Equivariant Graph Neural Networks

Kfir Eliyahu Ben Eliav Jonathan Kouchly

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Outline

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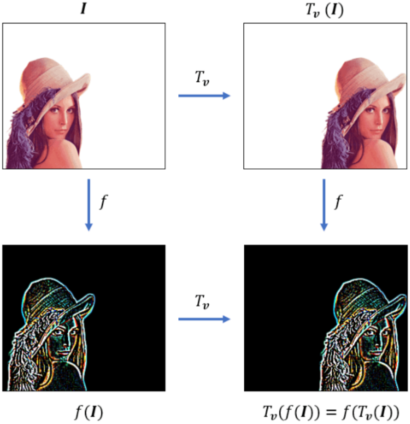

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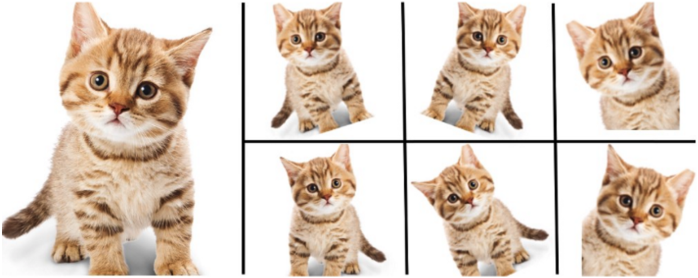
- A cat is a cat no matter how you look at it.



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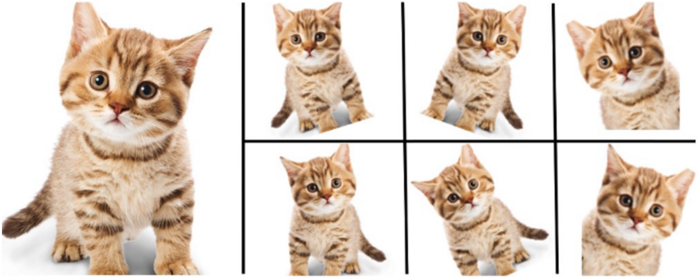
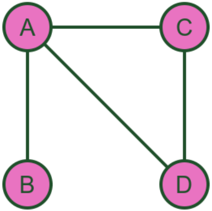


- It is acceptable to assume that being invariant to the rotation of the cat is a good property for a classification network.

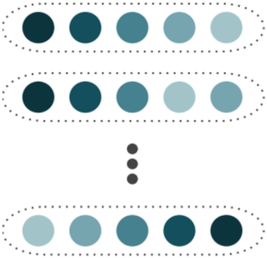
Motivation

- 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



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 $\pi x = (x_3, x_1, x_2)$.

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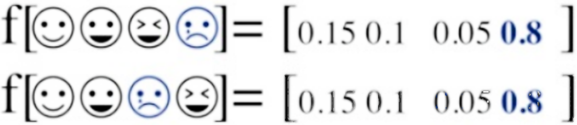

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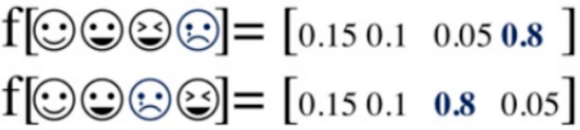

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- An equivariant neural network is a function $f : \mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d`}$ such that $\boldsymbol{P}f(X) = f(\boldsymbol{P}X)$.

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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.
- The action of $\boldsymbol{P}$ on (A, X) is $(\boldsymbol{P}^{\boldsymbol{T}} A \boldsymbol{P}, \boldsymbol{P} X)$.

Conclusion

- end

Thank You!