The strength of a simplex is the key to a continuous isometry classification of Euclidean clouds of unlabelled points

Vitaliy Kurlin
Computer Science department
University of Liverpool, UK
vitaliy.kurlin@gmail.com

Abstract

This paper solves the continuous classification problem for finite clouds of unlabelled points under Euclidean isometry. The Lipschitz continuity of required invariants in a suitable metric under perturbations of points is motivated by the inevitable noise in measurements of real objects.

The best solved case of this isometry classification is known as the SSS theorem in school geometry saying that any triangle up to congruence (isometry in the plane) has a continuous complete invariant of three side lengths.

However, there is no easy extension of the SSS theorem even to four points in the plane partially due to a 4-parameter family of 4-point clouds that have the same six pairwise distances. The computational time of most past metrics that are invariant under isometry was exponential in the size of the input. The final obstacle was the discontinuity of previous invariants at singular configurations, for example, when a triangle degenerates to a straight line.

All the challenges above are now resolved by the Simplexwise Centred Distributions that combine inter-point distances of a given cloud with the new strength of a simplex that finally guarantees the Lipschitz continuity. The computational times of new invariants and metrics are polynomial in the number of points for a fixed Euclidean dimension.

1. Isometry classification problem for clouds

The rigidity of many real objects motivates the most practical equivalence of *rigid motion*, which is a composition of translations and high-dimensional rotations in $\mathbb{R}^n$. We also study *isometry*, which maintains inter-point distances and allows reflections. Any orientation-preserving isometry can be realised as a continuous rigid motion.

Often there is no sense to distinguish rigid objects that are related by rigid motion or isometry. Hence we can define the *rigid shape* of a cloud C as its *isometry class* consisting of all infinitely many clouds isometric to C.

The only reliable tool for distinguishing clouds up to isometry is an *invariant* defined as a function or property preserved by any isometry. Since any isometry is bijective, the number of points is an isometry invariant, but the coordinates of points are not invariants even under translation. This simple invariant is *incomplete* (non-injective) because non-isometric clouds can have different numbers of points.

In Computer Science, an invariant I is a descriptor with *no false negatives* that are pairs (of different representations) $C \cong C'$ of equivalent objects with $I(C) \neq I(C')$. Isometry invariants are also called *equivariant descriptors*.

A *complete* invariant I should distinguish all non-isometric clouds, so if $C \not\cong C'$ then $I(C) \neq I(C')$. Equivalently, I has *no false positives* that are pairs $C \not\cong C'$ of non-equivalent objects with $I(C) = I(C')$. A complete invariant I can be considered a DNA-style code or a genome that uniquely identifies any object up to given equivalence.

Since real data are always noisy and motions of rigid objects are important to track, a useful complete invariant must be also continuous under the movement of points.

A complete and continuous invariant for $m = 3$ consists of three pairwise distances (sides of a triangle) and is studied at school as the SSS theorem [63]. But pairwise distances are incomplete for $m \geq 4$ even in $\mathbb{R}^2$ [8], see Fig. 1.

Problem 1.1 (complete isometry invariants with computable continuous metrics)**.** *For any cloud of m unlabelled points in $\mathbb{R}^n$, find an invariant I satisfying the properties*

(a) completeness *: C, C' are isometric $\Leftrightarrow I(C) = I(C')$;*

(b) Lipschitz continuity *: if any point of C is perturbed within its ε-neighbourhood then $I(C)$ changes by at most $\lambda\varepsilon$ for a constant λ and a metric d satisfying these axioms:*
1) $d(I(C), I(C')) = 0$ if and only if $C \cong C'$ are isometric,
2) symmetry *: $d(I(C), I(C')) = d(I(C'), I(C))$,*
3) $d(I(C), I(C')) + d(I(C'), I(C'')) \geq d(I(C), I(C''))$;

(c) computability *: I and d are computable in a polynomial time in the number m of points for a fixed dimension n.* ■

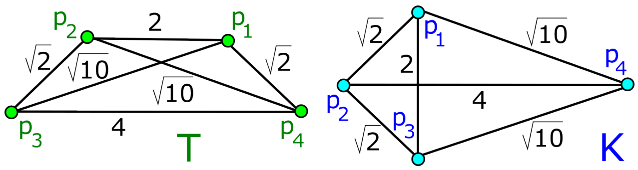

Figure 1. **Left**: the cloud $T = \{(1,1),(-1,1),(-2,0),(2,0)\}$. **Right**: the kite $K = \{(0,1),(-1,0),(0,-1),(3,0)\}$. T and K have the same 6 pairwise distances $\sqrt{2},\sqrt{2},2,\sqrt{10},\sqrt{10},4$.

Condition (1.1b) asking for a continuous metric is stronger than the completeness in (1.1a). Detecting an isometry $C \cong C'$ gives a discontinuous metric, say $d = 1$ for all non-isometric clouds $C \not\cong C'$ even if C, C' are nearly identical. Any metric d satisfying the first axiom in (1.1b) detects an isometry $C \cong C'$ by checking if $d = 0$.

Problem 1.1 for any clouds of m unlabeled points in $\mathbb{R}^n$ will be solved by Theorems 3.10, 5.7 and Corollary 6.1, which essentially needs the new strength of a simplex whose continuity is proved in hardest Theorem 4.2.

This paper extends [67, section 4] whose 8-page version without proofs and big examples will appear soon. In the papers [65–67], the first author implemented all algorithms, the second author wrote all theory, proofs, and examples.

2. Related work on point cloud classifications

This section reviews the past attempts at Problem 1.1 starting from the simplest case when points are ordered.

The case of labelled clouds $C \subset \mathbb{R}^n$ is easy for isometry classification because the matrix of distances d_{ij} between indexed points p_i, p_j allows us to reconstruct C by using the known distances to the previously constructed points [34, Theorem 9]. For any clouds of the same number m of labelled points, the difference between $m \times m$ matrices of distances (or Gram matrices of $p_i \cdot p_j$) can be converted into a continuous metric by taking a matrix norm. If given points are unlabelled, comparing $m \times m$ matrices requires $m!$ permutations of points, which makes this approach impractical, see the faster order types for labelled points in [13].

Multidimensional scaling (MDS). For a given $m \times m$ distance matrix of any m-point cloud A, MDS [55] finds an embedding $A \subset \mathbb{R}^k$ (if it exists) preserving all distances of M for a dimension $k \leq m$. A final embedding $A \subset \mathbb{R}^k$ uses eigenvectors whose ambiguity up to signs gives an exponential comparison time that can be close to $O(2^m)$.

