ASGN: an Active Semi-supervised Graph Neural Network for Molecular Property Prediction

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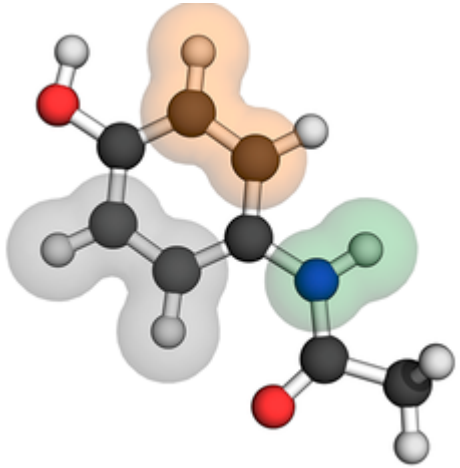
Introduction

- Our task: Molecular property prediction



Input: Molecule

Properties:
U0 (Atomization energy at 0K)
U (Atomization energy at room temperature)
G (Free energy of atomization)
HOMO
LUMO

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Output: Properties

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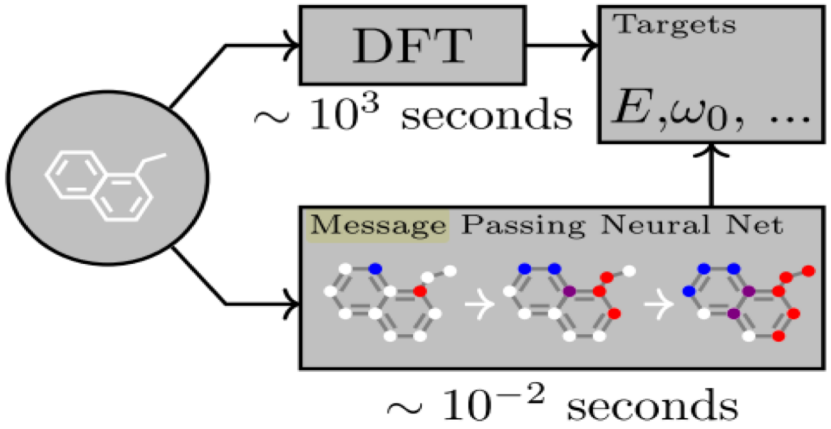
- Applications: Drug discovery, material engineering…

Introduction



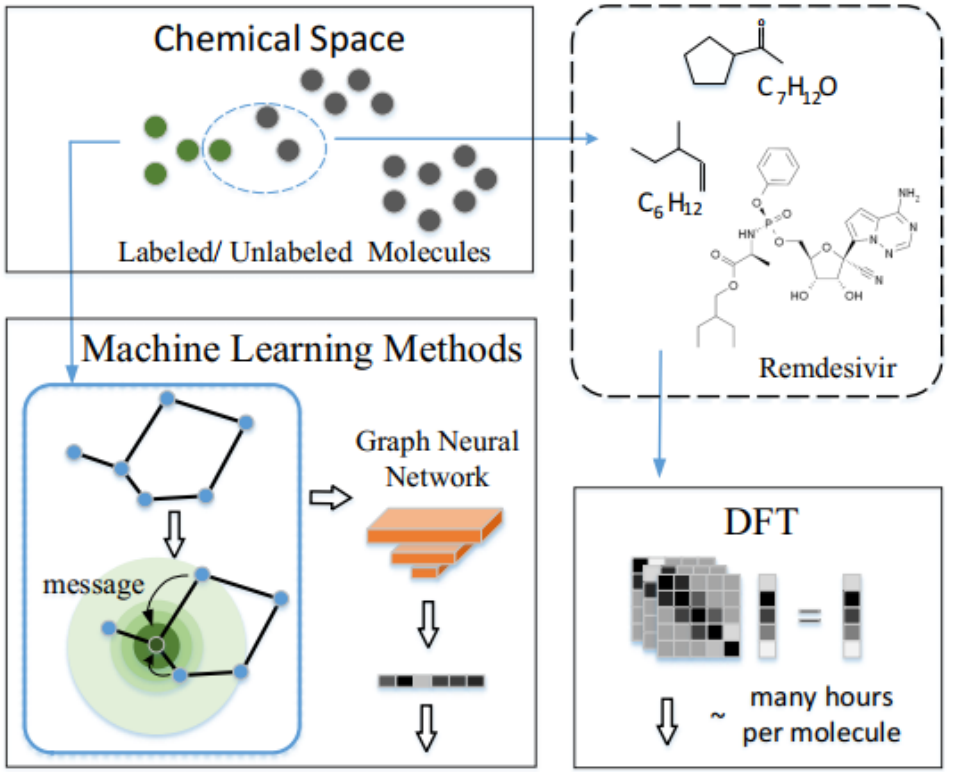
- Measure properties by experiments
- Density Functional Theory
- Modern: Machine learning methods

