E(n)-EQUIVARIANT GRAPH NEURAL NETWORKS

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INTRODUCTION

- Deep learning should exploit symmetry in data.
- Examples of network with symmetries: Translation in CNNs, Permutation in GNNs.
- 3D data has Euclidean group symmetries (E(3)) that can be exploited.
- Current methods: Require higher-order representations; computationally expensive.
- This work: Presents a simpler, computationally efficient model with E(3). Also scalable to higher dimensions beyond 3D without a significant increase in computation.

BACKGROUND: E(3) EQUIVARIANCE

- **Equivariance:** Function $\phi : X \to Y$ respects transformations in its input space X, mirroring them in output space Y:
  - $\phi(T_g(\mathbf{x})) = T_g(\phi(\mathbf{x}))$ where T_g and S_g are equivalent transformations associated with group g.
- **Key equivariance properties:** Translation, Rotation (Reflection), and Permutation Equivariance.

BACKGROUND: GRAPH NEURAL NETWORKS

- Graphs defined by nodes ($\mathcal{V}$) and edges ($\mathcal{E}$).
- Node embeddings evolve through layers using a message-passing scheme:

$$\begin{aligned} \mathbf{m}_{ij} &= \phi_e\left(\mathbf{h}_i^l, \mathbf{h}_j^l, a_{ij}\right) \\ \mathbf{m}_i &= \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij} \\ \mathbf{h}_i^{l+1} &= \phi_h\left(\mathbf{h}_i^l, \mathbf{m}_i\right) \end{aligned} \tag{1}$$

- ϕ_e and ϕ_h are the edge and node operations often being MLPs. Aggregation of messages and transformation are applied per node.

EQUIVARIANT GRAPH NEURAL NETWORKS

- The paper's model enhances traditional GNNs by incorporating equivariance.
- Updates node positions and features while maintaining structural and transformational integrity.
- **Key operation:** Equivariant updates of node positions using edge embeddings.

$$\mathbf{m}_{ij} = \phi_e\left(\mathbf{h}_i^l, \mathbf{h}_j^l, \left\|\mathbf{x}_i^l - \mathbf{x}_j^l\right\|^2, a_{ij}\right) \tag{2}$$

$$\mathbf{x}_i^{l+1} = \mathbf{x}_i^l + C\sum_{j \neq i}\left(\mathbf{x}_i^l - \mathbf{x}_j^l\right)\phi_x\left(\mathbf{m}_{ij}\right) \tag{3}$$

ANALYSIS ON $E(n)$ EQUIVARIANCE

- Proof of equivariance under the $E(n)$ group:

$$Q\mathbf{x}^{l+1} + g, \mathbf{h}^{l+1} = \text{EGCL}\left(Q\mathbf{x}^{l} + g, \mathbf{h}^{l}\right)$$

  .

- Focus on translational and rotational symmetry for node coordinates: invariance translation, equivariance of rotation, etc.

EXTENDING EGNNS FOR VECTOR TYPE REPRESENTATIONS

- Incorporation of momentum for dynamic systems, enhancing the prediction of particle movement, extending such that $\mathbf{h}^{l+1}, \mathbf{x}^{l+1}, \mathbf{v}^{l+1} = \text{EGCL}\left[\mathbf{h}^{l}, \mathbf{x}^{l}, \mathbf{v}^{\text{init}}, \mathcal{E}\right]$.
- Coordinate update (eq. 3) in two steps: compute the velocity and then update the position:

$$\begin{aligned} \mathbf{v}_i^{l+1} &= \phi_v\left(\mathbf{h}_i^l\right)\mathbf{v}_i^{\text{init}} + C\sum_{j\neq i}\left(\mathbf{x}_i^l - \mathbf{x}_j^l\right)\phi_x\left(\mathbf{m}_{ij}\right) \\ \mathbf{x}_i^{l+1} &= \mathbf{x}_i^l + \mathbf{v}_i^{l+1} \end{aligned} \tag{4}$$

- Observations: ϕ_V maps $\mathbf{h}_i^l$ to a scalar value scaling velocity. Zero initial velocity $\left(\mathbf{v}_i^{\text{init}} = 0\right)$, equation becomes same as eq. 3.

