Geometric Transformer with Interatomic Positional Encoding

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Project URL: https://github.com/microsoft/AI2BMD/tree/Geoformer

Preliminary – Introduction to ACE theory

The expansion of atomic potential energy could be written by:

$$E_i = \sum_{j_1} \sum_{v_1} c_{v_1} \phi_{v_1}(\hat{r}_{ij_1}) + \sum_{j_1 j_2} \sum_{v_1 v_2} c_{v_1 v_2} \phi_{v_1}(\hat{r}_{ij_1}) \phi_{v_2}(\hat{r}_{ij_2}) + \cdots$$

- $\phi_v(\hat{r}_{ij})$ is a set of orthogonal basis functions to describe the spatial relations between two atoms.
- $\hat{r}_{ij}$ denotes the relative position pointing from atom i to atom j.
- v indicates the functions' polynomial degree.
- c_v indicates the expansion coefficients.

Preliminary – Introduction to ACE theory

ACE leverages the ***density trick*** to reduce the computational overhead.

Atomic base $A_{i,\upsilon}$:

$$A_{i,\upsilon} = \sum_{j \in N(i)} \phi_{\upsilon}(\hat{r}_{ij})$$

A-basis $A_{i,\mathbf{v}}$:

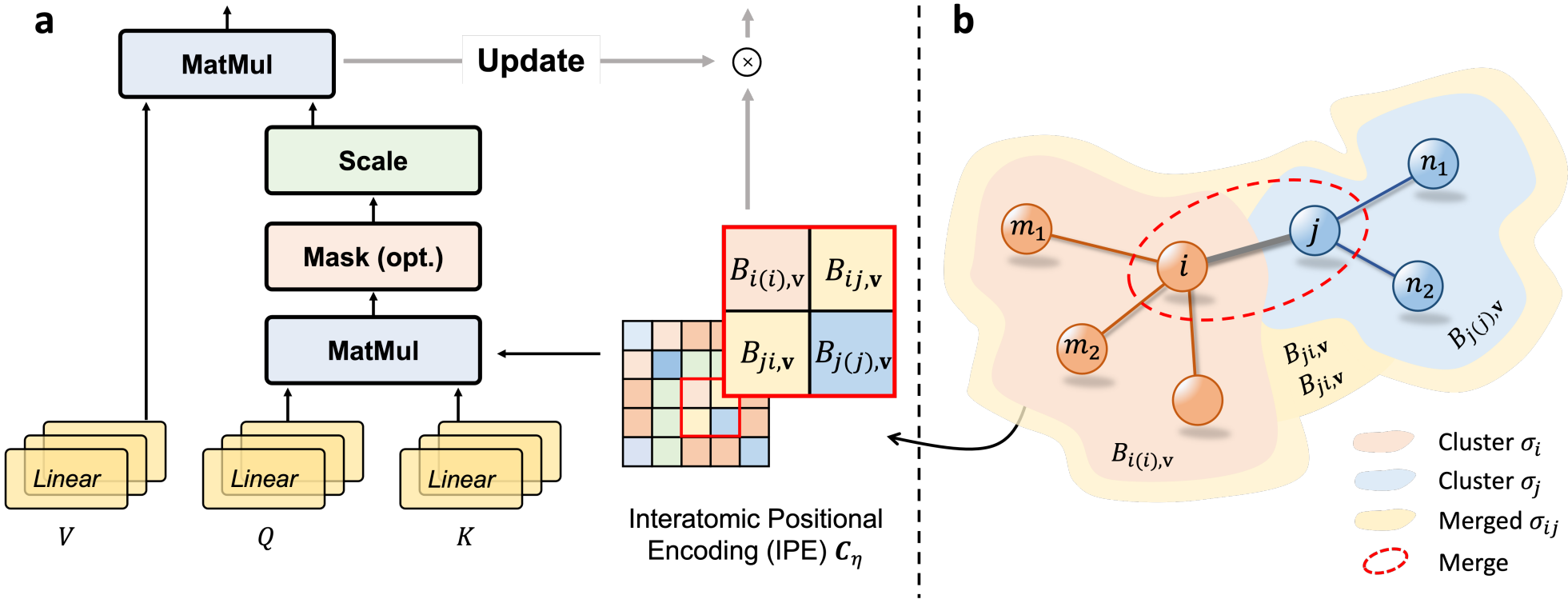
$$A_{i,\mathbf{v}} = \prod_{t=1}^{\epsilon} A_{i,\upsilon}\,, \mathbf{v} = (\upsilon_1, \ldots, \upsilon_\epsilon)$$

