Google Summer of Code

ML4SCI

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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Overview

1. Data Structure
2. Model Theory: Invariance and Equivariance
3. Model Theory: Graph Neural Networks
4. Model Implementation
5. Results and Analysis
6. Resources, Software, and Code

Dataset [7]

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

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

$$
\begin{matrix}
(\mathbf{2},\mathbf{1},\mathbf{1}) & (\mathbf{2},\mathbf{2},\mathbf{1}) & \cdots & (\mathbf{2},\mathbf{m_2},\mathbf{1}) \\
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$$

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

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

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

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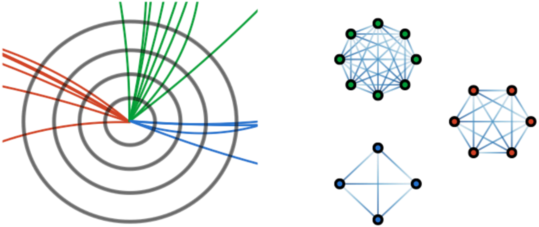
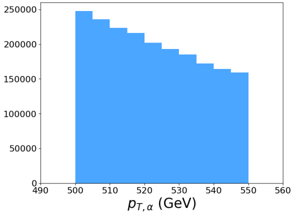
$$\boxed{x_\alpha^{(il)} \in \{p_T, \eta, \phi, m_p\}} \tag{1}$$

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

$$\boxed{y_n \in \{0, 1\} \text{ for Binary Classification}} \tag{2}$$



Data Distributions & Feature Engineering @ ML4SCI



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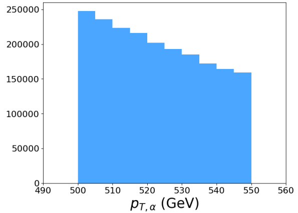

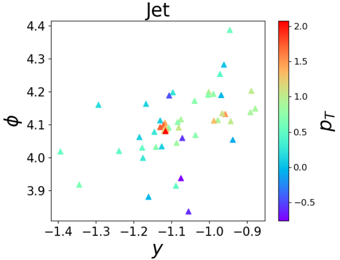

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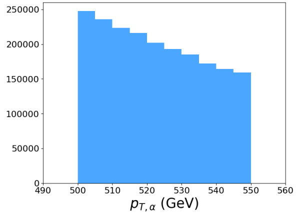

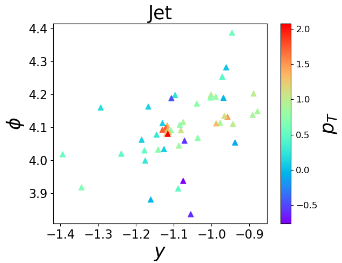

Feature set $h_\alpha^{(il)}$ with $l = 0, 1, 2, \ldots, 7$:

$$h_\alpha^{(il)} \equiv \{p_{T,\alpha}^{(i)}, y_\alpha^{(i)}, \phi_\alpha^{(i)},$$

$$m_{T,\alpha}^{(i)} = \sqrt{m_\alpha^{(i)2} + p_{T,\alpha}^{(i)2}},$$

$$E_\alpha^{(i)} = m_{T,\alpha}^{(i)} \cosh(y_\alpha^{(i)}),$$

$$p_{x,\alpha}^{(i)} = p_{T,\alpha}^{(i)} \cos(\phi_\alpha^{(i)}),$$

$$p_{y,\alpha}^{(i)} = p_{T,\alpha}^{(i)} \sin(\phi_\alpha^{(i)}),$$

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

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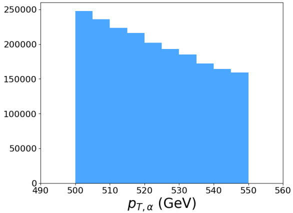

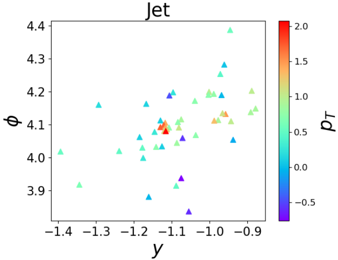

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\end{aligned}
$$

Edge Connections a_{ij}

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

Training, Validation, and Testing

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Data Splits

	N	$N_{quark:1}$	$N_{gluon:0}(0)$
Training	$10,000$	$4,982$	$5,018$
Validation	$1,250$	658	592
Testing	$1,250$	583	667