- A molecule as a graph($G = (V, E)$)
- Pass it to a message passing Graph Neural Networks
- Get the result after 10^{-2} seconds

Introduction

- ML model is data hungry, requires many **labelled** data
- Unlabelled data (molecular graph) is everywhere
- Labelling is expensive
- Our goal: label efficient model

  $f: G \rightarrow R^n$
- Our Solution: **Active semi-supervised learning**



Property	Value
HOMO	-0.38eV
LUMO	0.08eV
U	-196.43eV

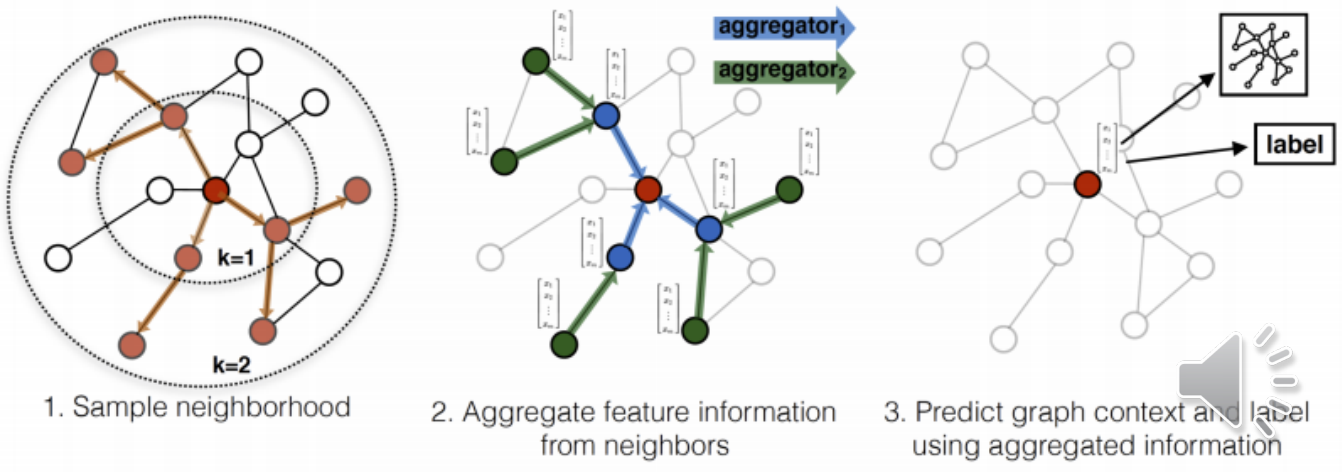
Preliminaries—GNN for molecular property prediction

