Machine learning for charged particle tracking

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Learning to discover, Institut Pascal, Université Paris-Saclay Workshop on representation learning, April 19th 2022



Acknowledgements

During the preparation of these slides, I have made extensive use of the following talks:

- Charline Rougier, "Towards a realistic track reconstruction algorithm based on graph neural networks for the HL-LHC", vCHEP 2021, May 17-21 2021
 (link)
- Catherine Biscarat et Sylvain Caillou, « Comment la future phase de haute luminosité du collisionneur LHC du CERN, qui doit permettre l'étude des interactions du boson de Higgs, bouscule notre façon de calculer », Séminaire SFP de la section Midi-Pyrénées, 29 octobre 2021 (link)
- Markus Elsing, "Pattern recognition in HEP (track reconstruction)", Learning to Discover: advanced pattern recognition, Institut Pascal, October 14-25 2019 (link)
- Material from Daniel Murnane (Berkeley LBL) and Charline Rougier (L2IT)

Charged particle tracking – 1960s style



The 80 inch (2.0 m) bubble chamber at BNL



Discovery of the Omega-minus baryon in 1964

Electronic readout !

Multi-wire proportional chamber





Nobel prize in physics (1992)

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

File: Charpek charbers

THE USE OF MULTIWIRE PROPORTIONAL COUNTERS TO SELECT AND LOCALIZE CHARGED PARTICLES



11.00

(A)

Atuc

G. Charpak, R. Bouclier, T. Bressani, J. Favier and Č. Zupančič

CERN, Geneva, Switzerland.

ABSTRACT

Properties of chambers made of planes of independent wires placed between two plane electrodes have been investigated. A direct voltage is applied to the wires. It has been checked that each wire works as an independent proportional counter down to separation of 0.1 cm between wires.

- Counting rates of 10⁵/wire are easily reached.
- Time resolutions of the order of 100 nsec have been obtained in some gases.
- It is possible to measure the position of the tracks between the wires using the time delay of the pulses.
- Energy resolution comparable to the one obtained with the best cylindrical chambers is observed.
- The chambers can be operated in strong magnetic fields.

Geneva - 23 February, 1968 (Submitted to Nucl. Instrum. and Methods)

Messrs. G. Amato and J.P. Papis were of great help in the research into very low-cost amplifiers and were successful in this respect. They showed that less than two dollars of equipment per wire was sufficient to bring the pulses to a level close to 1 volt, where their utilization

by logic circuits is easy.

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Today: silicon trackers





Integration test in 2007

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LHC, discovery of the Higgs boson

Large Hadron Collider (LHC) at CERN

- Explore small structures -> high energy
- Study rare processes -> high frequency of collisions (40 MHz)
- Two general-purpose detectors: CMS and ATLAS



Discovery of the Higgs boson (2012)

- Counting experiment in bins (intervals) of mass
- Comparison to theory prediction



And since then ?



- Since 2012, higher beam energy, accumulation of much more statistics
- Study of the coupling strength of the Higgs boson to many other particles: demonstration of clear correlation between the mass of a given particle and its coupling to the Higgs boson
- Key goal for HL-LHC: first experimental probe of the Higgs potential
 - -> expect to gain insight on the first instants of the universe
 - Study Higgs self-coupling: h -> hh
 - Very rare process



Fifteen times more data



Computing resources

Resources used today:

- O(1) million de CPU cores running continuously

- O(1) exabyte of storage

At HL-LHC: with our current computing model, we would face a significant shortage of computing resources

\rightarrow need to make important changes

\rightarrow ... or live with cuts into our physics programme

ML for track pattern recognition ?

Challenge on Kaggle platform (in 2018): <u>(link)</u> Article in proceedings of CHEP 2018: <u>(link)</u>

622 * 415 pixels

a large fraction carries information about the person

Can't use the same tools How to present tracking data to a neural network ?

ATLAS tracker for HL-LHC:

- 5 * 10⁹ readout channels
- ~3 * 10⁵ 3D space-points per event

=> data are *sparse*

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Representing tracking data using graphs

S. Farrell *et al.*, "Novel deep learning methods for track reconstruction", proceedings of *Connecting the Dots* conference 2018 (link)

Charged particles leave hits in the detector

Represent the data using a graph

Goal: classify the edges of the graph

High classification score

=> high probability that the edge is part of a track

Low classification score => low probability that the edge is part of a track

One node of the graph = one hit in the detector

Connect two nodes using an edge if "it seems possible" that the two hits are two (consecutive) hits on a track

Graph creation

A classic use case for graph neural networks: Study molecules and their chemical bonds

"I suppose I'll be the one to mention the elephant in the room."

