Google Summer of Code

ML
4
SCI

Quantum Invariant and Equivariant Graph Neural Networks for HEP Analysis

Google Summer of Code (GSOC) Contributor under the Machine Learning for Science (ML4SCI) Organization

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Department of Physics

October 23, 2023

Dataset [7]

Graphically Structured Data $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$

$$\begin{matrix} (\alpha,\mathbf{1},\mathbf{1}) & (\alpha,\mathbf{2},\mathbf{1}) & \cdots & (\alpha,\mathbf{m}_\alpha,\mathbf{1}) \\ (\alpha,\mathbf{1},\mathbf{2}) & (\alpha,\mathbf{2},\mathbf{2}) & \cdots & (\alpha,\mathbf{m}_\alpha,\mathbf{2}) \\ \vdots & \vdots & \ddots & \vdots \\ & & & (\alpha,\mathbf{m}_\alpha,\mathbf{l}) \end{matrix}$$

$$\begin{matrix} (\mathbf{2},\mathbf{1},\mathbf{1}) & (\mathbf{2},\mathbf{2},\mathbf{1}) & \cdots & (\mathbf{2},\mathbf{m_2},\mathbf{1}) \\ (\mathbf{2},\mathbf{1},\mathbf{2}) & (\mathbf{2},\mathbf{2},\mathbf{2}) & \cdots & (\mathbf{2},\mathbf{m_2},\mathbf{2}) \\ \vdots & \vdots & \ddots & \vdots \\ & & & (\mathbf{2},\mathbf{m_2},\mathbf{l}) \end{matrix}$$

$$\underbrace{\begin{matrix} (\mathbf{1},\mathbf{1},\mathbf{1}) & (\mathbf{1},\mathbf{2},\mathbf{1}) & \cdots & (\mathbf{1},\mathbf{m_1},\mathbf{1}) \\ (\mathbf{1},\mathbf{1},\mathbf{2}) & (\mathbf{1},\mathbf{2},\mathbf{2}) & \cdots & (\mathbf{1},\mathbf{m_1},\mathbf{2}) \\ \vdots & \vdots & \ddots & \vdots \\ (\mathbf{1},\mathbf{1},\mathbf{l}) & (\mathbf{1},\mathbf{2},\mathbf{l}) & \cdots & (\mathbf{1},\mathbf{m_1},\mathbf{l}) \end{matrix}}$$

(Jet (*n*), Multiplicity (*m*), Feature (*l*))

Dataset [7]

Graphically Structured Data $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$

$$
\begin{pmatrix}
(\alpha,1,1) & (\alpha,2,1) & \cdots & (\alpha,m_\alpha,1) \\
(\alpha,1,2) & (\alpha,2,2) & \cdots & (\alpha,m_\alpha,2) \\
\vdots & \vdots & \ddots & \vdots \\
 & & & (\alpha,m_\alpha,l)
\end{pmatrix}
$$

$$
\begin{pmatrix}
(2,1,1) & (2,2,1) & \cdots & (2,m_2,1) \\
(2,1,2) & (2,2,2) & \cdots & (2,m_2,2) \\
\vdots & \vdots & \ddots & \vdots \\
 & & & (2,m_2,l)
\end{pmatrix}
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\underbrace{\begin{pmatrix}
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(1,1,l) & (1,2,l) & \cdots & (1,m_1,l)
\end{pmatrix}}
$$

(Jet (n), Multiplicity (m), Feature (l))

Multiplicity $(m) \equiv$ Nodes with Features (l)

$$\boxed{x_\alpha^{(il)} \in \{p_T, \eta, \phi, m_p\}} \tag{1}$$

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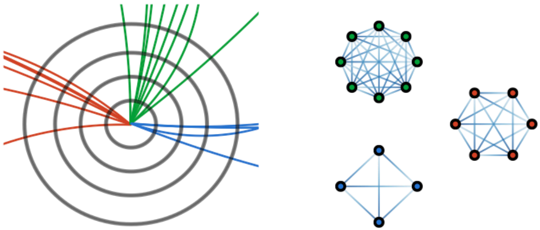
(Jet (n), Multiplicity (m), Feature (l))

