Extending persistence to stronger and faster invariants of clouds under isometry

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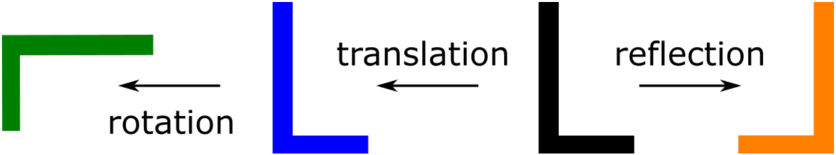
THE ROYAL SOCIETY

Equivalence by rigid motion

Many real-life objects are rigid and should be considered equivalent under **rigid motion**:



Compositions of translations and rotations in $\mathbb{R}^n$ form the group $\mathrm{SE}(n)$. If we allow reflections, we get the Euclidean group $\mathrm{E}(n)$ of **isometries**.

In a general metric space, an **isometry** is any map that preserves all inter-point distances.

Persistence and isometry

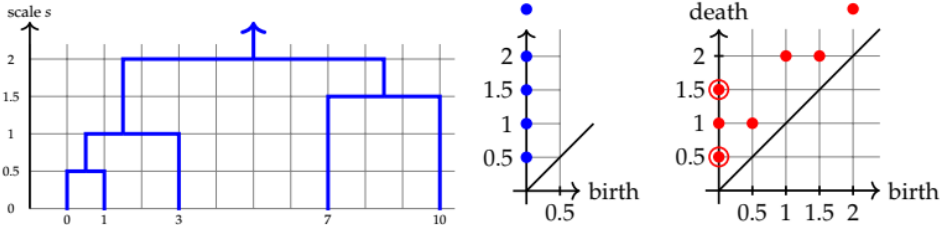
We can reconstruct any *ordered* $p_1, \dots, p_m \in \mathbb{R}^n$ from the matrix of distances $d_{ij} = |p_i - p_j|$ or $p_i \cdot p_j$, uniquely under isometry (Annals of Maths, 1935). Unordered points have $m!$ permutations.

For the Vietoris-Rips (VR), Cech, α-filtrations on a point set A in a metric space or $\mathbb{R}^n$, *persistent homology* is an invariant of A **under isometry**.

Questions: How strong is persistence under isometry? If incomplete, is it invariant under any weaker geometric *relation on point clouds* in $\mathbb{R}^n$?

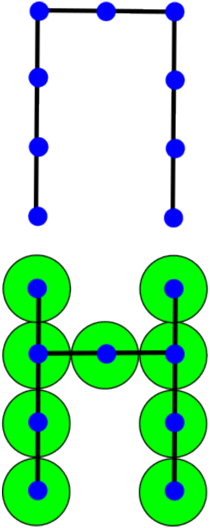
0D persistence $<<$ mergegram

$\{0,4,6,9,10\} \not\approx \{0,1,3,7,10\}$ have the same 0D persistence (edge-lengths of a Minimum Spanning Tree), but are distinguished by the stronger *mergegram*: also continuous in the bottleneck distance, the same asymptotic time.

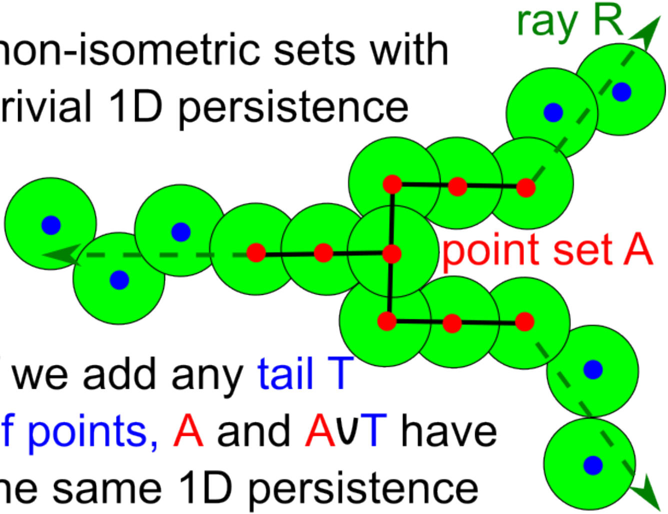


Yury Elkin, VK. Mathematics v.9(17), 2121 (2021).

P.Smith, VK. Generic families of metric spaces with identical or trivial 1D persistence, APCT'24.



non-isometric sets with trivial 1D persistence



if we add any tail T of points, A and A∨T have the same 1D persistence

Geo-mapping problem: point sets

Find a (complete, bi-continuous, and poly-time) *geocode* I for discrete sets of *unordered points*.