In our tracking example, using the TrackML dataset, we have O(100k) hits per event.

 \Rightarrow A fully connected graph would have O(100k) nodes and O(10¹⁰) edges. This is not going to fly.

Keep in mind that we want to run this at high throughput. Efficient graph creation becomes an area of study on its own.

Graph creation: "module map"

Results for TrackML detector

C. Biscarat *et al.*, "Towards a realistic track reconstruction algorithm based on graph neural networks for the HL-LHC", proceedings of the *vCHEP2021* conference (link)

New data-driven graph construction method:

- build graphs starting from a list of possible connections from a zone to another zone: the module map
- done using 1000 $t\bar{t}$ events considering tracks with p_T >0.5 GeV and leaving at least 3 hits

239 699 module connections found

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Graph creation: "module map"

Results for TrackML detector

C. Biscarat *et al.*, "Towards a realistic track reconstruction algorithm based on graph neural networks for the HL-LHC", proceedings of the *vCHEP2021* conference (link)

Moon number of adams

• Graphs created with this module map have $O(10^5)$ nodes and $O(10^7)$ edges

Edge selection on geometric parameters:

- $z_0 = z_{h1} r_{h1} \times \left(\frac{\Delta z}{\Delta r}\right)$ $\Delta \phi = \phi_{h2} \phi_{h1}$
- $\phi_{\text{slope}} = \frac{\Delta \phi}{\Delta r}$ $\Delta \eta = \eta_{h2} \eta_{h1}$

 $h_{1,2}$ being the hits connected by a given edge

Input graph

Node features = (r, ϕ, z) Edge features = $(\Delta \eta, \Delta \phi, \Delta r, \Delta z)$

• Target graph

Edge features = (boolean truth flag)

	Mean number of euges	ε
Initial	18.5×10^{6}	
z_0	3.56×10^{6}	19%
z_0, ϕ_{slope}	1.32×10^{6}	7.1%
$z_0, \phi_{slope}, \Delta \phi$	1.10×10^{6}	5.8%
$z_0, \phi_{slope}, \Delta \phi, \Delta \eta$	1.05×10^{6}	5.6%

Graph creation: metric learning

First Step: metric learning

- > For all hits, embed features (coordinates, cell direction, ...) with multi-layer perceptron (MLP) into N-dimensional space
- ➤ Associate hits on same track as close as N-dimensional distance
- ➤ Score each neighbour hit within embedding neighbourhood against the "source" hit at centre
- ➤ Create edges between the source hit at centre and the neighbouring hits above a given threshold on the score.

Second step: filtering

Reduce the number of edges using an MLP that looks separately at each edge (the features of the two nodes).

GNN architectures

S. Farrell *et al.*, "Novel deep learning methods for track reconstruction", proceedings of *Connecting the Dots* conference 2018 (link)

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Also used in Biscarat et al. (vCHEP2021).

An alternative GNN architecture ("Recurrent Attention Message Passing") is presented in N. Choma *et al.* (CTD 2020) (link)

Edge-level performance

C. Biscarat *et al.*, "Towards a realistic track reconstruction algorithm based on graph neural networks for the HL-LHC", proceedings of the *vCHEP2021* conference (link)

Cut	0.5	0.7	0.8
Per-edge efficiency	0.992	0.987	0.982
Per-edge purity	0.916	0.937	0.950

Results for TrackML dataset

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Track building starting from graph with edge scores

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Inference speed

Accelerating the Inference of the Exa.TrkX Pipeline

In many studies, no attempt is made to optimise execution speed (demonstrate feasibility first).

Constraints imposed by the need to run the final algorithm at high throughput are kept in mind.

Competitive execution speed has been demonstrated for one complete chain of algorithms.

Substantial gains expected from future implementations with custom CUDA kernels.

(Any volunteer for coding the module map in CUDA ?)

