3D Infomax improves GNNs for Molecular Property Prediction

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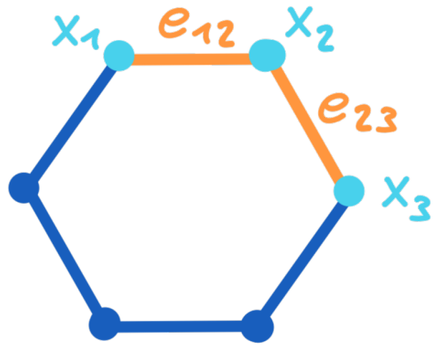
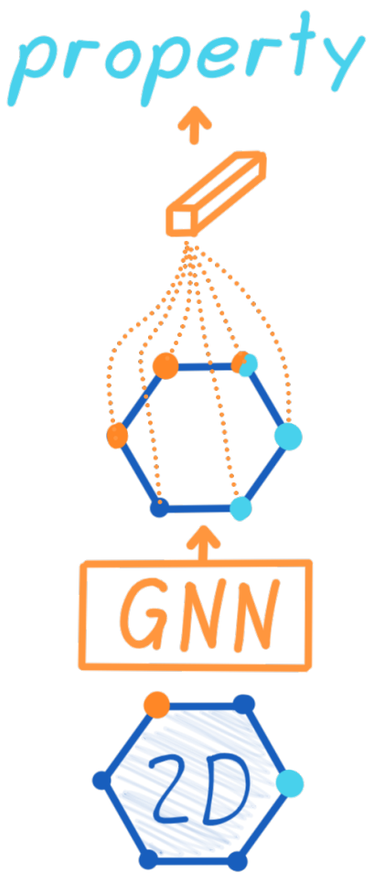
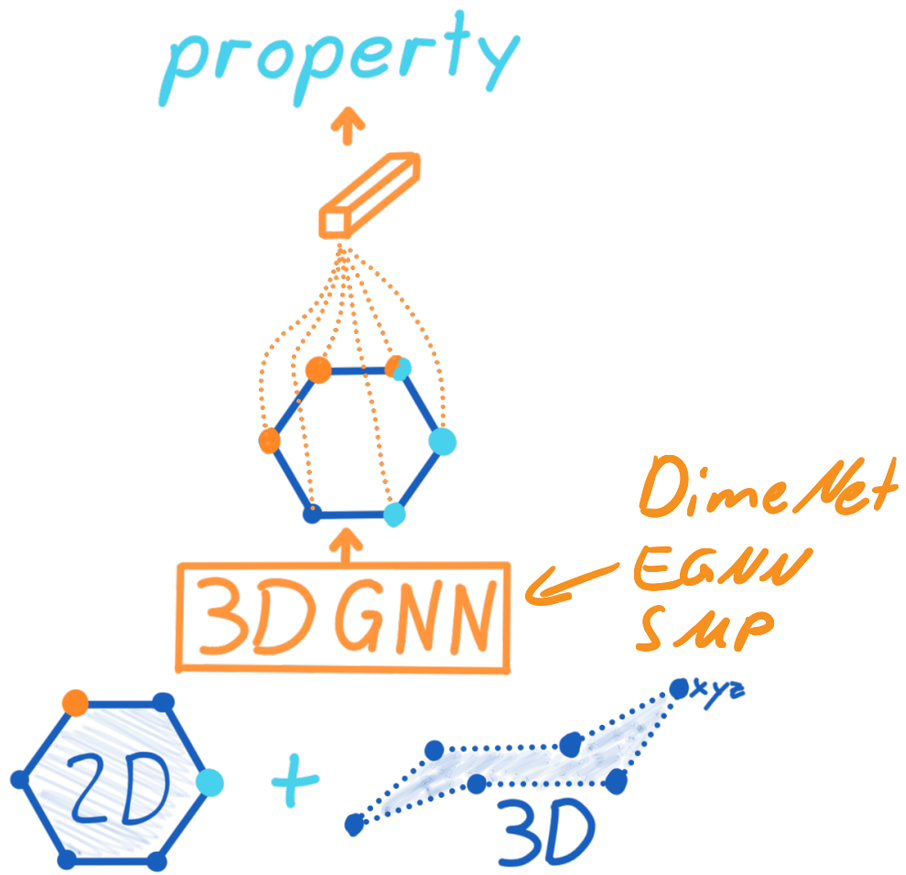
2D Graph