- Pass message from nodes to nodes
- Aggregate node to get the graph representation

$$z_i^{l+1} = \sigma(\boldsymbol{W}^l \cdot \mathrm{AGG}(z_i^l, \{\boldsymbol{e}(v_i, v_j) : v_j \in \boldsymbol{N}(v_i)\})),$$

$$z_{\mathcal{G}} = \mathrm{Pool}(\{z_i^L : v_i \in \mathcal{V}\}).$$

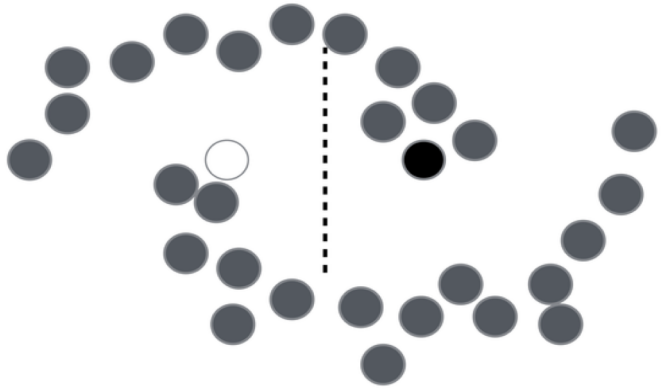
GraphSAGE: A popular MPNN



Related Work—Semi-supervised Learning

- Number of labeled data ≪ unlabeled data
- How can we make use of unlabeled data ?

- Create pseudo labels and predict them!

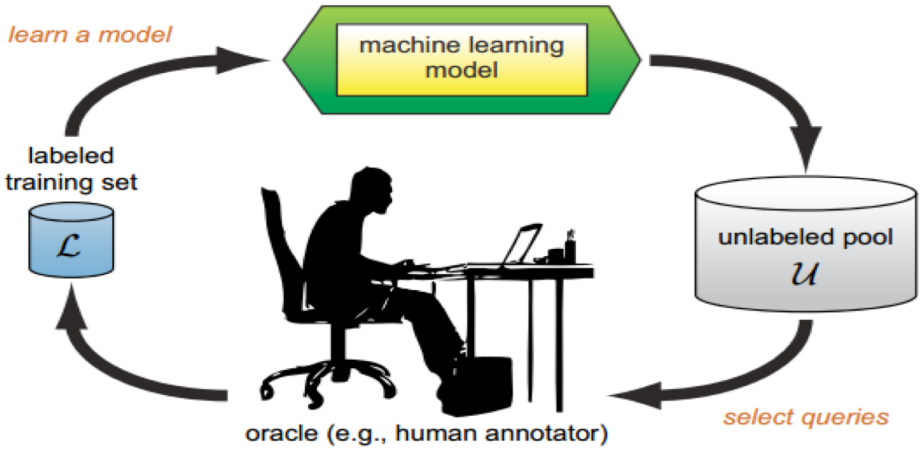


The influence of unlabeled data

Related Work—Active Learning

- Active learning is to improve the value of these labels
- Choose data that is helpful to the model and retrain the model
- Solution: most **representative** and **diversified** subset in the dataset

Framework of active learning.

