Equivariant Graph Neural Networks

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Outline

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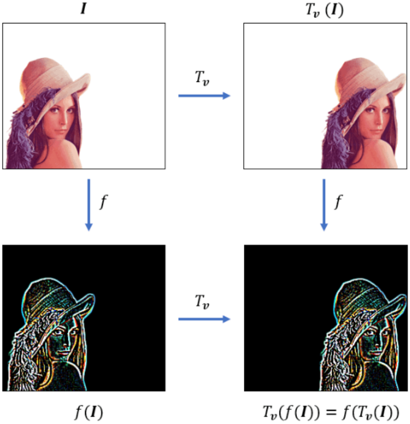

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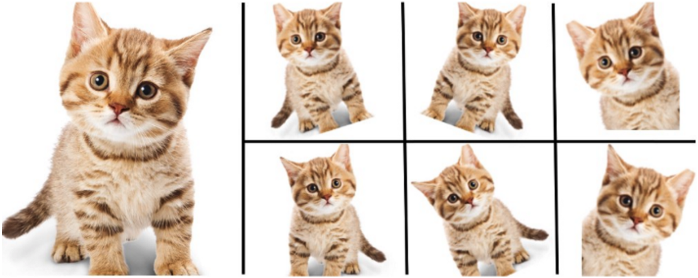
- A cat is a cat no matter how you look at it.



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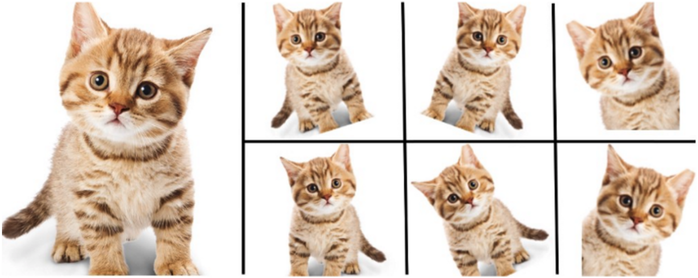
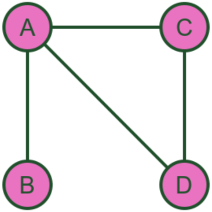


- It is acceptable to assume that being invariant to the rotation of the cat is a good property for a classification network.

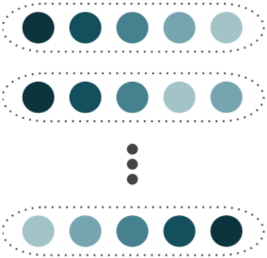
Motivation

- Our focus today is on sets and graph data.



Simple graph

	A	B	C	D
A	0	1	1	1
B	1	0	0	0
C	1	0	0	1
D	1	0	1	0



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  1. The symmetries of the data:
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  2. The space of functions learnable by the network:
     Are we fully utilizing the space of functions that are equivariant

The Permutation Group S_n

- The permutation group S_n is the group of all permutations of n elements.
- It has $n!$ elements, representing the $n!$ ways to order n elements.
- Given a set $X = \{x_1, x_2, \ldots, x_n\}$, a permutation $\pi \in S_n$ is a bijection $\pi : X \to X$
- e.g. $x = (x_1, x_2, x_3)$, and $\pi = (1, 2, 3) \in S_3$ is the permutation that maps $1 \to 2$, $2 \to 3$ and $3 \to 1$.
- We denote the **action** of π on x as $\pi x = (x_3, x_1, x_2)$.

Permutation Invariance

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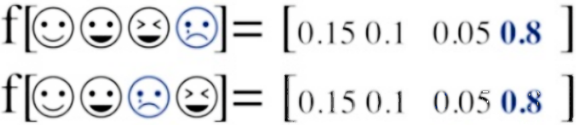

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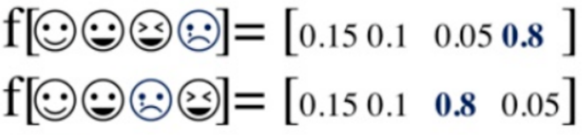

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- An invariant neural network is a function $f : \mathbb{R}^{n \times d} \to \mathbb{R}^{d'}$ such that $f(X) = f(\boldsymbol{P}X)$.
- An equivariant neural network is a function $f : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d'}$ such that $\boldsymbol{P}f(X) = f(\boldsymbol{P}X)$.

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- A permutation matrix $\boldsymbol{P} \in \mathbb{R}^{n \times n}$ acts on the adjacency matrix A and the feature matrix X.

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$$gL(\sigma(L(\sigma(\dots L(x)\dots)))) = gf(x)$$

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$\square$

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- Recall the two properties we mentioned earlier (symmetries of the data and the space of functions learnable by the network).
- *DeepSets* is an architecture that is equivariant to set permutations and is maximmally expressive in the space of permutation equivariant functions.
- We are going to see the construction and prove it satisfies equivariance and expressiveness.

DeepSets Layer

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Consider a set $x = \{x_1, x_2, \ldots, x_n\}$, where $x_i \in \mathbb{R}$.
A *DeepSets* layer is defined as

$$L(x) = \lambda \mathrm{I}\mathbf{x} + \mathbf{x}\mathbf{1}$$

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- It is easy to see that ϕ is permutation invariant, and thus f is permutation invariant.
- For a classification network, take some classification module ρ (e.g. an MLP), and define the final network as:

$$h(x) = \rho(f(x))$$

DeepSets Network

- Notice that the network is only defined for sets with elements in $\mathbb{R}$.

- We can extend this to a set $X \in \mathbb{R}^{n \times d}$ by defining L as:

$$L(x) = \mathbf{X} W_1 + \mathbf{1}\mathbf{1}^T \mathbf{X} W_2$$

- Ths keeps the general structure of the layer: a linear transformation of the distinct elements of the set summed with the mean of the set.

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Proof.

H.W. (using standard results from approximation theory). □

Conclusion

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Thank You!