Geometric Invariants on Position-Orientation Space

with application in equivariant machine learning

Gijs Bellaard, Bart M. N. Smets, and Remco Duits

16 April 2025

Outline

Motivation

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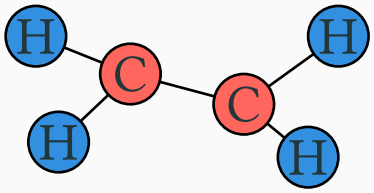

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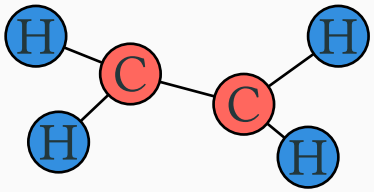

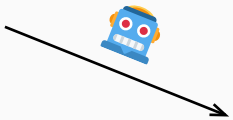

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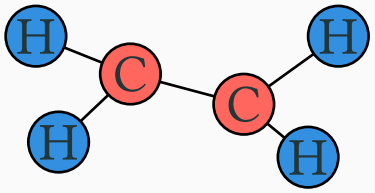

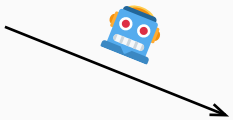

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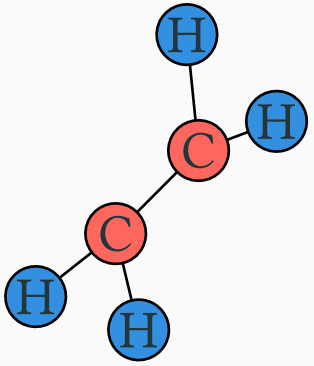

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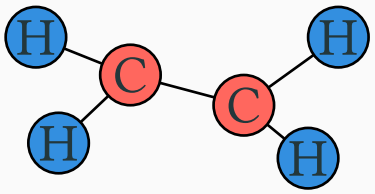

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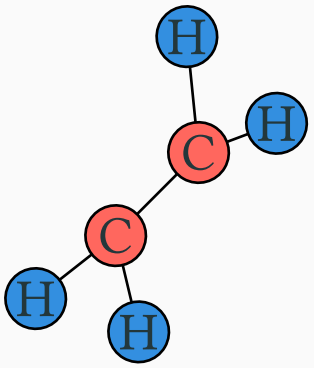

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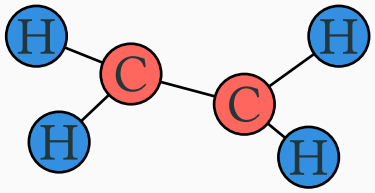

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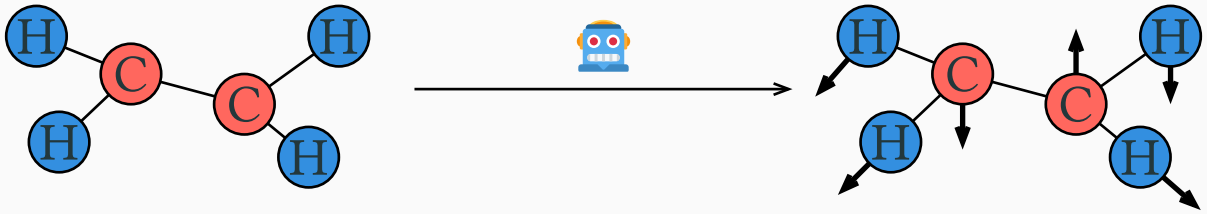

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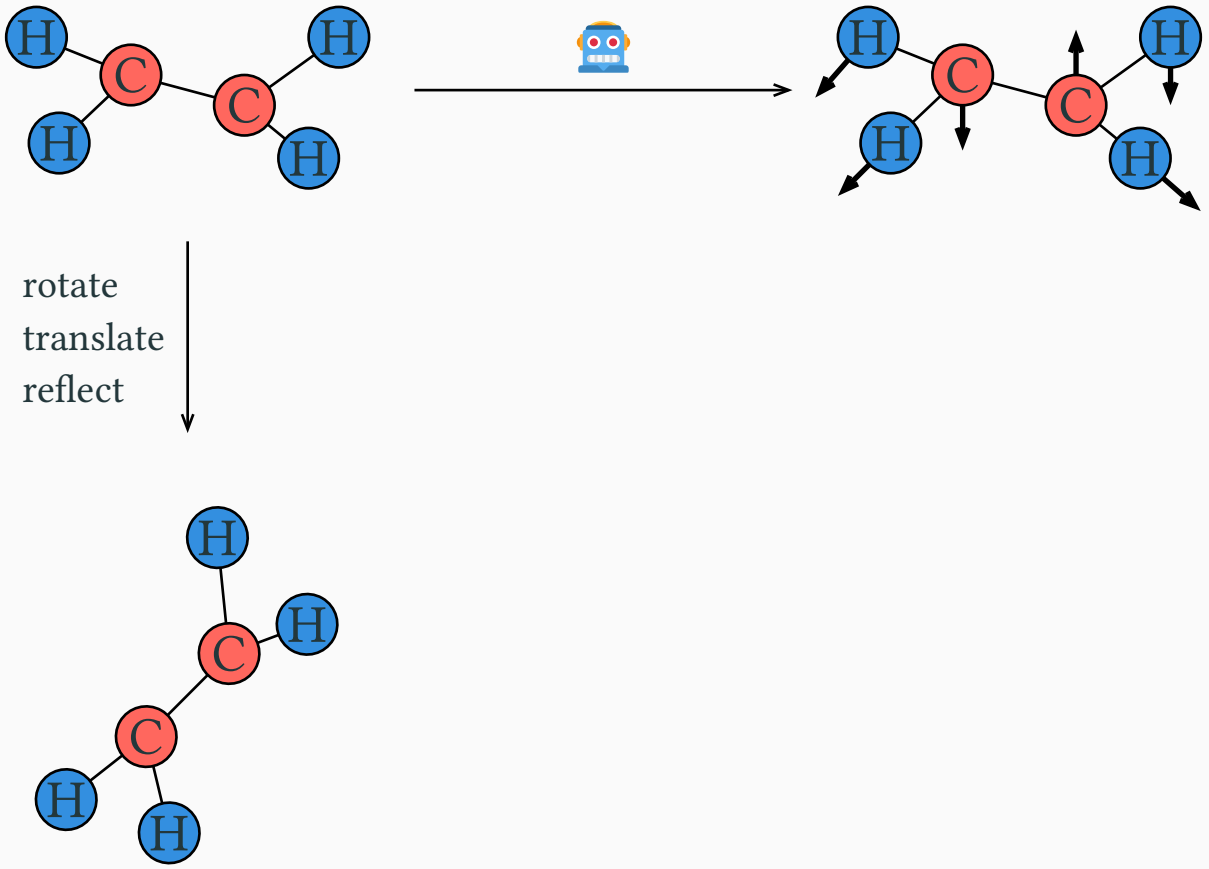

