Pin-Tuning: Parameter-Efficient In-Context Tuning for Few-Shot Molecular Property Prediction

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TL;DR

To achieve effective fine-tuning of pre-trained molecular encoders, we propose a parameter-efficient in-context tuning method, named `Pin-Tuning`, for few-shot molecular property prediction (FSMPP).

Motivation

Pilot study: ineffective fine-tuning of pre-trained molecular encoders

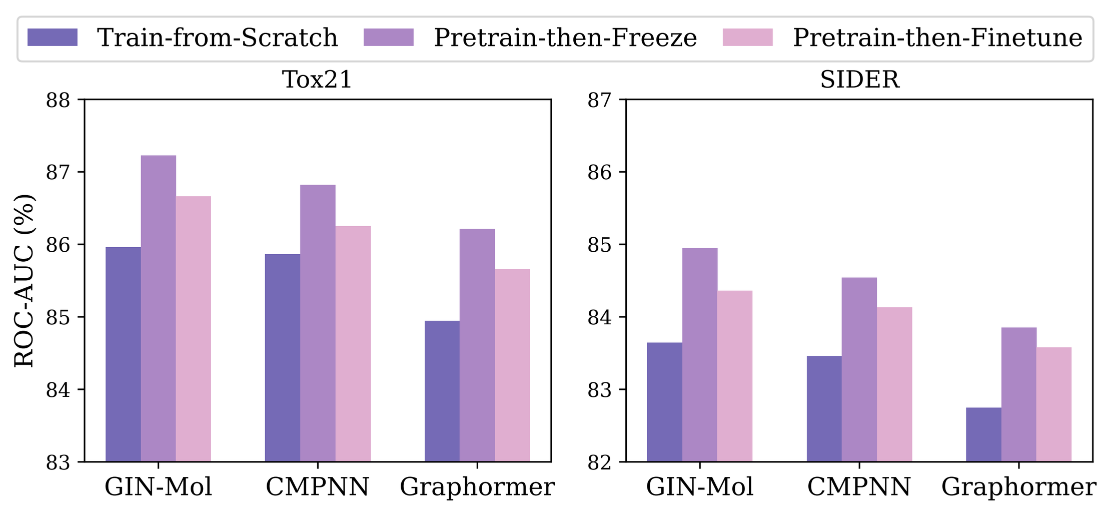

Figure 1. Comparison of molecular encoders trained via different paradigms: train-from-scratch, pretrain-then-freeze, and pretrain-then-finetune.

The results consistently demonstrate that while pre-training outperforms training from scratch, the current methods do not yet effectively facilitate fine-tuning of pre-trained molecular encoders.

The following question arises:

How to effectively adapt pre-trained molecular encoders to downstream tasks, especially in few-shot scenarios?

The Reasons of the Observation

- The imbalance between the abundance of tunable parameters and the scarcity of labeled molecules.
- The lack of contextual perceptiveness in the encoders.

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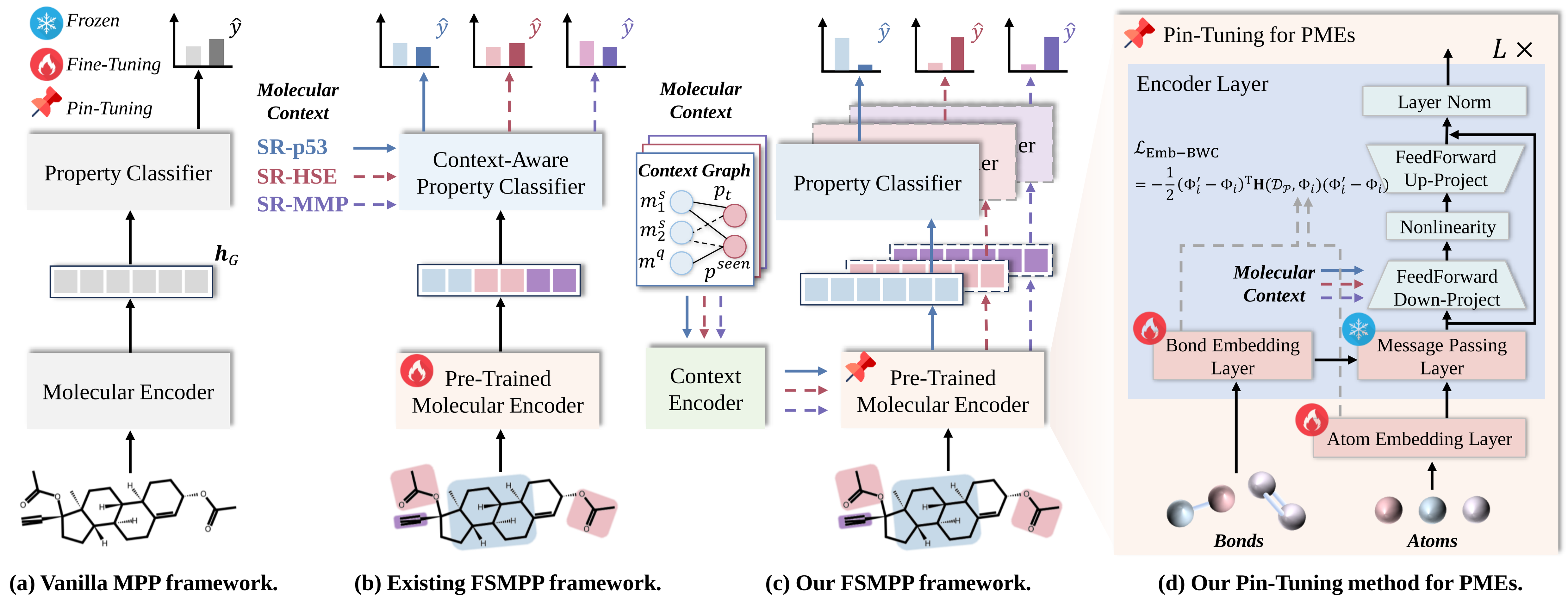

