Data Driven Engineering II: Advaced Topics

Graph Neural Networks II

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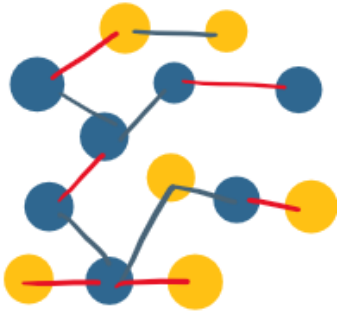
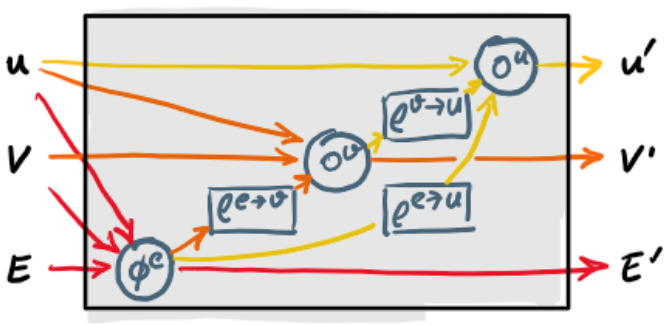
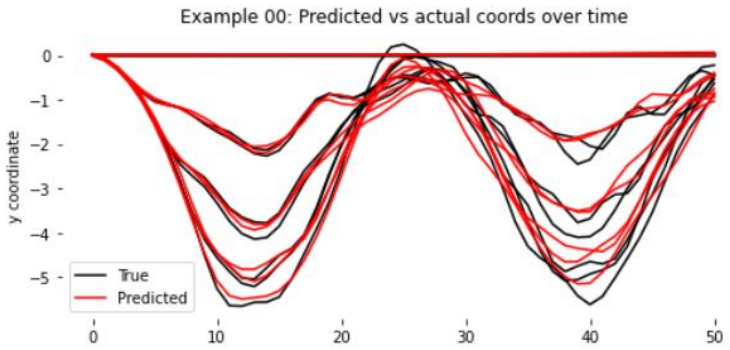


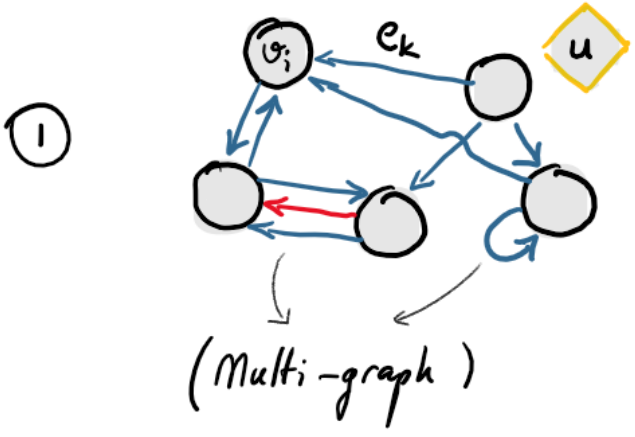




Graph Neural Networks :

1) GNN Basics
2) How GNN works
3) Basic architectures
4) Coding : Graph Nets library

Understanding the Graph :



Embedded

u ⇨ Global attributes - - - ->

v_i ⇨ Nodes - - - ->

e_k ⇨ Edges - - ->

v_{s_k} "sender" v_{r_k} "receiver"

Understanding the Graph:

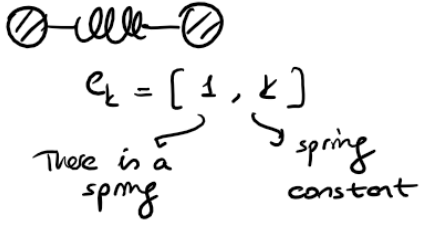
② Graph := 3-tuple ; $G = (u, V, E)$

- u is for the whole graph ⇨ label, parameter ($\vec{g}$) ...
- $V = \{v_i\}_{i=1,N^v}$ $\quad v_i \Rightarrow$ "particle i" ⇨ [x, y, z, u, v, w, m]
- $E = \{e_k, r_k, s_k\}_{k=1,N^e}$

$e_k \Rightarrow$ Edge attribute

$r_k \Rightarrow$ receiver index

$s_k \Rightarrow$ sender index



Understanding Graph Network :

idea ⇒ hidden states of nodes v_i updated (I) according to the info. passed (II) from neighbours (III)

* $$h_i^{(k+1)} = \phi_{update}\left(h_A^{(k)}, \phi_{aggregate}^{(k)}\left(\{ h_j^{(k)}, \forall k \in \mathcal{N}(i) \} \right) \right)$$

- ϕ_{update}: arbitrary differentiable function
- $\phi_{aggregate}$: arbitrary differentiable function
- $h_j^{(k)}$: message from neighbour

Understanding Graph Network :