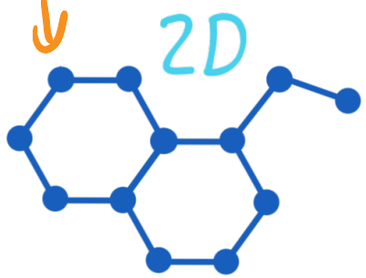
3D Conformers

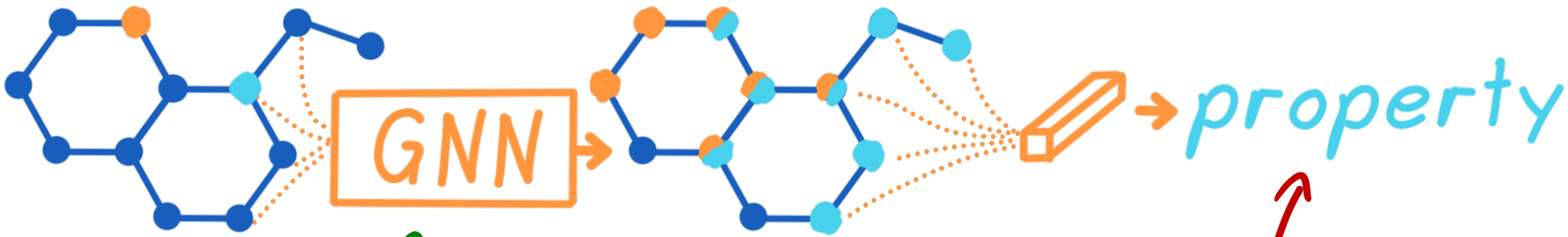


vs.



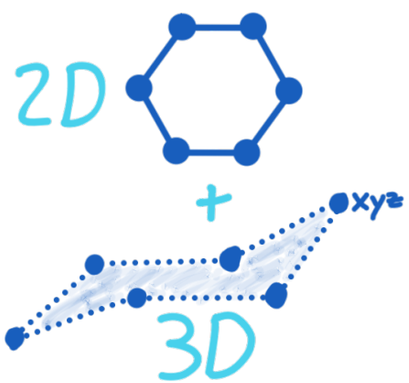
property ?



