Karlsruhe Institute of Technology

Autonome Lernende Roboter (ALR)

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Minimize the Distribution Shift in Graph Network Simulators

Project Type

- ☐ Master Thesis
- ☑ Bachelor Thesis
- ☐ Research Project

Supervisors

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Difficulty

Algorithmic

Math

Application

Description

Simulating dynamic physical interactions poses a significant challenge across various scientific domains, finding applications from robotics to material science. In the realm of mesh-based simulations, Graph Network Simulators (GNSs) emerge as an efficient alternative to traditional physics-based simulators. A key method in mesh-based simulation is MeshGraphNet (MGN) [2]. The paper employs a training strategy involving a 1-step prediction and an iterative roll-out for inference. This leads to a distribution shift between training and inference phases, as training consistently employs ground truth input, while inference may involve arbitrary and potentially inaccurate inputs based on the simulator's past accuracy.

To address this issue, two existing approaches are noteworthy. MGN introduces input noise during training to enhance stability. Additionally, a recent proposal [1] introduces a "push-forward trick," involving a single simulator step to generate ground truth for predicting the subsequent step, thereby training the model solely on the second step.

This bachelor thesis aims to evaluate and explore the effectiveness of the latter approach. Specifically, the focus is on implementing multi-step prediction training by creating a buffer of previously predicted steps. The objective is to establish a distribution over the training data that aligns more closely with the desired predictions.

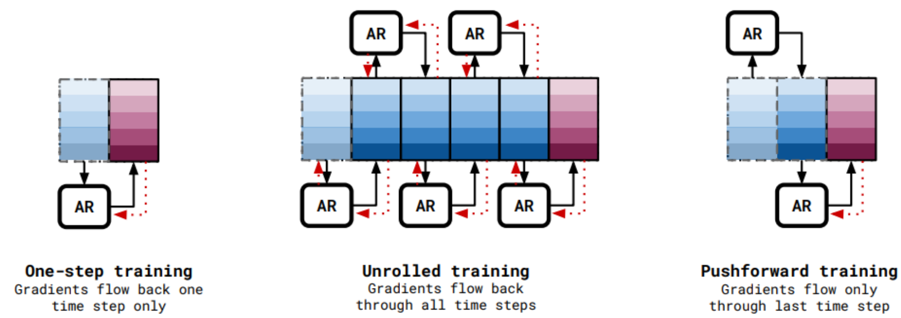

Figure 1: Different training schemes for GNSs

Tasks

- Get familiar with the theory Graph Network Simulators and the current code base
- Implement the push-forward trick
- Develop and finalize the proposed multi-step prediction method using a buffer
- Evaluate the different methods

References

[1] Johannes Brandstetter, Daniel E. Worrall, and Max Welling. Message passing neural PDE solvers. In *The Tenth International Conference on Learning Representations, ICLR 2022, Virtual Event, April 25-29, 2022*. OpenReview.net, 2022.

[2] Tobias Pfaff, Meire Fortunato, Alvaro Sanchez-Gonzalez, and Peter W. Battaglia. Learning mesh-based simulation with graph networks. In *9th International Conference on Learning Representations, ICLR 2021, Virtual Event, Austria, May 3-7, 2021*. OpenReview.net, 2021.