Roto-Translation Invariant Metrics on Position-Orientation Space

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Motivation

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- Data from a MRI machine can be described as a scalar field $f : \mathbb{M}_3 \to \mathbb{R}$ on *position-orientation space* $\mathbb{M}_3 := \mathbb{R}^3 \times S^2$. (High angular resolution diffusion imaging).
- This data can be enhanced/denoised using (nonlinear) PDEs defined on $\mathbb{M}_3$ (Portegies et al. [1], Duits et al. [2] Smets et al. [3]):

$$\begin{aligned} \text{Diffusion} \quad & \frac{\partial f}{\partial t} = \frac{1}{2}\Delta f \\ \text{Dilation/Erosion} \quad & \frac{\partial f}{\partial t} = \pm\frac{1}{2}\|\nabla f\|^2 \\ \text{Total Variation Flow} \quad & \frac{\partial f}{\partial t} = \nabla \cdot \frac{\nabla f}{\|\nabla f\|} \end{aligned}$$

- ...where gradient ∇, norm $\|\cdot\|$, Laplacian Δ, and divergence $\nabla \cdot$, *all* depend on the *Riemannian metric* $\mathcal{G}$ that is chosen on $\mathbb{M}_3$.
- For this processing to be *roto-translation group* $\mathrm{SE}(3)$ *equivariant* the Riemannian metric $\mathcal{G}$ on $\mathbb{M}_3$ needs to be $\mathrm{SE}(3)$ *invariant*.

Can we **classify all** roto-translation group $\mathrm{SE}(3)$ invariant Riemannian metrics on position-orientation space $\mathbb{M}_3$?

Definitions

Definitions

Definition: The *special Euclidean group* or *roto-translation group* is

$$\mathrm{SE}(3) := \left\{(t, R) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \;\middle|\; R^\top R = I, \det R = 1\right\},$$

where t is the *translation vector* and R the *rotation matrix*.

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

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

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

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

$$(t, R) \triangleright (x, n) = (t + Rx, Rn).$$

Which induces an action $\triangleright\colon \mathrm{SE}(3) \times T\mathbb{M}_3 \to T\mathbb{M}_3$ on tangent vectors

$$(t, R) \triangleright (\dot{x}, \dot{n}) = (R\dot{x}, R\dot{n}).$$

Invariant metrics

Invariant metrics

Definition: A Riemannian metric $\mathcal{G}$ on $\mathbb{M}_3$ is SE(3)-*invariant* if

$$\mathcal{G}(g \triangleright \dot{p}, g \triangleright \dot{p}) = \mathcal{G}(\dot{p}, \dot{p}) \text{ for all } \dot{p} \in T\mathbb{M}_3 \text{ and } g \in \mathrm{SE}(3)$$

Theorem: In Bellaard et al. [4] we show that **every** SE(3)-invariant Riemannian metric $\mathcal{G}$ on $\mathbb{M}_3$ yields a norm of the form

$$\|(p, \dot{p})\|_{\mathcal{G}} = w_1 |\dot{x} \cdot n|^2 + w_2 \|\dot{x} \times n\| + w_3 \|\dot{n}\|^2 + 2w_4 \dot{x} \cdot \dot{n} + 2w_5 \dot{x} \cdot (\dot{n} \times n),$$

where $p = (x, n) \in \mathbb{M}_3$, $\dot{p} = (\dot{x}, \dot{n}) \in T_p\mathbb{M}_3$, and $w_i \in \mathbb{R}$ *metric parameters* that satisfy the positivity constraints $w_1, w_2, w_3 > 0$ and $w_2 w_3 > w_4^2 + w_5^2$.

We can **classify all** roto-translation group $\mathrm{SE}(3)$ invariant metrics on position-orientation space $\mathbb{M}_3$ through five **metric parameters** $w_1, \ldots, w_5 \in \mathbb{R}$.