Alina Lazar¹, Xiangyang Ju², Daniel Murnane², Paolo Calafiura², Steven Farrell², Yaoyuan Xu³, Maria Spiropulu⁴, Jean-Roch Vlimant⁴, Giuseppe Cerati⁵, Lindsey Gray⁵, Thomas Klijnsma⁵, Jim Kowalkowski⁵, Markus Atkinson⁶, Mark Neubauer⁶, Gage DeZoort⁷, Savannah Thais⁷, Shih-Chieh Hsu⁸, Adam Aurisano⁹, Jeremy Hewes⁹, Alexandra Ballow¹, Nirajan Acharya¹, Chun-yi Wang¹⁰, Emma Liu¹¹, Alberto Lucas¹²

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Table 1. Wall time of the Python-based Inference pipeline for the baseline and optimized implementations. The time is calculated with 500 events on an Nvidia Volta 100 GPU with a memory of 16 GB. The reported times are the average time and the standard deviation of the time in the unit of seconds.

	Baseline	Faiss	$\operatorname{cuGraph}$	AMP	FRNN
Data Loading	0.0022 ± 0.0003	0.0021 ± 0.0003	0.0023 ± 0.0003	0.0022 ± 0.0003	0.0022 ± 0.0003
Embedding	0.02 ± 0.003	0.02 ± 0.003	0.02 ± 0.003	0.0067 ± 0.0007	0.0067 ± 0.0007
Build Edges	12 ± 2.64	0.54 ± 0.07	0.53 ± 0.07	0.53 ± 0.07	0.04 ± 0.01
Filtering	0.7 ± 0.15	0.7 ± 0.15	0.7 ± 0.15	0.37 ± 0.08	0.37 ± 0.08
GNN	0.17 ± 0.03	0.17 ± 0.03	0.17 ± 0.03	0.17 ± 0.03	0.17 ± 0.03
Labeling	2.2 ± 0.3	2.1 ± 0.3	0.11 ± 0.01	0.09 ± 0.008	0.09 ± 0.008
Total time	$15 \pm 3.$	3.6 ± 0.6	1.6 ± 0.3	1.2 ± 0.2	0.7 ± 0.1

Triggering (ATLAS)

"Recording data at the LHC is like drinking from a fire hose"

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Simplify GNN -> inference on FPGA

Computing and Software for Big Science (2021) 5:26 https://doi.org/10.1007/s41781-021-00073-z (link)

ORIGINAL ARTICLE

Charged Particle Tracking via Edge-Classifying Interaction Networks

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Abstract

Recent work has demonstrated that geometric deep learning methods such as graph neural networks (GNNs) are well suited to address a variety of reconstruction problems in high-energy particle physics. In particular, particle tracking data are naturally represented as a graph by identifying silicon tracker hits as nodes and particle trajectories as edges, given a set of hypothesized edges, edge-classifying GNNs identify those corresponding to real particle trajectories. In this work, we adapt the physics-motivated interaction network (IN) GNN toward the problem of particle tracking in pileup conditions similar to those expected at the high-luminosity Large Hadron Collider. Assuming idealized hit filtering at various particle momenta thresholds, we demonstrate the IN's excellent edge-classification accuracy and tracking efficiency through a suite of meas-urements at each stage of GNN-based tracking: graph construction, edge classification, and track building. The proposed IN architecture is substantially smaller than previously studied GNN tracking architectures; this is particularly promising as a reduction in size is critical for enabling GNN-based tracking in constrained computing environments. Furthermore, the IN may be represented as either a set of explicit matrix operations or a message passing GNN. Efforts are underway to accelerate each representation via heterogeneous computing resources towards both high-level and low-latency triggering applications.

Work has also been done to accelerate the inference of deep neural networks with heterogeneous resources beyond GPUs, like field-programmable gate arrays (FPGAs) [49–57]. This work extends to GNN architectures [29, 58]. Specifically, in Ref. [29], a compact version of the IN was implemented for $p_{\rm T} > 2$ GeV segmented geometric graphs with up to 28 nodes and 37 edges, and shown to have a latency less than 1 μ s, an initiation interval of 5 ns, reproduce the floating-point precision model with a fixed-point precision of 16 bits or less, and fit on a Xilinx Kintex UltraScale FPGA.