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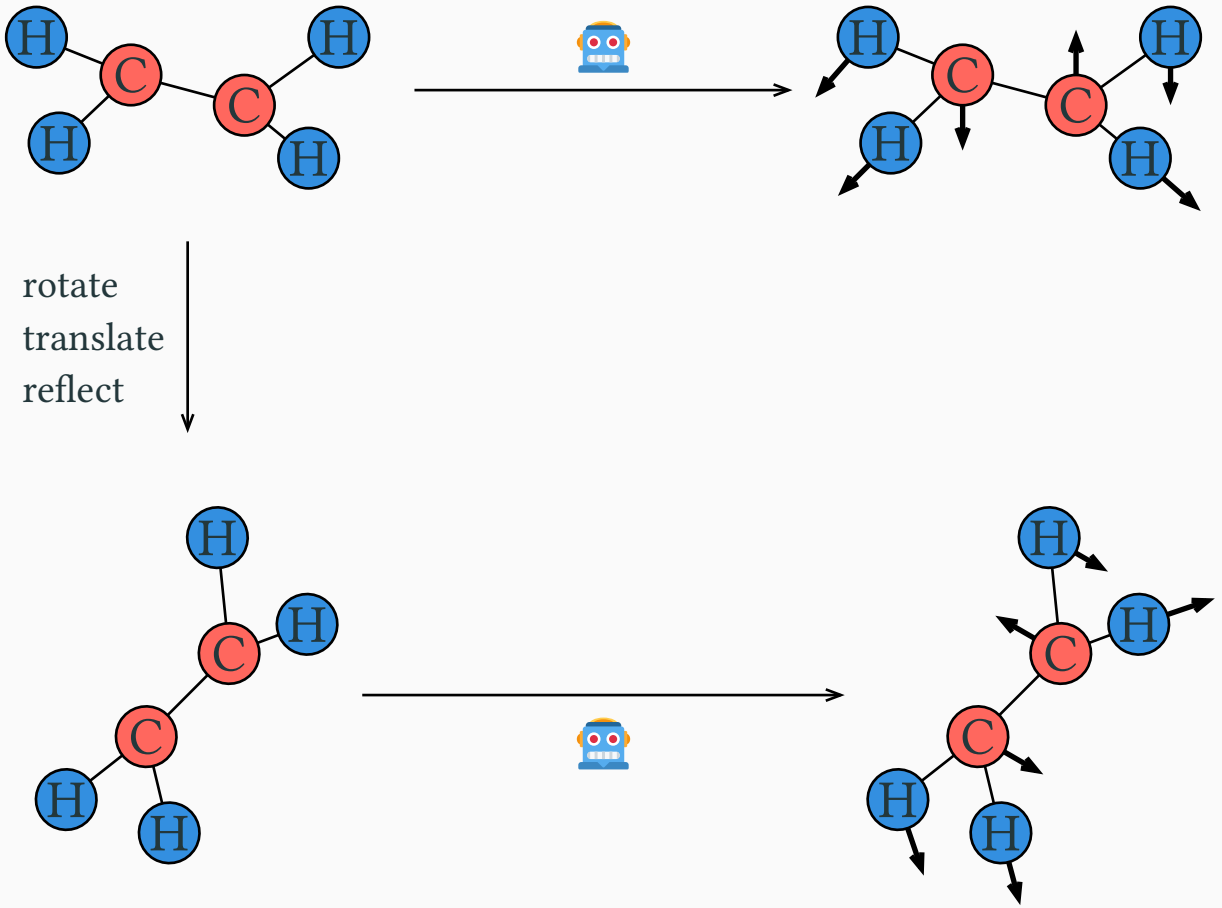

