Summer 2024 IRIS-HEP Fellowship Proposal: Towards Differentiable Jet Clustering

Nishank Gite
University of California, Berkeley

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Jet clustering algorithms play a crucial role in the field of high-energy physics as they aid in the interpretation of data obtained from particle collisions. However, the existing methodologies encounter certain limitations due to their non-differentiable nature. These limitations arise from the discrete decision processes employed, which are inherently unsuitable for gradient-based optimization. This proposal presents an approach to redefine jet clustering algorithms, making them differentiable. This advancement will enable the integration of jet clustering into larger gradient optimized systems, such as into neural networks or design optimization pipelines.

Traditional methods for jet clustering, like the anti-k_t algorithm, rely hard minimum distance selections that are non-differentiable because of their discrete characteristics. [2] This lack of differentiability hinders the application of modern computational methods that depend on gradient descent for optimization. The ability to differentiate is essential for incorporating jet clustering into neural network frameworks or gradient-based optimization pipelines. The primary objective of this project is to create a differentiable jet clustering framework that enhances the clustering procedure through a continuous, gradient-oriented learning approach.

Our strategy involves transitioning from deterministic to probabilistic clustering by establishing the likelihood of particle merges based on a distance metric. This enables us to convert these decisions into a probabilistic space. Subsequently, we can compute the gradient of this expectation with respect to the model's parameters using stochastic gradient estimation techniques. To achieve this, we will employ Gumbel-Softmax functions, which allow us to transform distance metrics into probabilities that can be smoothly adjusted and differentiated. By utilizing Gumbel distributions, we introduce noise to the softmax probabilities, ensuring differentiability during sampling. [1] This approach facilitates the computation of gradients, even when selecting specific clustering configurations, which is crucial for effective backpropagation. As a result, down stream optimization objectives defined over expectations of jet properties can subsequently be optimised with respect to the inputs to, or parameters of, the jet clustering algorithm using gradient based methods.

My extensive experience in jet physics, particularly in optimizing jet tagging models as demonstrated in my senior honors thesis, has turned this project into a natural progression, focusing on enhancing the foundational aspect of jet physics by improving jet data creation. With nearly 3 years of involvement in machine learning applications in particle physics within the ATLAS collaboration, I am well-equipped to lead this innovative initiative. By combining my technical expertise and theoretical understanding, I aim to address a crucial research gap. I am fortunate to have the guidance of Dr. Michael Aaron Kagan from SLAC and Professor Lukas Alexander Heinrich from the Technical University of Munich, with whom I will have regular weekly meetings for mentorship.

The expected timeline of this project is as follows:

- **Weeks 1-2:** Comprehensive review of existing jet clustering algorithms and current implementations. Study the mathematical foundations relevant to differentiable programming and probabilistic modeling.
- **Weeks 3-5:** Prototype development with current jet clustering algorithms, adapting them to include probabilistic decision metrics.
- **Weeks 6-8:** Implementation of the Gumbel-Softmax function and development of the framework for computing expected values of the clustering configurations.

- **Weeks 9-10:** Integration of the developed models into a gradient-based optimization pipeline, enabling backpropagation and automatic differentiation.
- **Weeks 11-12:** Systematic studies of the gradient-based optimization pipeline and preparation of a detailed research paper documenting the findings and methodologies.

This endeavor holds the potential to significantly advance the realm of jet physics through the introduction of a novel approach to jet clustering. Embracing a differentiable framework will embed jet clustering within the wider scope of machine learning and artificial intelligence, thereby paving the way for fresh opportunities in both research and practical applications within the domain of particle physics.

References

[1] Yang, G., et al. "Incorporating Gumbel-Softmax into Probabilistic Graph Models for Differentiable Learning." *arXiv preprint arXiv:2010.04838*, 2020. Available: `https://arxiv.org/abs/2010.04838`

[2] Cacciari, M., Salam, G. P., and Soyez, G. "The Anti-k_t Jet Clustering Algorithm." *Journal of High Energy Physics, Gravitation and Cosmology*, vol. 73, Article 2480, 2013. Available: `https://arxiv.org/abs/1304.2394`