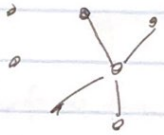
More NN architectures beyond CNNs

Another popular framework, also permutation inv't:
graph neural networks "message passing NN"

View each data pt as a graph — more flexible than image!
↳ no discretization
better for sparse images


← e.g. jet constituents

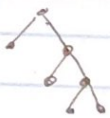
graphs have nodes and edges
↓
attributes (p_x, p_y, p_z) e.g.

Diff types of graphs: fully connected

sets (no connections)

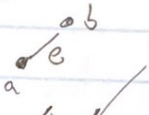
hierarchical trees

locally connected
- each node connected to nearest neighbors (by some dist metric)



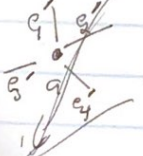
Message passing framework

∀ edge



$\phi^{edge}(e, a, b) = e'$

∀ node



$\phi^{node}(\rho(e_1', e_2', \dots), a) = a'$

ρ → symmetric fn e.g. sum, mean, max
↓
perm inv'ce

ϕ^{edge}, ϕ^{node} → MLPs usually

Same ∀ edge/node weights sharing like CNN filters!

- So output another graph w/ updated edge & node info!

↓

again, stackable!

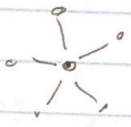
graph → MP layer1 → MP layer2 → ...

before final layer, must involve perm inv't aggregation
e.g. sum or max pool.
e.g. $\sum_{\text{nodes}}$

→ MLP → out

- example: dynamic graph CNN (1801.07829)

kNN edges → new edges based on kNN of learned features



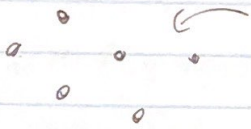
$$\begin{cases} e'_{ab} = \phi^{edge}(\widetilde{a,b}^{kNN}) \\ \phi a' = \square_{\text{max, sum, ...}} e'_{ac} \end{cases} \rightarrow \text{new edges}$$

- Particle Net based on DGCNN won top tagging competition ca 2019! (10% better R30 than ResNext)
- Graph nets — very flexible & powerful framework!
- Downside: compute scales w/ N_{nodes}^2 for DGCNN — kNN is expensive ($N_{nodes} = N_{particles}$ @ LHC ...)

Another application of GNNs

good ref: Batzner et al Nature Comm. 13 (2022)

Regression for "inter-atomic potential" in materials science



← atoms positions $\vec{r}_i$, atomic # Z_i

→ wat total pot'l energy ϵ_{pot} & forces acty on atoms $\vec{F}_i$

good approx (?)

$$\epsilon_{pot} = \sum_i \epsilon_{i,\text{atomic}}$$ sum of individual local atomic energies

$$\vec{F}_i = -\nabla_i \epsilon_{pot}$$

can be calculated using Density Functional Theory but very computationally expensive.

A lot of data to play with: Materials Project website

A growing literature on regressing DFT w/ NNs → GNNs especially well-suited!

system already in the form of a graph!

- node attributes r_i, Z_i
- edge attributes r_{ij}

(+ rotational & translational symmetry)

MP-NN → final graph output gives $\epsilon_{i,\text{atomic}}$ at each node → ϵ_{pot} from final sum over nodes

Fully differentiable! → forces