Since $A_{i,\mathbf{v}}$ is not rotationally invariant, we need additional Clebsch-Gordan coefficients C_{υ} to construct fully permutation and isometry-invariant basis functions (B-basis):

$$B_{i,\mathbf{v}} = \sum_{\mathbf{v}'} C_{\mathbf{v}\mathbf{v}'} A_{i,\mathbf{v}'}$$

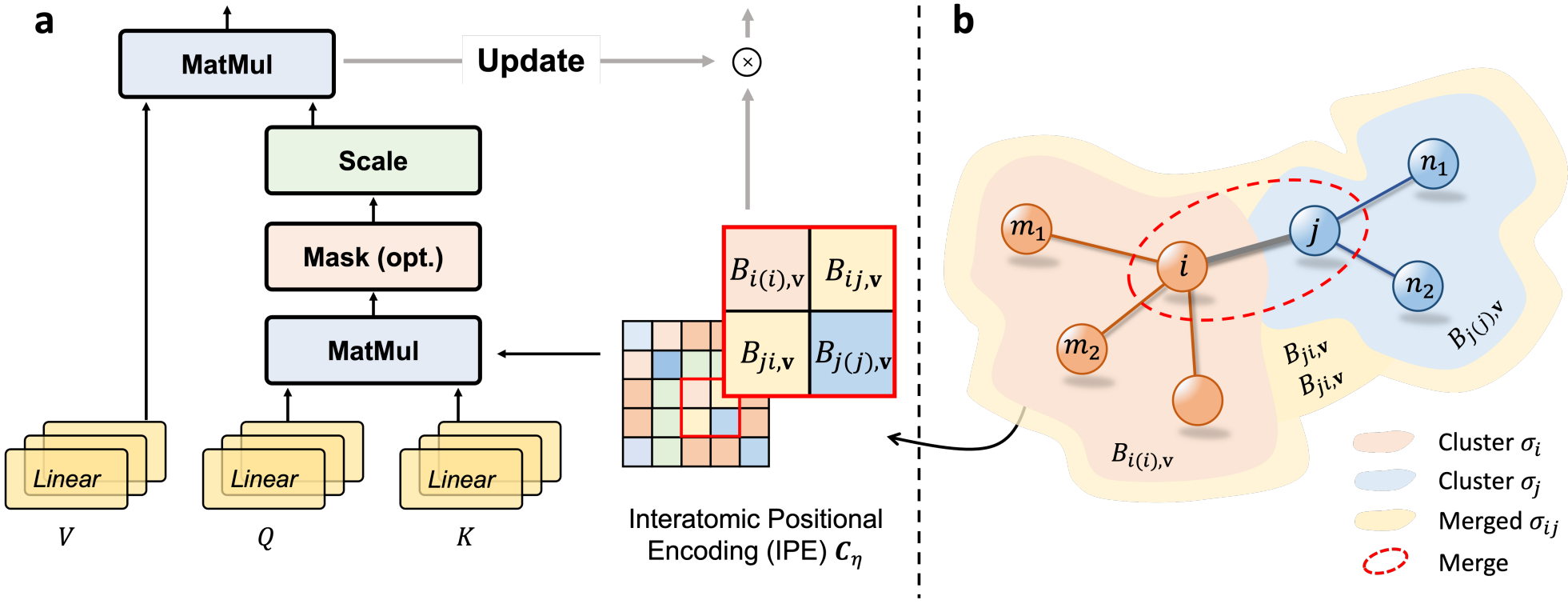
$$E_i = \sum_{\epsilon} c_{i,\mathbf{v}} B_{i,\mathbf{v}} = c_i \cdot B_i$$