Riemannian Distance

Riemannian Distance

- Both the diffusion and dilation/erosion PDEs on $\mathbb{M}_3$ can be (approximately) solved using the *Riemannian distance* $d : \mathbb{M}_3 \times \mathbb{M}_3 \to \mathbb{R}_{\geq 0}$:

$$\frac{\partial f}{\partial t} = \frac{1}{2}\Delta f \qquad \longrightarrow \qquad f_t(p) \approx \int_{\mathbb{M}_3} \exp\left(-\frac{d(p,q)^2}{2t}\right) \cdot f_0(q)\,\mathrm{d}q$$

$$\frac{\partial f}{\partial t} = -\frac{1}{2}\|\nabla f\|^2 \qquad \longrightarrow \qquad f_t(p) = \inf_{q \in \mathbb{M}_3} \frac{d(p,q)^2}{2t} + f_0(q)$$

- However, the Riemannian distance d is **expensive** to compute.
- In Portegies et al. [1] it is suggested to use the *mav distance* as a **cheap** alternative.
- We saw an application of the mav distance as a *learnable* invariant in the PONITA architecture [5] by Bekkers et al. [6], with the metric parameter $w_1, \ldots, w_5$ acting as trainable weights.

More Definitions

More Definitions

Definition: The *Lie algebra* of the roto-translation group is

$$\mathfrak{se}(3) := \left\{(v,\omega) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \;\middle|\; \omega^\top + \omega = 0\right\},$$

where v is the *translation velocity vector* and ω the *angular velocity tensor*.

Definition: The *angular velocity* of a generator $(v,\omega) \in \mathfrak{se}(3)$ is given by $\sqrt{\omega_1^2 + \omega_2^2 + \omega_3^2}$ where ω is parametrized as

$$\omega = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix},$$

Definition: The action $\triangleright\colon \mathrm{SE}(3) \times \mathbb{M}_3 \to \mathbb{M}_3$ induces a *Lie algebra action* $\triangleright\colon \mathfrak{se}(3) \times \mathbb{M}_3 \to T\mathbb{M}_3$

$$(v,\omega) \triangleright (x,n) = (v + \omega x, \omega n).$$

Mav Distance

Mav Distance

Definition: The *length* $L(\gamma)$ of a curve $\gamma : [0, 1] \to \mathbb{M}_3$ with respect to a Riemannian metric $\mathcal{G}$ is given by $L(\gamma) := \int_0^1 \|\dot{\gamma}(t)\| \, \mathrm{d}t$.

Definition: The *Riemannian distance* is

$$d(p_1, p_2) = \inf_{\gamma \in \Gamma} L(\gamma)$$

where Γ is the set of piecewise continuously differentiable curves between $\gamma(0) = p_1$ and $\gamma(1) = p_2$.

Definition: The *mav generator* $M(p_1, p_2) \in \mathfrak{se}(3)$ is the unique generator between two position-orientations $p_1, p_1 \in \mathbb{M}_3$, i.e. $\exp(M) \triangleright p_1 = p_2$, with *minimal angular velocity*.