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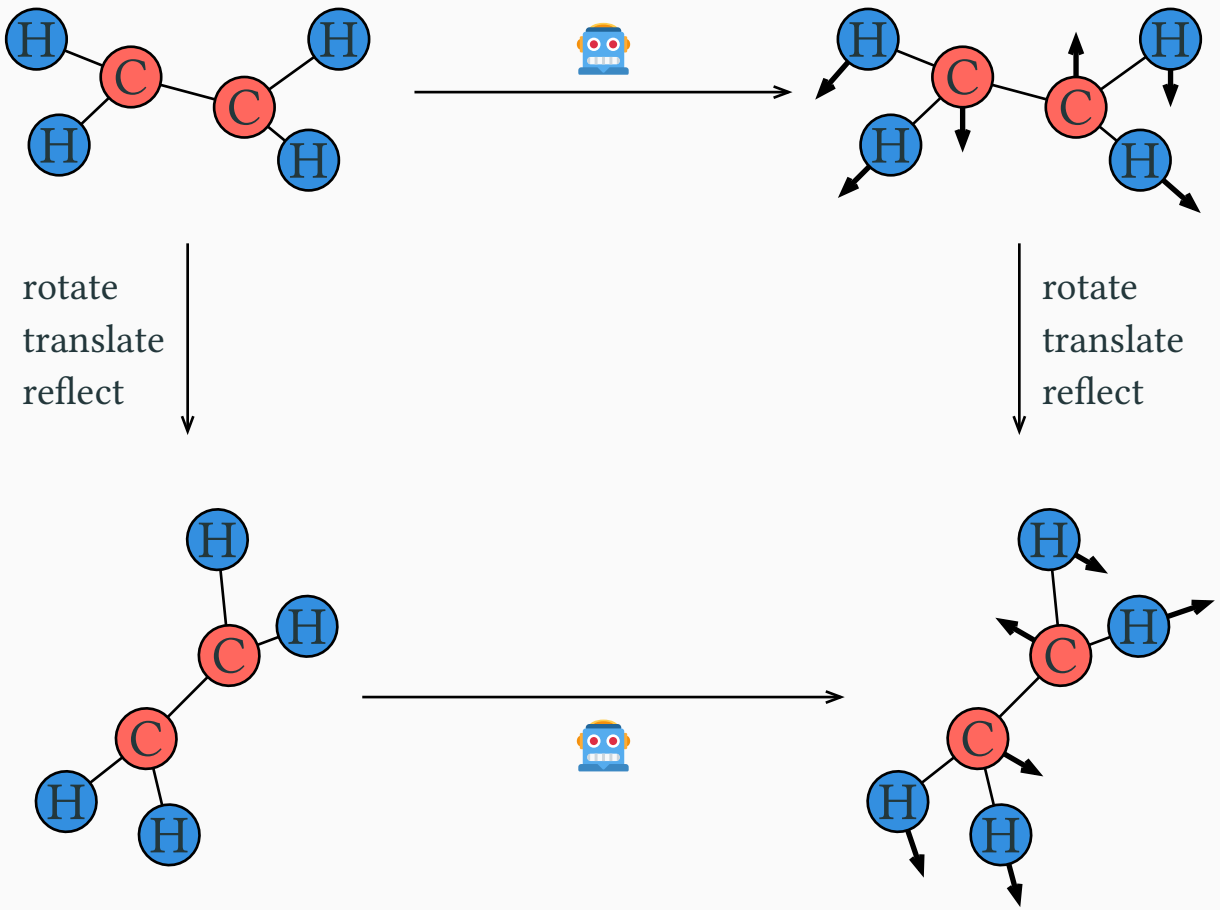
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- Actually interested in the **equivariant machine learning** part.
- We build on architectures that were benchmarked on chemical datasets so we follow suit to see if our modifications improve performance.
- While our main applications of interest are in image processing, much of our work is very general and applies to a wide range of problems.

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

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

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- Consider a linear operator Φ to process such a field f, as is common in neural networks:

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- So, to make PONITA respect certain 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

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

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- This observation has an immediate application in PONITA: we can decide to parameterize the kernels k by, for example, a multi-layer perceptron $\text{MLP}_\theta : \mathbb{R}^n \to \mathbb{R}$ with (trainable) parameters θ, and plugging in a predesigned collection of n invariants: $k = \text{MLP}_\theta(\iota_1, ..., \iota_n)$.

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- 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.

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- 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**?

$\mathrm{E}(3)$ 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. [1] propose the following collection of three invariants:

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

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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}
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Theorem: In Bellaard et al. [4] is it shown our invariants are universal and independent.

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

Experiment

- QM9: predict chemical properties of small organic molecules from their graph.
- PONITA: original invariants (3) versus our universal set (4).

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

Target	Unit	Original	Universal (Ours)	Difference %
μ	D	0.0195	0.0166	−15.0
α	a_0^3	0.0557	0.0489	−12.1
$\varepsilon_{\text{homo}}$	eV	0.0226	0.0202	−10.4
$\varepsilon_{\text{lumo}}$	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 [5], [6]). Mean absolute error on the test set is reported (lower is better). Our universal invariants perform better.

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

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...where gradient ∇, norm $\|\cdot\|$, Laplacian Δ, and divergence $\nabla\cdot$, *all* depend on $\mathcal{G}$.

Can we **classify all** $\mathrm{E}(3)$ invariant metrics on $\mathbb{M}_3$?

