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XAI FOR ML JET TAGGERS

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INTRODUCTION
- Explain ML decisions of a jet classifier using expert augmented (XAUG) variables
- General method: provide XAUG inputs to a jet tagging network, apply LRP to network and compare results to same network without XAUG vars.
- Due to a conservation of relevance, the backwards propagation process does not alter the prediction

- LRP attributes the entirety of the network’s decision to the inputs, which can be visualized as a heat map for images
TOY MODEL
Toy events simulated to mimic particle level events with 1 jet consisting of 20 particles, divided evenly between 2 subjets.

- Goal is to have a small number of variables capture all the information in the event.
- The $z$ and $\theta$ ($\Delta R$) values are sampled from a normal distribution for "signal-like" images and from exponential distribution for "background-like" images.
Architecture inspired by DeepAK8 jet tagging algorithm
More relevance is given along the $\phi$ axis in the signal images.
TOY 2DCNN RESULTS

- **Mean Normalized Relevance**
  - Find feature with max absolute LRP score and divide all scores by this max value
  - For each image, sum absolute value of normalized pixels to get a single number for each image
  - Average absolute relevance scores across all events for each feature
Profile plots show the relevances vs the corresponding input variables.

For some profiles, relevance appears to reflect input distribution, but other don’t — networks’ decision boundaries live in a higher dimensional space.
Darker markers correspond to higher relevance scores.

Sharp gradient shows decision boundary for these variables.

Differences in boundary shape show how trainings vary.
Most relevant features are same as 2DCNN.

Error bars show standard deviation of relevance after multiple trainings.

More robust "substructure" within relevance of the top two variables.
Simulated with pythia8, SM ZZ and QCD

- AK8 jets from fastjet
- pT > 200 GeV
- mMDT from fastjet-contrib
  - z = 0.1, β = 0
- Preprocessing for images: rotation and scaling so that lower pT subjet is always at (0,-1), and normalize inputs w.r.t. jet pT, parity flip
Use same network structures as Toy Model, replacing inputs with equivalent counterparts.
LRP HEATMAPS

Signal is given mostly positive relevance, primarily along $\phi$ axis.

Background is given mostly negative relevance, and is more dispersed.
Darker markers correspond to higher abs. relevance scores.

Decision boundaries not as clear as toy case.
CONCLUSIONS

- Introducing XAUG variables and performing LRP can shed light on network decisions and relevant subspaces in the training.
- XAUG variables can be used to boost classification performance.
- XAUG variables can capture the information of lower level networks entirely, and a set of XAUG variables can replace long lists of particle-level information while producing comparable network performance.
- Use of these techniques together can be used to quantify numerical uncertainty in training of DNNs.
Machine Learning (ML) is commonly used for classification of boosted jets

- Convolutional Neural Networks (CNNs) take greyscale jet images as inputs
- A special case of the CNN is a 1-dimensional CNN which takes list-like input
- Decision-making process of the networks is not well understood

**Fig 1: Greyscale jet image**

MOTIVATION

- Most ML models behave as black boxes
- Augment the inputs to various types of jet classifying NNs with expert variables
- Extract classifying information using Layerwise Relevance Propogation (LRP)
- Understand what subset of information from the inputs and expert variables is relevant to the NN
DNN FORWARD PROPAGATION

\[ z_j = \sum_i x_i w_i + b \]
DNN FORWARD PROPAGATION

\[ z_j = \sum_i x_i w_i + b \]
DNN FORWARD PROPAGATION

\[ z_1 = x_1 w_1 + x_2 w_2 + x_3 w_3 + b \]
DNN FORWARD PROPAGATION
Want to ensure that predictions are supported by meaningful patterns in the data.
LRP is one technique that can be used to tease out if the networks learned patterns are following the intended categorisation.
LRP PROPAGATION RULES

- **LRP-z:**
  - Redistributes the relevance in proportion to the contributions to the neuron activation.
  - Gradient $\times$ Input $\rightarrow$ Noisy

  \[ R_j = \sum_k \frac{a_j w_{jk}}{\sum_{0,j} a_j w_{jk}} R_k \]

- **LRP-$\epsilon$:**
  - $\epsilon$ absorbs some relevance for weak and/or contradictory contributions.
  - For large $\epsilon$ only salient explanation factors survive the absorption $\rightarrow$ Less Noisy

  \[ R_j = \sum_k \frac{a_j w_{jk}}{\epsilon + \sum_{0,j} a_j w_{jk}} R_k \]

- **LRP-$\alpha \beta$:**
  - Limiting effect on how large positive and negative relevance can grow $\rightarrow$ Stable Explanations
  - $\alpha(\beta)$ controls by how much positive(negative) contributions are favored.

  \[ R_j = \sum_k \left( \alpha \frac{(a_j w_{jk})^+}{\sum_{0,j} (a_j w_{jk})^+} - \beta \frac{(a_j w_{jk})^-}{\sum_{0,j} (a_j w_{jk})^-} \right) R_k \]
TOY MODEL

Toy Model $z$ Distribution

Toy Model $\theta$ Distribution

Toy Model $\phi_1$ Distribution

Toy Model $\phi_{1,\text{hll}}$ Distribution

Toy Model $\eta$ Distribution

Toy Model $\alpha_1$ Distribution

Toy Model $\delta_{1,\text{hll}}$ Distribution
1. Cut on softdrop mass: keep jets with $m_{SD}$ 50-150 GeV

2. Numerical rescaling
   1. Rebin outliers to $mean + 3(\text{std})$ and $mean - 3(\text{std})$
   2. Input distributions are then rescaled from 0 to 1:
      $$\frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$
Profiles do not show a clear decision boundary, prompting the creation higher dimensional plots.
## Particle List Inputs

<table>
<thead>
<tr>
<th>Variable</th>
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<tbody>
<tr>
<td>$\log(p_T)$</td>
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<tr>
<td>$\log(p_T/p_{T_{jet1}})$</td>
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<td>$\log(E)$</td>
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<td>$</td>
</tr>
<tr>
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<tr>
<td>$\Delta \eta(jet)$</td>
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<td>$d_{xy}$</td>
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