In this paper, we present a cutting-edge approach that combines Graph Neural Networks (GNNs) with AutoML for reconstructing ground-based cosmic ray (CR) observational data. Our novel method accurately estimates primary cosmic ray energy and enhances proton/gamma identification. We have achieved convincing results by using full Monte Carlo simulation data to simulate the Tibet ASgamma experiment (Tibet III+MD). By utilizing the powerful functions of AutoML and GNNs, our integrated approach achieves a significant improvement of 31% energy resolution in data reconstruction above 100 TeV, surpassing the performance of traditional methods in reconstructing the primary energy and arriving direction of the particles. Additionally, our method effectively reduces the cosmic ray background by 30% compared to traditional methods, while preserving the crucial gamma events. The outstanding accuracy of our GNN-based energy reconstruction is further amplified through AutoML, which enables the assimilation of critical information, such as air shower size, secondary cosmic ray lateral distributions, density distributions on the detector, core position, zenith angle distributions, and more. Beyond cosmic ray observation, our versatile machine learning approach holds promise for tackling a wide range of particle physics and astrophysics challenges, making substantial contributions to these fields and paving the way for exciting future advancements.
1. Introduction

The Tibet ASgamma experiment, positioned at 4300 meters altitude in Yangbajing, Tibet, China, covering a total area of 65,700 m$^2$ [1]. It consists of three sub-arrays: Tibet air-shower array (Tibet-III), air-shower-core detector-grid (YAC-II), and underwater Cherenkov muon detector array (MD) covering a total area of 3,400 m$^2$ [2, 3].

![Figure 1: Schematic view of (Tibet-III+MD) array(left) and a MD detector structure(right).](image)

Machine learning (ML) has transformed particle physics, aiding data collection, physics object reconstruction, identification, and new physics searches [4]. Traditional ML methods depended on manually derived high-level features and algorithms like decision trees, support vector machines, and shallow neural networks. However, advancements, particularly in deep neural networks like CNNs, RNNs, and GNNs, leverage raw detector data directly [5], bypassing laborious feature extraction and yielding superior outcomes.

Graph neural networks, especially, have made significant strides, finding applications across domains such as recommendation systems, medical biology, risk control, and optimization.

With a profusion of ML techniques, selecting the right methods and optimal hyperparameters can be time-intensive. AutoML emerges as a robust, efficient solution for this challenge, ensuring fault tolerance.

The hexagonal detector configuration of the Tibet ASgamma experiment introduces internal and external variations, rendering direct matrix representations challenging. Furthermore, data translation symmetry is imperfect, hindering the performance of convolutional neural networks. However, graph neural networks excel in non-Euclidean data spaces. This article proposes utilizing GNNs for feature extraction and combining their outcomes with traditionally derived features. Event reconstruction and identification will be achieved through the autoML approach.

2. Graph Neural Network

Graph Neural Networks (GNNs) excel at capturing intricate relationships in diverse datasets, such as social networks, maps, and knowledge graphs. In the realm of particle physics, graph representations offer advantages over traditional matrices, adeptly handling variable-sized data...
without unnecessary zero-padding. These graphs effectively manage sparse, heterogeneous detector
data that may not seamlessly translate into images[6].

Formally, a graph $G = (u, V, E)$ is defined with $N_v$ vertices and $N_e$ edges. $u$ denotes overall
graph features, $V = v_i$ comprises node sets ($v_i$ represents the i-th node’s features), and $E = e_{ij}$
signifies edges ($e_{ij}$ holds edge features between the i-th and j-th nodes).

For graph neural networks, the computation in the $(l+1)^{th}$ iteration of graph $G = (u^{l+1}, V^{l+1}, E^{l+1})$
is as follows:

Edge feature update: $e^{l+1}_{ij} = \phi^e(v^l_i, v^l_j, e^{l-1}_{ij})$, where $\phi^e$ aggregates information from adjacent
nodes via edges. Node feature update: $v^{l+1}_i = \rho(e^{l+1}_{ij})$ for all $j \in N_i$, with $\rho$ processing aggregated
edge features. Global graph feature update: $u^{l+1} = \phi^v(v^{l+1}_i, v^l_i, u^{l+1})$, as $\phi^v$ updates node and global
graph features. Choice of $\phi^e$, $\phi^v$, and $\rho$ yields varied GNN structures, accommodating diverse
patterns and data dependencies. These operations iteratively equip GNNs to learn and represent
complex relationships within graph-structured data, effectively addressing tasks in particle physics
and beyond[6–8].

3. Automated Machine Learning

Automated Machine Learning (AutoML) simplifies model selection, configuration, and optimization, streamlining the machine learning process. Unlike traditional methods that demand expert intervention, AutoML empowers non-experts to harness machine learning proficiently[9].

AutoML aims to automate common tasks like data preprocessing, feature engineering, model
selection, hyperparameter tuning, and ensemble creation. By utilizing AutoML tools, manual effort
is minimized, expediting the development of high-performing models. These tools automatically
identify suitable models, fine-tune hyperparameters, and enhance performance through model
fusion[10, 11].

4. Monte Carlo simulation

The extensive air showers (EAS) development in the atmosphere and the response in the
Tibet hybrid experiment array have been comprehensively studied using full Monte Carlo (MC)
simulation. The widely-used simulation code, CORSIKA[12], is employed to generate both gamma
events and cosmic ray events. And all detector responses are calculated using Geant4[13].

