

ML4Science Hackathon

Happy Holmes

K. Ganesh Chandan, Kartik Majila



Inputs	Representation	Architecture	Loss
SMILES	SMILES2vec	SVM	MSE/ RMSE
		Linear layers	
		ResNet	Metrics
	Fingerprints	Transformer Decoder	
		MPNN	

Architecture

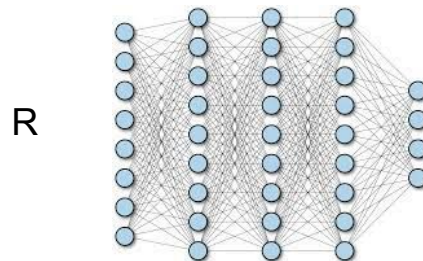
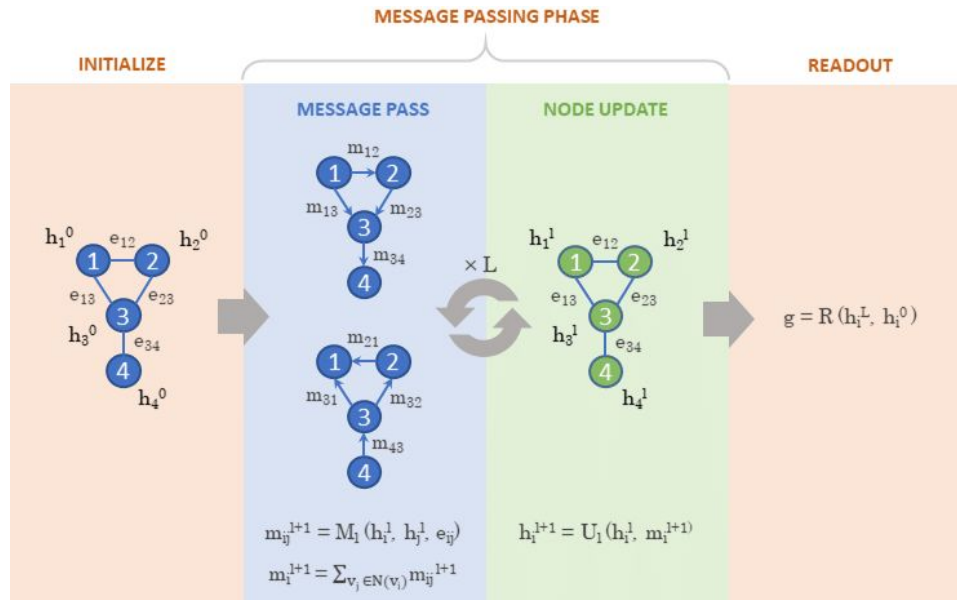
MPNN (Message Passing Neural Networks) based approach produced the best results.

Given a Graph G with node features such as atom type, #bonds, charge etc and bond features (e_{vw}).

$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

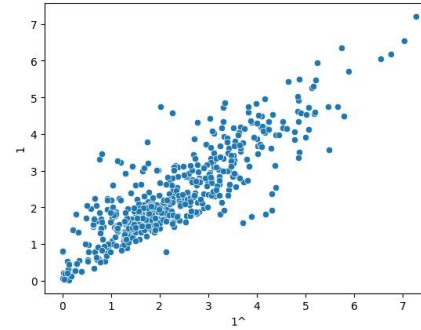
$$\hat{y} = R(\{h_v^T | v \in G\})$$



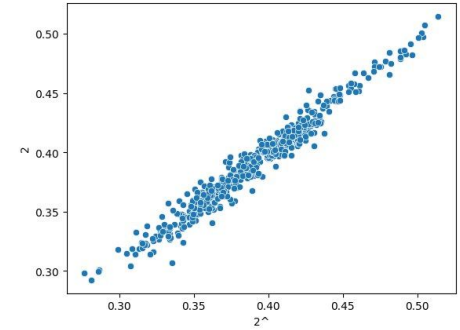
Results

Property	R2	Pearson R
1	0.690	0.860
2	0.958	0.981
3	0.921	0.961
4	0.970	0.985

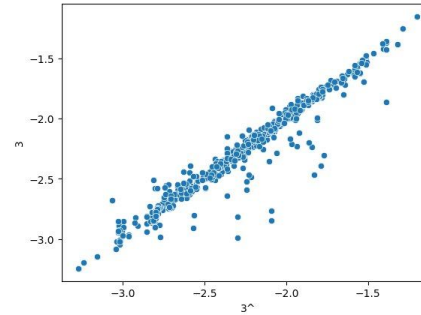
Property 1



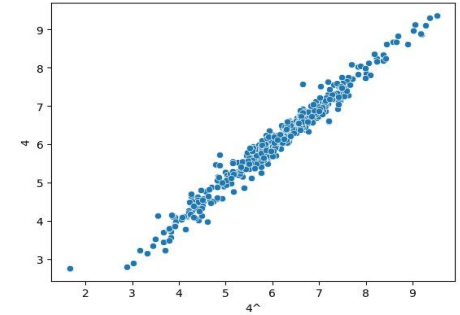
Property 2



Correlation plots



Property 3



Property 4