While this preliminary FPGA acceleration work is promising, there are several limitations of the current FPGA implementation of the IN:

- 1. This fully pipelined design cannot easily scale to beyond O(100) nodes and O(1000) edges. However, if the initiation interval requirements are loosened, it can scale up to O(10, 000) nodes and edges.
- 2. The neural network itself is small, and while it is effective for $p_T > 2$ GeV graphs, it may not be sufficient for lower- p_T graphs.
- 3 The FDGA design makes no assumptions about the nos-

Triggering (ATLAS)

ATLAS

Technical Design Report for the Phase-II Upgrade of the ATLAS Trigger and Data Acquisition System - EF Tracking Amendment

The ATLAS Collaboration

Reference:

Created:March 1, 2022Last modified:March 1, 2022Prepared by:The ATLAS Collaboration

v1.2

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Abstract

This Technical Design Report Amendment describes revised plans for Event Filter Tracking in the upgrade of the ATLAS Trigger and Data Acquisition system for the High Luminosity LHC. The motivation to change the baseline for Event Filter Tracking is explained. Next, a description of the requirements for Event Filter Tracking and the definition of the proposed baseline to meet these requirements are presented. Several demonstrations using various hardware and software are reported in support of this proposal. Finally, the organization and resources needed to deliver the new baseline are set out. TDAQ Phase-II Upgrade Project

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From the TrackML dataset to the real world

At least two major complications have been (deliberately) omitted from the TrackML dataset.

Secondary particles from interactions with material in detector

electron knocked out of atom

hadronic interactions: (lots of relatively high-Z material in modern trackers [support, cooling, readout])

Silicon strip detectors

strip (one strip = 1 readout channel)

- hit from a charged particle
- "ghost" (accidental crossing of strips)

It would be extremely useful to have a new open dataset that includes these effects. Maybe even a dataset released by CMS and/or ATLAS ?

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Comment on GNN design

In this region, it is relatively clear in which direction to look for the next hit.

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Conclusion

- Lots of exciting physics results since the Higgs boson discovery in 2012; the Higgs boson as new tool for precision tests of the standard model
- Even more exciting outlook for the HL-LHC: among others, probe the first moments of the Universe right after the Big Bang (EW baryogenesis)
- TrackML challenge in 2018 was huge boost to get the "ML for tracking" effort going. The dataset from then is still being used today.
- Feasibility of complete GNN-based tracking solutions has been demonstrated in 2021.
- These conceptual solutions are trying to face the real world right now.
 - A new open dataset that is close to the real world would really help.
- Lot's of variants:
 - Fast, use in trigger decision
 - Seeding only
 - Large radius tracking
 - ..

Backup material

La physique des particules et le boson de Higgs

 Comprendre les constituants fondamentaux de la matière et les interactions qui les régissent

Séminaire SFP MP, Jan Stark (L2IT), déc. 2019

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Higgs potential

A measurement of the Higgs self-coupling is the only way to experimentally reconstruct the Higgs potential (reconstruct its shape close to the minimum).

Jan Stark

Electroweak baryogenesis ?

To get the observed baryon asymmetry of the universe from an initially baryon-symmetric universe, Sacharow's conditions must be satisfied.

Baryon number (B) violation
 C and CP violation
 Out of equilibrium

It is not easy to construct a credible mechanism that meets these conditions.

The mechanism that meets these conditions and that is considered to be the most credible one is electroweak baryosynthesis.

An effective potential (free energy density) is used to describe the Higgs potential during the electroweak phase transition.

Electroweak baryosynthesis can only work if the electroweak phase transition is a a first order phase transition (PT).

First order PTs imply a system that is out of equilibrium (violent transition, large creation of entropy).

« Computing enables physics »

Photography: C. Biscarat

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Annonce de la découverte du maillon manquant de notre Modèle Standard, le boson de Higgs.

CERN seminar, July 4th 2012, retransmitted at ICHEP (Melbourne)

10 ans pour nous préparer

- Community white paper (2017)
 - Algorithmes, infrastructures, data access...
- Des actions concrètes :
 - HEP Software Foundation (HSF)
 - Software Institute for Data-Intensive Sciences (SIDIS)
 - Création d'une revue scientifique « Computing and software for big Science » (Springer)
 - IRIS-HEP (Projet NSF U.S.A.)
 - Projet international Data Organization, Management and Access (DOMA)

• The 2020 update of the EU strategy for particle physics

D. Large-scale data-intensive software and computing infrastructures are an essential ingredient to particle physics research programmes. The community faces major challenges in this area, notably with a view to the HL-LHC. As a result, the software and computing models used in particle physics research must evolve to meet the future needs of the field. *The community must vigorously pursue common, coordinated R&D efforts in collaboration with other fields of science and industry, to develop software and computing infrastructures that exploit recent advances in information technology and data science. Further development of internal policies on open data and data preservation should be encouraged, and an adequate level of resources invested in their implementation.*