For the gamma events, the primary particle’s energy ranges from 300 GeV to 100 PeV, with a
spectral index of $-\frac{1}{2}$. In total, $10^9$ gamma events are generated to capture a broad range of energy
levels.

Regarding the primary cosmic-ray composition model, the model spectrum proposed by M.
Shibata et al. [14] is adopted to determine their chemical composition and energy spectrum.
The low-energy hadronic interactions are simulated using FLUKA [15], while the high-energy
interactions are modeled using EPOS LHC [16]. A significant number of $4 \times 10^9$ cosmic ray events
are generated to ensure robust and statistically significant results.

3
Table 1: Parameters used in the CORSIKA air shower simulation

<table>
<thead>
<tr>
<th>Primary type</th>
<th>Spectral</th>
<th>Energy range (TeV)</th>
<th>Events</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gamma rays</td>
<td>Power law with index -2</td>
<td>$0.3 \times 10^3$</td>
<td>$10^9$</td>
</tr>
<tr>
<td>Cosmic rays</td>
<td>M. Shibata et al. [14]</td>
<td>$0.3 \times 10^5$</td>
<td>$4 \times 10^9$</td>
</tr>
</tbody>
</table>

5. Method

The cut condition employed closely follows the approach used in the Crab study [17], with the omission of $N_\mu$ cut condition and the removal of age cut condition to increase the dataset. The traditional method refers to the method in ref [17, 18].

Figure 2: Algorithm flowchart

The algorithm flowchart for our method showed in Figure 2. First, the Monte Carlo simulation data is transformed into graph-structured data based on the relative positions of the detectors. The detector data are converted into graph data, and a GNN is utilized for feature extraction from the graph data. In the case of data reconstruction, two additional fully connected layers are added after the pooling layer of GNN. The extracted features are combined with the features obtained from the Monte Carlo simulation data using traditional method. Subsequently, the combined features are fed into an autoML system to obtain the reconstruction or discrimination results.

6. Result

6.1 Event Reconstruction

For reconstructing (Tibet III+MD) raw experimental data, it is discussed in two parts, angle-resolved and energy-resolved. The angle resolution and energy resolution obtained in this work are compared with the traditional method at different energies.

Comparing the angular resolution obtained by this work with the traditional method, as shown in the figure 3, the angular resolution obtained by this work is better than the traditional method in each energy range.
For the reconstruction of energy, it can be seen in the figure.4 that compared with the traditional method, the image obtained by the reconstruction of this work is narrower, and as can be seen in the table.2, the energy resolution we obtained is at different energies and different zenith angles are superior to traditional methods. And we achieve a 31% improvement in energy resolution for event about 100 TeV in all zenith angle, compared to traditional methods.

![Figure 3: Comparison of arrival directions between traditional method and this work](image)

**Table 2:** Comparison of energy resolution between traditional method and this work

<table>
<thead>
<tr>
<th>Energy</th>
<th>about 50 TeV</th>
<th>about 100 TeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>sec(theta)</td>
<td>1.0-1.1</td>
<td>1.1-1.3</td>
</tr>
<tr>
<td>Traditional method</td>
<td>0.33</td>
<td>0.47</td>
</tr>
<tr>
<td>This work</td>
<td>0.22</td>
<td>0.30</td>
</tr>
</tbody>
</table>

![Figure 4: Comparison of energy fitting results between traditional method and this work.](image)
6.2 Gamma/Proton Identification

For different energy ranges, we define Signal-to-Noise Ratio (SNR) and use the results from this work and traditional methods to calculate the optimal cut conditions that maximize SNR. Then, we compare the SNR values across all energy ranges. Gamma/Proton identification of this work is better than our traditional methods at each energy bin, especially for high energy ranges. At about 100 TeV, this work achieves a third higher SNR than conventional methods, roughly reducing the cosmic ray background by 30% improvement compare to traditional methods, while preserving the same gamma events.

![Figure 5: Comparison of SNR between traditional method and this work.]

7. Discussion

The integration of Graph Neural Networks (GNNs) and Automated Machine Learning (AutoML) holds remarkable potential for enhancing event reconstruction and identification in the Tibet ASgamma experiment. This innovative fusion promises significant improvements in processing cosmic ray (CR) observational data.

By harnessing the capabilities of GNNs and AutoML, our combined approach achieves a substantial 31% enhancement compare to traditional methods in energy resolution for data reconstruction beyond 100 TeV. This outperforms conventional techniques in primary energy reconstruction and particle arrival direction estimation. Notably, our method reduces cosmic ray background by 30% while effectively preserving essential gamma events compare to traditional methods. The success owes much to GNN-based energy reconstruction, further enhanced by AutoML’s ability to assimilate critical details like air shower size, secondary cosmic ray distributions, detector density patterns, core position, zenith angles, and more.

GNNs excel in handling complex relationships within graph-structured data, as illustrated by the hexagonal detector configuration of the Tibet ASgamma experiment. This sets them apart from traditional matrix representations and bridges gaps left by convolutional neural networks.

Moreover, AutoML emerges as a robust tool to navigate the array of machine learning techniques available. It simplifies model selection, configuration, and optimization, making machine learning more accessible and efficient for non-experts. Automation streamlines data preprocessing, feature
engineering, model selection, hyperparameter tuning, and ensemble creation, reducing manual intervention and accelerating model development.

The success achieved in the Tibet ASgamma experiment extends beyond, offering insights for particle physics and astrophysics. The combined power of GNNs and AutoML demonstrated here lays the groundwork for future advances in a variety of research domains, showcasing their potential for addressing the challenges of event reconstruction and identification.

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References


