Covariant Compositional Neural Networks For Learning Graphs

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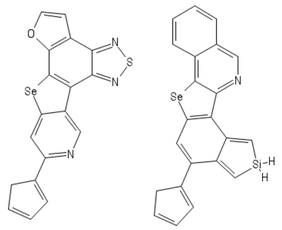
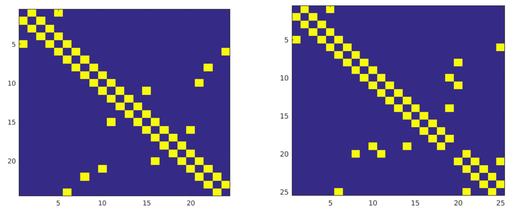
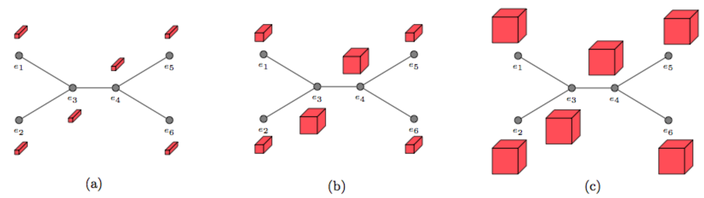
Molecular representation

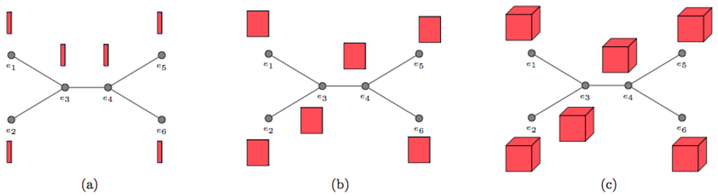




Higher order Message Passing

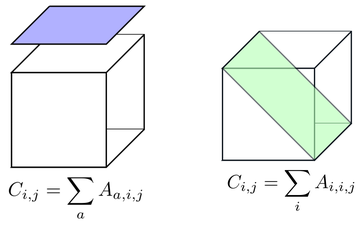


Tensor activations for our CCN-2D architecture applied to a C_2H_4 molecular graph. The tensor activations of each vertex in a CCN 2D model are shown after 0, 1, and 2 rounds of message passing in (a), (b) and (c). Here the rows and columns correspond to the size of the receptive field, whereas the depth of the tensor is determined by the number of channels.



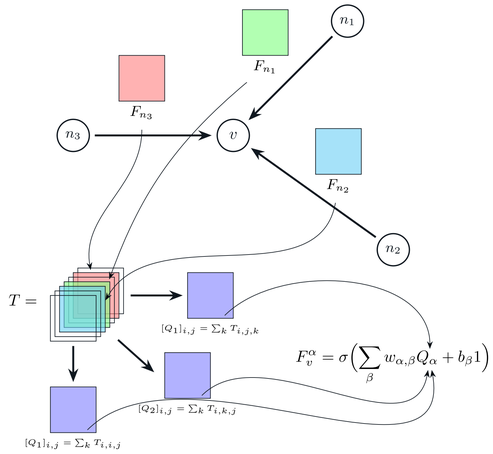
Geometry of the tensor activations in zeroth (CCN 0D), first (CCN 1D), and second (CCN 2D) order message passing algorithms. Vertices have a vector (zeroth order), matrix (first order), and second order tensor representations corresponding as shown in (a), (b), and (c).

Tensor Contractions



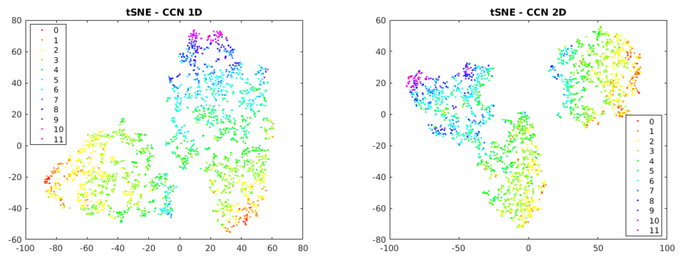
$$C_{i,j} = \sum_a A_{a,i,j} \qquad C_{i,j} = \sum_i A_{i,i,j}$$

General Structure



Molecular representation produced by CCNs

2D t-SNE visualization of learned CCNs molecular features on Harvard Clean Energy Project (HCEP) dataset:



Result

MAE and RMSE results of each model on predicting the Power Conversion Efficiency (PCE) for graphs on the test set of HCEP. Lower values are better.

	Test MAE	Test RMSE
Lasso	0.867	1.437
Ridge regression	0.854	1.376
Random forest	1.004	1.799
Gradient boosted trees	0.704	1.005
WL graph kernel	0.805	1.096
Neural graph fingerprints	0.851	1.177
PSCN	0.718	0.973
CCN 1D	**0.216**	**0.291**
CCN 2D	**0.340**	**0.449**

Regression results of CCN-1D architecture applied to QM9(b). A comparison between CCN prediction error and DFT error known as "chemical accuracy."

Target	CCNs	DFT error	Physical unit
alpha	**0.19**	0.4	Bohr^3
Cv	**0.06**	0.34	cal/mol/K
G	**0.05**	0.1	eV
gap	**0.11**	1.2	eV
H	**0.05**	0.1	eV
HOMO	**0.08**	2.0	eV
LUMO	**0.07**	2.6	eV
mu	0.43	**0.1**	Debye
omega1	**2.54**	28	cm^{-1}
R2	5.03	-	Bohr^2
U	**0.06**	0.1	eV
U0	**0.05**	0.1	eV
ZPVE	**0.0043**	0.0097	eV

Reference

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