* Algorithm of a graph network

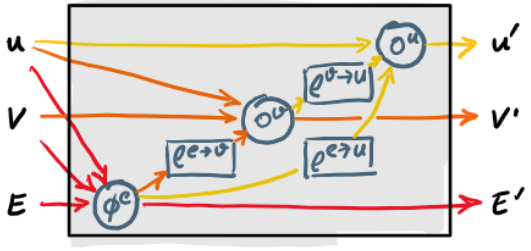
edges
nodes
global

(i) 3 update functions → edge, nodes, global
(ii) 3 aggregate functions → edge, nodes, global

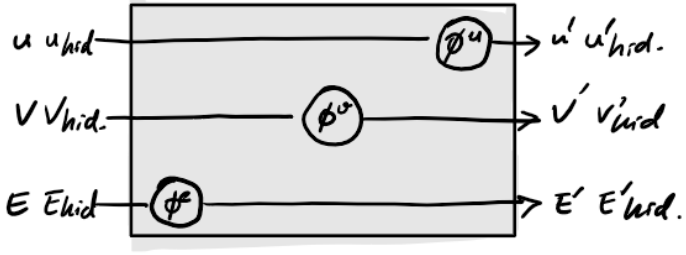
1) Update edge attributes $e'_k = \phi^e\left(e_k, v_{r_k}, v_{s_k}, u\right)$

2) Aggregate edge att. per node $\bar{e}'_i = \rho^{e\to v}\left\{\left(e'_k, r_k, s_k\right)\right\}_{r_k=i,\, k=1:N^e}$

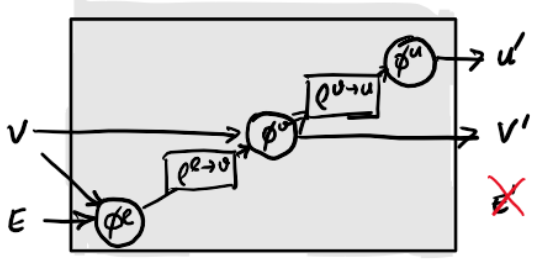
Graph Neural Networks



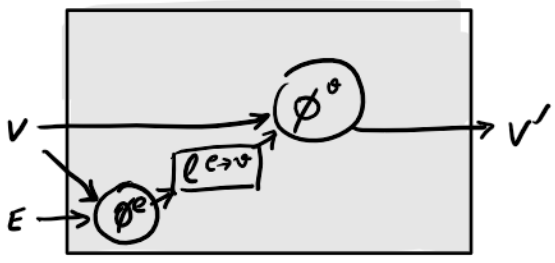
Full GN block



Independent recurrent block



Message-passing NN.



Non-local N.N.