The Hausdorff distance [36] can be defined for any subsets A, B in an ambient metric space as $d_H(A,B) = \max\{\vec{d}_H(A,B), \vec{d}_H(B,A)\}$, where the directed Hausdorff distance is $\vec{d}_H(A,B) = \sup\limits_{p\in A}\inf\limits_{q\in B}|p-q|$. To take into account isometries, one can minimize the Hausdorff distance over all isometries [18, 20, 38]. For $n = 2$, the Hausdorff distance minimized over isometries in $\mathbb{R}^2$ for sets of at most m point needs $O(m^5 \log m)$ time [19]. For a given $\varepsilon > 0$ and $n > 2$, the related problem to decide if $d_H \leq \varepsilon$ up to translations has the time complexity $O(m^{\lceil (n+1)/2 \rceil})$ [64, Chapter 4, Corollary 6]. For general isometry, only approximate algorithms tackled minimizations for infinitely many rotations initially in $\mathbb{R}^3$ [33], now in $\mathbb{R}^n$ [4, Lemma 5.5].

The Gromov-Wasserstein distances can be defined for metric-measure spaces, not necessarily sitting in a common ambient space. The simplest Gromov-Hausdorff (GH) distance cannot be approximated with any factor less than 3 in polynomial time unless P = NP [54, Corollary 3.8]. Polynomial-time algorithms for GH were designed for ultrametric spaces [48]. However, GH spaces are challenging even for finite clouds in the line $\mathbb{R}$, see [45] and [69].

Topological Data Analysis studies persistent homology [14, 26], which was finally recognised as an isometry invariant of a given cloud C, at least for standard filtrations such as Vietoris-Rips, Cech, and Delaunay complexes on C. This invariant turned out to be rather weak and informally comparable to classical homology, which is insufficient to classify even graphs up to homeomorphism, see the non-trivial extensions of 0D persistence [28, 29] and generic families of different scalar functions [15, 23] and finite metric spaces [58] that cannot be distinguished by persistence in dimensions 0 and 1, likely in all higher dimensions.

Geometric Data Science studies analogues of Problem 1.1, where rigid motion on clouds is replaced by any practical equivalence on real data objects. Another attempt at Problem 1.1 produced a complete invariant [40] of unlabelled clouds by using principal directions, which discontinuously change when a basis degenerates to a lower dimensional subspace but inspired Complete Neural Networks [37].

The earlier work has studied the following important cases of Problem 1.1: 1-periodic discrete series [5, 6, 40], 2D lattices [10, 42], 3D lattices [9, 39, 41, 49], periodic point sets in $\mathbb{R}^3$ [25, 59] and in higher dimensions [2–4].

The applications of to crystalline materials [7, 52, 62, 70] led to the *Crystal Isometry Principle* [65, 66, 68] extending Mendeleev's table of chemical elements to the *Crystal Isometry Space* of all periodic crystals parametrised by complete invariants like a geographic map.

Experimental approaches tested invariant features [51, 60, 61, 71] or optimised equivariant descriptors for clouds from specific datasets [17, 50, 56] without theoretical proofs of completeness, continuity, and time complexity, though sometimes beyond the Euclidean case as in the axiomatically rigorous Geometric Deep Learning [11, 12]. The widely known concerns [1, 22, 24, 35, 44] motivated us to state and solve Problem 1.1 in a mathematical way.

3. Simplexwise Centred Distribution (SCD)

This section introduces the Oriented Simplexwise Distribution (OSD) and its simplified version SCD (Simplexwise Centred Distribution) to solve Problem 1.1.

The *lexicographic* order $u < v$ on any vectors $u = (u_1, \dots, u_n)$ and $v = (v_1, \dots, v_n)$ means that if the first i (possibly, $i = 0$) coordinates of u, v coincide then $u_{i+1} < v_{i+1}$. Let S_n denote the permutation group on indices $1, \dots, n$.

Definition 3.1 (matrices $D(A)$ and $M(C; A)$ for $A \subset C$)**.** *Let C be a cloud of m unordered points in $\mathbb{R}^n$ with a fixed orientation. Let $A = (p_1, \dots, p_n) \in C^n$ be an ordered sequence consists of n distinct points. Let $D(A)$ be the $n \times n$* distance *matrix whose entry $D(A)_{i,j}$ is Euclidean distance $|p_i - p_j|$ for $1 \le i < j \le n$, all other entries are zeros.*

For any other point $q \in C - A$, write distances from q to $p_1, \dots, p_n$ as a column. For the $n \times (m-n)$-matrix by these $m - n$ lexicographically ordered columns. At the bottom of the column of a $q \in C - A$, add the sign of the determinant consisting of the vectors $q - p_1, \dots, q - p_n$. The resulting $(n+1) \times (m-n)$-matrix with signs in the bottom $(n+1)$-st row is the oriented relative distance *matrix* $M(C; A)$. ■

Any permutation $\xi \in S_n$ is a composition of some t transpositions $i \leftrightarrow j$ and has $\text{sign}(\xi) = (-1)^t$.

Definition 3.2 (distributions $\text{ORD}(C; A)$ and $\text{OSD}(C)$ for $C \subset \mathbb{R}^n$)**.** *Any permutation $\xi \in S_n$ acts on $D(A)$ by mapping $D(A)_{ij}$ to $D(A)_{kl}$, where $k \le l$ is the pair $\xi(i), \xi(j) - 1$ written in increasing order. Then ξ acts on $M(C; A)$ by mapping any i-th row to the $\xi(i)$-th row and by multiplying the $(n+1)$-st row by $\text{sign}(\xi)$, after which all columns are written in the lexicographic order.*

The Oriented Relative Distribution $\text{ORD}(C; A)$ *is the equivalence class of the pair $[D(A); M(C; A)]$ up to all permutations $\xi \in S_n$. The* Oriented Simplexwise Distribution $\text{OSD}(C)$ *is the unordered collection of* $\text{ORD}(C; A)$ *for all $\binom{m}{n}$ unordered subsets $A \subset C$ of n points.* ■

Any mirror reflection in $\mathbb{R}^n$ reverses the sign of the $n \times n$ determinant consisting of vectors $v_1, \dots, v_n \in \mathbb{R}^n$, hence reverses all signs in the $(n + 1)$-st rows of the matrices $M(C; A)$ in Oriented Relative Distributions. $\overline{\text{ORD}}(C; A)$ and $\overline{\text{OSD}}(C)$ denote the 'mirror images' of $\text{ORD}(C; A)$ and $\text{OSD}(C)$, respectively, with all signs reversed.

