Universal Collection of Euclidean Invariants between Pairs of Position-Orientations

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Motivation

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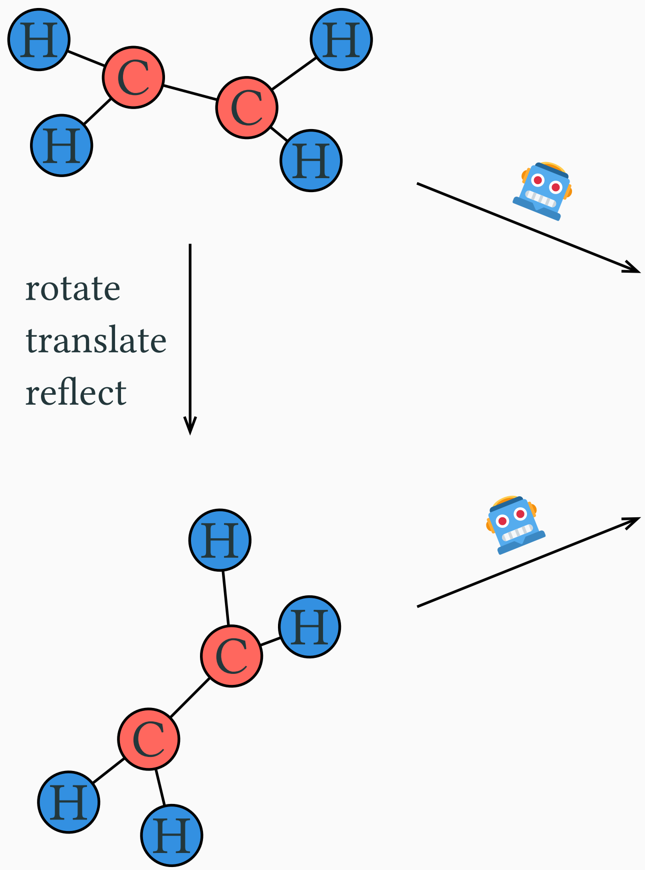