Multiplicity $(m) \equiv$ Nodes with Features (l)

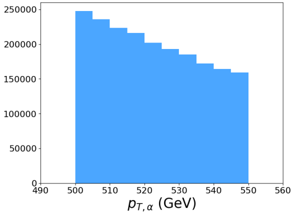
$$\boxed{x_\alpha^{(il)} \in \{p_T, \eta, \phi, m_p\}} \quad (1)$$

Jet $(n) \equiv$ Graph with Labels (not shown)

$$\boxed{y_n \in \{0,1\} \text{ for Binary Classification}} \quad (2)$$



Data Distributions & Feature Engineering @ ML4SCI



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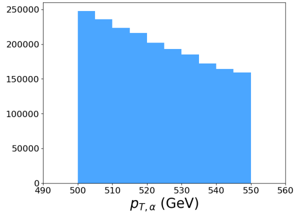

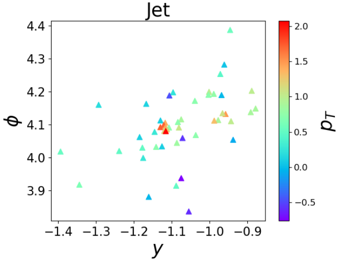

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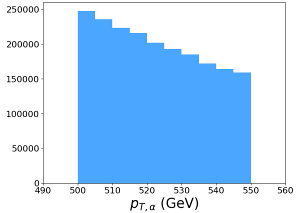
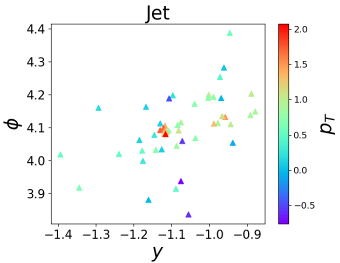
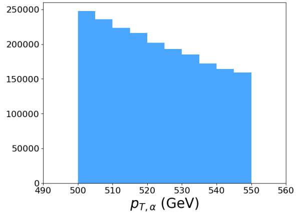


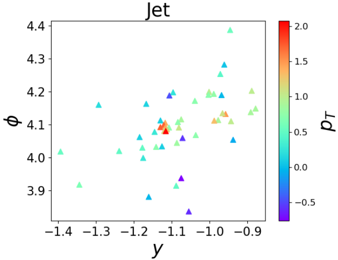


Feature set $h_\alpha^{(il)}$ with $l = 0, 1, 2, \ldots, 7$:

$$
\begin{aligned}
h_\alpha^{(il)} \equiv \{ p_{T,\alpha}^{(i)}, y_\alpha^{(i)}, \phi_\alpha^{(i)},\\
m_{T,\alpha}^{(i)} &= \sqrt{m_\alpha^{(i)2} + p_{T,\alpha}^{(i)2}},\\
E_\alpha^{(i)} &= m_{T,\alpha}^{(i)} \cosh(y_\alpha^{(i)}),\\
p_{x,\alpha}^{(i)} &= p_{T,\alpha}^{(i)} \cos(\phi_\alpha^{(i)}),\\
p_{y,\alpha}^{(i)} &= p_{T,\alpha}^{(i)} \sin(\phi_\alpha^{(i)}),\\
p_{z,\alpha}^{(i)} &= m_{T,ij} \sinh(y_\alpha^{(i)}) \}
\end{aligned}
$$

Data Distributions & Feature Engineering @ ML4SCI





Feature set $h_\alpha^{(il)}$ with $l = 0, 1, 2, \ldots, 7$:

$$h_\alpha^{(il)} \equiv \{p_{T,\alpha}^{(i)}, y_\alpha^{(i)}, \phi_\alpha^{(i)},$$
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$$p_{z,\alpha}^{(i)} = m_{T,ij} \sinh(y_\alpha^{(i)})\}$$