Example 3.3 (OSD for mirror clouds)**.** *In $\mathbb{R}^2$ with the counter-clockwise orientation, the cloud R on the vertices $p_1 = (0, 0)$, $p_2 = (4, 0)$, $p_3 = (0, 3)$ of the triangle in Fig. 2 (middle) has* $\text{OSD}(R)$ *consisting of* $\text{ORD}(R; (p_1, p_2)) = [4, \begin{pmatrix} 3 \\ 5 \\ + \end{pmatrix}]$, $\text{ORD}(R; (p_2, p_3)) = [5, \begin{pmatrix} 4 \\ 3 \\ + \end{pmatrix}]$, $\text{ORD}(R; (p_3, p_1)) = [3, \begin{pmatrix} 5 \\ 4 \\ + \end{pmatrix}]$. *If we swap the points $p_1 \leftrightarrow p_3$, the last* ORD *above changes to the equivalent form* $\text{ORD}(R; (p_1, p_3)) = [3, \begin{pmatrix} 4 \\ 5 \\ - \end{pmatrix}]$, *without affecting other* ORDs. *If we reflect R with respect to the x-axis, the new cloud $\bar{R}$ of the points $p_1, p_2, \bar{p}_3 = (0, -3)$ has* $\text{OSD}(\bar{R}) = \overline{\text{OSD}}(R)$ *with* $\text{ORD}(\bar{R}; (p_1, p_2)) = [4, \begin{pmatrix} 3 \\ 5 \\ - \end{pmatrix}]$, $\text{ORD}(\bar{R}; (p_2, \bar{p}_3)) = [5, \begin{pmatrix} 4 \\ 3 \\ - \end{pmatrix}]$, $\text{ORD}(\bar{R}; (p_3', p_1)) = [3, \begin{pmatrix} 5 \\ 4 \\ - \end{pmatrix}]$, *which differs from* $\text{OSD}(R)$ *even if we swap points in each pair.* ■

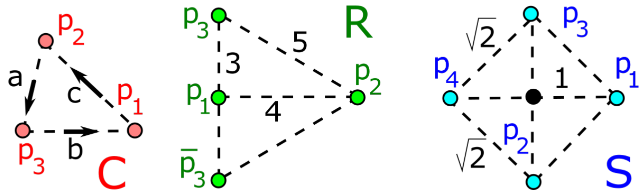

Figure 2. **Left**: a cloud $C = \{p_1, p_2, p_3\}$ with distances $a \le b \le c$. **Middle**: the triangular cloud $R = \{(0, 0), (4, 0), (0, 3)\}$. **Right**: the square cloud $S = \{(1, 0), (-1, 0), (0, 1), (-1, 0)\}$.

Example 3.4 (OSD for T, K)**.** *Fix the* counter-clockwise *orientation on $\mathbb{R}^2$ so that if a vector v is obtained from u by a counter-clockwise rotation then $\det(u, v) > 0$. Then Table 1 shows the Oriented Simplexwise Distribution for the 4-point clouds $T, K \subset \mathbb{R}^2$ in Fig. 1.* ■

The book "Euclidean Distance Geometry" [**?**, Chapter 3] discusses realizations of a complete graph given by a full distance matrix in $\mathbb{R}^n$. Lemma 3.5 and later resuts in the appendices hold for all cases including degenerate ones, for example, when 3 points are in a straight line in $\mathbb{R}^3$.

Lemma 3.5 (reconstructing from $D(A)$)**.** *Any finite ordered set $A \subset \mathbb{R}^n$ is reconstructed (uniquely up to isometry) from the distance matrix $D(A)$ in Definition 3.2.* ■

Proof. Let $A \subset \mathbb{R}^n$ consist of n points $p_1, \dots, p_n$ as in Definition 3.1. A translation allows us to put p_1 at the origin $0 \in \mathbb{R}^n$. A rotation allows us to put p_2 in the (positive half of the) 1st coordinate axis at the distance $|p_2 - p_1|$ from $p_1 = 0$. A further rotation around the 1st coordinate axis allows us to put p_3 in the (positive half-) plane on the first two coordinates axes by using the distances $|p_3 - p_1|$ and $|p_3 - p_2|$ from the given distance matrix $D(A)$, and so on.

In a degenerate situation, a point p_{k+1} might belong to the subspace spanned by $p_1, \dots, p_k$. For example, if $k = 2$

ORDs in OSD(T)	ORDs in OSD(K)
$[\sqrt{2}, \begin{pmatrix} 2 & \sqrt{10} \\ \sqrt{10} & 4 \\ - & - \end{pmatrix}]$	$[\sqrt{2}, \begin{pmatrix} 2 & \sqrt{10} \\ \sqrt{2} & 4 \\ - & - \end{pmatrix}]$
$[\sqrt{2}, \begin{pmatrix} 2 & \sqrt{10} \\ \sqrt{10} & 4 \\ + & + \end{pmatrix}]$	$[\sqrt{2}, \begin{pmatrix} 2 & \sqrt{10} \\ \sqrt{2} & 4 \\ + & + \end{pmatrix}]$
$[2, \begin{pmatrix} \sqrt{2} & \sqrt{10} \\ \sqrt{10} & \sqrt{2} \\ - & - \end{pmatrix}]$	$[2, \begin{pmatrix} \sqrt{2} & \sqrt{10} \\ \sqrt{2} & \sqrt{10} \\ - & + \end{pmatrix}]$
$[\sqrt{10}, \begin{pmatrix} \sqrt{2} & 4 \\ 2 & \sqrt{2} \\ + & - \end{pmatrix}]$	$[\sqrt{10}, \begin{pmatrix} \sqrt{2} & 2 \\ 4 & \sqrt{10} \\ - & - \end{pmatrix}]$
$[\sqrt{10}, \begin{pmatrix} \sqrt{2} & 4 \\ 2 & \sqrt{2} \\ - & + \end{pmatrix}]$	$[\sqrt{10}, \begin{pmatrix} \sqrt{2} & 2 \\ 4 & \sqrt{10} \\ + & + \end{pmatrix}]$
$[4, \begin{pmatrix} \sqrt{2} & \sqrt{10} \\ \sqrt{10} & \sqrt{2} \\ + & + \end{pmatrix}]$	$[4, \begin{pmatrix} \sqrt{2} & \sqrt{2} \\ \sqrt{10} & \sqrt{10} \\ + & - \end{pmatrix}]$

Table 1. The Oriented Simplexwise Distributions from Definition 3.2 for the 4-point clouds $T, K \subset \mathbb{R}^2$ in Fig. 1.

and $|p_3 - p_1| \pm |p_3 - p_2| = \pm|p_2 - p_1|$, then the point p_3 belongs to the 1st coordinate axes through $p_1 = 0$ and p_2. Then we have more flexibility with rotations, so p_4 can be rotated around the 1st coordinate axes through p_1, p_2, p_3.

So we continue until either all h points of A are fixed or all already fixed points affinely span $\mathbb{R}^n$. If the former case, A is reconstructed uniquely up to isometry of $\mathbb{R}^n$ that keeps invariant the low dimensional subspace spanned by A. In the latter case, any next point $q \in A$ is uniquely located in $\mathbb{R}^n$ by at least $n+1$ distances to the already fixed points. □

Lemma 3.5 doesn't hold for stricter rigid motion instead of isometry. A 3-point cloud with inter-point distances $3, 4, 5$ can be reconstructed in $\mathbb{R}^2$ as two triangles related by reflection, not by rigid motion, see Fig. 2 (middle).