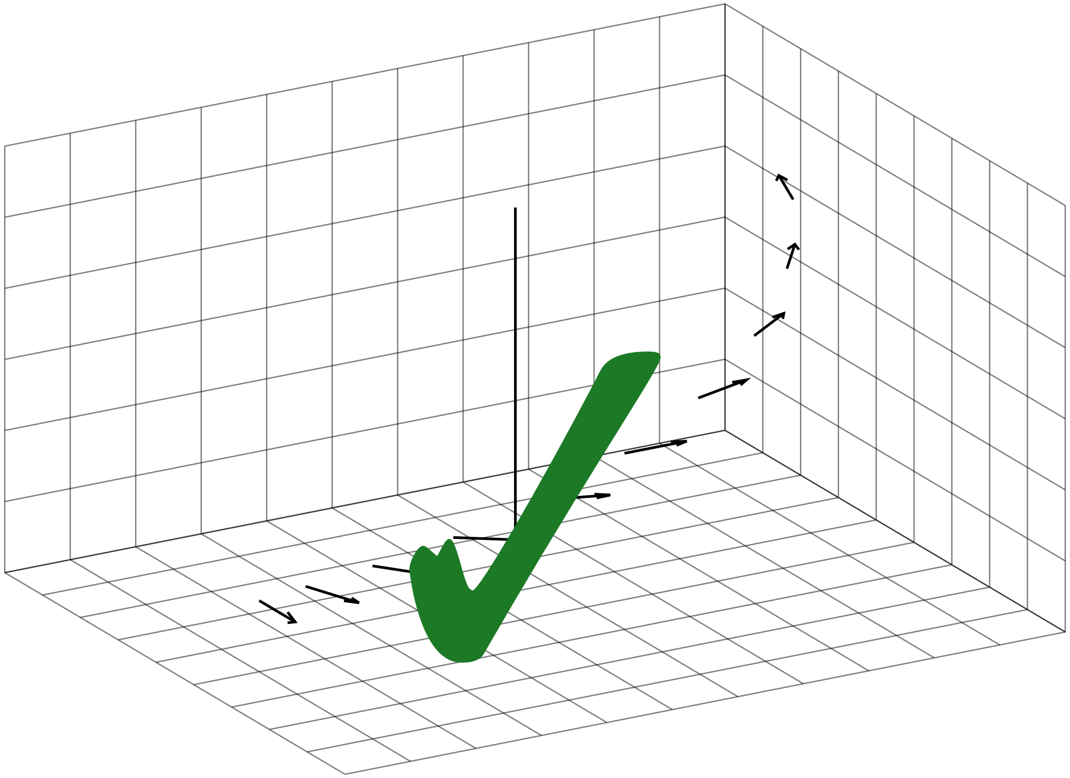
Definition: The *mav distance* is

$$\mu(p_1, p_2) = L(\eta)$$

where $\eta : [0, 1] \to \mathbb{M}_3$ is the *mav curve* defined by $\eta(t) = \exp(tM) \triangleright p_1$, and $M = M(p_1, p_2) \in \mathfrak{se}(3)$ the mav generator.

Mav Distance

$$t \mapsto \exp(tM) \rhd p_1$$



Mav Distance

- But why is the mav distance μ cheap to compute?

Proposition: Let $X \in \mathfrak{se}(3)$, $p \in \mathbb{M}_3$, and $\mathcal{G}$ an SE(3) invariant Riemannian metric on $\mathbb{M}_3$. Then the length of the curve $\eta : t \mapsto \exp(tX) \triangleright p$ is

$$L(\eta) = \|X \triangleright p\|.$$

- So more specifically

Proposition: Let $\mathcal{G}$ be an SE(3) invariant Riemannian metric on $\mathbb{M}_3$. The mav distance μ can be computed as

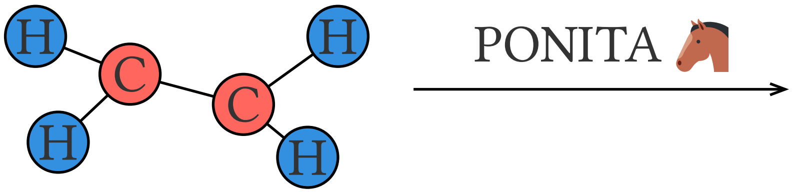
$$\mu(p_1, p_2) = \|M(p_1, p_2) \triangleright p_1\|$$

The mav distance μ is **cheap** because the length of the mav curve w.r.t. a roto-translation group $\mathrm{SE}(3)$ invariant metric $\mathcal{G}$ is straightforward.

Experiment

Experiment

- QM9: predict chemical properties of small organic molecules.
- PONITA: original architecture versus our mav distance with trainable metric parameters.
- Code can be found at [7].



PONITA 🐴

Dipole moment: 0.05 D
Isotropic polarizability: 1.55 a_0^3
Internal energy at 0K: 1.30 eV
$\vdots$

Experiment

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 Ramakrishan 2014, Ruddigkei 2012). 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 chemical properties.

Thank you for your attention!

Questions?

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