Methods - Positional Encoding for Geometric Molecule Modeling



Theorem 1 *Given two cluster σ_i and σ_j and their basis functions, there exists a set of invariant basis functions for the merged cluster σ_{ij} to describe integrated cluster potentials $\tilde{E}_{ij}$.*

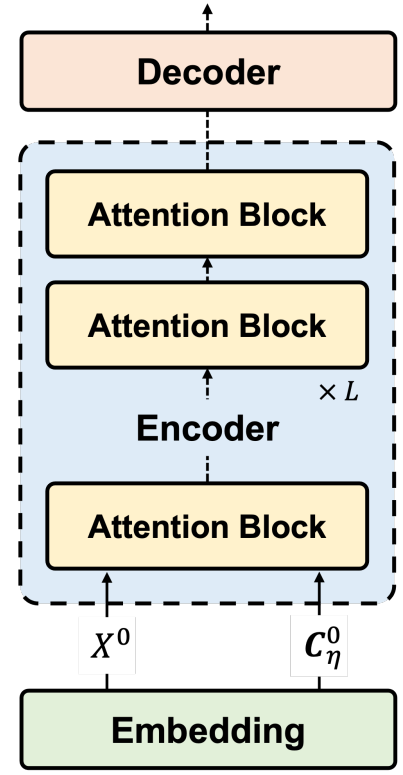
Methods - Positional Encoding for Geometric Molecule Modeling



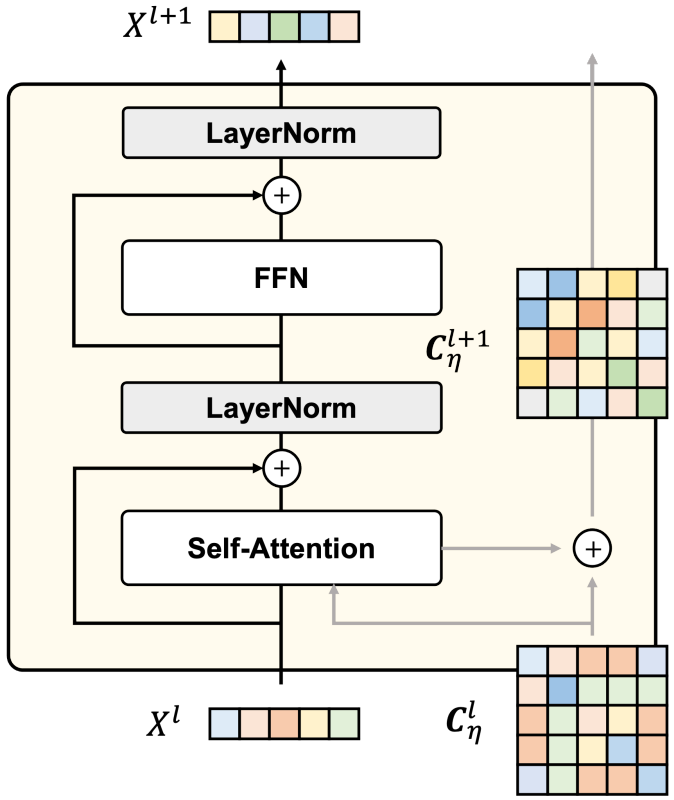
Theorem 2 *Given one molecule with N atoms, there exists a positional encoding matrix $C_\eta \in \mathbb{R}^{N\times N}$, which naturally describes the interatomic potentials. In particular, C_η is directly multiplied with Query and Key before scaling, serving as the positional encoding in Transformer:*

$$\alpha = (XW_Q)(XW_K)^\top \odot C_\eta$$

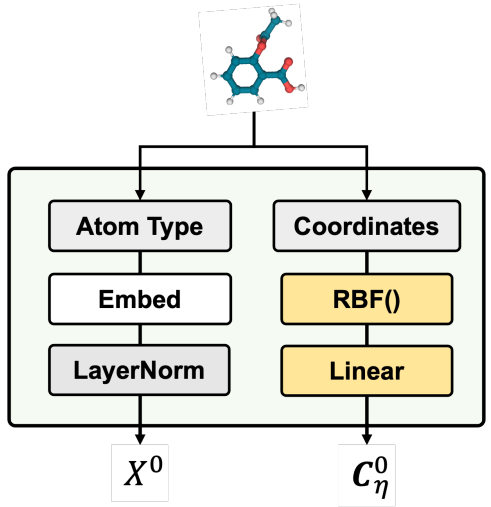
Methods - Geometric Transformer for molecules