The *affine dimension* $\text{aff}(C)$ of a cloud $C = \{p_1, \dots, p_m\} \subset \mathbb{R}^n$ is the maximum dimension of the vector space generated by all inter-point vectors $p_i - p_j$, $i, j \in \{1, \dots, m\}$. Then $\text{aff}(C)$ is an isometry invariant and is independent of an order of points of C. Any cloud C of 2 distinct points has $\text{aff}(C) = 1$. Any cloud C of 3 points that are not in the same straight line has $\text{aff}(C) = 2$. Let $S(p; d)$ be the sphere with a centre p and a radius d.

Lemma 3.6 (reconstructing from ORD)**.** *A cloud $C \subset \mathbb{R}^n$ of $m > n$ unlabelled points can be reconstructed (uniquely up to rigid motion) from* $\text{ORD}(C; A)$ *in Definition 3.2 for any ordered subset $A \subseteq C$ with* $\text{aff}(A) = n - 1$. ■

Proof. By Lemma 3.5 any subset $A \subseteq C$ can be uniquely reconstructed up to isometry from the triangular distance matrix $D(A)$ in Definition 3.2. Since $\text{aff}(A) = n - 1$, the subset A has $h \geq n$ points. We may assume that the first n points $p_1, \dots, p_n$ of A span the subspace of the first $n - 1$ coordinate axes of $\mathbb{R}^n$, all unique up to rigid motion.

We prove that any point $q \in C - A \subset \mathbb{R}^n$ has a location determined by the n distances $|q - p_1|, \dots, |q - p_n|$ written in a column of the matrix $\text{ORD}(C; A)$. The n spheres $S(p_i; |q - p_i|)$, $i = 1, \dots, n$, contain q and intersect in one or two points. We can uniquely choose q among these two options due to the sign of the determinant (in the bottom row of $\text{ORD}(C; A)$) of the vectors $q - p_1, \dots, q - p_n$. □

Lemma 3.6 implies that $\text{ORD}(C; A)$ can have identical columns only for degenerate subsets $A \subset C$ with $\text{aff}(A) < n - 1$. For example, let $n = 3$ and A consist of three points p_1, p_2, p_3 in the same straight line $L \subset \mathbb{R}^3$. The three distances $|q - p_i|$, $i = 1, 2, 3$, to any other point $q \in C$ outside L define three spheres $S(p_i; |q - p_i|)$ that share a common circle in $\mathbb{R}^3$, so the position of q is not uniquely determined in this case.

Though one $\text{ORD}(C; A)$ with $\text{aff}(A) = n - 1$ suffices to reconstruct $C \subset \mathbb{R}^n$ up to rigid motion, the dependence on a subset $A \subset C$ required us to consider the larger Oriented Simplexwise Distribution $\text{OSD}(C)$ for all n-point subsets $A \subset C$ to get a complete invariant in Theorem 3.7.

An equality $\text{OSD}(C) = \text{OSD}(C')$ is interpreted as a bijection $\text{OSD}(C) \to \text{OSD}(C')$ matching all ORDs.

Theorem 3.7 (completeness of OSD)**.** *The Oriented Simplexwise Distribution* $\text{OSD}(C)$ *in Definition 3.2 is a complete isometry invariant and can be computed in time $O(m^{n+1}/(n-3)!)$. So any clouds $C, C' \subset \mathbb{R}^n$ of m unlabelled points are related by rigid motion (isometry, respectively) if and only if* $\text{OSD}(C) = \text{OSD}(C')$ *(*$\text{OSD}(C) = \text{OSD}(C')$ *or its mirror image* $\overline{\text{OSD}}(C')$*, respectively).*

Proof. Part *if* $\Leftarrow$. Any bijection $\text{OSD}(C) \to \text{OSD}(C')$ matches $\text{ORD}(C; A)$ with $\text{ORD}(C'; A')$ for some subsets $A \subset C$ and $A' \subset C'$ of n points. By Lemma 3.6 any equality $\text{ORD}(C; A) = \text{ORD}(C'; A')$ for n-point subsets A, A' with $\text{aff} = n - 1$ guarantees that C, C' are related by rigid motion in $\mathbb{R}^n$. In the degenerate case, when all subsets have $\text{aff} < n - 1$, hence C, C' belong to a k-dimensional subspace of $\mathbb{R}^n$ for $k < n$, we apply the reconstruction of Lemma 3.6 to $\mathbb{R}^k$ instead of $\mathbb{R}^n$. In the case $\text{OSD}(C) = \overline{\text{OSD}}(C')$, we get an equality $\text{ORD}(C; A) = \text{ORD}(\bar{C}'; A')$, where $\bar{C}'$ is a mirror image of C', hence C, C' are related by an orientation-reversing isometry.

Part *only if* $\Rightarrow$. Any rigid motion f of $\mathbb{R}^n$ bijectively maps C to C' and any subset $A \subseteq C$ to $A' = f(A) \subseteq C' = f(C)$, hence induces a bijection $\mathrm{OSD}(C) \to \mathrm{OSD}(C')$. Similarly, any orientation-reversing isometry $C \to C'$ induces a bijection $\mathrm{OSD}(C) \to \overline{\mathrm{OSD}}(C') = \mathrm{OSD}(\bar{C}')$.

To compute $\mathrm{OSD}(C)$, we consider $\binom{m}{n} = \frac{m!}{n!(m-n)!}$ subsets $A \subset C$ of n points. For each fixed A, the matrix $D(A)$ of $\frac{n(n-1)}{2}$ pairwise distances needs $O(n^2)$ time. The Oriented Relative Distribution $\mathrm{ORD}(C; A) = [D(A); M(C; A)]$ includes $n(m-n)$ distances, and also $m-n$ signs and strengths that each requires determinant computations in time $O(n^3)$ by Gaussian elimination. So $\mathrm{ORD}(C; A)$ can be computed in time $O(n^3 m)$.

Multiplying the last time by the number $\binom{m}{n} = \frac{m!}{n!(m-n)!}$ of n-point subsets $A \subset C$, we estimate the final time for $\mathrm{OSD}(C)$ as $O(\frac{m! n^3 m}{n!(m-n)!}) = O(m^2(m-1)\dots(m-n+1)n^2/(n-1)!) = O(m^{n+1}/(n-3)!)$. □

Now we simplify the OSD invariant to the Simplexwise Centred Distribution (SCD) by using the centre of mass of C as a useful anchor reducing the ambiguity.