A Roadmap for HEP Software and Computing R&D for the 2020s	 Download: PDF Other formats 			
Is Albrecht, Antonio Augusto Alves Jr, Guilherme Amadio, Giuseppe Andronico, Nguyen Anh-Ky, Laurent che, John Apostolakis, Makoto Asai, Luca Atzori, Marian Babik, Giuseppe Bagliesi, Marilena Bandieramonte, a Banerjee, Martin Barisits, Lothar A.T. Bauerdick, Stefano Belforte, Douglas Benjamin, Catrin Bernius, Wahid Riccardo Maria Bianchi, Ian Bird, Catherine Biscarat, Jakob Blomer, Kenneth Bloom, Tommaso Boccali, Brian ian, Tomasz Bold, Daniele Bonacorsi, Antonio Boveia, Concezio Bozzi, Marko Bracko, David Britton, Andy , Predrag Buncic, Paolo Calafiura, Simone Campana, Philippe Canal, Luca Canali, Gianpaolo Carlino, Nuno Marco Cattaneo, Gianluca Cerminara, Javier Cervantes Villanueva, Philip Chang, John Chapman, Gang Chen, , Piders, Peter Clarke, Marco Clemencic, Eric Cogneras, Jeremy Coles, Ian Collier, David Collino, Gloria Corti	Current browse context: physics.comp.ph <prev next="" =""> new recent 1712 Change to browse by: hep-ex. physics</prev>			
Gabriele Cosmo, Davide Costanzo, Ben Couturier, Kyle Cranmer, Jack Cranshaw, Leonardo Cristella, David Crooks, Sabine Crépé-Renaudin, Robert Currie, Sünje Dallmeier-Tiessen, Kaushik De, Michel De Cian, Albert De Roeck, Antonio Delgado Peris, Frédéric Derue, Alessandro Di Girolamo, Salvatore Di Guida, Gancho Dimitrov, Caterina	References & Citations INSPIRE HEP (refers to cited by) NASAADS 			
Doglioni, Andrea Dotti, Dirk Duellmann, Laurent Duflot, Dave Dykstra, Katarzyna Dziedziniewicz-Wojcik, Agnieszka Dziurda, Ulrik Egede, Peter Elmer, Johannes Elmsheuser, V. Daniel Elvira, Giulio Eulisse, Steven Farrell, Torben	Export citation Google Scholar			
Ferber, Andrej Filipcic, Ian Fisk, Conor Fitzpatrick, José Flix, Andrea Formica, Alessandra Forti, Giovanni Franzoni, James Frost, Stu Fuess, Frank Gaede, Gerardo Ganis, Robert Gardner, Vincent Garonne, Andreas Gellrich et al. (210 additional authors not shown)	Bookmark X 💀 😤 🚟			
(Submitted on 18 Dec 2017 (v1) Jast revised 19 Dec 2018 (this version v5))				

Particle physics has an ambitious and broad experimental programme for the coming decades. This programme requires large investments in detector hardware, either to build new facilities and experiments, or to upgrade existing ones. Similarly, it requires commensurate investment in the R&D of software to acquire, manage, process, and analyse the shear amounts of data to be recorded. In planning for the HL-LHC in particular, it is critical that all of the collaborating stakeholders agree on the software goals and priorities, and that the efforts complement each other. In this spirit, this white paper describes the R&D activities required to prepare for this software upgrade.

Contraintes et opportunités

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The TrackML dataset

- Generation (Pythia8): 1000 $t\bar{t}$ events from pp collisions
 - $\sqrt{s} = 14 \, TeV$, $\mu = 200$ (HL-LHC conditions), pile-up modeling using A3 tune
- Simulation: Generic detector simulated with fast simulation of ACTS framework

18 728 silicon modules

Le défi de HL-LHC pour la reconstruction de traces

- Reconstruction actuellement résolu par des algorithmes basés sur des filtres de Kalman
- Estimation des paramètres de la trajectoire hélicoïdal
- Très bonne performance et optimisé depuis des années
- La partie la plus coûteuse en complexité de calcul (donc en ressources CPU) dans la reconstruction d'un événement
- La combinatoire va exploser avec HL-LHC (pileup ~20 => pileup ~200)
- Va entrainer une augmentation très importante du volume et de la complexité des données
- Les algorithmes actuels ne suffiront pas

LHC (pileup ~20)

HL-LHC (pileup ~200)

Qk Come Come 27

I. propagate $p_{k,l}$ and its covariance $C_{k,l}$: $q_{k|k-1} = f_{k|k-1}(q_{k-1|k-1})$ $C_{k|k-1} = F_{k|k-1}C_{k-1|k-1}F_{k|k-1}^{T} + Q_k$ with $Q_k \sim \text{noise term (M.S.)}$