Invariance and Equivalence

Definition

A function $\varphi : X \to Y$ is **equivariant** with respect to a set of group transformations $T_g : X \to X$, $g \in G$, acting on the input vector space X, if there exists a set of transformations $S_g : Y \to Y$ which similarly transform the output space Y, i.e.

$$\varphi(T_g x) = S_g \varphi(x). \tag{3}$$

A function is said to be **invariant** when for all $g \in G$, S_g becomes the set containing only the trivial mapping, i.e. $S_g = \{\mathbb{I}_G\}$, where $\mathbb{I}_G \in G$ is the identity element of the group G .

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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Input Embedding

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

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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

$$\varphi(g \cdot x) = g' \cdot \varphi(x) \tag{5}$$

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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

$\mathcal{U}(gx) \rightarrow$

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

Equivariant coordinate update function

Proposition

Let $T_g : X \to X$ be the set of translational and rotational group transformations with elements $g \in T_g \subset G$ which act on the vector space X. The function $\varphi : X \to X$ defined by

$$\varphi(x) = x_i + C \sum_{j \neq i} (x_i - x_j) \tag{6}$$

is equivariant with respect to T_g.

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Proof

Let a general transformation $g \in T_g$ of this form act on X by $gX = RX + T$,

$$\begin{aligned}
\varphi(gx) &= (gx_i) + C \sum_{j \neq i} (gx_i - gx_j) \\
&= (Qx_i + T) + C \sum_{j \neq i} (Qx_i + T - Qx_j - T) \\
&= Qx_i + C \sum_{j \neq i} Q(x_i - x_j) + T \\
&= Q[x_i + C \sum_{j \neq i} (x_i - x_j)] + T \\
&= g\varphi(x),
\end{aligned}$$

where $\varphi(gx) = g\varphi(x)$ shows φ transforms equivariantly under transformations $g \in T_g$ acting on X.

Graph Neural Network Theory [3, 2, 6]

Graph Neural Network (GNN)

Message Passing GCNN Layer

Nodes $v_i \in \mathcal{V}$, edges $e_{ij} \in \mathcal{E}$

$$\mathbf{m}_{ij} = \phi_e(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}) \tag{7}$$

$$\mathbf{m}_i = \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij} \tag{8}$$

$$\mathbf{h}_i^{l+1} = \phi_h(\mathbf{h}_i^l, \mathbf{m}_i) \tag{9}$$

where $\mathbf{h}_i$ are node features, a_{ij} are edge attributes, $\mathcal{N}(i)$ is the set of neighbors of node v_i, and ϕ_e, ϕ_h are edge and node operations typically approximated using Multiplayer Perceptrons (MLPs) (Kipf & Welling 2016, Gilmer et al. 2017).

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SE(2) Equivariant GNN (EGNN)

Message Passing EGCNN Layer

Nodes $v_i \in \mathcal{V}$, edges $e_{ij} \in \mathcal{E}$

$$\mathbf{m}_{ij} = \phi_e(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}, |\mathbf{x}_i^l - \mathbf{x}_j^l|) \tag{10}$$

$$\mathbf{m}_i = \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij} \tag{11}$$

$$\mathbf{x}_i^{l+1} = \mathbf{x}_i^l + C \sum_{j \neq i} (\mathbf{x}_i^l - \mathbf{x}_j^l) \phi_x(\mathbf{m}_{ij}) \tag{12}$$

$$\mathbf{h}_i^{l+1} = \phi_h(\mathbf{h}_i^l, \mathbf{m}_i) \tag{13}$$

where we update the coordinates via x_i^{l+1}, include the invariant distance $|\mathbf{x}_i^l - \mathbf{x}_j^l|$ in ϕ_e, and ϕ_x is the coordinate MLP. The equivariant regularization parameter $C(n) < 1$.