The Euclidean structure of $\mathbb{R}^n$ allows us to translate the *center of mass* $\dfrac{1}{m}\sum\limits_{p \in C} p$ of a given m-point cloud $C \subset \mathbb{R}^n$ to the origin $0 \in \mathbb{R}^n$. Then Problem 1.1 reduces to only rotations around 0 from the orthogonal group $\mathrm{O}(\mathbb{R}^n)$.

Definition 3.2 introduced the Oriented Simplexwise Distribution (OSD) as an ordered collection of $\mathrm{ORD}(C; A)$ for all $\binom{m}{n}$ unordered subsets $A \subset C$ of n points. Including the centre of mass, allows us to consider the smaller number of $\binom{m}{n-1}$ subsets $A \subset C$ of $n-1$ points instead of n.

Though the centre of mass is uniquely determined by any cloud $C \subset \mathbb{R}^n$ of unlabelled points, real applications may offer one or several labelled points of C that substantially speed up metrics on invariants. For example, an atomic neighbourhood in a solid material is a cloud $C \subset \mathbb{R}^3$ of atoms around a central atom, which may not be the centre of mass of C, but is suitable for all methods below.

For any basis sequence $A = \{p_1, \dots, p_{n-1}\} \in C^{n-1}$ of $n-1$ ordered points, add the origin 0 as the n-th point and consider the $n \times n$ distance matrix $D(A \cup \{0\})$ and the $(n+1) \times (m-n)$ matrix $M(C; A \cup \{0\})$ in Definition 3.1. Any n vectors $v_1, \dots, v_n \in \mathbb{R}^n$ can be written as columns in the $n \times n$ matrix whose determinant has a *sign* ± 1 or 0 if the vectors $v_1, \dots, v_n$ are linearly dependent.

Any permutation $\xi \in S_{n-1}$ of $n-1$ points of A acts on $D(A)$, permutes the first $n-1$ rows of $M(C; A \cup \{0\})$ and multiplies every sign in the $(n+1)$-st row by $\mathrm{sign}(\xi)$.

Definition 3.8 (Simplexwise Centred Distribution SCD)**.** *Let $C \subset \mathbb{R}^n$ be any cloud of m unlabelled points. For any basis sequence $A = (p_1, \dots, p_{n-1}) \in C^{n-1}$, the* Oriented Centred Distribution $\mathrm{OCD}(C; A)$ *is the equivalence class of pairs $[D(A \cup \{0\}), M(C; A \cup \{0\})]$ considered up to permutations $\xi \in S_{n-1}$ of points of A.*

The Simplexwise Centred Distribution $\mathrm{SCD}(C)$ *is the unordered set of the distributions $\mathrm{OCD}(C; A)$ for all $\binom{m}{n-1}$ unordered $(n-1)$-point subsets $A \subset C$. The mirror image $\overline{\mathrm{SCD}}(C)$ is obtained from $\mathrm{SCD}(C)$ by reversing signs.* ■

Definition 3.8 needs no permutations for any $C \subset \mathbb{R}^2$ as $n-1 = 1$. Columns of $M(C; A \cup \{0\})$ can be lexicographically ordered without affecting future metrics.

Some of the $\binom{m}{n-1}$ OCDs in $\mathrm{SCD}(C)$ can be identical as in Example 3.9(b). If we collapse any $l > 1$ identical OCDs into a single OCD with the *weight* $l/\binom{m}{h}$, SCD can be considered as a weighted probability distribution of OCDs.

Example 3.9 (SCD for clouds in Fig. 2)**.** ***(a)*** *Let $R \subset \mathbb{R}^2$ consist of the vertices $p_1 = (0,0)$, $p_2 = (4,0)$, $p_3 = (0,3)$ of the right-angled triangle in Fig. 2 (middle). Though $p_1 = (0,0)$ is included in R and is not its centre of mass,* $\mathrm{SCD}(R)$ *still makes sense. In* $\mathrm{OCD}(R; p_1) = [0, \begin{pmatrix} 4 & 3 \\ 4 & 3 \\ 0 & 0 \end{pmatrix}]$, *the matrix $D(\{p_1, 0\})$ is $|p_1 - 0| = 0$, the top row has $|p_2 - p_1| = 4$, $|p_3 - p_1| = 3$. In* $\mathrm{OCD}(R; p_2) = [4, \begin{pmatrix} 4 & 5 \\ 0 & 3 \\ 0 & - \end{pmatrix}]$, *the first row has $|p_1 - p_2| = 4$, $|p_3 - p_2| = 5$, the second row has $|p_1 - 0| = 0$, $|p_3 - 0| = 3$,* $\det \begin{pmatrix} -4 & 0 \\ 3 & 3 \end{pmatrix} < 0$. *In* $\mathrm{OCD}(R; p_3) = [3, \begin{pmatrix} 3 & 5 \\ 0 & 4 \\ 0 & + \end{pmatrix}]$, *the first row has $|p_1 - p_3| = 3$, $|p_2 - p_3| = 5$, the second row has $|p_1 - 0| = 0$, $|p_2 - 0| = 4$,* $\det \begin{pmatrix} 4 & 4 \\ -3 & 0 \end{pmatrix} > 0$. *So* $\mathrm{SCD}(R)$ *consists of the three* OCDs *above.*

If we reflect R with respect to the x-axis, the new cloud $\bar{R}$ of the points $p_1, p_2, \bar{p}_3 = (0, -3)$ has $\mathrm{SCD}(\bar{R}) = \overline{\mathrm{SCD}}(R)$ *with* $\mathrm{OCD}(\bar{R}; p_1) = \mathrm{OCD}(R)$, $\mathrm{OCD}(\bar{R}; p_2) = [4, \begin{pmatrix} 4 & 5 \\ 0 & 3 \\ 0 & + \end{pmatrix}]$, $\mathrm{OCD}(R; \bar{p}_3) = [3, \begin{pmatrix} 3 & 5 \\ 0 & 4 \\ 0 & - \end{pmatrix}]$ *whose signs changed under reflection, so* $\mathrm{SCD}(R) \neq \mathrm{SCD}(\bar{R})$.

(b) *Let $S \subset \mathbb{R}^2$ consist of $m = 4$ points $(\pm 1, 0)$, $(0, \pm 1)$ that are vertices of the square in Fig. 2 (right). The centre of mass is $0 \in \mathbb{R}^2$ and has a distance 1 to each point of S.*

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

$(1, 0)$, *we have* $M(S; \begin{pmatrix} p_1 \\ 0 \end{pmatrix}) = \begin{pmatrix} \sqrt{2} & \sqrt{2} & 2 \\ 1 & 1 & 1 \\ - & + & 0 \end{pmatrix}$, *where the columns are ordered according to* $p_2 = (0, -1)$, $p_3 = (0, 1)$, $p_4 = (-1, 0)$ *in Fig. 2 (right). The sign in the bottom right corner is 0 because the points* $p_1, 0, p_4$ *are in a straight line. Due to the rotational symmetry,* $M(S; \{p_i, 0\})$ *is independent of* $i = 1, 2, 3, 4$*. So* $\mathrm{SCD}(S)$ *can be considered as one* $\mathrm{OCD} = [1, M(S; \begin{pmatrix} p_1 \\ 0 \end{pmatrix})]$ *of weight 1.* ■

Example 3.9(b) illustrates the key discontinuity challenge: if $p_4 = (-1, 0)$ is perturbed, the corresponding sign can discontinuously change to $+1$ or -1. To get a continuous metric on OCDs, we will multiply each sign by a continuous *strength* function that vanishes for any zero sign.

