Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds

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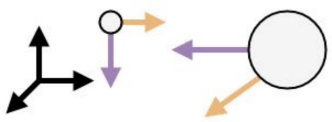
Agenda

Motivation

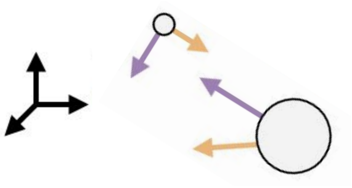
Goal: utilize symmetries of the point clouds, graphs and physical world in the NN design

Approach: equivariance with respect to group of isometries in 3D

Two point **masses** with **velocity** and **acceleration**



Same system, with rotated coordinates.



Source: NeurIPS Workshop

Wigner D-Matrix

Definition

A representation of a group G is a function $D : G \to \mathbb{R}^{n \times n}$, such that for all $g, h \in G$,

$$D(g)D(h) = D(gh)$$

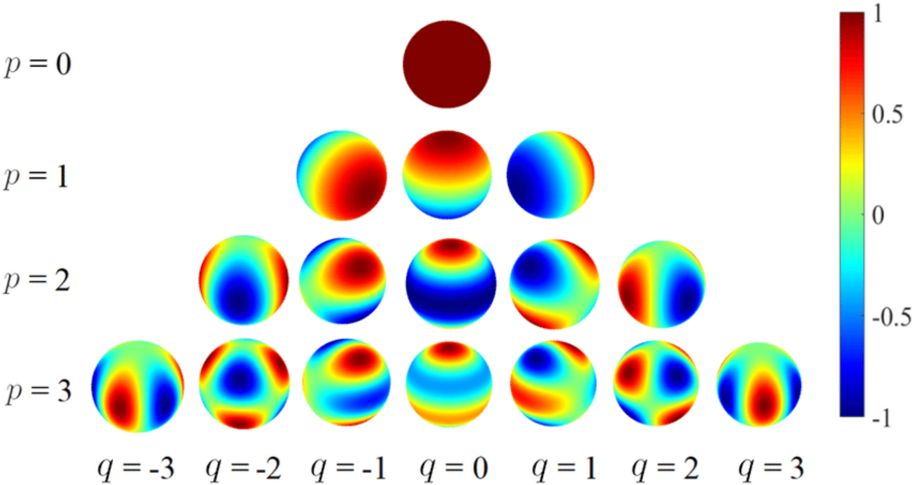
The elements of *3D rotation group* can be represented by $(2l+1) \times (2l+1)$-dimensional matrices $D^{(l)}$, which are called Wigner D-matrices.

Example

For scalars and 3-space vectors, the Wigner D-matrices are

$$D^{(0)}(g) = 1 \qquad \text{and} \qquad D^{(1)}(g) = \mathcal{R}(g).$$

Spherical Harmonics



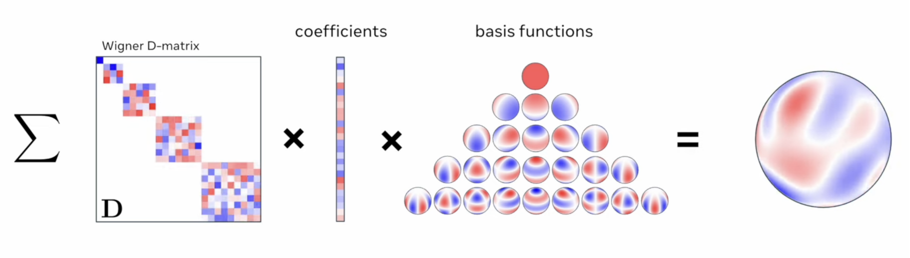
Source: Guezenoc, Corentin (2021) Binaural Synthesis Individualization based on Listener Perceptual Feedback

Spherical Harmonics

Definition

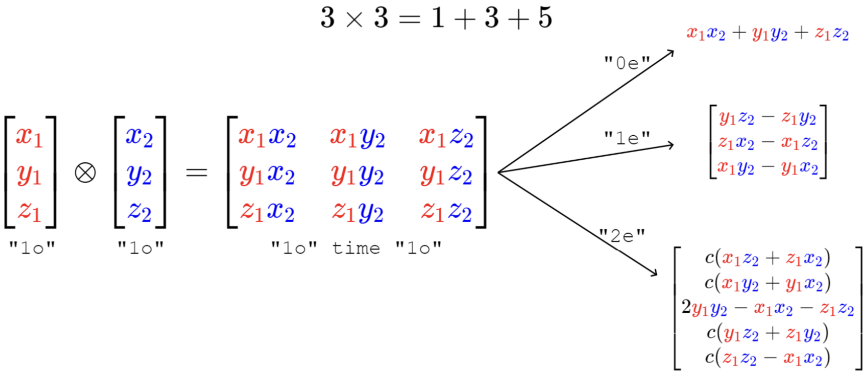
A function $\mathcal{L} : \mathcal{X} \to \mathcal{Y}$ is equivariant with respect to a group G and group representations $D^{\mathcal{X}}$ and $D^{\mathcal{Y}}$ if for all $g \in G$,