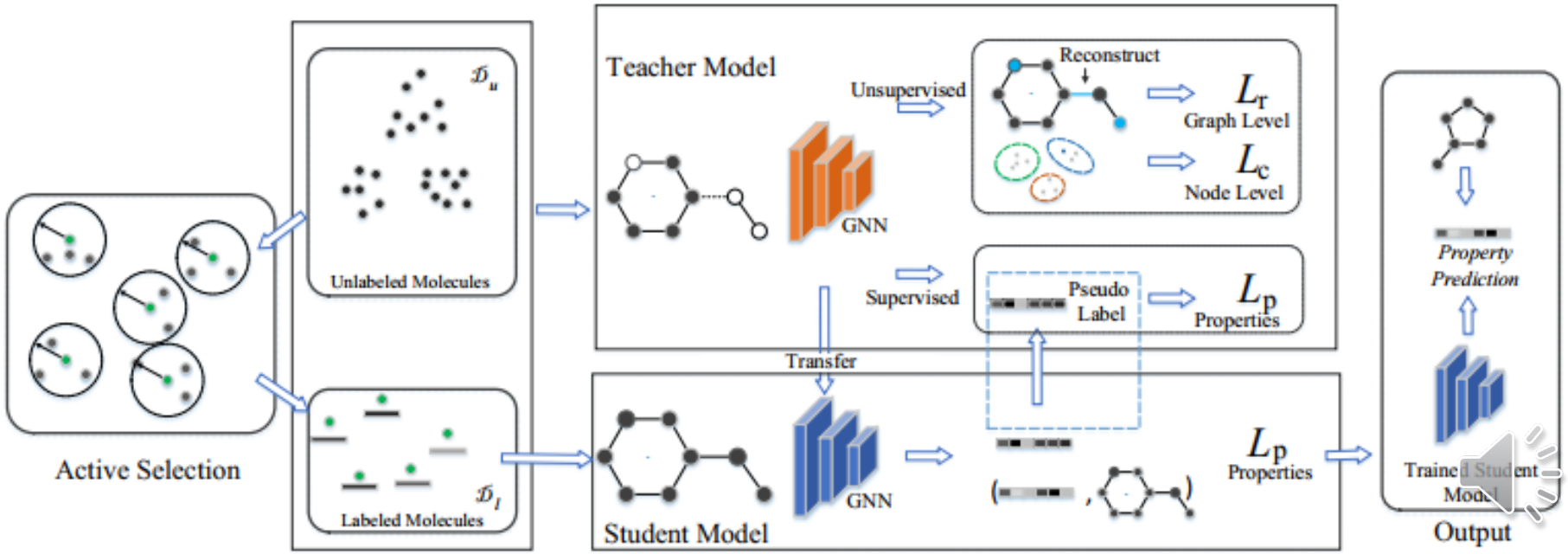


Challenges

- Data structure of molecules is different from traditional images/text/…
- Few works on semi-supervised learning of molecules
- Low training efficiency because of the imbalance data

Model Framework

- Two GNN, a teacher and a student model
- Train the teacher with semi-supervised learning
- Train the student with fully supervised learning for downstream property prediction

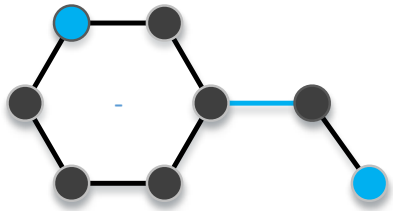


Teacher Model

- Local(node) level pseudo labels—reconstruction
- We believe a good property predictor is able to recover the atom itself from its embedding
- A loss function to reconstruct atom and their distance

$$\mathcal{L}_r = -\mathbb{E}_{v_i \sim \mathcal{V}} \left[\sum_{m=1}^{K_n} f_{im} \log(g_{\theta_n}(z_i)) \right] - \mathbb{E}_{e_{ij} \sim \mathcal{E}} \left[\sum_{m=1}^{K_e} e_{ijm} \log(g_{\theta_e}(z_i, z_j)) \right],$$