Theorem 3.10 (completeness of SCD)**.** ***(a)*** *The Simplexwise Centred Distribution* $\mathrm{SCD}(C)$ *in Definition 3.8 is a complete isometry invariant of clouds* $C \subset \mathbb{R}^n$ *of* m *unlabelled points with a centre of mass at the origin* $0 \in \mathbb{R}^n$*, and can be computed in time* $O(m^n/(n-4)!)$*.*

So any clouds $C, C' \subset \mathbb{R}^n$ *are related by rigid motion (isometry, respectively)* if and only if $\mathrm{SCD}(C) = \mathrm{SCD}(C')$ *(*$\mathrm{SCD}(C)$ *equals* $\mathrm{SCD}(C')$ *or its mirror image* $\overline{\mathrm{SCD}}(C')$*, respectively). For any* m*-point clouds* $C, C' \subset \mathbb{R}^n$*, let* $\mathrm{SCD}(C)$ *and* $\mathrm{SCD}(C')$ *consist of* $k = \binom{m}{n-1}$ OCDs*.*

Proof of Theorem 3.10. All arguments follow the proof of Theorem 3.7 after replacing n with $n-1$. □

4. The new continuous strength of a simplex

This section resolves the discontinuity of signs of determinants by introducing the multiplicative factor below.

Definition 4.1 (*strength* $\sigma(A)$ of a simplex)**.** *For a set* A *of* $n+1$ *points* $q = p_0, p_1, \dots, p_n$ *in* $\mathbb{R}^n$*, let* $p(A) = \frac{1}{2}\sum\limits_{i \neq j}^{n+1} |p_i - p_j|$ *be half of the sum of all pairwise distances. Let* $V(A)$ *denote the volume the* n*-dimensional simplex on the set* A*. Define the* strength $\sigma(A) = V^2(A)/p^{2n-1}(A)$*.*

For $n = 2$ *and a triangle* A *with sides* a, b, c *in* $\mathbb{R}^2$*, Heron's formula gives* $\sigma(A) = \dfrac{(p-a)(p-b)(p-c)}{p^2}$*,* $p = \dfrac{a+b+c}{2} = p(A)$ *is the half-perimeter of* A*.* ■

For $n = 1$ and a set $A = p_0, p_1 \subset \mathbb{R}$, the volume is $V(A) = |p_0 - p_1| = 2p(A)$, so $\sigma(A) = 2|p_0 - p_1|$.

The strength $\sigma(A)$ depends only on the distance matrix $D(A)$ from Definition 3.1, so the notation $\sigma(A)$ is used only for brevity. In any $\mathbb{R}^n$, the squared volume $V^2(A)$ is expressed by the Cayley-Menger determinant [57] in pairwise distances between points of A. Importantly, the strength $\sigma(A)$ vanishes when the simplex on a set A degenerates.

Corollary 6.1 will need the continuity of $s\sigma(A)$, when a sign $s \in \{\pm 1\}$ from a bottom row of ORD changes while passing through a degenerate set A. In appendices, the proof of the continuity of $\sigma(A)$ in Theorem 4.2 gives an explicit upper bound for a Lipschitz constant c_n below.

Theorem 4.2 (Lipschitz continuity of the strength σ)**.** *Let a cloud* A' *be obtained from another* $(n+1)$*-point cloud* $A \subset \mathbb{R}^n$ *by perturbing every point within its* ε*-neighbourhood. The strength* $\sigma(A)$ *from Definition 4.1 is Lipschitz continuous so that* $|\sigma(A') - \sigma(A)| \leq 2\varepsilon c_n$ *for a constant* c_n*.* ■

Proof of Theorem 4.2 for dimension $n = 2$ *and* $c_2 = 2\sqrt{3}$*.* Let a 3-point cloud $A \subset \mathbb{R}^2$ have pairwise distances a, b, c. Using the half-perimeter $p = \dfrac{a+b+c}{2}$, the variables $\tilde{a} = p - a$, $\tilde{b} = p - b$, $\tilde{c} = p - c$ are independent and bijectively expressed via a, b, c, so $a = \tilde{b} + \tilde{c}$, $b = \tilde{a} + \tilde{c}$, $c = \tilde{a} + \tilde{b}$, $p = \tilde{a} + \tilde{b} + \tilde{c}$. The Jacobian of this change of variables is $\dfrac{\partial(a, b, c)}{\partial(\tilde{a}, \tilde{b}, \tilde{c})} = \begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = 2$.

If each point of A is perturbed within its ε-neighbourhood in the Euclidean distance on $\mathbb{R}^2$, then any pairwise distance between points of A changes by at most 2ε.

By the mean value theorem [30], this bound 2ε gives $|\sigma(A') - \sigma(A)| \leq 2\varepsilon \sup |\nabla \sigma|$, where $\nabla \sigma = (\frac{\partial \sigma}{\partial a}, \frac{\partial \sigma}{\partial b}, \frac{\partial \sigma}{\partial c})$ is the gradient of the first order partial derivatives of $\sigma(A)$ with respect to the three distances between points of A.