Learning to Simulate Complex Physics with Graph Networks

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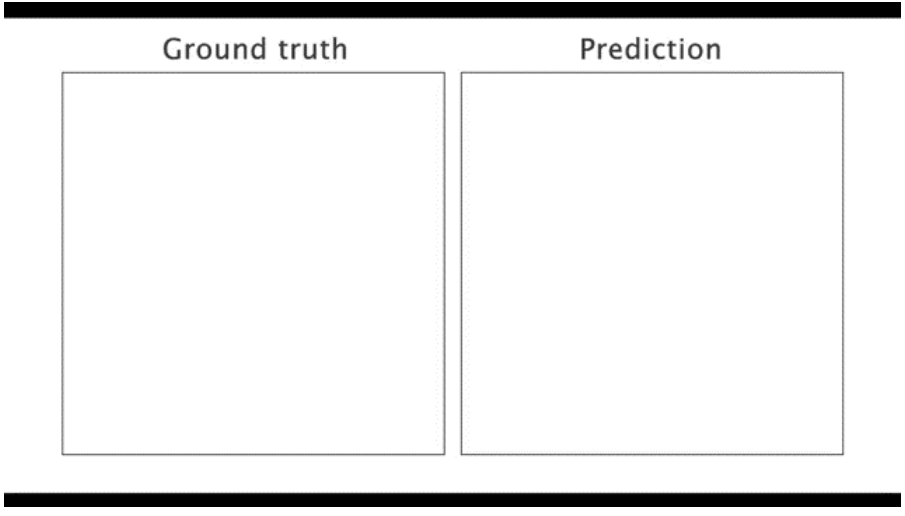
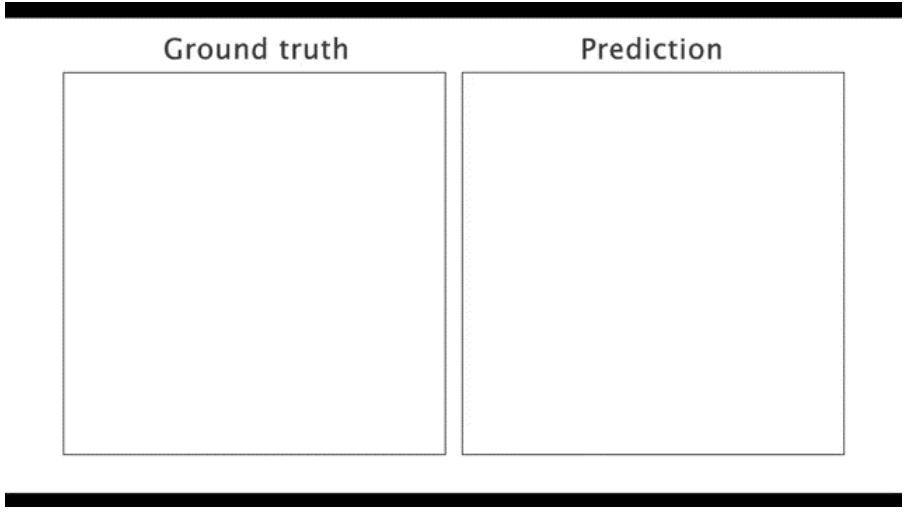
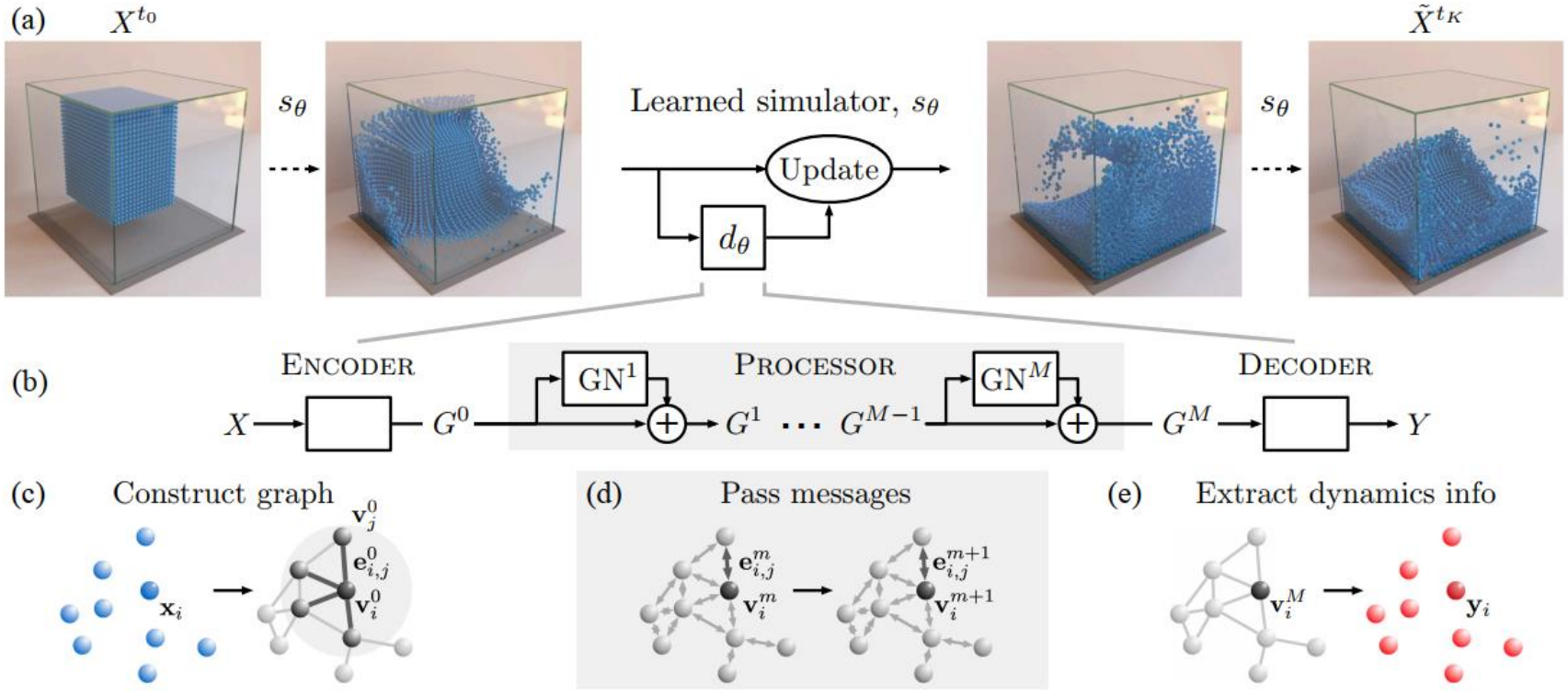
Peter W. Battaglia [1]





Graph Neural Networks



Data for training

WaterDrop
Water
Sand
Goop
MultiMaterial
RandomFloor
WaterRamps
SandRamps
FluidShake
FluidShakeBox
Continuous
WaterDrop-XL
Water-3D
Sand-3D
Goop-3D

Check

- "download_dataset.sh"
- "WaterDrop"

colab