# Equivariant Graph Neural Networks

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# Outline

1. Motivation
2. Mathematical Backoground
3. Deep Sets

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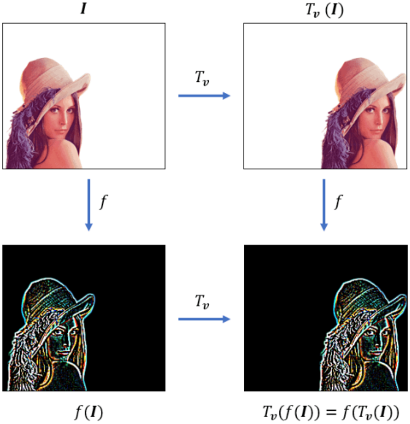

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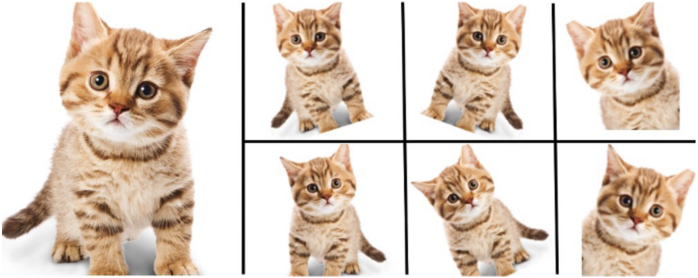
- A cat is a cat no matter how you look at it.



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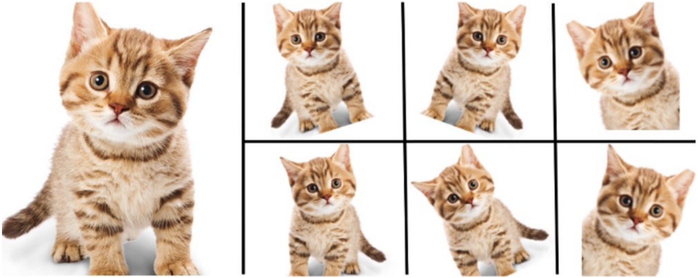
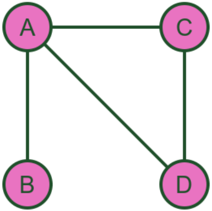


- It is acceptable to assume that being invariant to the rotation of the cat is a good property for a classification network.

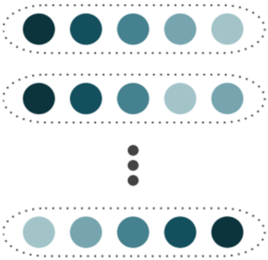
# Motivation

- 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:
     What inherent structure should our model be oblivious to?
  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 $\pi$ on $x$ as $\pi x = (x_3, x_1, x_2)$.

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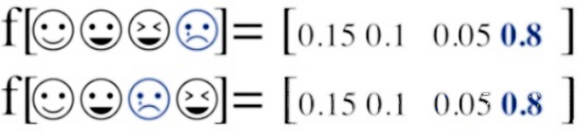

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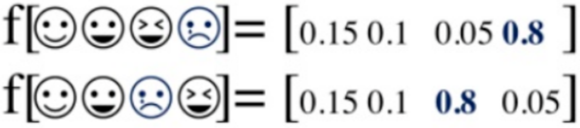

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- An invariant neural network is a function $f : \mathbb{R}^{n \times d} \to \mathbb{R}^{d`}$ such that $f(X) = f(\boldsymbol{P}X)$.
- An equivariant neural network is a function $f : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d`}$ such that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

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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 $X$.

# Equivariant Network Construction

**Theorem**

*Let $L$ be a linear equivariant layer, and let $f$ be a neural network constructed be stacking $L$ and non-linearities $\sigma$. Then $f$ is permutation equivariant.*

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$$f(gx) = L(\sigma(L(\sigma(\ldots L(gx)\ldots)))) = L(\sigma(L(\ldots g\sigma(L(x))\ldots))) = \ldots$$

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

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$$h(gx) = \phi(f(gx)) = \phi(gf(x)) = \phi(f(x)) = h(x)$$

$\square$

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- A seminal work in the field of equivariant neural networks.
- 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

- We saw a general structure of an invariant and equivariant network.
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## Definition

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

$$L(x) = \lambda \mathrm{I}\mathbf{x} + \mathbf{x1}$$

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

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- It is easy to see that $\phi$ is permutation invariant, and thus $f$ is permutation invariant.
- For a classification network, take some classification module $\rho$ (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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H.W. (using standard results from approximation theory). □

# Conclusion

- end

Thank You!