$\mathrm{E}(3)$ Invariant Metrics on $\mathbb{M}_3$

Theorem: In Bellaard et al. [10] it is shown that every $\mathrm{E}(3)$ invariant Riemannian metric tensor field $\mathcal{G}$ on $\mathbb{M}_3$ yields a norm of the form

$$\|(p, \dot{p})\|_{\mathcal{G}}^2 = (w_1 \, |\dot{x} \cdot n|)^2 + (w_2 \, \|\dot{x} \times n\|)^2 + (w_3 \, \|\dot{n}\|)^2 + w_4 \, \dot{x} \cdot \dot{n}$$

where $p = (x, n) \in \mathbb{M}_3$, $\dot{p} = (\dot{x}, \dot{n}) \in T_p\mathbb{M}_3$, and $w_i \in \mathbb{R}$ constants called the *metric parameters*.

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- However, the Riemannian distance d, in general, is **expensive** to compute.
- In Portegies et al. [7] it is instead suggested to use the **cheap** *mav distance*.
- We saw an application of the mav distance as a *learnable* invariant in PONITA, with the metric parameter $w_1, \ldots, w_4$ acting as trainable weights.

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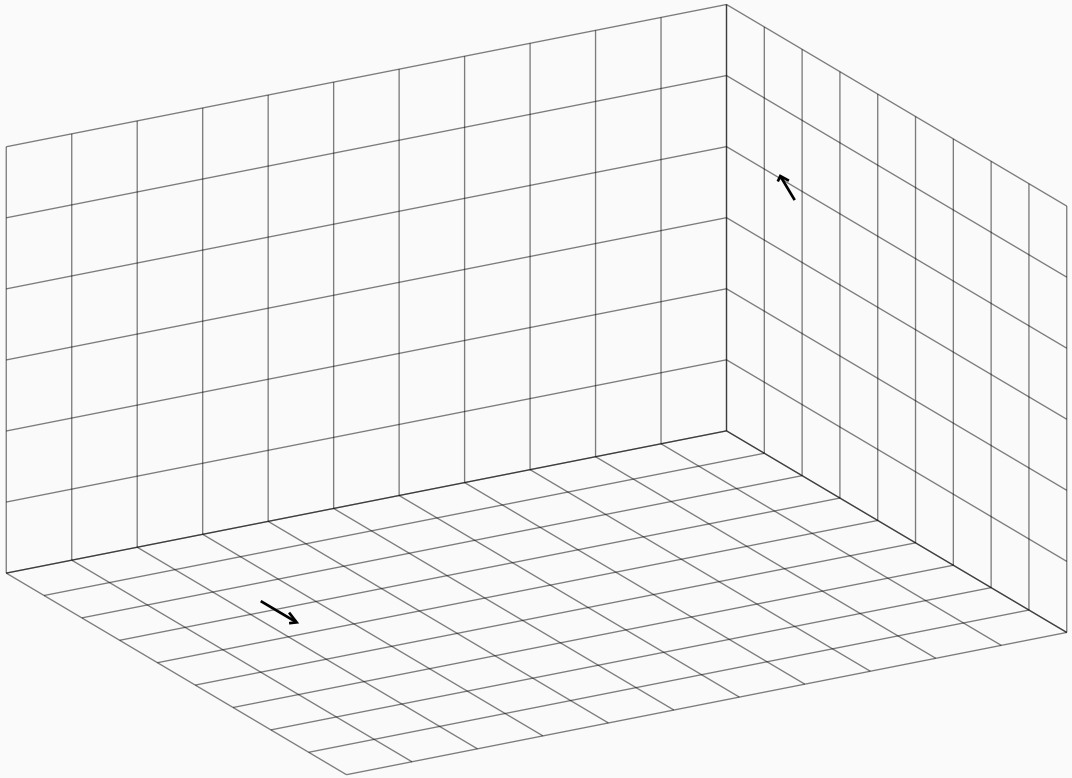

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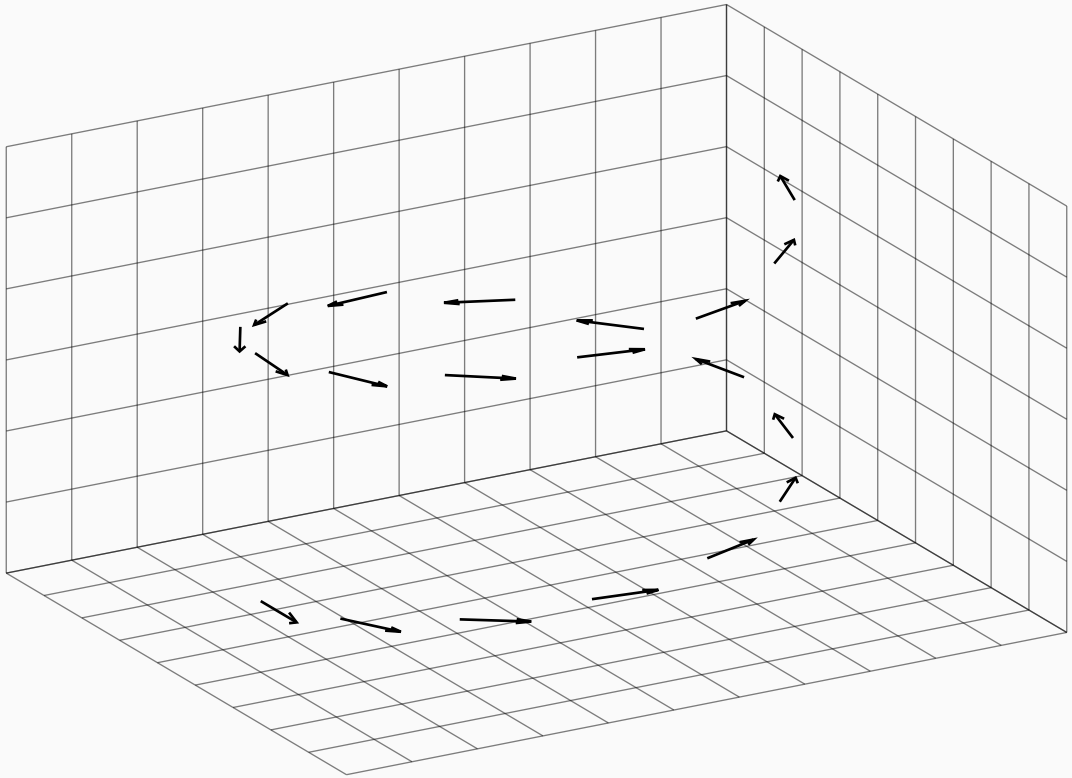