2. update prediction to get $q_{k|k}$ and $C_{k|k}$: $q_{k|k} = q_{k|k-1} + K_k[m_k - h_k(q_{k|k-1})]$ $C_{k|k} = (I - K_k H_k)C_{k|k-1}$

with $K_k \sim \text{gain matrix}$: $K_k = C_{k|k-1} H_k^{\mathrm{T}} (G_k + H_k C_{k|k-1} H_k^{\mathrm{T}})^{-1}$

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Apprentissage des patterns de traces avec des GNNs

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Graph (neural) networks

Oct 2018 (link)

Relational inductive biases, deep learning, and graph networks

Peter W. Battaglia¹*, Jessica B. Hamrick¹, Victor Bapst¹, Alvaro Sanchez-Gonzalez¹, Vinicius Zambaldi¹, Mateusz Malinowski¹, Andrea Tacchetti¹, David Raposo¹, Adam Santoro¹, Ryan Faulkner¹, Caglar Gulcehre¹, Francis Song¹, Andrew Ballard¹, Justin Gilmer², George Dahl², Ashish Vaswani², Kelsey Allen³, Charles Nash⁴, Victoria Langston¹, Chris Dyer¹, Nicolas Heess¹, Daan Wierstra¹, Pushmeet Kohli¹, Matt Botvinick¹, Oriol Vinyals¹, Yujia Li¹, Razvan Pascanu¹

¹DeepMind; ²Google Brain; ³MIT; ⁴University of Edinburgh

A GN block contains three "update" functions, ϕ , and three "aggregation" functions, ρ ,

$$\begin{aligned} \mathbf{e}'_{k} &= \phi^{e} \left(\mathbf{e}_{k}, \mathbf{v}_{r_{k}}, \mathbf{v}_{s_{k}}, \mathbf{u} \right) & \mathbf{\bar{e}}'_{i} &= \rho^{e \to v} \left(E'_{i} \right) \\ \mathbf{v}'_{i} &= \phi^{v} \left(\mathbf{\bar{e}}'_{i}, \mathbf{v}_{i}, \mathbf{u} \right) & \mathbf{\bar{e}}' &= \rho^{e \to u} \left(E' \right) \\ \mathbf{u}' &= \phi^{u} \left(\mathbf{\bar{e}}', \mathbf{\bar{v}}', \mathbf{u} \right) & \mathbf{\bar{v}}' &= \rho^{v \to u} \left(V' \right) \end{aligned}$$

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where $E'_i = \{(\mathbf{e}'_k, r_k, s_k)\}_{r_k=i, \ k=1:N^e}, V' = \{\mathbf{v}'_i\}_{i=1:N^v}, \text{ and } E' = \bigcup_i E'_i = \{(\mathbf{e}'_k, r_k, s_k)\}_{k=1:N^e}.$

Graph (neural) networks

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¹DeepMind; ²Google Brain; ³MIT; ⁴University of Edinburgh

Interaction networks

Interaction Networks (Battaglia et al., 2016; Watters et al., 2017) and the Neural Physics Engine Chang et al. (2017) use a full GN but for the absence of the global to update the edge properties:

$$\begin{split} \phi^{e}\left(\mathbf{e}_{k},\mathbf{v}_{r_{k}},\mathbf{v}_{s_{k}},\mathbf{u}\right) &\coloneqq f^{e}\left(\mathbf{e}_{k},\mathbf{v}_{r_{k}},\mathbf{v}_{s_{k}}\right) = \mathrm{NN}_{e}\left(\left[\mathbf{e}_{k},\mathbf{v}_{r_{k}},\mathbf{v}_{s_{k}}\right]\right) \\ \phi^{v}\left(\overline{\mathbf{e}}_{i}',\mathbf{v}_{i},\mathbf{u}\right) &\coloneqq f^{v}\left(\overline{\mathbf{e}}_{i}',\mathbf{v}_{i},\mathbf{u}\right) &= \mathrm{NN}_{v}\left(\left[\overline{\mathbf{e}}_{i}',\mathbf{v}_{i},\mathbf{u}\right]\right) \\ \rho^{e \to v}\left(E_{i}'\right) &\coloneqq &= \sum_{\{k: r_{k}=i\}} \mathbf{e}_{k}' \end{split}$$