Edge Connections a_{ij}

$$\Delta R_\alpha^{(ij)} = \sqrt{\left(\phi_\alpha^{(i)} - \phi_\alpha^{(j)}\right)^2 + \left(y_\alpha^{(i)} - y_\alpha^{(j)}\right)^2}$$

Invariance vs. Equivariance [6, 5]

@

Invariance

Invariance

A function φ is invairant with respect to a group G transformation $g \in T_g \subset G$ if

$$\varphi(g \cdot x) = \varphi(x) \tag{4}$$

best for

$\downarrow$

Invariance vs. Equivariance [6, 5]

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Invariance

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A function φ is invairant with respect to a group G transformation $g \in T_g \subset G$ if

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best for

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Input Embedding

Classical	**Quantum**
$\mathbf{m}_{ij}(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}) \rightarrow$	$\mathcal{U}_{ij}(x_i, x_j) \rightarrow$
$\mathbf{m}_{ij}(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}, \boxed{\lvert\mathbf{x}_i - \mathbf{x}_j\rvert})$	$\mathcal{U}_{ij}(\boxed{\lvert\mathbf{x}_i - \mathbf{x}_j\rvert})$

Invariance vs. Equivariance [6, 5]

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Input Embedding

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$\mathbf{m}_{ij}(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}) \rightarrow$

$\mathbf{m}_{ij}(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}, \boxed{|\mathbf{x}_i - \mathbf{x_j}|})$

Quantum

$\mathcal{U}_{ij}(x_i, x_j) \rightarrow$

$\mathcal{U}_{ij}(\boxed{|\mathbf{x}_i - \mathbf{x_j}|})$

Equivariance

Equivariance

A function φ is equivariant with respect to group G, G' transformations $g \in T_g \subset G, g' \in S_g \subset G'$ if

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best for

$\downarrow$

Invariance vs. Equivariance [6, 5]

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A function φ is invairant with respect to a group G transformation $g \in T_g \subset G$ if

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Layer Structure

Classical

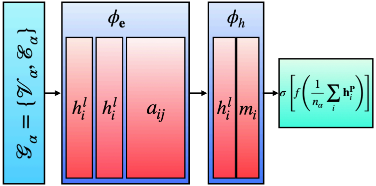
$$gx_i^l \rightarrow$$
$$gx_i^l + C\sum_{j \neq i}(gx_i^l - gx_j^l)\phi_x(\mathbf{m}_{ij})$$

Quantum

$$\mathcal{U}(gx) \rightarrow$$
$$\mathcal{U}_g \mathcal{U}(x) \mathcal{U}_g^{\dagger}$$

