Momentum conserved GNN

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1 Introduction

A GNN takes as inputs initial node and edge features, $\mathbf{h}_i^{(0)}$ and $\mathbf{e}_{ij}^{(0)}$ respectively, and updates them after L layers, to get $\mathbf{h}_i^{(L)}$ and $\mathbf{e}_{ij}^{(L)}$. Then, the output acceleration $\mathbf{a}_i$ is computed from them. We assume that external forces (e.g. gravity) are applied afterwards. Therefore, $\mathbf{a}_i$ only includes the contribution from interaction with other particles. Naively, we can just perform for instance

$$\mathbf{a}_i = \phi(\mathbf{h}_i^{(L)}) \tag{1}$$

To ensure conservation of momentum, we need to ensure that

$$\sum_i \mathbf{a}_i = 0 \tag{2}$$

Note that Eq. 1 does not guarantees momentum conservation.

To fulfill that condition, we can write that as

$$\mathbf{a}_i = \sum_{j \in \mathcal{N}_i} \mathbf{f}_{ji} \tag{3}$$

where $\mathbf{f}_{ij} = -\mathbf{f}_{ji}$ is antisymmetric. The above could be understood as forces acting on node i. To show that the above prescription actually allows to conserve momentum, it is useful to define the function θ_{ji} such that it is 1 if $j \in \mathcal{N}_i$ and 0 otherwise. Note that j being in the neighborhood of i implies that i is also in the neighborhood of j (since the graph is bidirectional), so θ_{ij} is symmetric: $\theta_{ij} = \theta_{ji}$. Therefore,

$$\sum_i \mathbf{a}_i = \sum_i \sum_{j \in \mathcal{N}_i} \mathbf{f}_{ji} = \sum_{i,j} \theta_{ji} \mathbf{f}_{ji} = \frac{1}{2} \sum_{i,j} (\theta_{ij} \mathbf{f}_{ij} + \theta_{ji} \mathbf{f}_{ji}) = \frac{1}{2} \sum_{i,j} \mathbf{f}_{ij} (\theta_{ij} - \theta_{ji}) = 0 \tag{4}$$

The feature vector $\mathbf{f}_{ij}$ could be given by any antisymmetric combination of node or edge features. We propose the following form:

$$\mathbf{f}_{ij} = \mathbf{e}_{ij}^{(L)} - \mathbf{e}_{ji}^{(L)} \tag{5}$$

In these cases, $\mathbf{e}_{ij}^{(L)}$ should have the shape $(N_e, 3)$, with N_e the number of edges.

What about the boundaries?

To account for external forces and boundary forces, we could add updated node features.

1.1 Energy conservation

$$E = \sum_i T_i + U_i \tag{6}$$

$$\frac{dE}{dt} = \frac{1}{m} \sum_{ij} \left(\mathbf{p}_i \cdot \mathbf{f}_{ji} - \frac{1}{2} \mathbf{f}_{ji} \cdot (\mathbf{p}_i - \mathbf{p}_j) \right) = 0 \tag{7}$$

2 Symmetries

- Euclidean

$$\begin{aligned} \mathbf{x}_i &\rightarrow \mathbf{R}\mathbf{x}_i + \mathbf{T} && (8) \\ \mathbf{v}_i &\rightarrow \mathbf{R}\mathbf{v}_i && (9) \\ \mathbf{a}_i &\rightarrow \mathbf{R}\mathbf{a}_i && (10) \end{aligned}$$

- Galilean

$$\begin{aligned} \mathbf{x}_i &\rightarrow \mathbf{R}\mathbf{x}_i + \mathbf{V}t && (11) \\ \mathbf{v}_i &\rightarrow \mathbf{R}\mathbf{v}_i + \mathbf{V} && (12) \\ \mathbf{a}_i &\rightarrow \mathbf{R}\mathbf{a}_i && (13) \end{aligned}$$

3 Integration

$$\mathbf{a}_i^t = GNN(\{\mathbf{x}_i^t, \mathbf{v}_i^t\}_{i \in G}) \quad (14)$$

- Symplectic Euler

$$\begin{aligned} \mathbf{v}_i^{t+1} &= \mathbf{v}_i^t + \mathbf{a}_i^t \Delta t && (15) \\ \mathbf{x}_i^{t+1} &= \mathbf{x}_i^t + \mathbf{v}_i^{t+1} \Delta t = \mathbf{x}_i^t + \mathbf{v}_i^t \Delta t + \mathbf{a}_i^t \Delta t^2 && (16) \end{aligned}$$

- Leapfrog

$$\begin{aligned} \mathbf{v}_i^{t+1} &= \mathbf{v}_i^t + \frac{1}{2}\left(\mathbf{a}_i^t + \mathbf{a}_i^{t+1}\right) \Delta t && (17) \\ \mathbf{x}_i^{t+1} &= \mathbf{x}_i^t + \mathbf{v}_i^t \Delta t + \frac{1}{2}\mathbf{a}_i^t \Delta t^2 && (18) \end{aligned}$$

Note that in this case one computes first $\mathbf{x}_i^{t+1}$ and the use that result to get $\mathbf{a}_i^{t+1}$ and $\mathbf{v}_i^{t+1}$.

Symplectic Euler and leapfrog fulfill equivariance under Galilean and Euclidean transformations.