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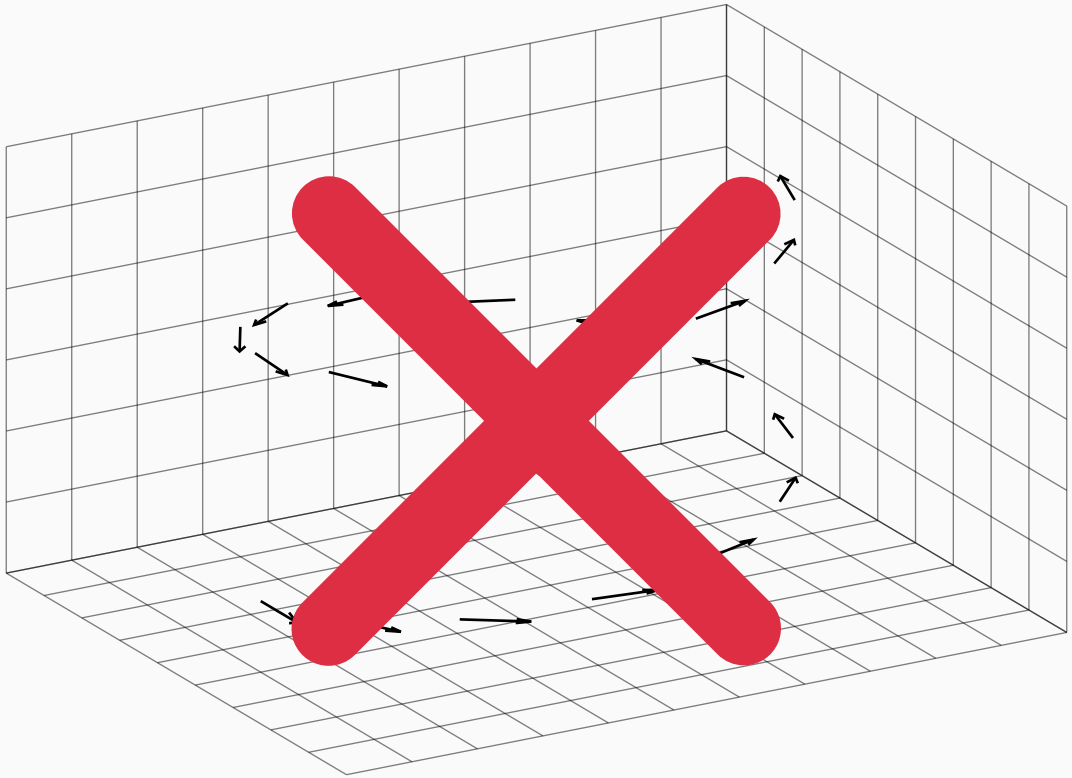

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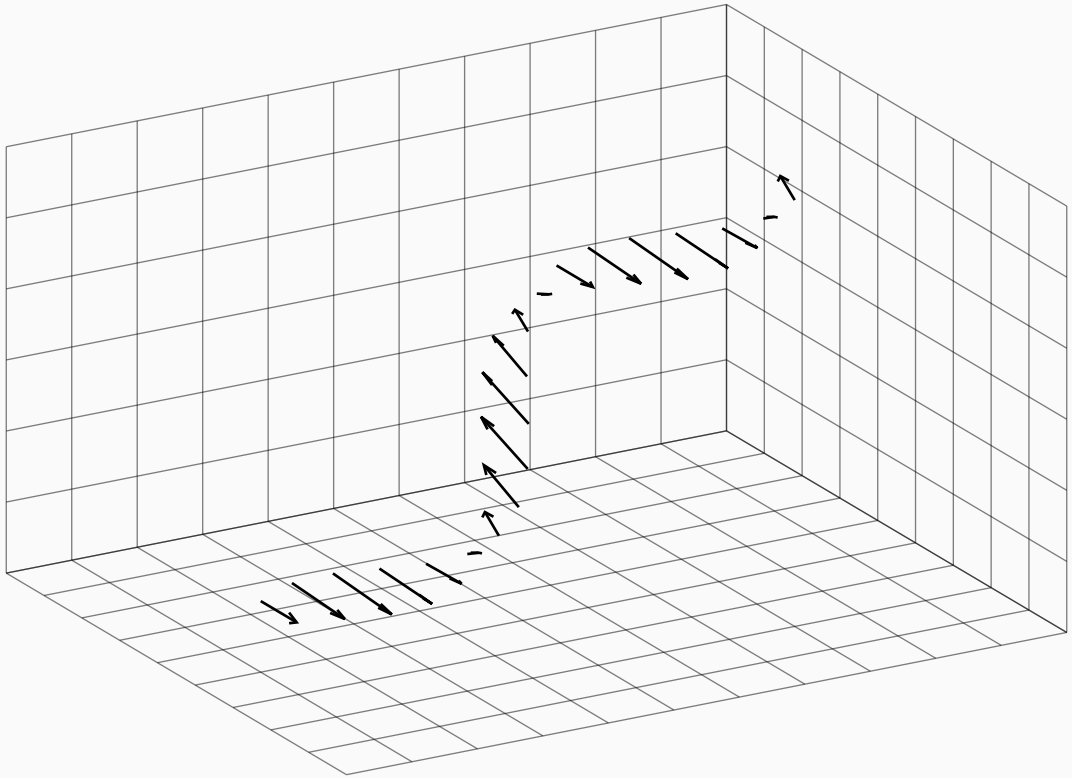