Since $|\nabla \sigma| = \left| \dfrac{\partial(a, b, c)}{\partial(\tilde{a}, \tilde{b}, \tilde{c})} \left(\dfrac{\partial \sigma}{\partial \tilde{a}}, \dfrac{\partial \sigma}{\partial \tilde{b}}, \dfrac{\partial \sigma}{\partial \tilde{c}} \right) \right| \leq 2 \left| \left(\dfrac{\partial \sigma}{\partial \tilde{a}}, \dfrac{\partial \sigma}{\partial \tilde{b}}, \dfrac{\partial \sigma}{\partial \tilde{c}} \right) \right|$, it remains to estimate the first order partial derivatives of the strength from Definition 4.1 $\sigma = \dfrac{\tilde{a}\tilde{b}\tilde{c}}{(\tilde{a} + \tilde{b} + \tilde{c})^2}$ with respect to the variables $\tilde{a}, \tilde{b}, \tilde{c}$. Since σ is symmetric $\tilde{a}, \tilde{b}, \tilde{c}$, it suffices to consider $\dfrac{\partial \sigma}{\partial \tilde{a}} = \dfrac{\tilde{b}\tilde{c}}{(\tilde{a} + \tilde{b} + \tilde{c})^2} - \dfrac{2\tilde{a}\tilde{b}\tilde{c}}{(\tilde{a} + \tilde{b} + \tilde{c})^3} = \dfrac{\tilde{b}\tilde{c}(\tilde{b} + \tilde{c} - \tilde{a})}{(\tilde{a} + \tilde{b} + \tilde{c})^3} = \dfrac{(p-b)(p-c)(2a-p)}{p^3} = \left(1 - \dfrac{b}{p}\right)\left(1 - \dfrac{c}{p}\right)\left(2\dfrac{a}{p} - 1\right)$. By the triangle inequalities for a, b, c, we have $\max\{a, b, c\} \leq p = \frac{a+b+c}{2}$. Then $\frac{a}{p}, \frac{b}{p}, \frac{c}{p} \in (0, 1]$, and $1 - \frac{b}{p}, 1 - \frac{c}{p} \in [0, 1)$, and $2\frac{a}{p} - 1 \in (-1, 1]$, so $|\frac{\partial \sigma}{\partial \tilde{a}}| \leq 1$. The similar upper bounds $|\frac{\partial \sigma}{\partial \tilde{b}}|, |\frac{\partial \sigma}{\partial \tilde{c}}| \leq 1$ imply that $|\nabla \sigma| \leq 2\sqrt{3}$ and $|\sigma(A') - \sigma(A)| \leq 2\varepsilon \sup |\nabla \sigma| \leq 2\varepsilon c_2$ for $c_2 = 2\sqrt{3}$. □

The used inequality $\max\{a, b, c\} \leq p$ extends to $n \geq 3$.

Lemma 4.3 (upper bound for edge ratios)**.** *For any $(n+1)$-point set $A \subset \mathbb{R}^n$ with pairwise distances d_{kl}, we have $\dfrac{d_{kl}}{p(A)} \le \dfrac{2}{n}$ for any k,l, where $p(A) = \dfrac{1}{2}\sum\limits_{i,j=1}^{n+1} d_{ij}$.* ■

Proof. Use the triangle inequalities: $2p(A) = \sum\limits_{i,j=1}^{n+1} d_{ij} \ge d_{kl} + \sum\limits_{i\neq k,l}(d_{ik}+d_{il}) = d_{kl} + (n-1)d_{kl} = nd_{kl}$. □

We express a Lipschitz constant c_n of the strength $\sigma(A)$ in Theorem 4.2 via the *rencontre* number $r_n = n!\sum\limits_{k=0}^{n}\dfrac{(-1)^k}{k!}$ counting permutations of $1,\dots,n$ without a fixed point [16], e.g. $r_2=1, r_3=2, r_4=9, r_5=44$.

The proof of Theorem 4.2 for $n \ge 3$ below gives the following rough upper bound of a Lipschitz constant

$$c_n = \left(4r_n + 2r_{n+1} + \frac{n(2n-1)}{4}r_{n+2}\right)\frac{2^{n-0.5}\sqrt{n+1}}{(n!)^2 n^{2n-1.5}}.$$

The convergence $c_n \to 0$ as $n \to +\infty$ illustrates the curse of dimensionality meaning that the change of volume is tiny for big n. The bounds above give $c_2 \approx 4.7$, $c_3 \approx 0.43$.

Proof of Theorem 4.2 for $n \ge 3$. The Cayley-Menger determinant [57] expresses the squared volume of the n-dimensional simplex on any $(n+1)$-point set $A = \{p_1,\dots,p_{n+1}\} \subset \mathbb{R}^n$ as $V^2(A) = \dfrac{(-1)^{n-1}}{2^n(n!)^2}\det\hat{B}$, where the $(n+2)\times(n+2)$ matrix $\hat{B}$ is obtained from the $(n+1)\times(n+1)$ matrix $B_{ij} = |p_i - p_j|^2$ of squared Euclidean distances by bordering B with a top row $(0,1,\dots,1)$ and a left column $(0,1,\dots,1)^T$. For $n=3$, the squared volume is $V^2(A) = \dfrac{1}{288}\begin{vmatrix} 0 & 1 & 1 & 1 & 1\\ 1 & 0 & d_{12}^2 & d_{13}^2 & d_{14}^2\\ 1 & d_{21}^2 & 0 & d_{23}^2 & d_{24}^2\\ 1 & d_{31}^2 & d_{32}^2 & 0 & d_{34}^2\\ 1 & d_{41}^2 & d_{42}^2 & d_{43}^2 & 0\end{vmatrix}$, where $d_{ij} = d_{ji}$ is the Euclidean distance between p_i, p_j.

Similarly to $n=2$, the mean value theorem [30] for the strength $\sigma(A) = V^2(A)/p^{2n-1}(A)$, where $p(A) = \frac{1}{2}\sum\limits_{i\neq j}^{n+1} d_{ij}$, implies for any cloud A and its perturbation A'

$$|\sigma(A') - \sigma(A)| \le 2\varepsilon \sup|\nabla\sigma| \le 2\varepsilon\sqrt{\tfrac{n(n+1)}{2}}\sup_{i,j}\left|\tfrac{\partial\sigma}{\partial d_{ij}}\right|.$$

To find an upper bound of $\left|\dfrac{\partial\sigma}{\partial d_{ij}}\right|$ for $\sigma = \dfrac{V^2(A)}{p^{2n-1}(A)}$, we initially ignore the numerical factor in $V^2(A) = \dfrac{(-1)^{n-1}}{2^n(n!)^2}\det\hat{B}$ and differentiate only $\det\hat{B}\cdot\dfrac{1}{p^{2n-1}(A)}$ by the product rule as follows: $\dfrac{\partial}{\partial d_{ij}}\left(\dfrac{\det\hat{B}}{p^{2n-1}(A)}\right) = \dfrac{\partial\det\hat{B}}{\partial d_{ij}}\dfrac{1}{p^{2n-1}(A)} - \det\hat{B}\dfrac{n-\frac{1}{2}}{p^{2n-2}(A)}$. Lemmas 4.4 and 4.5 below imply the upper bound $\left|\dfrac{\partial}{\partial d_{ij}}\dfrac{\det\hat{B}}{p^{2n-1}(A)}\right| \le (4r_n + 2r_{n+1})\left(\dfrac{2}{n}\right)^{2n-1} + (n-\frac{1}{2})r_{n+2}\left(\dfrac{2}{n}\right)^{2n-2} = (4r_n + 2r_{n+1} + \frac{n(2n-1)}{4}r_{n+2})\left(\dfrac{2}{n}\right)^{2n-1}$. Taking into account the factors $\dfrac{(-1)^{n-1}}{2^n(n!)^2}$ in $V^2(A)$ and $\sqrt{\frac{n(n+1)}{2}}$ for estimating the length of the gradient $\nabla\sigma$ of $\frac{n(n+1)}{2}$ first order partial derivatives $\frac{\partial\sigma}{\partial d_{ij}}$, the final Lipschitz constant is $c_n = (4r_n + 2r_{n+1} + \frac{n(2n-1)}{4}r_{n+2})\dfrac{2^{n-0.5}\sqrt{n+1}}{(n!)^2 n^{2n-1.5}}$. □

Lemma 4.4. $\left|\dfrac{\det\hat{B}}{(p(A))^{2n-2}}\right| \le r_{n+2}\left(\dfrac{2}{n}\right)^{2n-2}$.