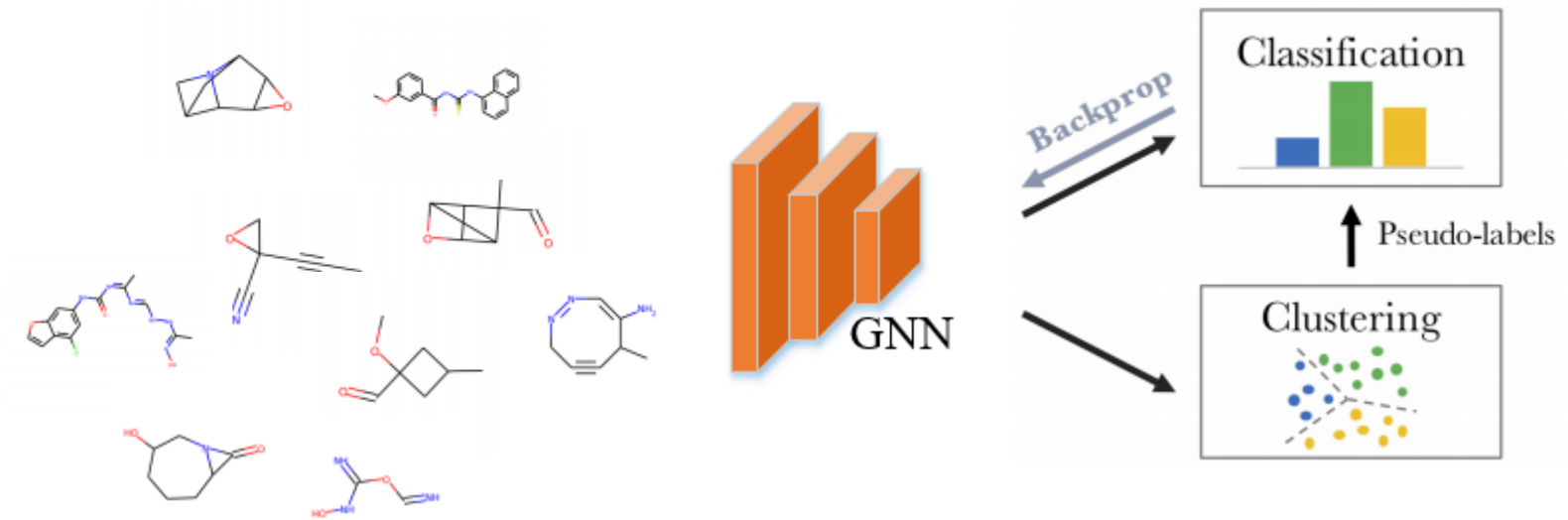
GNN



Sample and reconstruct

Teacher Model

- Global level pseudo labels—clustering loss
- Implicit clustering via optimal transport
- Predict these clusters and repeat iteratively



Teacher model

- Summary of the teacher model
- Add these three loss terms to guide its optimization

(1).property loss

(2).reconstruction loss

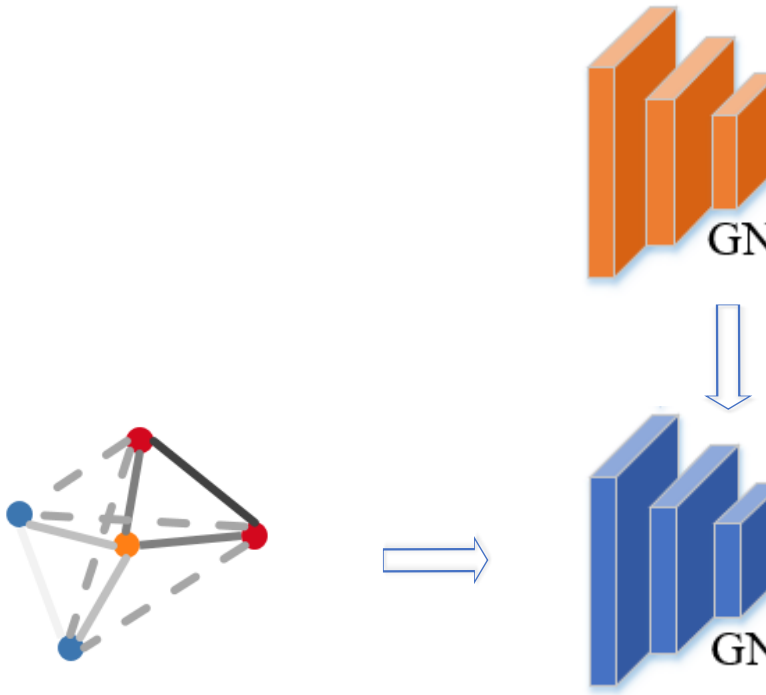
(3).clustering loss

$$\mathcal{L}_t = \sum_{\mathcal{G} \in \mathcal{D}_l} \mathcal{L}_p + \sum_{\mathcal{G} \in \mathcal{D}_u \cup \mathcal{D}_l} \mathcal{L}_r + \sum_{\mathcal{G} \in \mathcal{D}_u \cup \mathcal{D}_l} \mathcal{L}_c .$$