$$\mathcal{L} \circ D^{\mathcal{X}}(g) = D^{\mathcal{Y}}(g) \circ \mathcal{L}$$



Source: Equivariant Models — Open Catalyst Intro Series

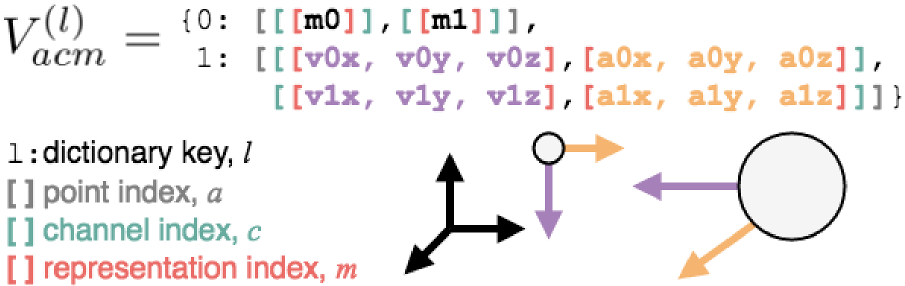
Tensor product reduction



Source: Chaoran Cheng blog

Clebsch-Gordan coefficients are used to calculate tensor products.

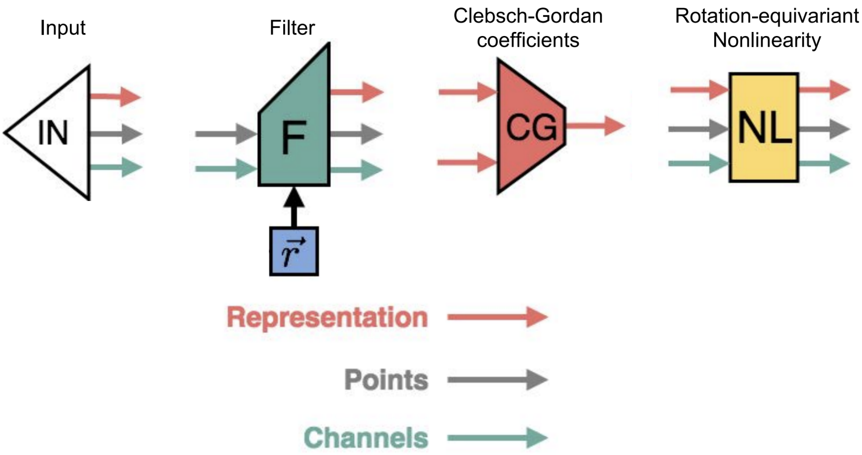
TFN Architecture



Source: NeurIPS Workshop presentation

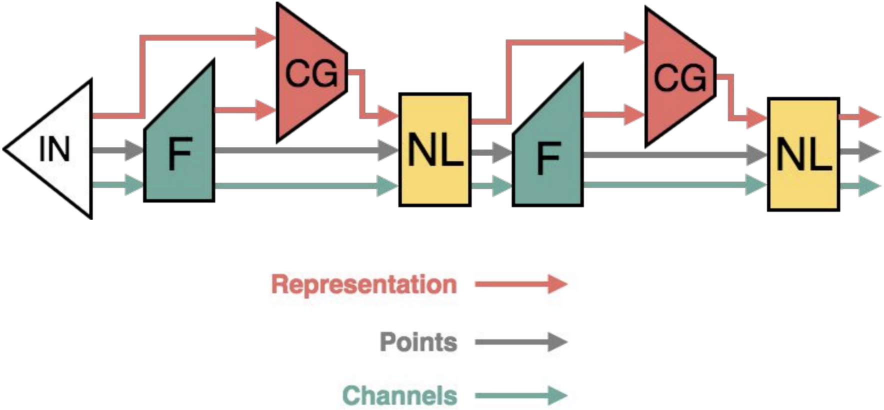
Inputs and outputs of a layer: 3D coordinates of points and features at those points(scalars, vectors, and higher-order tensors).

TFN Architecture



Source: NeurIPS Workshop presentation

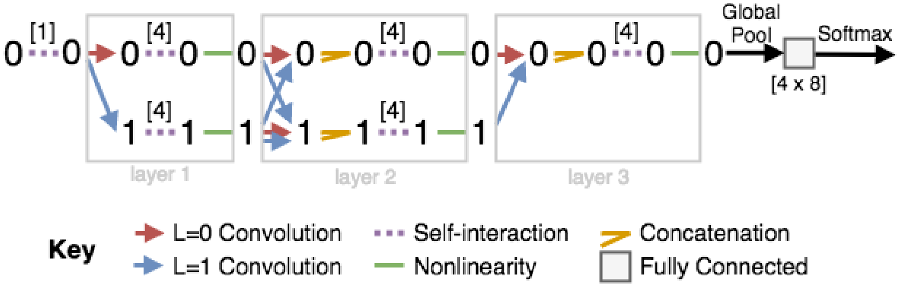
TFN Architecture



Source: NeurIPS Workshop presentation

Filters are the products of a learnable radial function and a spherical harmonic

TFN Architecture



Source: Original paper

Proving equivariance

- **Permutation** equivariance (by design)
- **Translation** equivariance (use only differences between vectors)
- **Rotation** equivariance (see below)