Invariance: if point sets $S \simeq Q$ are isometric, then $I(S) = I(Q)$, so I should be well-defined on isometry classes or I has *no false negatives*.

Completeness: if $I(S) = I(Q)$, then $S \simeq Q$ are isometric, hence I has *no false positives*.

Continuity: find a *metric* d and a constant λ such that if any point of S is perturbed within its ε-neighborhood, then $I(S)$ changes by max $\lambda\varepsilon$.

Harder practical requirements

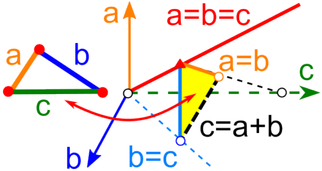
Invertibility: any $S \subset \mathbb{R}^n$ can be reconstructed from its invariant $I(S)$ in a *continuous* way.

Computability: the invariant I, the metric d, and a reconstruction of $S \subset \mathbb{R}^n$ from $I(S)$ can be obtained in polynomial time in the size of S, forbidding *infinite or exponential size* invariants.

Geo-style maps: describe all *realizable values* $I(S)$ that allow us to reconstruct a cloud $S \subset \mathbb{R}^n$. Then I defines *geographic-style coordinates* on the moduli space of point clouds under isometry.

Euclid's ideal solution for triangles

SSS theorem for $m = 3$ points in any $\mathbb{R}^n$. Two triangles are congruent (isometric) *if and only if* they have the same triple of sides a, b, c (under all 6 permutations). For rigid motion (without reflections), allow only 3 cyclic permutations.



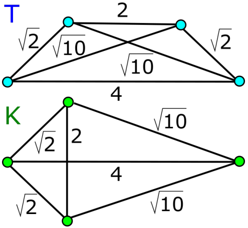
The **Cloud Isometry Space** $\mathrm{CIS}(\mathbb{R}^n; 3)$ is the cone in $\mathbb{R}^3$ $\{0 < a \leq b \leq c \leq a + b\}$ continuously parametrized by three inter-point distances a, b, c.

Generically complete invariants

Is the problem *open for quadrilaterals* in $\mathbb{R}^2$?

One can train neural networks to experimentally output isometry invariants but it can be hard to prove their completeness and continuity.

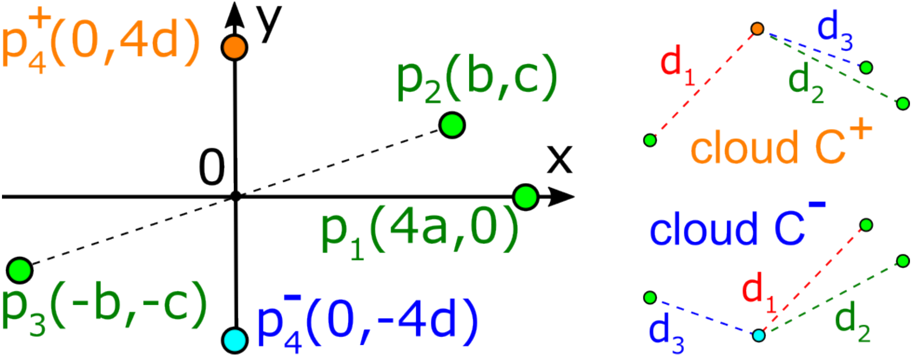
Boutin, Kemper, 2004: the vector of all sorted pairwise distances is *generically complete* in $\mathbb{R}^n$



distinguishing almost all clouds of unordered points except singular examples. These non-isometric clouds have the same 6 pairwise distances.

Clouds with the same 6 distances

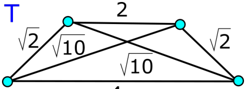
Pairs of non-isometric clouds $\{p_1, p_2, p_3, p_4^{\pm}\}$ in $\mathbb{R}^2$ (depending on 4 parameters $a, b, c, d > 0$) have the same 6 pairwise distances below.



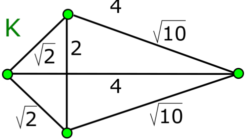
What invariant can distinguish these clouds?

Pointwise Distance Distributions

For a set S of m points $p_1, \dots, p_m$ in a metric space, choose any number $1 \leq k < m$ of neighbors and build the $m \times k$ matrix $D(S;k)$.



