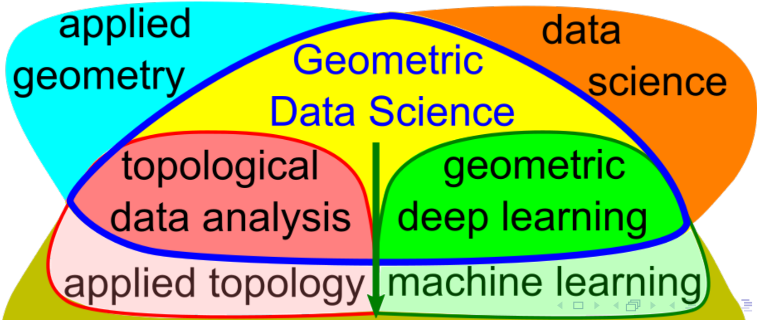
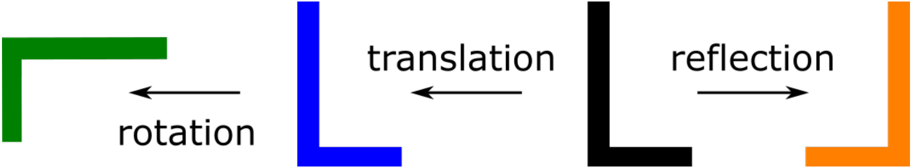
CVPR 2023 paper : Recognizing rigid patterns of unlabeled point clouds by *complete and continuous isometry invariants* with **no false negatives** and **no false positives** for all data.

Authors: Daniel Widdowson, Vitaliy Kurlin.
Materials Innovation Factory, Liverpool, UK



A **cloud** consists of *m unlabeled* points in $\mathbb{R}^n$, or in a metric space (given by pairwise distances).

An **isometry** is any map preserving inter-point distances. In any Euclidean $\mathbb{R}^n$, all isometries are compositions of translations, rotations, and reflections, and form the Euclidean group $E(n)$.



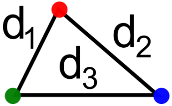
If reflections are excluded, we get *rigid motions* that form the group $SE(n)$. The **rigid pattern** of a cloud C is its class under $SE(n)$ or $E(n)$.

Isometry problem for clouds

Design an invariant I : {isometry classes of clouds in $\mathbb{R}^n$} $\to$ {a simpler space} satisfying

completeness: any clouds A, B are isometric if and only if $I(A) = I(B)$, so I is a DNA-style code with *no false negatives* and *no false positives*;

Lipschitz continuity : there is a constant λ, if any point of A is perturbed up to ε, then $I(A)$ changes by at most $\lambda\varepsilon$ in a *metric d* such that



$d(I(A), I(B)) = 0 \Leftrightarrow A, B$ are isometric,

$d(I(A), I(B)) = d(I(B), I(A))$, $d_1 + d_2 \geq d_3$.

Labeled vs unlabeled points in $\mathbb{R}^n$

If all m points of a cloud $C \subset \mathbb{R}^n$ are labeled $p_1, \dots, p_m$, then C is reconstructed (uniquely up to isometry) from the distances $d_{ij} = |p_i - p_j|$.

If m points are unlabeled, C can be uniquely represented by $m!$ distance matrices obtained by $m!$ permutations of points, it's impractical.

The isometry problem has one more condition **computability**: the invariant I and the metric d are computable in a polynomial time in the number m of points for a fixed dimension n.

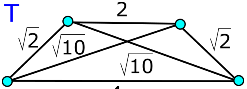
Generically complete invariants

Geometric Deep Learning (GDL) trains neural networks to output isometry invariants but without proofs of completeness and continuity while ignoring the known geometric invariants.

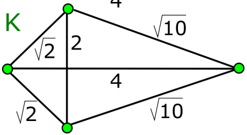
Boutin, Kemper, 2004: the vector of all sorted pairwise distances is *generically complete* in $\mathbb{R}^n$ distinguishing almost all clouds of unlabeled points except singular examples. We extend this invariant instead of trying to reinvent the wheel.