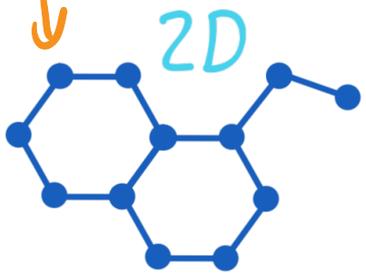


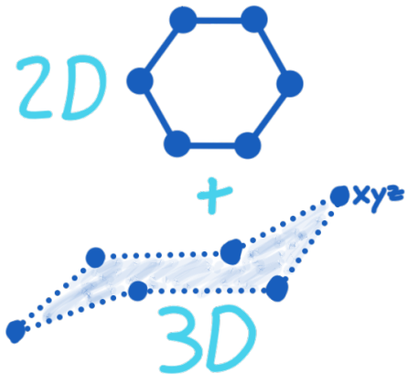
fast

2D accuracy

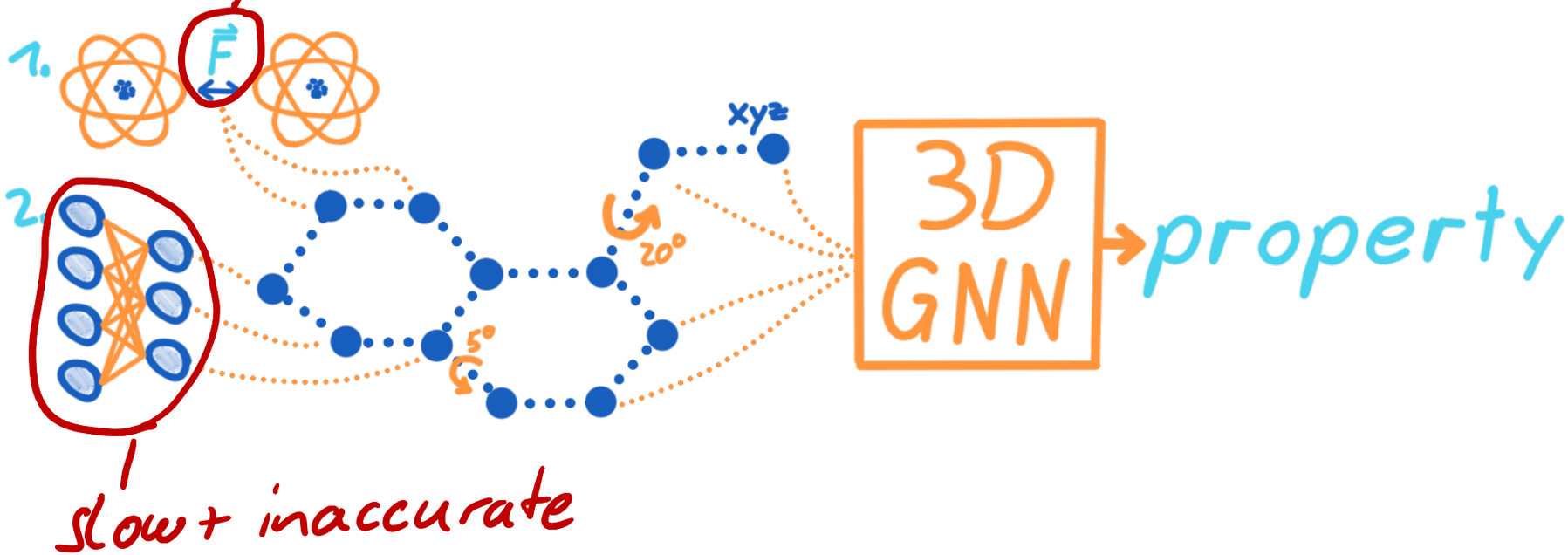


property?



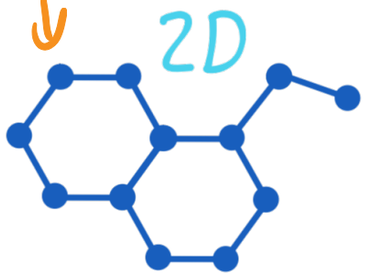


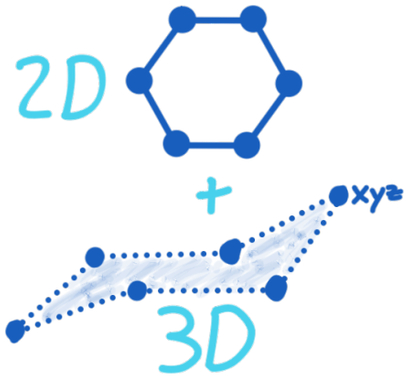
very slow



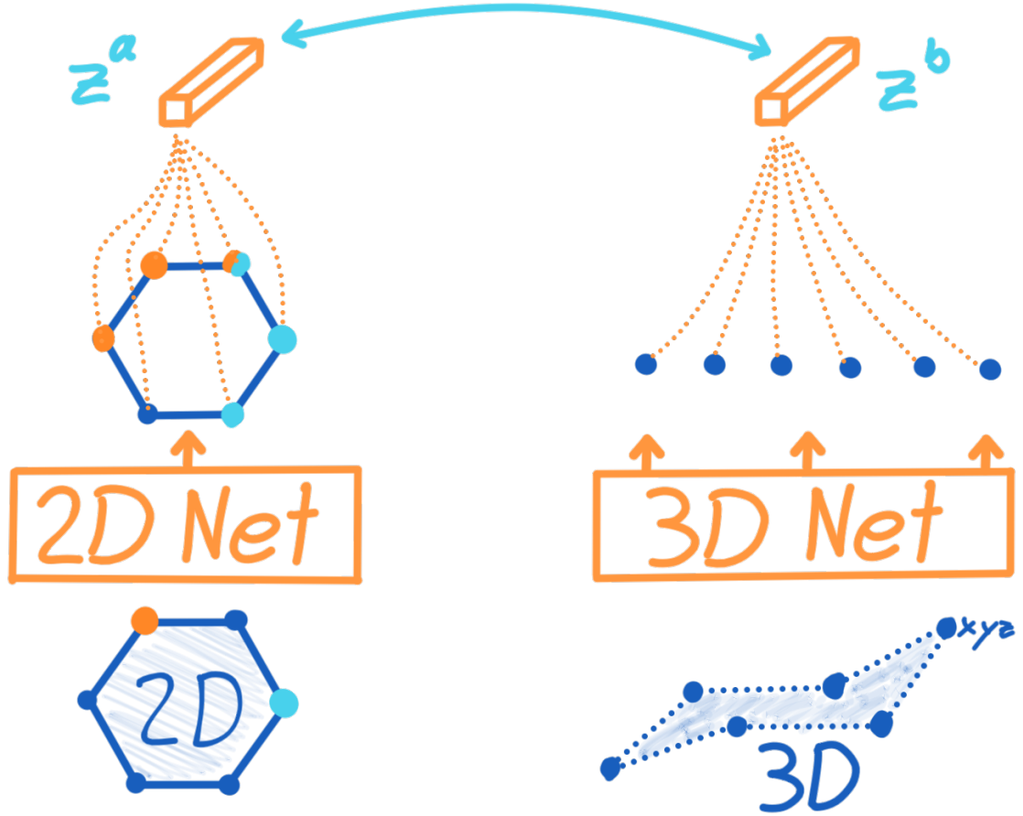
slow + inaccurate

property ?