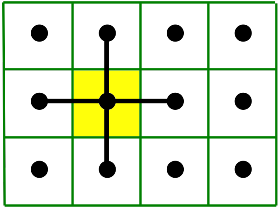
$$\mathrm{PDD}(T;3) = \left(\begin{array}{c|ccc} 1/2 & \sqrt{2} & 2 & \sqrt{10} \\ 1/2 & \sqrt{2} & \sqrt{10} & 4 \end{array}\right) \neq$$



$$\mathrm{PDD}(K;3) = \left(\begin{array}{c|ccc} 1/4 & \sqrt{2} & \sqrt{2} & 4 \\ 1/2 & \sqrt{2} & 2 & \sqrt{10} \\ 1/4 & \sqrt{10} & \sqrt{10} & 4 \end{array}\right).$$

Collapse identical rows and assign weights. The matrices PDDs are continuously compared by *Earth Mover's Distance* (EMD), NeurIPS 2022.

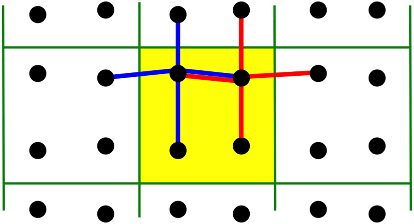
Earth Mover's Distance (EMD)



any small perturbation

→

continuously affects PDD



[Widdowson, VK. NeurIPS 2022] If we perturb all points of a set S up to ε, the perturbed set S' has $\mathrm{EMD}(\mathrm{PDD}(S;k),\mathrm{PDD}(S';k)) \leq 2\varepsilon$.

PDD(S;4)=

weight 1	1	1	1	1

PDD(S';4)=

weight 0.5	0.8	1.005	1.005	1.2
weight 0.5	1	1	1.005	1.005

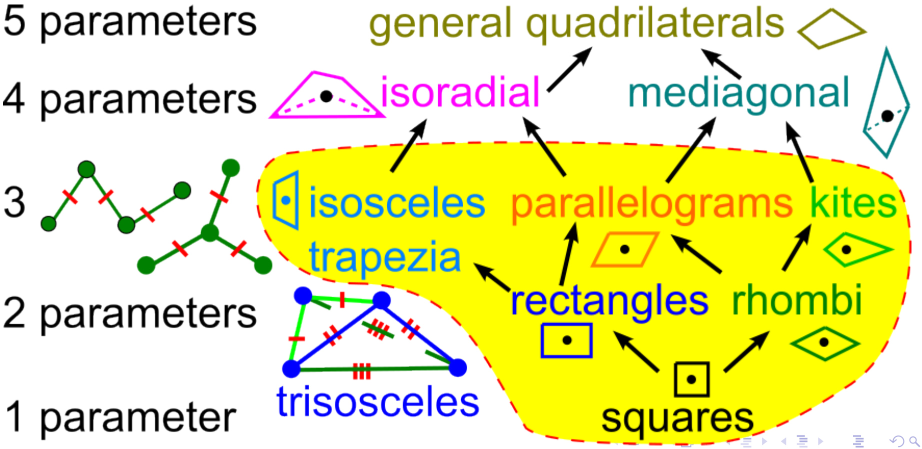
EMD = 0.5 (0.2+0.005) = 0.1025 ⩽ 0.2 bound

EMD minimizes a cost of matching weighted rows.

New types of 4-point clouds in $\mathbb{R}^2$

Thm 5.3 in arxiv:2108.04798v3 (July 2025):

PDD is *complete* for any $m \leq 4$ points in $\mathbb{R}^n$.



Invariants stronger than PDD

Conjecture: PDD is complete for any m in $\mathbb{R}^2$.

Some clouds in $\mathbb{R}^3$ have equal PDDs. We have extended the PDD to a *complete* SCD in $\mathbb{R}^n$.

simplest invariants **SRD** and **SPD**
Sorted Radial/Pairwise Distances

near-linear time invariant **PDD**
Pointwise Distance Distribution

in any metric space

in any Euclidean space

strongest isometry invariants **SDD**
Simplexwise Distance Distribution

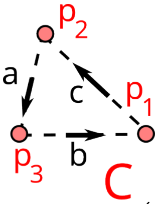
complete isometry invariants **SCD**
Simplexwise Centered Distribution

All these invariants are Lipschitz continuous with constant 2 [Widdowson, VK. CVPR 2023]. Extended in arxiv:2303.13486 and 2303.14161.

Towards complete invariants

Let C be a cloud of m unordered points in a *metric space*. $\mathrm{SDD}(C;h)$ for $h=1$ is $\mathrm{PDD}(C)$.