Pointwise Distance Distributions

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



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



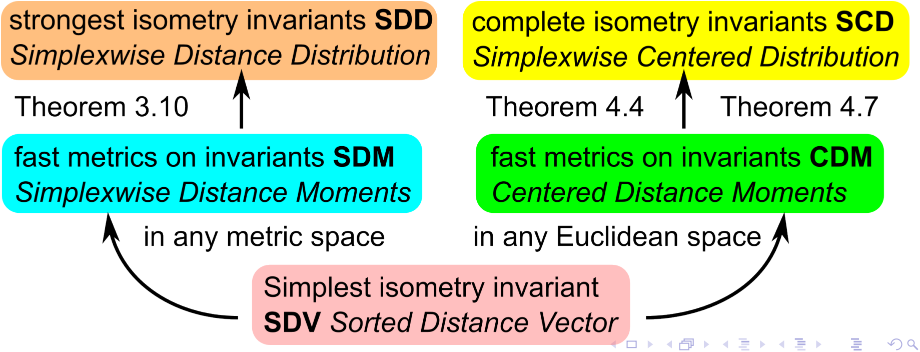
$$\mathrm{PDD}(K;3) = \left(\begin{array}{c|ccc} 1/4 & \sqrt{2} & \sqrt{2} & 4 \\ 1/2 & \sqrt{2} & 2 & \sqrt{10} \\ 1/4 & \sqrt{10} & \sqrt{10} & 4 \end{array}\right).$$

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

Invariants stronger than PDD

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

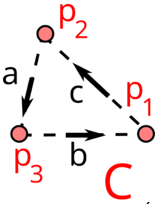
PDD is not complete for some clouds in $\mathbb{R}^3$, but the *stronger invariants* below distinguish them.



Relative Distance Distribution

Let C be a cloud of m unlabeled 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

$$A = \begin{pmatrix} p_2 \\ p_3 \end{pmatrix} \text{ is } \mathrm{RDD}(C; A) = [a; \begin{pmatrix} c \\ b \end{pmatrix}].$$

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

Simplexwise Distance Distribution

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

Theorem 3.10: 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 $O(h!(h^2 + m^{1.5}\log^h m)l^2 + l^3 \log l)$.

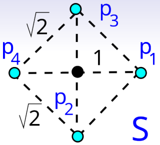
Simplexwise Centered Distribution

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 $D(A)$ and matrix M with $m - n + 1$ permutable columns of n distances $|q - p_i|$ for $q \in C - A$.

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

$\mathrm{SCD}(C)$ is the unodered 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

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

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,

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

The strength $\sigma(B)$ of a simplex B

The discontinuity of a sign in degenerate cases such as 3 points in a line is resolved by the new *strength* of a simplex $\sigma(B) = V^2/p^{2n-1}$, where V is the volume, p is the half-perimeter of B.

The strength of a triangle $B \subset \mathbb{R}^2$ with sides a, b, c is $\sigma(B) = \dfrac{(p-a)(p-b)(p-c)}{p^2}$, which is 'roughly linear' unlike the 'quadratic' area of B.

Theorem 4.4: in $\mathbb{R}^n$, the strength σ is Lipschitz continuous with constants $c_2 = 2\sqrt{3}$, $c_3 \approx 0.43$.

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

Theorem 4.7: for any cloud C of m unlabeled points in $\mathbb{R}^n$, the Simplexwise Centered Distribution $\mathrm{SCD}(C)$ is a *complete invariant* under rigid motion, and is computable in time $O(m^n/(n-4)!)$, has Lipschitz constant 2 in the Earth Mover's Distance (EMD), computable in time $O((n-1)!(n^2+m^{1.5}\log^n m)l^2+l^3\log l)$, l is the number of different OCDs in SCDs.

The complete isometry invariant is the pair of $\mathrm{SCD}(C)$ and $\overline{\mathrm{SCD}}(C)$ with reversed signs.

Geometric Data Science

The **major breakthroughs** are the continuous isometry classifications for discrete point sets: *finite* (CVPR 2023), *periodic* (NeurIPS 2022).