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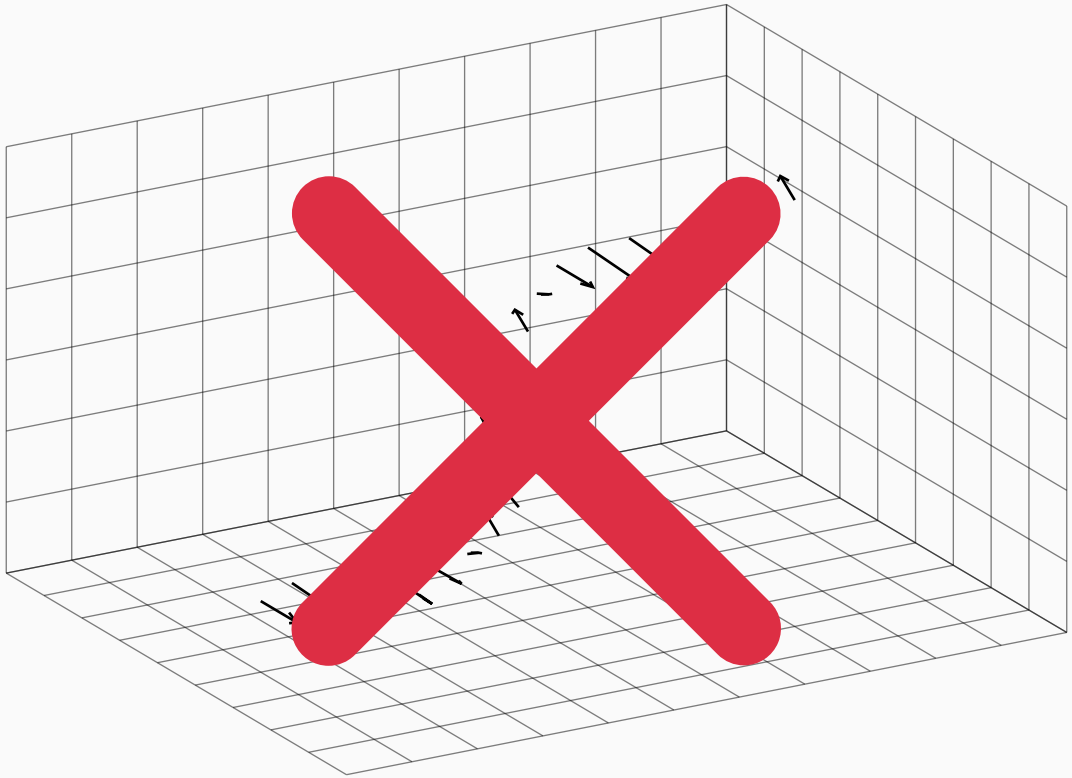

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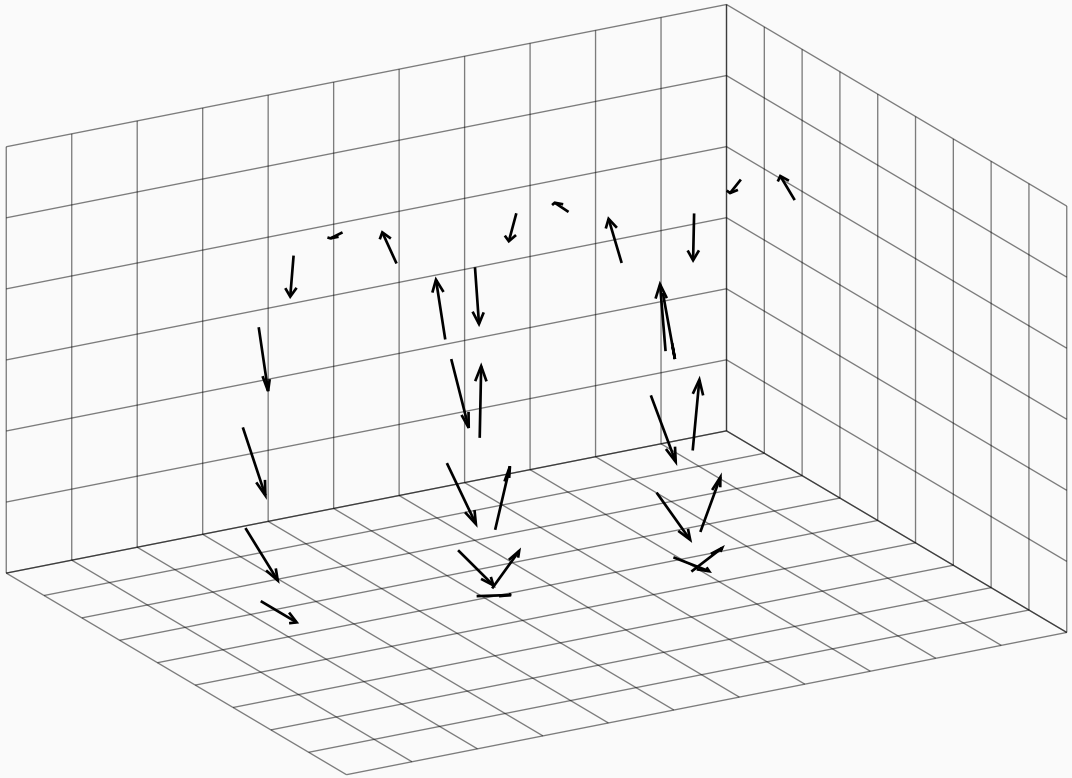