INFERRING EDGES IN POINT CLOUDS

- Addressing edge detection in unstructured data.
- Use of a soft-attention mechanism to infer connections:

$$\mathbf{m}_i = \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij} = \sum_{j \neq i} e_{ij} \mathbf{m}_{ij} \tag{5}$$

$$e_{ij} \approx \phi_{inf}(\mathbf{m}_{ij})$$

- Facilitates dynamic and adaptive network topology.

RELATED WORK OVERVIEW - TABLE 1

- **General Equivariance:** (Cohen et al., 2016; Weiler et al., 2019).
- **E(3) and SE(3) Equivariance:**
  - Utilizing spherical harmonics for higher-order transformations (Thomas et al., 2018; Fuchs et al., 2020).
  - Computational expense and limitation to 3D spaces.
- **Message Passing in Molecular Data:**
  - Has permutation equivariance, but lacks translation or rotation (Gilmer et al., 2017).
  - E(n) invariant networks considering relative distances (Schütt et al., 2017).
- **Innovative Methods:** Incorporating angles and directional information through modified message passing (Klicpera et al., 2020).

COMPARISON WITH EXISTING METHODS

- **Distinguishing Features of EGNN:**
  - Unlike other methods, EGNN updates both node embeddings and coordinates.
  - Maintains E(n) equivariance efficiently without costly operations like spherical harmonics.
- **Some Comparisons:**
  - Radial Field (Kohler et al., 2019) method focuses solely on positional data, limiting feature dynamics across nodes.
  - Tensor Field Networks (Thomas et al., 2018) offer comprehensive feature propagation but at a high computational cost.

EXPERIMENT 1: MODELLING A DYNAMICAL SYSTEM - N-BODY SYSTEM

- **Context:** Dynamical systems are fundamental in various domains such as control systems and physical simulations.
- **Experiment Setup:** Extended the Charged Particles N-body experiment to 3D. System involves 5 particles with charges, interacting through basic physical laws.
- **Data:** 3,000 trajectories for training, 2,000 for validation, and 2,000 for testing. Each trajectory spans 1,000 timesteps.
- **Task:** Predict positions of particles after 1,000 timesteps based on initial conditions.

N-BODY SYSTEM: IMPLEMENTATION AND RESULTS

- **Implementation:** Utilized EGNN with velocity extension. Charges input as edge attributes. Compared with several baselines and other equivariant methods.
- **Performance:** Achieved the lowest MSE, outperforming others by 32%.

EXPERIMENT 2: REPRESENTATION LEARNING - GRAPH AUTOENCODER

- **Objective:** Learn unsupervised representations of graphs in a continuous latent space.
- **Approach:** Used EGNN to construct an Equivariant Graph Autoencoder.
- **Dataset and Task:** Embedding of graphs into latent spaces; focused on reconstructing adjacency matrix without node features.

GRAPH AUTOENCODER: IMPLEMENTATION AND RESULTS

- **Implementation:** Autoencoder framework with EGNN encoder and a simple decoder for adjacency matrix reconstruction. Addressed symmetries in graphs without node features by introducing noise.
- **Results:** Demonstrated superior performance in embedding and reconstructing graphs, significantly reducing errors.

EXPERIMENT 2: MOLECULAR DATA PREDICTION - QM9 DATASET

- **Dataset:** QM9, standard for chemical property prediction. Contains small molecules with varied atomic properties.
- **Task:** Predict 12 chemical properties, which are invariant to spatial transformations of molecule configurations.

QM9: IMPLEMENTATION AND RESULTS

- **Implementation:** EGNN implemented without updating particle positions, focusing on edge inference and molecular properties prediction.
- Competitive results, achieving high accuracy across all tested properties, highlighting the model's efficacy and simplicity.