Quantum GNN Theory [8]

Quantum GNN (QGNN)

QGCNN Layer

Nodes $v_i \in \mathcal{V}$, edges $e_{ij} \in \mathcal{E}$

$$H(\mathcal{W}_{ij}, \mathcal{M}_i, \mathcal{Q}_0) = \underbrace{\sum_{(i,j)\in\mathcal{E}} \mathcal{W}_{ij}\sigma_i^z\sigma_j^z}_{\text{Interactions Between Nodes (qubits)}} + \underbrace{\sum_i \mathcal{M}_i\sigma_i^z}_{\text{Node (qubit) weights}} + \mathcal{Q}_0 \underbrace{\sum_i \sigma_i^x}_{\textit{Transverse}} \tag{14}$$

$$U_{ij} = \phi_u(\mathcal{W}_{ij}, \mathcal{M}_i, \mathcal{Q}_0) = e^{-i\sum_{q=1}^{Q}\gamma_{lq}H_q(\mathcal{W}_{ij},\mathcal{M}_i,\mathcal{Q}_0)}, \tag{15}$$

$$|\psi^{l+1}\rangle = \phi_{|\psi\rangle}(|\psi^l\rangle, U_{ij}) = U_\theta^l U_{ij} U_\theta^{l\dagger} |\psi^l\rangle \tag{16}$$

where $\mathcal{W}, \mathcal{M}, \mathcal{Q}$ are pre-determined or learned, γ_{lq} is a learnable infinitesimal parameter, $|\psi_i^l(\mathbf{h}_i)\rangle$ is the quantum state at layer l, and U_θ^l is a trainable unitary matrix. Applying this transformation Q times will correspond to running our network over P layers, thus, building up a full trainable unitary parameter transformation (Verdon et al. 2019).

Equivariant Quantum GNN Theory [4]

Equivariant Quantum GNN (EQGNN)

EQGCNN Layer

Nodes $v_i \in \mathcal{V}$, edges $e_{ij} \in \mathcal{E}$

$$H(A_{ij}, \mathcal{M}_i, \mathcal{Q}_0) = \underbrace{\sum_{(i,j)\in\mathcal{E}} A_{ij}\sigma_i^z\sigma_j^z}_{\substack{\text{Interactions}\\ \text{Between}\\ \text{Nodes (qubits)}}} + \underbrace{\sum_i \mathcal{M}_i\sigma_i^z}_{\substack{\text{Node}\\ \text{(qubit) weights}}} + \mathcal{Q}_0 \underbrace{\sum_i \sigma_i^x}_{\textit{Transverse}} \tag{17}$$

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$$|\psi^{l+1}\rangle = \phi_{|\psi\rangle}(|\psi^l\rangle, U_{ij}) = U_\theta^l U_{ij} U_\theta^{l\dagger} |\psi^l\rangle \tag{19}$$

$$U_{ij}(\mathcal{U}_g A_{ij} \mathcal{U}_g^\dagger) = \tilde{\mathcal{U}}_{g'} U_{ij}(A_{ij}) \tilde{\mathcal{U}}_{g'}^\dagger \implies U_{ij}(A_{ij}) = \tilde{\mathcal{U}}_{g'}^\dagger U_{ij}(\mathcal{U}_g A_{ij} \mathcal{U}_g^\dagger) \tilde{\mathcal{U}}_{g'} \tag{20}$$

where we restrict the trainable interaction matrix to the adjacency matrix of the graph, i.e. $\mathcal{W}_{ij} \to A_{ij}$, such that $\mathcal{U}_g \in \mathbb{C}^{n\times n}$ and $\tilde{\mathcal{U}}_{g'} \in \mathbb{C}^{2^n\times 2^n}$ are different representations of group $T_g \cong S_g$ elements $\mathcal{U}_g \in T_g, \tilde{\mathcal{U}}_{g'} \in S_g$.

A Note on Permutation Equivariance

Fact

A GNN is permutation equivariant with respect to the sum of the graphically transformed node features corresponding to each graph. This can be written as a map $\varphi : V^{m\times n} \to V^n$ which takes the node feature matrix of each graph to a single feature vector such that $\varphi(\mathbf{h}^P) = \sum_i \mathbf{h}_i^P$.