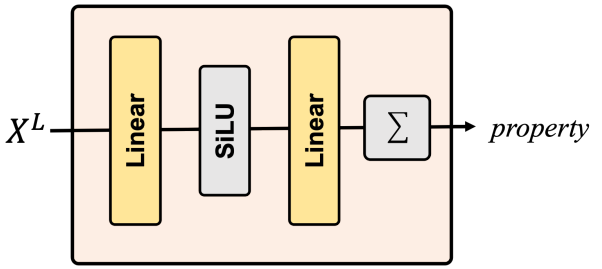
(a) Geoformer Architecture



(b) Attention Block with IPE



(c) Embedding Layer



(d) Decoder

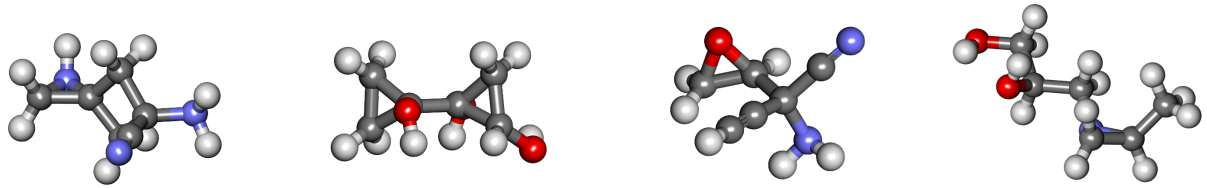
Experiments

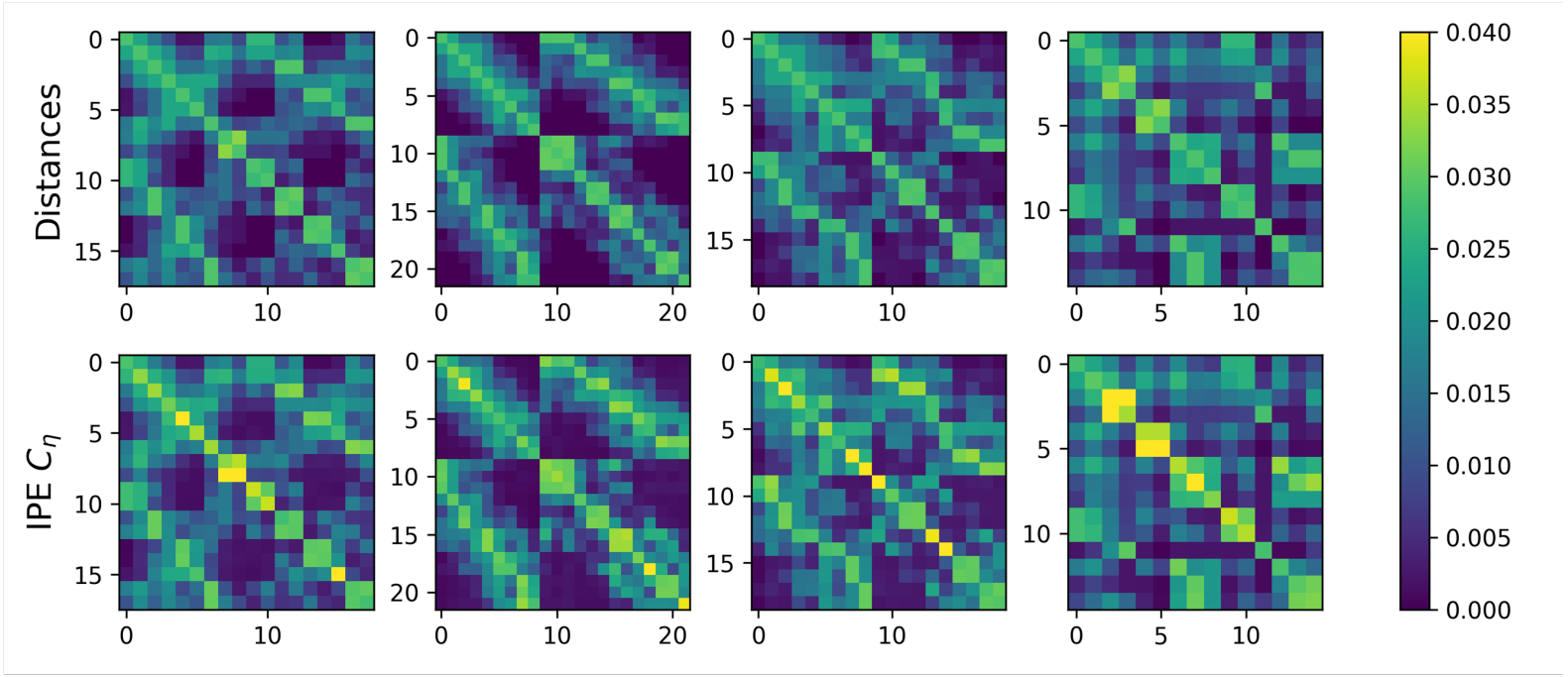
Mean absolute errors (MAE) of 12 kinds of molecular properties on QM9 compared with state-of-the-art algorithms.

