tree.
XGBoost Hyper Parameters

- **colsample_bynode** is the subsample ratio of columns for each node (split). Subsampling occurs once every time a new split is evaluated. Columns are subsampled from the set of columns chosen for the current level.

- **colsample_by* parameters** work cumulatively. For instance, the combination 'colsample_bytree':0.5, 'colsample_bylevel':0.5, 'colsample_bynode':0.5 with 64 features will leave 8 features to choose from at each split.

- On Python interface, when using hist, gpu_hist or exact tree method, one can set the **feature_weights** for DMatrix to define the probability of each feature being selected when using column sampling. There’s a similar parameter for fit method in sklearn interface.

- **λ [default=1, alias: reg_λ]:** L2 regularization term on weights. Increasing this value will make model more conservative.

- **α [default=0, alias: reg_α]:** L1 regularization term on weights. Increasing this value will make model more conservative.