Proposition

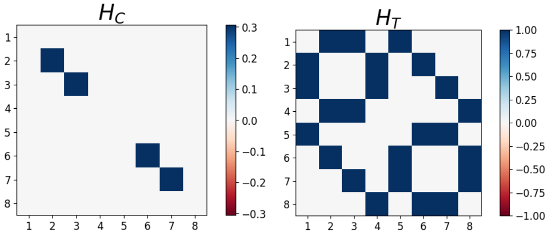
For V a commutable vector space, the product state $\bigotimes_{i=1}^m \mathbf{v}_i : V^n \times \cdots \times V^n \to V^{n^m}$ is permutation equivariant with respect to the sum of its entries. We prove the $n = 2$ case for all $m \in \mathbb{Z}_{>0}$.

Note: Here, m is the number of nodes per graph and n is the number of features.

Hamiltonian and its General Linear Form

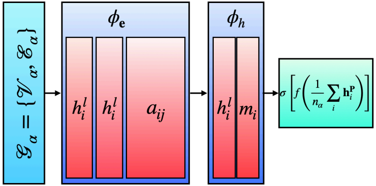
With inspiration from quantum unconstrained binary optimization (QUBO) problems which utilize Ising Hamiltonians, we choose a Hamiltonian which best exploits the properties of a graph by mapping the classical scalar form to the quantum operator form

$$H(a_{ij}) = \underbrace{\sum_{(i,j)\in\mathcal{E}} a_{ij} \left(\frac{\hat{\mathbb{I}}_i - \sigma_i^z}{2} - \frac{\hat{\mathbb{I}}_j - \sigma_j^z}{2} \right)^2}_{H_C} + \underbrace{\sum_{i\in\mathcal{V}} \sigma_i^x}_{H_T} \tag{21}$$



Model Architectures

GNN



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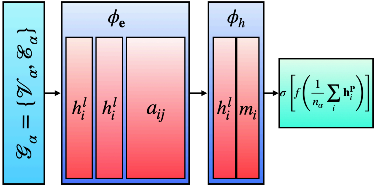
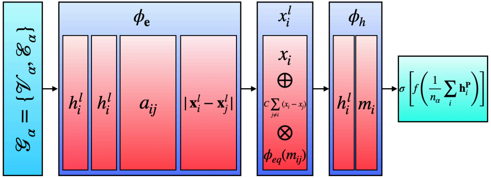


EGNN



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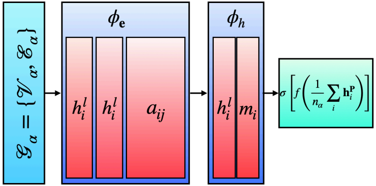

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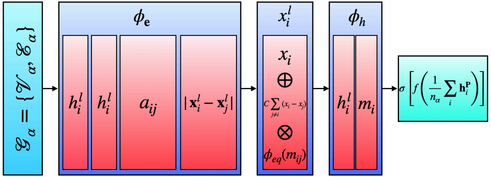
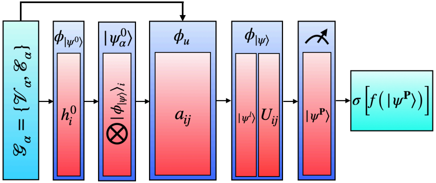


QGNN



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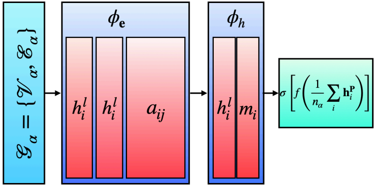
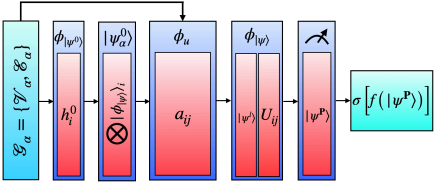
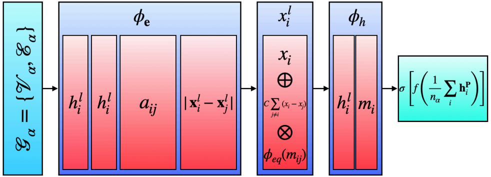