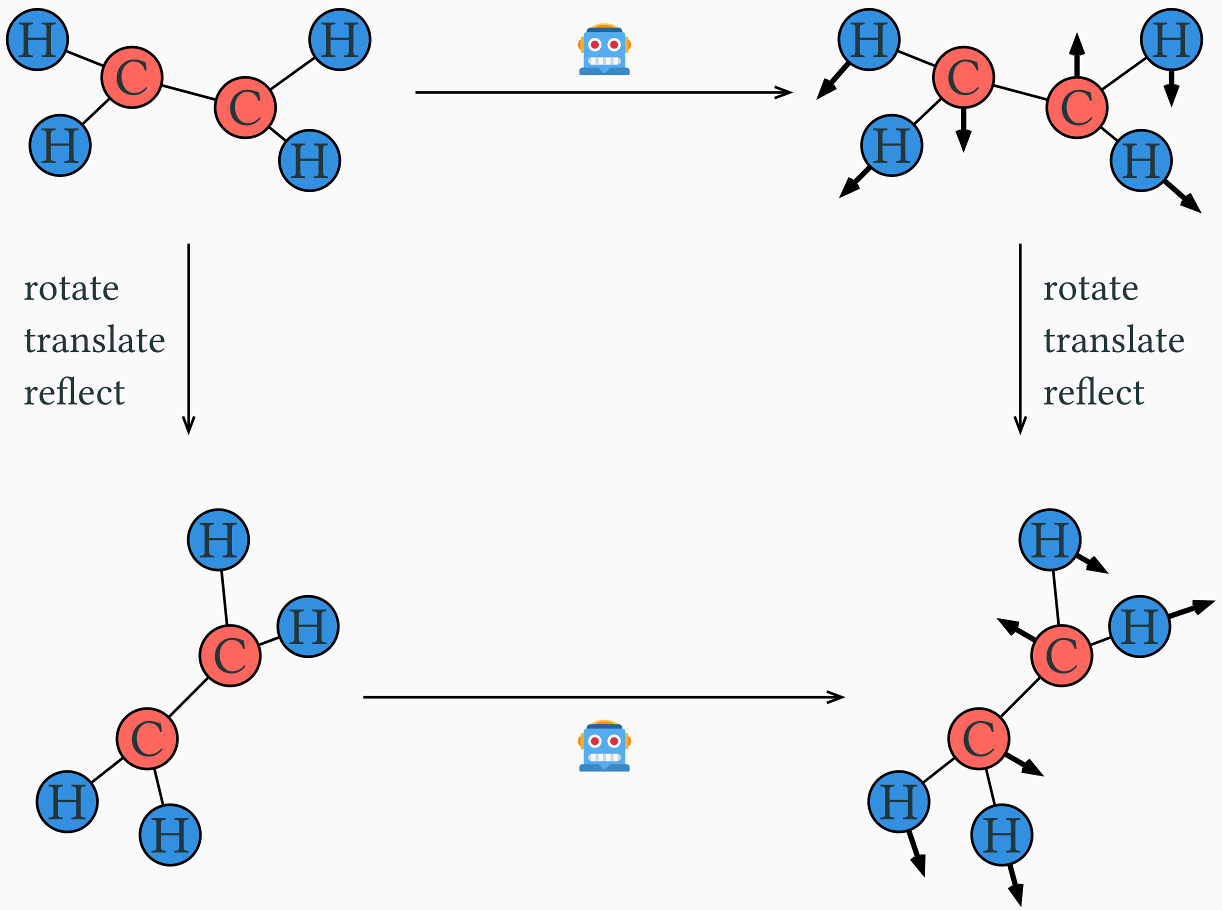
Dipole moment: 0.05 D

Isotropic polarizability: 1.55 a_0^3

Internal energy at 0K: 1.30 eV

$\vdots$

Motivation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rotate
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reflect

We should build models that **respect** translation, rotational, and reflectional transformations.

PONITA

PONITA

PONITA [1] is a neural network architecture by Bekkers et al. [2] that…

- respects translation, rotational, and reflectional transformations.
- uses scalar fields on *position-orientation space* $\mathbb{M}_3$.
- is faster than the typical steerable/tensor field network (Thomas et al. [3], Anderson et al. [4]).
- does not require any representation theory of $\mathrm{SO}(3)$ (no Clebsch-Gordan coefficients, Wigner D-matrices, etc…).
- achieves state-of-the-art accuracy when predicting molecular dynamics & properties.

Euclidean Group $\mathbb{E}(3)$ & Position-Orientation Space $\mathbb{M}_3$

Euclidean Group $\mathrm{E}(3)$ & Position-Orientation Space $\mathbb{M}_3$

Definition: The *Euclidean group* or *rigid transformation group* in 3 dimensions is

$$\mathrm{E}(3) := \{(t, Q) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \mid Q^\top Q = I\},$$

where t is the *translation vector* and Q the *rotoreflection matrix.*

Definition: The space of *three-dimensional position-orientations* is:

$$\mathbb{M}_3 := \{(x, n) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid \|n\| = 1\},$$

where x is the *position* and n the *orientation.*

Definition: We define the action $\triangleright\colon \mathrm{E}(3) \times \mathbb{M}_3 \to \mathbb{M}_3$

$$(t, Q) \triangleright (x, n) = (t + Qx, Qn)$$

$\mathrm{E}(3)$ **Invariants on** $\mathbb{M}_3 \times \mathbb{M}_3$

E(3) Invariants on $\mathbb{M}_3 \times \mathbb{M}_3$

- In the PONITA architecture all data (feature maps) is stored as scalar fields $f : \mathbb{M}_3 \to \mathbb{R}$ on position-orientation space $\mathbb{M}_3$.
- Consider a linear operator Φ to process such a field f, as is common in neural networks:

$$(\Phi f)(p) := \int_{\mathbb{M}_3} k(p, q) f(q) \,\mathrm{d}q,$$

  with kernel $k : \mathbb{M}_3 \times \mathbb{M}_3 \to \mathbb{R}$.
- To make the operator Φ *equivariant*, that is

$$\Phi(g \triangleright f) = g \triangleright \Phi(f) \text{ for all } f : \mathbb{M}_3 \to \mathbb{R} \text{ and } g \in \mathrm{E}(3)$$

  it suffices to make the kernel k *invariant*:

$$k(g \triangleright p, g \triangleright q) = k(p, q) \text{ for all } p, q \in \mathbb{M}_3 \text{ and } g \in \mathrm{E}(3)$$

- So, to make PONITA respect rigid transformations we are motivated to study **invariants** $\iota : \mathbb{M}_3 \times \mathbb{M}_3 \to \mathbb{R}$, that being functions with the property that

$$\iota(g \triangleright p, g \triangleright q) = \iota(p, q) \text{ for all } p, q \in \mathbb{M}_3 \text{ and } g \in \mathrm{E}(3)$$