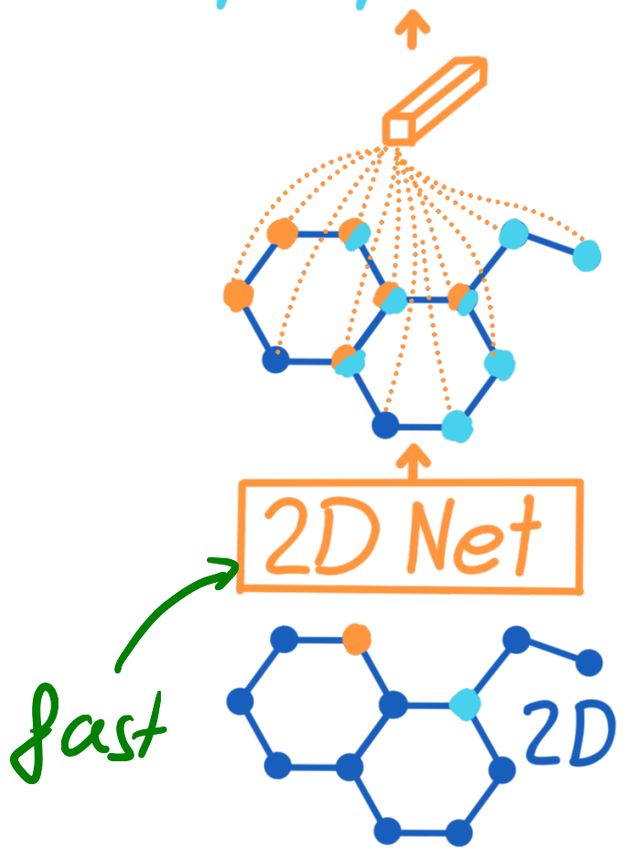


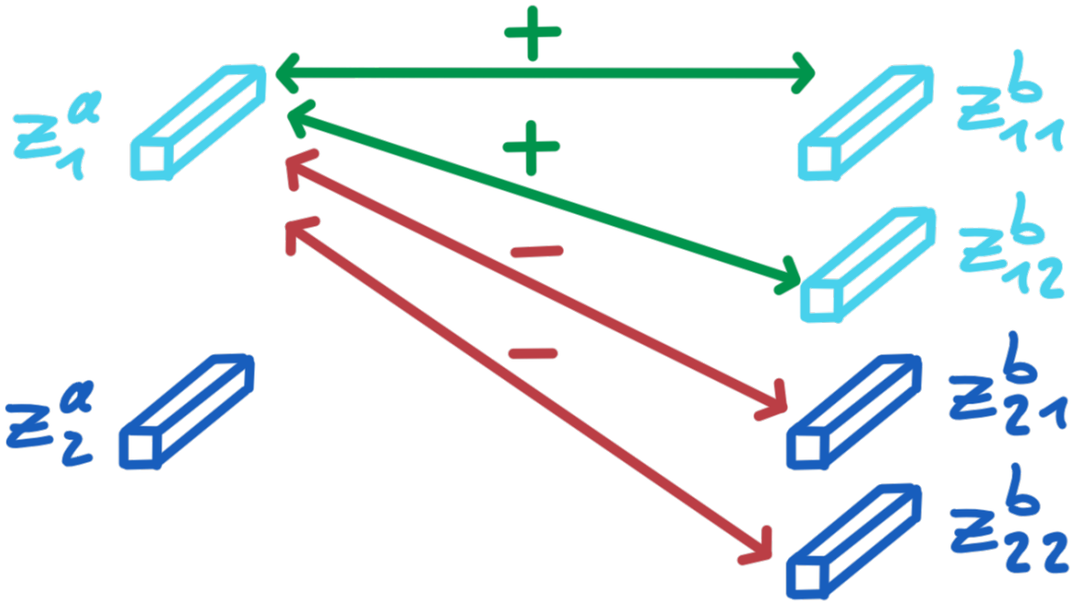
1. maximize MI

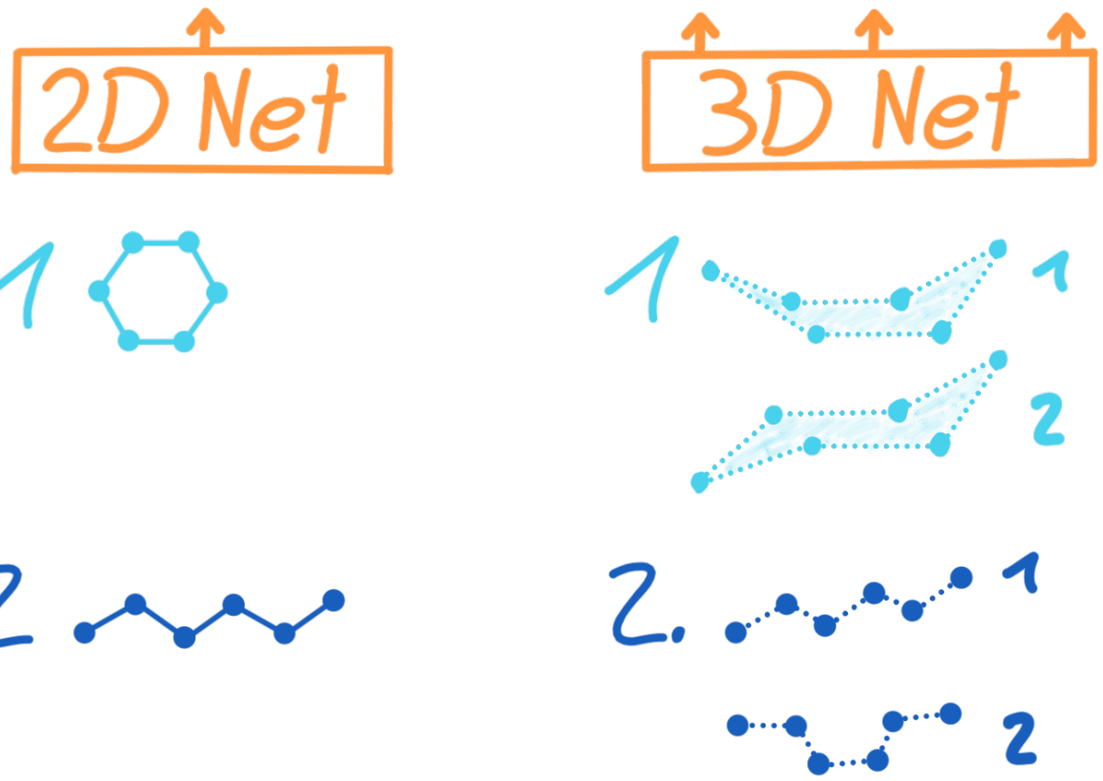


more accurate

2. property







for batchsize N
and c conformers

$$L_i = -\log \frac{\sum_{j=1}^{c} e^{sim(z_i^a, z_{i,j}^b)}}{\sum_{k=1}^{N} \sum_{j=1}^{c} e^{sim(z_i^a, z_{k,j}^b)}}$$

pre-training datasets

Target	Rand Init	Pre-training baselines GraphCL	Pre-training baselines PropPred	Our 3D Infomax QM9	Our 3D Infomax Drugs	Our 3D Infomax QMugs	RDKit SMP	*True 3D SMP*
μ	0.4133±0.003	0.3937	0.3975	**0.3507**	**0.3512**	0.3668	0.4344	0.0726
α	0.3972±0.014	0.3295	0.3732	0.3268	0.2959	**0.2807**	0.3020	0.1542
homo	82.10±0.33	79.57	93.11	**68.96**	70.78	70.77	82.51	56.19
lumo	85.72±1.62	80.81	99.84	**69.51**	71.38	78.10	80.36	43.58
gap	123.08±3.98	120.08	131.99	**101.71**	102.59	103.85	114.24	85.10
r2	22.14±0.21	21.84	29.21	**17.39**	18.96	18.00	22.63	1.51
ZPVE	15.08±2.83	12.39	11.17	7.966	9.677	12.06	**5.18**	2.69
c_v	0.1670±0.004	0.1422	0.1795	0.1306	0.1409	**0.1208**	0.1419	0.0498