Figure 2. (a) The vanilla encoder-classifier framework for MPP. (b) The framework widely adopted by existing FSMPP methods, containing a pre-trained molecular encoder and a context-aware property classifier. (c) Our proposed framework for FSMPP, in which we introduce a `Pin-Tuning` method to update the pre-trained molecular encoder followed by the property classifier. (d) The details of our proposed `Pin-Tuning` method for pre-trained molecular encoders.

Experiments

I. ROC-AUC scores (%) on benchmark datasets.

Model	Tox21		SIDER		MUV		ToxCast		PCBA	
	10-shot	5-shot	10-shot	5-shot	10-shot	5-shot	10-shot	5-shot	10-shot	5-shot
Siamese	80.40	-	71.10	-	59.96	-	-	-	-	-
ProtoNet	74.98	72.78	64.54	64.09	65.88	64.86	68.87	66.26	64.93	62.29
MAML	80.21	69.17	70.43	60.92	63.90	63.00	68.30	67.56	66.22	65.25
TPN	76.05	75.45	67.84	66.52	65.22	65.13	69.47	66.04	67.61	63.66
EGNN	81.21	76.80	72.87	60.61	65.20	63.46	74.02	67.13	69.92	67.71
IterRefLSTM	81.10	-	69.63	-	49.56	-	-	-	-	-
Pre-GNN	82.14	82.04	73.96	76.76	67.14	70.23	75.31	74.43	76.79	75.27
Meta-MGNN	82.97	76.12	75.43	66.60	68.99	64.07	76.27	75.26	72.58	72.51
PAR	84.93	83.95	78.08	77.70	69.96	68.08	79.41	76.89	73.71	72.79
GS-Meta	86.67	86.43	84.36	84.57	66.08	64.50	83.81	82.65	79.40	77.47
Pin-Tuning	**91.56**	**90.95**	**93.41**	**92.02**	**73.33**	**70.71**	**84.94**	**83.71**	**81.26**	**79.23**
Δ*Improve.*	5.64%	5.23%	10.73%	8.81%	4.82%	3.86%	1.35%	1.28%	2.34%	2.27%

Experiments (Cont.)

II. Tunable parameter size analysis.

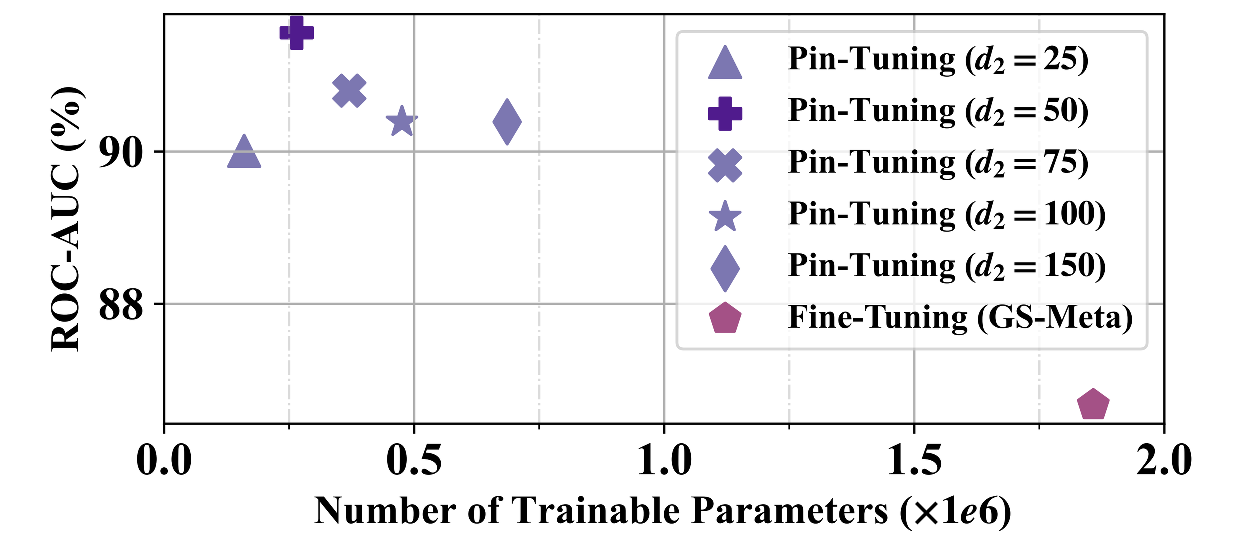

Figure 3. ROC-AUC (%) scores and number of trainable parameters of Pin-Tuning and full Fine-Tuning method on the Tox21 dataset.