Proving equivariance

Definition

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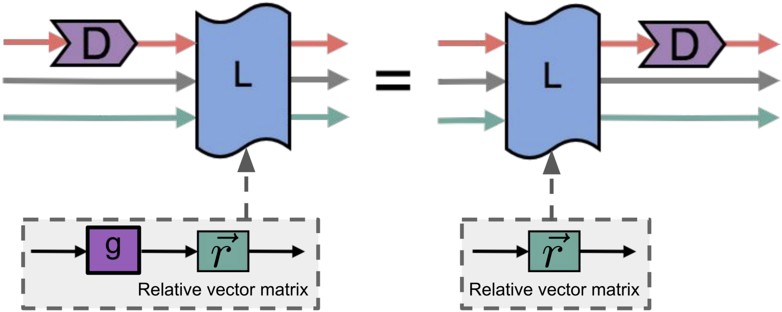
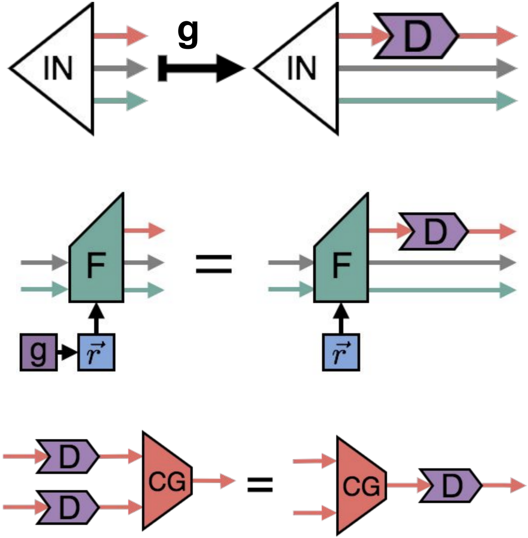
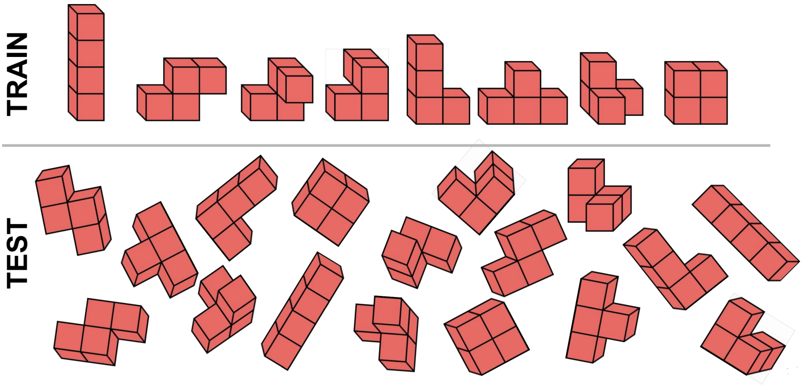


Proving equivariance



Source: NeurIPS Workshop presentation

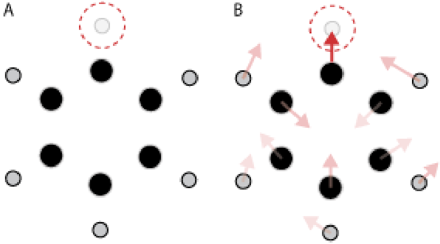
3D Tetris



Source: NeurIPS Workshop presentation

- Perfect classification score on rotated and translated figures after training on the figures in single orientation
- Networks relying only on distances and angles can not distinguish mirrored shapes, but TFN can

Molecular structures



Source: original paper

- Task is to locate randomly removed atom
- Output is a vector pointing to the missing point and a confidence probability for each point
- Over 95% prediction accuracy for structures with 20-30 atoms

Discussion

Pros

- data augmentation not needed
- universal architecture for equivariant deep learning on atomic systems and 3D graphs
- non-scalar features improve expressive power

Cons

- $O(L^6)$ complexity, where L is rotation order
- Computing spherical harmonics on the fly can be slow

References and credits for all illustrations

- Thomas, Nathaniel and Smidt, Tess and Kearnes, Steven and Yang, Lusann and Li, Li and Kohlhoff, Kai and Riley, Patrick (2018)
  Tensor Field Networks: Rotation- and Translation-Equivariant Neural Networks for 3D Point Clouds
- Github TNF
  https://github.com/tensorfieldnetworks/tensorfieldnetworks
- Github Euclidean neural networks
  https://github.com/e3nn/e3nn
- Chaoran Cheng
  Blog post
  https://github.com/e3nn/e3nn