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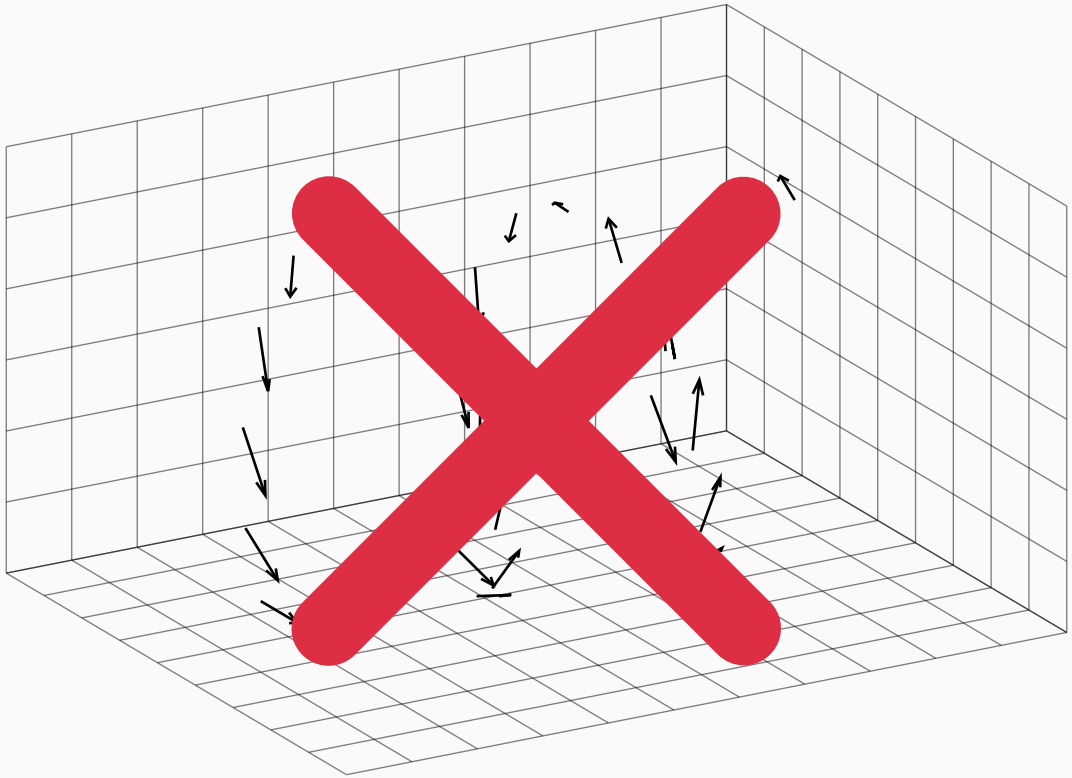

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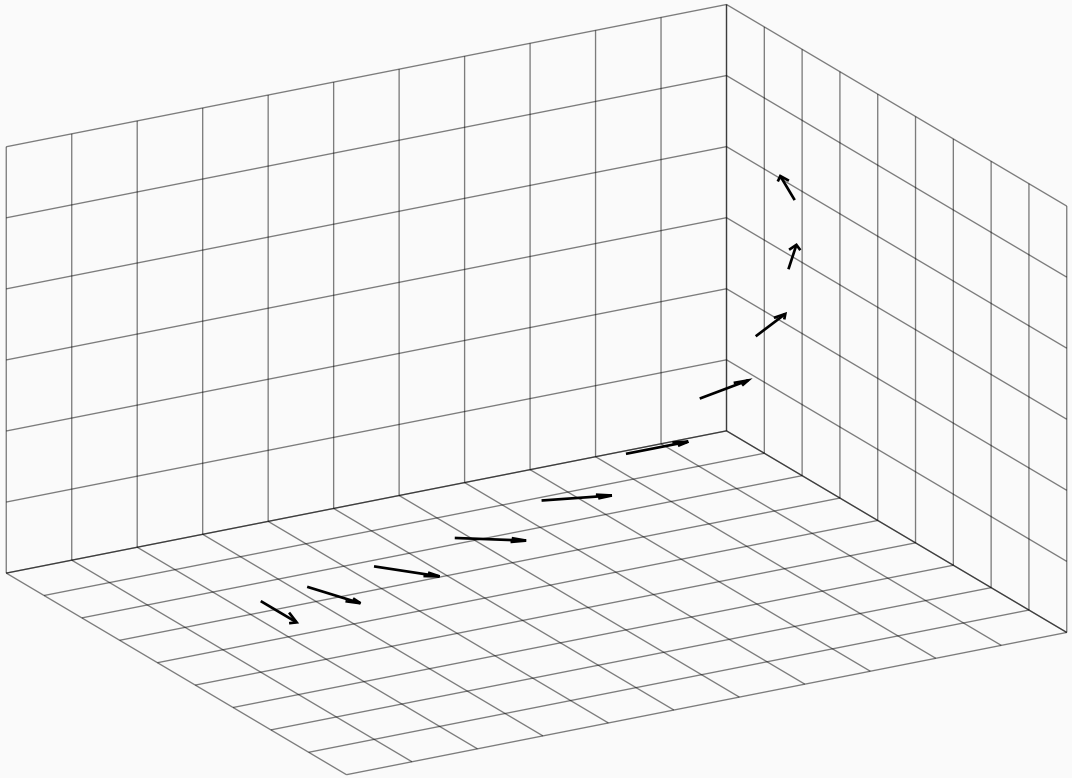