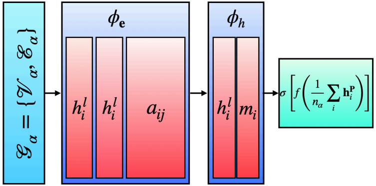
Model Architectures

GNN

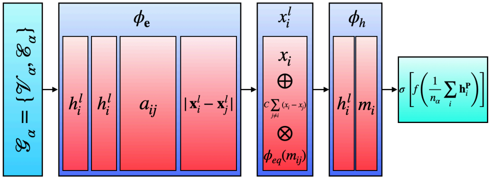


Model Architectures

GNN

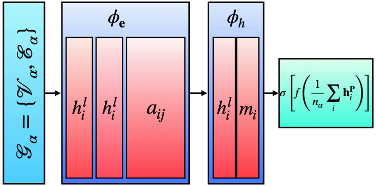


EGNN



Model Architectures

GNN



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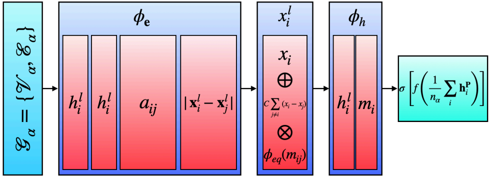
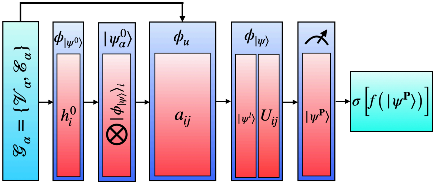
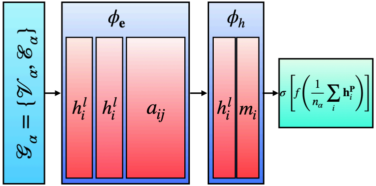


QGNN



Model Architectures

GNN



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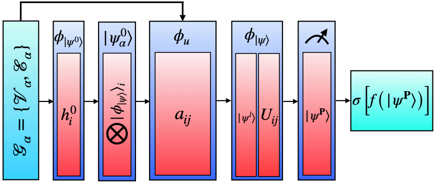
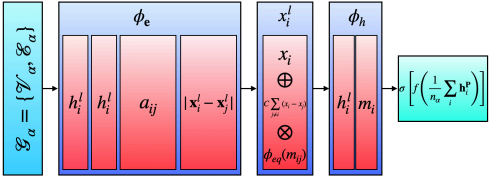
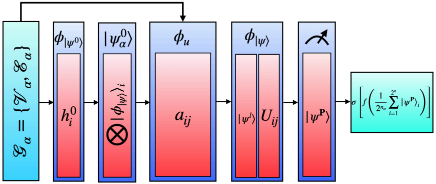


EGNN



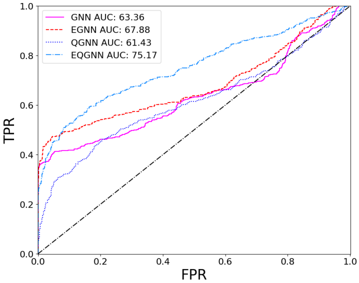
EQGNN

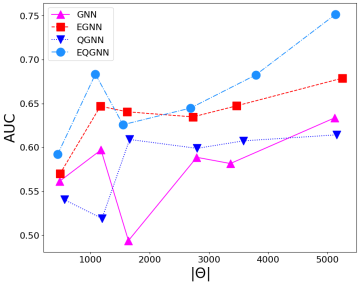


Results

Table: Metric comparison between the classical and quantum graph models.

Model	$\lvert\Theta\rvert$	N_h	P	Train ACC	Val ACC	Test AUC
GNN	5122	10	5	74.25%	74.80%	**63.36%**
EGNN	5252	10	4	73.66%	74.08%	**67.88%**
QGNN	5156	8	6	74.00%	73.28%	**61.43%**
EQGNN	5140	8	6	74.42%	72.56%	**75.17%**





Conclusion and Outlook

Takeaways

- **Statement: Quantum GNNs exhibit enhanced classifier performance over their classical GNN counterparts based on the best test AUC scores produced after the training of the models while relying on a similar number of parameters, hyperparameters, and model structures.**
- **However, the community requires a significant improvement in quantum APIs.**
  - E.g. Pennylane does not support broadcastable operators, i.e. train on one graph at a time.
  - Quantum algorithms took nearly 100 times as long to train.
  - Difficult to construct the quantum layers with enough trainable parameter flexibility.
- **Model improvements include**
  - Further theoretical foundations for complex quantum algorithms.
  - More general equivariance, e.g. unitary SU(2), Lorentz SO(1,3) etc.
  - Greater complexity, e.g. quantum attention mechanism (AT).
  - Testing among different tasks, e.g. classification, regression, etc.
  - Improved quantum optimizers and API integration.

Resources and Software

Developing and Documentation

Packages and APIs

Computing and Testing

Blogging and Connecting

Resources and Code

Figure: **Code** (left) and **website** (right).