Any sequence $A\subset C$ of h points has the matrix $\mathrm{RDD}(C;A)$ with $m-h$ permutable columns of distances from $q\in C-A$ to all points of A.



The **Relative Distance Distribution** for $A=\begin{pmatrix}p_2\\p_3\end{pmatrix}$ is $\mathrm{RDD}(C;A)=[a;\begin{pmatrix}c\\b\end{pmatrix}]$.

$\mathrm{RDD}(C;\begin{pmatrix}p_3\\p_1\end{pmatrix})=[b;\begin{pmatrix}a\\c\end{pmatrix}]$, $\mathrm{RDD}(C;\begin{pmatrix}p_1\\p_2\end{pmatrix})=[c;\begin{pmatrix}b\\a\end{pmatrix}]$

Simplexwise Distance Distribution

Classes of these RDD pairs with the distance matrix of A (under permutations of points in A) for all h-point unordered subsets $A \subset C$ form **SDD**$(C; h)$. For $h = 2$, the stronger invariant $\mathrm{SDD}(C; 2)$ *distinguished all counter-examples* to the completeness of easier past invariants in $\mathbb{R}^3$

Thm (CVPR'23): for any m-point cloud C in a *metric space*, $\mathrm{SDD}(C; h)$ is computable in time $O(m^{h+1}/(h-1)!)$ and has Lipschitz constant 2 in EMD, time $O(h!(h^2 + m^{1.5}\log^h m)l^2 + l^3 \log l)$.

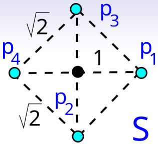
Simplexwise Centered Distribution

In $\mathbb{R}^n$, fix the center of a cloud C at $p_0 = 0 \in \mathbb{R}^n$.

For any *ordered* subset $A = (p_1, \dots, p_{n-1}) \subset C$, $\mathrm{OCD}(C; A)$ is the pair of the distance matrix $D(A \cup \{0\})$, matrix M with $m - n + 1$ permutable columns of n distances $|q - p_i|$ for $q \in C - A$.

To reconstruct $C \subset \mathbb{R}^n$ under rigid motion, we add the *sign of the determinant* on the vectors from each $q \in C - A$ to the points $p_0, \dots, p_{n-1}$.

SCD(C) is the *unordered set of classes* of $\mathrm{OCD}(C; A)$ for all $(n-1)$-point subsets $A \subset C$.



For each 1-point subset $A = \{p\} \subset S$, the distance matrix $D(A \cup \{0\})$ on two points is one number 1. Then $M(S; A \cup \{0\})$ has $m - n + 1 = 3$ columns. For $p_1 = (1, 0)$, we have

$$M\left(S; \begin{pmatrix} p_1 \\ 0 \end{pmatrix}\right) = \begin{pmatrix} \sqrt{2} & \sqrt{2} & 2 \\ 1 & 1 & 1 \\ - & + & 0 \end{pmatrix},$$

whose three columns are ordered as p_2, p_3, p_4. The sign in the bottom right corner is 0 because $p_1, 0, p_4$ are in a straight line. By the rotational symmetry,

$$\mathrm{SCD}(S) \text{ is one } \mathrm{OCD} = \left[1, \begin{pmatrix} \sqrt{2} & \sqrt{2} & 2 \\ 1 & 1 & 1 \\ - & + & 0 \end{pmatrix}\right].$$

Complete invariant SCD in $\mathbb{R}^n$

Theorem (CVPR 2023): for any n-dimensional cloud C of m unordered points, the *Simplexwise Centered Distribution* $\mathrm{SCD}(C)$ is a **complete invariant** under rigid motion in $\mathbb{R}^n$, computable in time $O(m^n/(n-4)!)$, and has Lipschitz constant 2 in the EMD, which is computable in time $O((n-1)!(n^2+m^{1.5}\log^n m)l^2+l^3\log l)$. Here l is the number of different OCDs in SCDs.

The **complete isometry invariant** of $C\subset\mathbb{R}^n$ is the pair $\{\mathrm{SCD}(C),\overline{\mathrm{SCD}}(C)\}$ with reversed signs.

Hierarchy of cloud invariants

Fast: *Sorted Radial Distances* SRD (decreasing distances from 0 to m points) in time $O(m)$.

Stronger: Sorted Pairwise Distances $\mathrm{SPD}(C)$.

Even stronger: $\mathrm{PDD}(C; m-1)$ in time $O(m^2)$.

Complete: $\mathrm{SCD}(C)$ in time $O(m^3)$ for $C \subset \mathbb{R}^3$.