E(3) Invariants on $\mathbb{M}_3 \times \mathbb{M}_3$

- Consider any collection of invariants $\iota_1, \ldots, \iota_n : \mathbb{M}_3 \times \mathbb{M}_3 \to \mathbb{R}$.
- We can create a new invariant ι' easily by considering any $h : \mathbb{R}^n \to \mathbb{R}$ and defining $\iota' = h(\iota_1, \ldots, \iota_n)$.
- This observation has an immediate application in PONITA: we can decide to parameterize the kernels k by, for example, a multi-layer perceptron $\mathrm{MLP}_\theta : \mathbb{R}^n \to \mathbb{R}$ with (trainable) parameters θ, and plugging in a predesigned collection of n invariants: $k = \mathrm{MLP}_\theta(\iota_1, \ldots, \iota_n)$.
- This motivates looking into what an **"optimal"** collection of invariants would be, so that we can construct networks that are as expressive and efficient as possible.

E(3) Invariants on $\mathbb{M}_3 \times \mathbb{M}_3$

- Suppose we have a collection of invariants where one of them is a function of the others. If this happens we say the collection of invariants is **dependent**.
- A dependent collection is *not* "optimal" in the sense that we could remove the dependent invariant and lose no expressiveness.
- Suppose we have a collection of invariants for which we know that *any* other invariant is a function of them. We say such a collection of invariants is **universal**.
- A universal collection of invariants is "optimal" in the sense that there is no reason to add another invariant because we gain no expressiveness.

Can we find a collection of $\mathrm{E}(3)$ invariants on $\mathbb{M}_3 \times \mathbb{M}_3$ that is both **independent** and **universal**?

E(3) Invariants on $\mathbb{M}_3 \times \mathbb{M}_3$

Definition (Original PONITA Invariants): Write $p_1 = (x_1, n_1)$, $p_2 = (x_2, n_2) \in \mathbb{M}_3$. Bekkers et al. [2] propose the following collection of three invariants:

$$\iota_1(p_1, p_2) = (x_2 - x_1) \cdot n_1$$
$$\iota_2(p_1, p_2) = \|(x_2 - x_1) - \iota_1 n_1\|$$
$$\iota_3(p_1, p_2) = n_1 \cdot n_2$$

Proposition: The original invariants are independent but *not* universal.

E(3) Invariants on $\mathbb{M}_3 \times \mathbb{M}_3$

Definition (Our Invariants): Write $p_1 = (x_1, n_1)$, $p_2 = (x_2, n_2) \in \mathbb{M}_3$. We propose the following collection of four invariants:

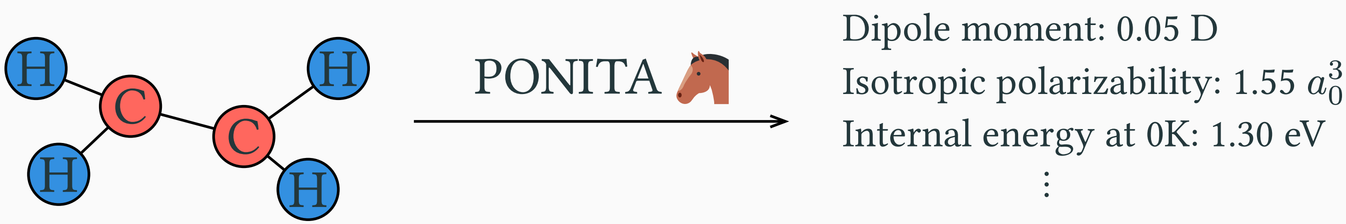
$$\begin{aligned}
\iota_1(p_1, p_2) &= (x_2 - x_1) \cdot n_1 \\
\iota_2(p_1, p_2) &= (x_2 - x_1) \cdot n_2 \\
\iota_3(p_1, p_2) &= (x_2 - x_1) \cdot (x_2 - x_1) \\
\iota_4(p_1, p_2) &= n_1 \cdot n_2
\end{aligned}$$

Theorem: In Bellaard et al. [5] we show that our invariants are universal and independent.

Experiment

Experiment

- QM9: predict chemical properties of small organic molecules.
- PONITA: original invariants versus our universal collection.
- Code can be found at [6].