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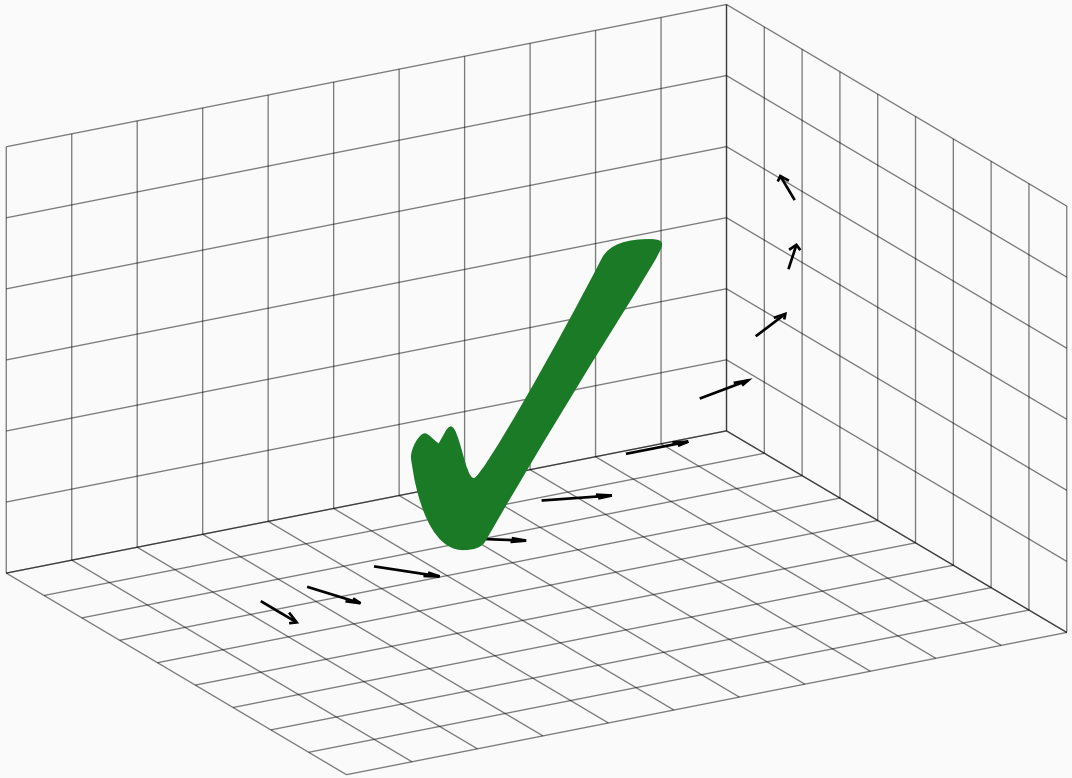

Mav Distance

Target	Unit	Original	Mav Distance (ours)	Difference %
μ	D	0.0195	0.0181	−07.2
α	a_0^3	0.0556	0.0540	−02.9
$\varepsilon_{\text{homo}}$	eV	0.0225	0.0229	+01.8
$\varepsilon_{\text{lumo}}$	eV	0.0205	0.0207	+01.0
$\Delta\varepsilon$	eV	0.0414	0.0431	+04.0
$\langle R^2 \rangle$	a_0^2	0.4160	0.4942	+18.8
ZPVE	meV	1.5647	1.5613	−00.2
U_0	eV	0.9920	0.7047	−28.9
U	eV	1.3593	1.0947	−19.5
H	eV	1.0204	1.0856	+06.4
G	eV	1.1856	0.9691	−18.3
c_v	cal/mol·K	0.0291	0.0283	−02.8

PONITA trained to predict chemical properties of various molecules (QM9 dataset [5], [6]). Mean absolute error on the test set is reported (lower is better).

Using the **mav distance** has a **marginal positive** impact on the accuracy of the PONITA model when predicting molecular properties.

Using the **mav distance** has a **marginal positive** impact on the accuracy of the PONITA model when predicting molecular properties.[1]

[1]However, it did have a significant negative impact on the financial situation of our group.

Thank you for your attention!

Questions?

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