The QM9 database has 130K+ molecules with atomic coordinates and 873,527,974 pairs of molecules of the same size. The hierarchy of the invariants above *distinguished all pairs in QM9* within a few hours on a desktop computer.

Principle of Molecular Rigidity

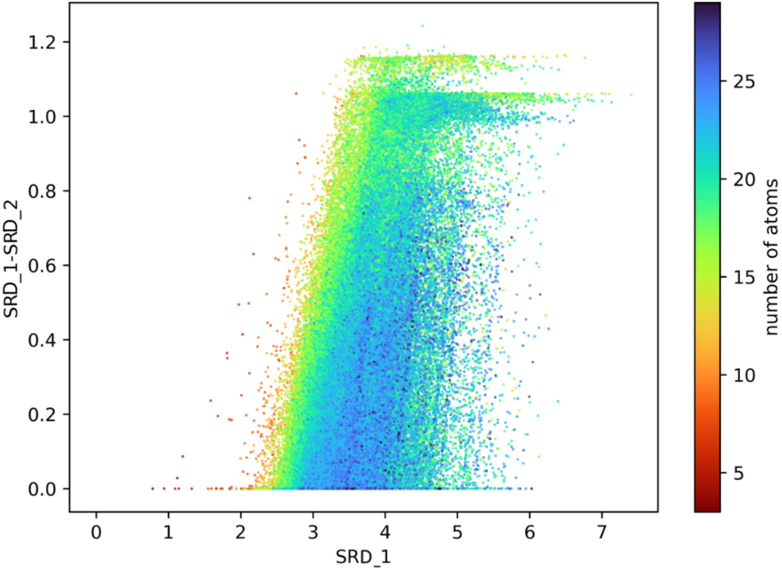
Chemically different molecules *differ rigidly*.

invariant	distance, Å	molecule A	molecule B
SRD	0.02057	$H_3C_4N_3O_2$	$H_4C_5N_2O_1$
SPD	0.05505	$H_3C_4N_5$	$H_3C_5N_3O_1$
PDD	0.05145	$H_3C_4N_5$	$H_3C_5N_3O_1$
SCD	0.07054	$H_4C_5N_4$	$H_4C_6N_2O_1$

The map: $\{$molecules$\} \to \{$clouds of atomic centers$\}$ is **injective** modulo rigid motion in $\mathbb{R}^3$.

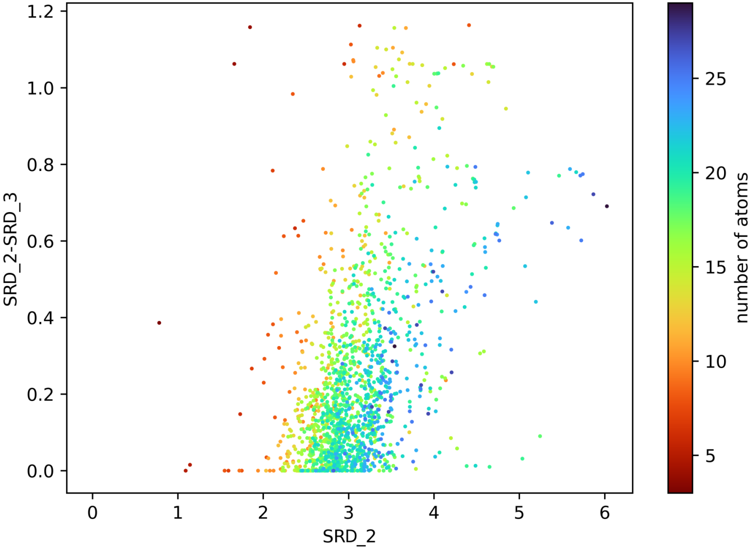
New definition: a *molecular structure* is a class of atomic clouds under rigid motion in $\mathbb{R}^3$.

Geo-graphic-style maps of QM9



All QM9 molecules. The units are Å $=10^{-10}$ m.

Use further invariants to zoom in

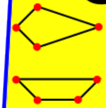


QM9 subset: $\mathrm{SRD}_1 = \mathrm{SRD}_2$ equal radii from a center.

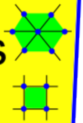
Collaborations are welcome!

We can similarly explore continuous spaces of other data objects (proteins, graphs, meshes) under rigid motion or other equivalences.

Geometric Data Science



geographic-style maps on spaces of data modulo an equivalence



rigid classification of unordered point clouds

Crystal Isometry Space of all **periodic** crystals

equivalence *metric* *continuity* *computability*