Target	Unit	Original	Universal (Ours)	Difference %
μ	D	0.0195	0.0166	−15.0
α	a_0^3	0.0557	0.0489	−12.1
$\varepsilon_{\mathrm{homo}}$	eV	0.0226	0.0202	−10.4
$\varepsilon_{\mathrm{lumo}}$	eV	0.0206	0.0187	−9.0
$\Delta\varepsilon$	eV	0.0415	0.0378	−8.9
$\langle R^2 \rangle$	a_0^2	0.4160	0.4251	+2.2
ZPVE	meV	1.5647	1.5241	−2.6
U_0	eV	0.9920	1.0285	+3.7
U	eV	1.3593	0.7362	−45.8
H	eV	1.0205	0.6934	−32.1
G	eV	1.1856	0.7721	−34.9
c_v	cal/mol·K	0.0292	0.0270	−7.4

PONITA trained to predict chemical properties of various molecules (QM9 dataset [7], [8]). Mean absolute error on the test set is reported (lower is better). Our universal invariants perform better.

Using a **universal** collection of invariants has a **significant positive** impact on the accuracy of the PONITA model when predicting chemical properties.

Thank you for your attention!

Questions?

References

[1] E. J. Bekkers, “PONITA.” Accessed: Oct. 20, 2025. [Online]. Available: https://github.com/ebekkers/ponita

[2] E. J. Bekkers, S. Vadgama, R. Hesselink, P. A. van der Linden, and D. W. Romero, “Fast, Expressive SE(3) Equivariant Networks through Weight-Sharing in Position-Orientation Space,” in *ICLR*, 2024. [Online]. Available: https://openreview.net/forum?id=dPHLbUqGbr

[3] N. Thomas *et al.*, “Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds,” *arXiv preprint*, 2018, [Online]. Available: https://arxiv.org/abs/1802.08219

[4] B. Anderson, T. S. Hy, and R. Kondor, “Cormorant: Covariant Molecular Neural Networks,” in *NeurIPS*, 2019, p. . [Online]. Available: https://papers.neurips.cc/paper_files/paper/2019/hash/03573b32b2746e6e8ca98b9123f2249b-Abstract.html

[5] G. Bellaard, B. M. N. Smets, and R. Duits, “Universal Collection of Euclidean Invariants Between Pairs of Position-Orientations,” in *Geometric Science of Information*, F. Nielsen and F. Barbaresco, Eds., Cham: Springer Nature Switzerland, 2025, pp. 24–33.

References

[6] G. Bellaard, “PONITA Invariants.” Accessed: Oct. 20, 2025. [Online]. Available: https://gitlab.com/gijsbel/ponita_invariants

[7] R. Ramakrishnan, P. O. Dral, M. Rupp, and O. A. von Lilienfeld, “Quantum chemistry structures and properties of 134 kilo molecules,” *Scientific Data*, vol. 1, no. 1, 2014, doi: 10.1038/sdata.2014.22.

[8] L. Ruddigkeit, R. van Deursen, L. C. Blum, and J.-L. Reymond, “Enumeration of 166 Billion Organic Small Molecules in the Chemical Universe Database GDB-17,” *Journal of Chemical Information and Modeling*, vol. 52, no. 11, pp. 2864–2875, Nov. 2012, doi: 10.1021/ci300415d.

Some PONITA Details

- QM9 has graphs $(\mathcal{V}_0 \subset \mathbb{R}^3, \mathcal{E}_0)$ with some scalar features $(f_x)_{x \in \mathcal{V}_0} \subset \mathbb{R}$.
- Discretize $S^2_n \subset S^2$ and let $\mathcal{V} := \mathcal{V}_0 \times S^2_n \subset \mathbb{M}_3$ be the vertices of a fully connected (lifted) graph.
- Lift features as $\tilde{f}_v = \tilde{f}_{(x,n)} = f_x$ for all $v \in \mathcal{V}$.
- A feature $(f_v)_{v \in \mathcal{V}} \subset \mathbb{R}$ can be represented in the continuous setting as

$$f := \sum_{v \in \mathcal{V}} f_v \delta_v.$$

- Consequently the linear operator works as

$$(\Phi f)(v) = \int_{\mathbb{M}_3} k_\theta(v, w) f(w) \, \mathrm{d}w = \sum_{w \in \mathcal{V}} k_\theta(v, w) f(w) \qquad \forall v \in \mathcal{V},$$

  which is a particular choice of *message passing* for a Graph Neural Network.
- For performance reasons reduce the graph based on spatial distance, i.e.

$$(\Phi f)(v) = \sum_{w \in \mathcal{N}(v)} k_\theta(v, w) f(w),$$

  with $\mathcal{N}(x, n) := \{(x', n') \in \mathcal{V} \mid \|x - x'\| < C\}$.