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E(n) equivariant graph neural networks & E(n) equivariant graph normalizing flows

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This paper introduces a new model to learn graph neural networks equivariant to rotations, translations, reflections and permutations called E(n)-Equivariant Graph Neural Networks (EGNNs). In contrast with existing methods, our work does not require computationally expensive higher-order representations in intermediate layers while it still achieves competitive or better performance. In addition, whereas existing methods are limited to equivariance on 3 dimensional spaces, our model is easily scaled to higher-dimensional spaces. We demonstrate the effectiveness of our method on dynamical systems modelling, representation learning in graph autoencoders and predicting molecular properties.