Target Unit	μ mD	α ma_0^3	ϵ_{HOMO} meV	ϵ_{LUMO} meV	$\Delta\epsilon$ meV	$\langle R^2 \rangle$ ma_0^2	$ZPVE$ meV	U_0 meV	U meV	H meV	G meV	C_v $\frac{\text{mcal}}{\text{mol K}}$
NMP	30	92	43	38	69	180	1.50	20	20	17	19	40
SchNet	33	235	41	34	63	73	1.70	14	19	14	14	33
Cormorant	38	85	34	38	61	961	2.03	22	21	21	20	26
LieConv	32	84	30	25	49	800	2.28	19	19	24	22	38
DimeNet++	30	44	25	20	33	331	1.21	6.32	6.28	6.53	7.56	23
EGNN	29	71	29	25	48	106	1.55	11	12	12	12	31
PaiNN	12	45	28	20	46	66	1.28	5.85	5.83	5.98	7.35	24
TorchMD-NET	11	59	20	18	36	33	1.84	6.15	6.38	6.16	7.62	26
GNS + NoisyNode	25	52	20	19	29	700	1.16	7.30	7.57	7.43	8.30	25
SphereNet	25	45	23	19	31	268	**1.12**	6.26	6.36	6.33	7.78	**22**
SEGNN	23	60	24	21	42	660	1.62	15	13	16	15	31
EQGAT	11	53	20	16	32	382	2.00	25	25	24	23	24
PaxNet	11	45	23	19	31	249	1.17	5.90	5.92	6.04	7.14	23
ComENet	25	45	23	20	32	259	1.20	6.59	6.82	6.86	7.98	24
Equiformer	11	46	**15**	**14**	**30**	251	1.26	6.59	6.74	6.63	7.63	23
AMP	12	67	26	23	45	93	4.10	11.3	11.4	11.3	12.4	32
Molformer	28	41	25	26	39	350	2.05	7.52	7.46	7.38	8.11	25
GeoT	29.7	52.7	25.0	20.2	43.9	300.8	1.73	11.1	11.7	11.3	11.7	27.6
Geometric Transformer	26.4	51	27.5	20.4	36.1	157	1.24	7.35	7.55	7.73	8.21	28.0
Transformer-M	37	41	17.5	16.2	27.4	75	1.18	9.37	9.41	9.39	9.63	**22**
Geoformer	**10**	**40**	18.4	15.4	33.8	**27.5**	1.28	**4.43**	**4.41**	**4.39**	**6.13**	**22**

Experiments

Visualization of IPE C_η on molecules GDB65488, GDB101712, GDB87153 and GDB56373 in QM9 test set.





Microsoft

Thanks