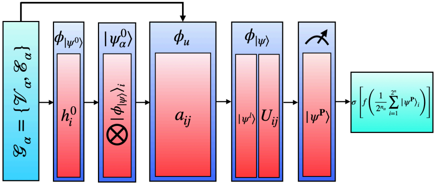
QGNN



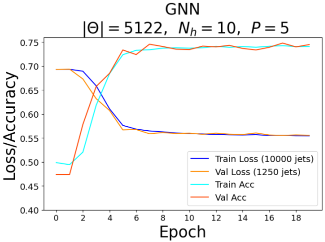
EGNN



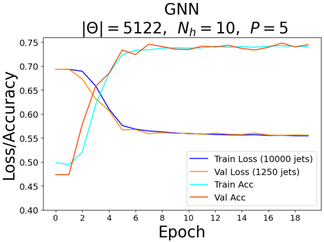
EQGNN

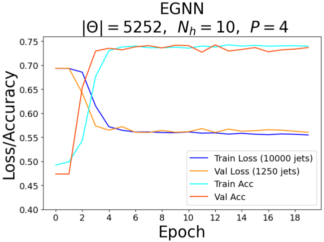


Model Performances

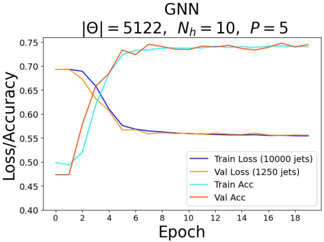


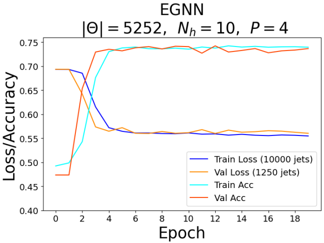
Model Performances

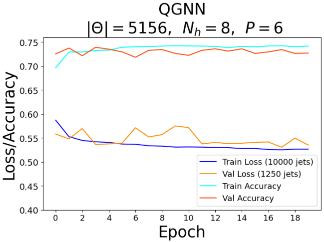




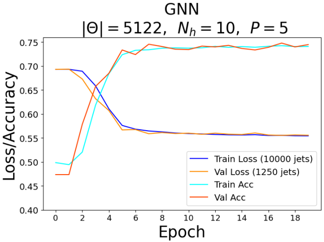
Model Performances

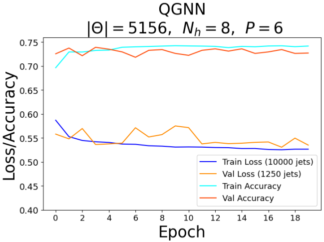


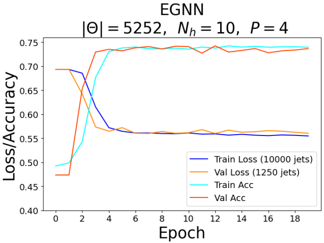


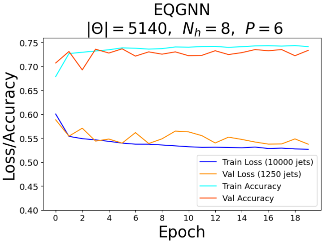


Model Performances





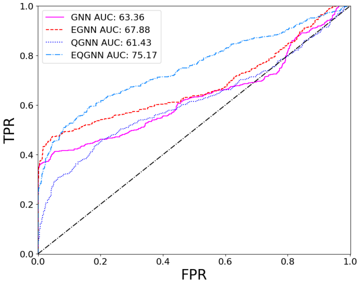


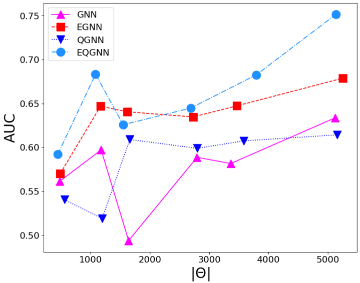


Results

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 Code

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

Resources and Software

Developing and Documentation

Packages and APIs

Computing and Testing

Blogging and Connecting

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