III. Representation visualization.

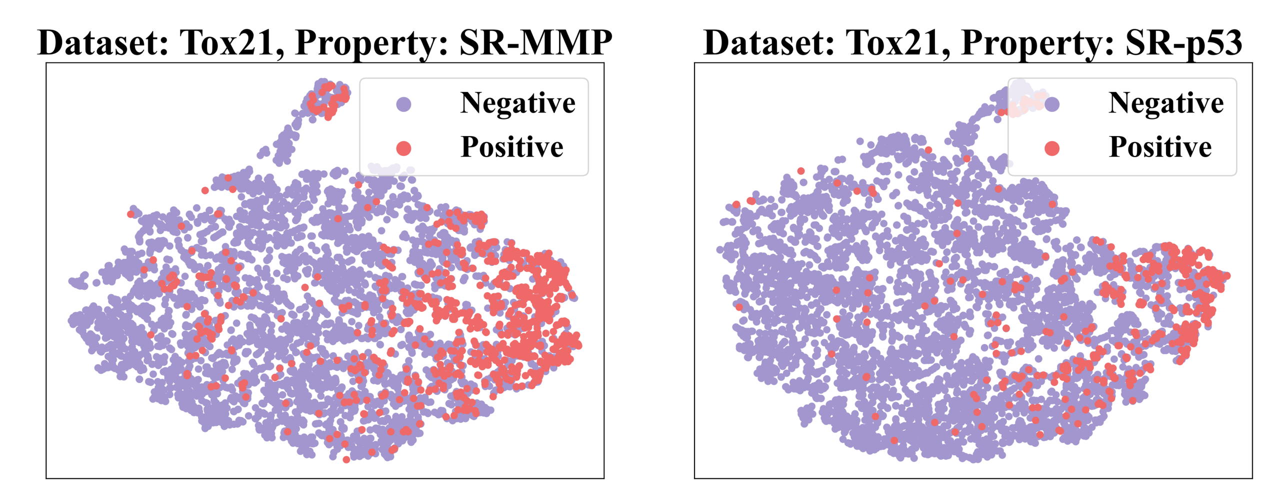

Figure 4. Molecular representations encoded after Fine-Tuning.

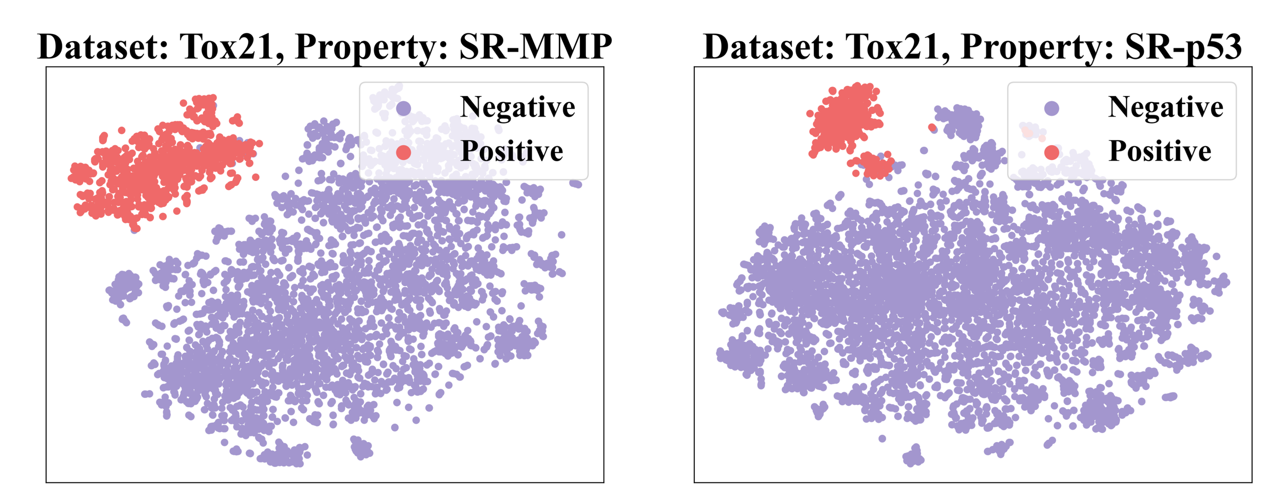

Figure 5. Molecular representations encoded after Pin-Tuning.