D_l:labeled data D_u:unlabeled data

Student model

- Weight transfer from the teacher model
- Fine tune on property prediction task
- Accelerate convergence and alleviate loss conflict



Property	Value
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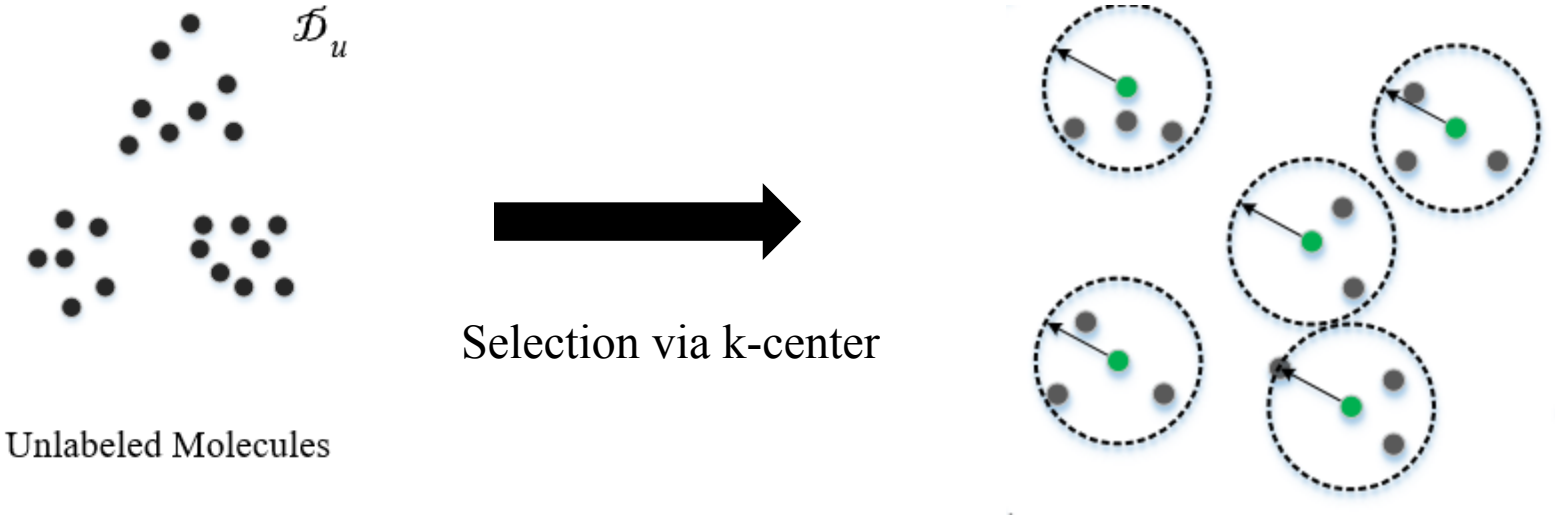
Active Data Selection

- Choose most informative data
- K center to choose one molecule from one cluster
- Add them into the labeled dataset

- Repeat the process until label budget is used up



Experiments

- Datasets

(1) QM9: 130,000 molecules, <9 heavy atoms

(2) OPV: 100,000 medium sized molecules

- Properties (All calculated by DFT)

(1) QM9:

U_0	U	G	H	C_v	HOMO	LUMO	gap	ZPVE	R^2	μ	α
eV	eV	eV	eV	Cal/MolK	eV	eV	eV	eV	Bohr^2	Debye	Bohr^3

(2) OPV:

HOMO	LUMO
Hatree	

Experiments

- Effectiveness, compare error on test dataset
- Baselines

(1).Supervised

(2).Mean-teachers

(3).InfoGraph

Experiments

- Results

Properties	U_0	U	G	H	C_v	HOMO	LUMO	gap	ZPVE	R^2	μ	α
Unit	eV	eV	eV	eV	Cal/MolK	eV	eV	eV	eV	Bohr^2	Debye	Bohr^3
Supervised	0.3204	0.2934	0.2948	0.2722	0.2368	0.1632	0.1686	0.2475	0.0007	10.05	0.3201	0.5792
Mean-Teachers	0.3717	0.2730	0.2535	0.2150	0.2036	0.1605	0.1686	0.2394	0.00054	5.22	0.3488	0.5792
InfoGraph	0.1410	0.1702	0.1592	0.1552	0.1965	0.1605	0.1659	0.2421	0.00036	4.92	0.3168	0.5444
ASGN (Ours)	**0.0562**	**0.0594**	**0.0560**	**0.0583**	**0.0984**	**0.1190**	**0.1061**	**0.2012**	**0.00017**	**1.38**	**0.1947**	**0.2818**

Results on QM9

Property	HOMO	LUMO
Unit	Hatree	
Supervised	0.080	0.078
Mean-Teacher	0.078	0.075
InfoGraph	0.077	0.076
ASGN (Ours)	**0.059**	**0.057**

Results on OPV

Experiments

- Efficiency, the label efficiency at a certain error
- Baselines:

(1).Random

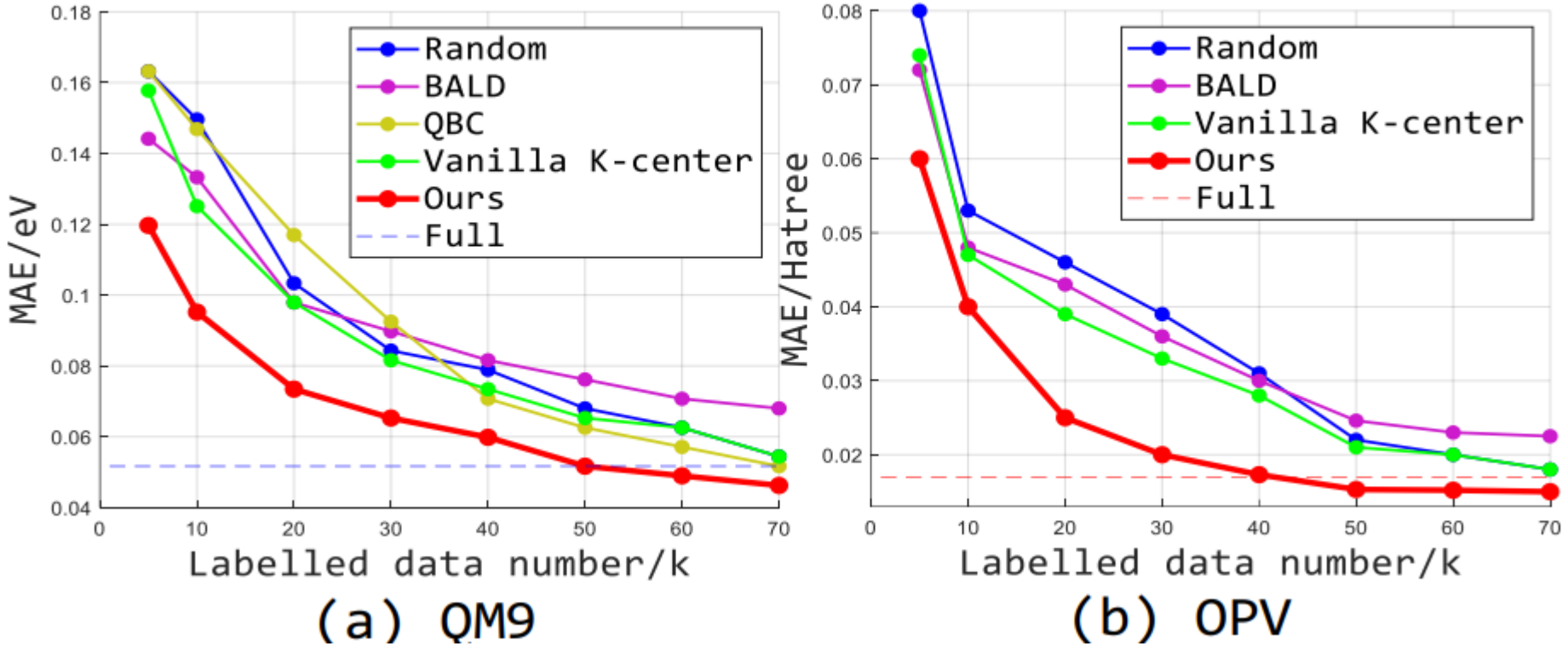
(2).Query by Committee

(3).Deep Bayesian Active Learning

(4).Vanilla K-center

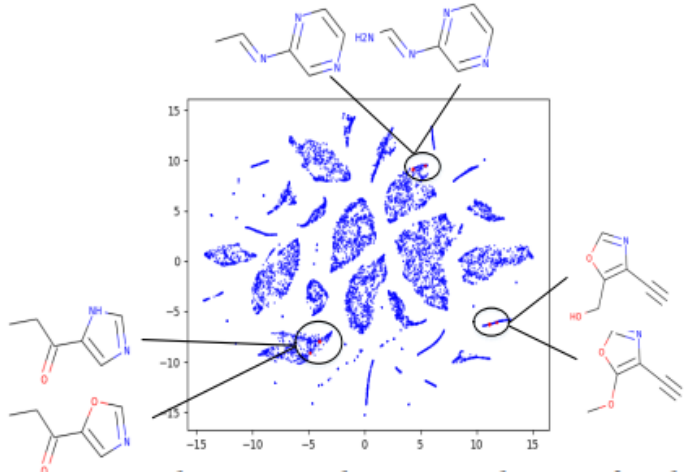
Experiments

- Results



Experiments

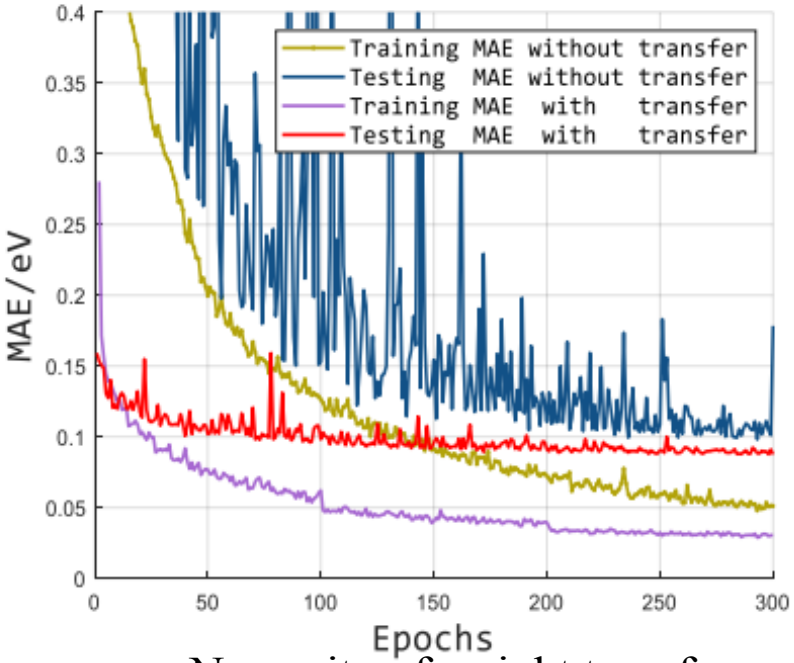
- Ablation Study
- Why using two models (a teacher and a student)
- Why transferring weight from the teacher to the student
- Visualization experiment



Visualization

Name/Dataset	Homo(QM9)			Homo(OPV)		
Unit	eV			Hatree		
Number of data	5k	10k	50k	5k	10k	50k
ASGN-T	0.1668	0.1523	0.0682	0.080	0.053	0.020
ASGN-S	0.1632	0.1252	0.0653	0.076	0.049	0.019
ASGN	**0.1190**	**0.0951**	**0.0517**	**0.060**	**0.039**	**0.015**

Necessity of teacher and student



Necessity of weight transfer

Many thanks!