Proof. The determinant $\det\hat{B}$ is a polynomial of maximum degree $2(n-1)$ in all distances d_{ij}. The determinant formula $\det\hat{B} = \sum\limits_{\xi\in S_{n+2}}(-1)^{\text{sign}(\xi)}\alpha_{1,\xi(1)}\dots\alpha_{n,\xi(n)}$ excludes all zeros on the diagonal, so $k \neq \xi(k)$ for $k = 1,\dots,n+2$ and all permutations ξ of $1,\dots,n+2$ have no fixed points. Then $\det\hat{B}$ is a sum of (the rencontre number) r_{n+2} terms. Each term is a product of at most $2n-2$ distances. Divide by $p^{2n-2}(A)$ and use Lemma 4.3. □

Lemma 4.5. *In the above notations for fixed i,j, we have* $\left|\dfrac{\partial\det\hat{B}}{\partial d_{ij}}\dfrac{1}{p^{2n-1}(A)}\right| \le (4r_n + 2r_{n+1})\left(\dfrac{2}{n}\right)^{2n-1}$.

Proof. Since $\det\hat{B}$ has d_{ij}^2 in exactly two cells in different rows and columns, $\det\hat{B}$ is a quadratic polynomial $\alpha d_{ij}^4 + \beta d_{ij}^2 + \gamma$, where α,β,γ depend on other fixed distances $d_{kl} \neq d_{ij}$. Then $\dfrac{\partial\det\hat{B}}{\partial d_{ij}} = 4\alpha d_{ij}^3 + 2\beta d_{ij}$.

The coefficient α is the determinant of the $n\times n$ submatrix (α_{ij}) obtained from $\hat{B}$ by removing two rows and columns $i+1, j+1$. Since this submatrix has zeros on the main diagonal, its determinant $\alpha = \sum\limits_{\xi\in S_n}(-1)^{\text{sign}(\xi)}\alpha_{1,\xi(1)}\dots\alpha_{n,\xi(n)}$ is a sum over all permutations $\xi \in S_n$ such that $k \neq \xi(k)$ for $k = 1,\dots,n$, so ξ has no fixed points and the sum α is over (the rencontre number) r_n permutations ξ. If $n=3$ and $d_{ij} = d_{34}$, then $\alpha = \begin{vmatrix} 0 & 1 & 1\\ 1 & 0 & d_{12}^2\\ 1 & d_{21}^2 & 0\end{vmatrix} = 2d_{12}^2$. Each product $\alpha_{1,\xi(1)}\dots\alpha_{n,\xi(n)}$ has a total degree $2(n-2)$ in distances d_{kl}. After dividing αd_{ij}^3 of degree $2n-1$ by $(p(A))^{2n-1}$, we use the upper bound $\dfrac{d_{kl}}{p(A)} \le \dfrac{2}{n}$, which follows from . Since each product inside αd_{ij}^3, after dividing by $p^{2n-1}(A)$, has the upper bound $(\frac{2}{n})^{2n-1}$, we get $\left|\dfrac{\alpha d_{ij}^3}{p^{2n-1}(A)}\right| \le r_n \left(\dfrac{2}{n}\right)^{2n-1}$.

The coefficient β in $\det \hat{B} = \alpha d_{ij}^4 + \beta d_{ij}^2 + \gamma$ is the sum of products included into two determinants of the submatrices obtained from $\hat{B}$ by removing the row $i+1$ and column $j+1$ (for one submatrix), then the row $j+1$ and column $i+1$ (for another submatrix). Since each $(n+1)\times(n+1)$ submatrix includes one entry d_{ij}^2, all products with this entry are excluded as there were counted in αd_{ij}^4.

For example, if $n = 3$ and $d_{ij} = d_{13}$, then

$$\beta = \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & d_{21}^2 & 0 & d_{24}^2 \\ 1 & d_{31}^2 & d_{32}^2 & d_{34}^2 \\ 1 & d_{41}^2 & d_{43}^2 & 0 \end{vmatrix} + \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & d_{12}^2 & d_{13}^2 & d_{14}^2 \\ 1 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix},$$

where $d_{13}^2 = d_{31}^2$ should be replaced by 0, hence $\beta = \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & d_{21}^2 & 0 & d_{24}^2 \\ 1 & 0 & d_{32}^2 & d_{34}^2 \\ 1 & d_{41}^2 & d_{43}^2 & 0 \end{vmatrix} + \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & d_{12}^2 & 0 & d_{14}^2 \\ 1 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix}$. Up to a permutation of indices, each submatrix can be rewritten with the diagonal that has one d_{ij}^2, while all other diagonal elements are zeros. The example above gives

$$\beta = -\begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & d_{32}^2 & d_{34}^2 \\ 1 & d_{21}^2 & 0 & d_{24}^2 \\ 1 & d_{41}^2 & d_{43}^2 & 0 \end{vmatrix} - \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & d_{23}^2 & d_{24}^2 \\ 1 & d_{12}^2 & 0 & d_{14}^2 \\ 1 & d_{42}^2 & d_{43}^2 & 0 \end{vmatrix}.$$

Similarly to the argument for the determinant α, the sum βd_{ik} contains $2r_{n+1}$ products of total degree $2n-1$, so $\left|\dfrac{\beta d_{ik}}{p^{2n-1}(A)}\right| \le 2r_{n+1}\left(\dfrac{2}{n}\right)^{2n-1}$. Then the required inequality follows: $\left|\dfrac{\partial \det \hat{B}}{\partial d_{ij}} \dfrac{1}{p^{2n-1}(A)}\right| = \dfrac{|4\alpha d_{ij}^3 + 2\beta d_{ij}|}{p^{2n-1}(A)} \le (4r_n + 2r_{n+1})\left(\dfrac{2}{n}\right)^{2n-1}$. □

Example 4.6 (strength $\sigma(A)$ and its upper bounds)**.** *For $n \ge 2$, the proved upper bounds for the Lipschitz constant of the strength: $c_2 = 2\sqrt{3}$, $c_3 \approx 0.43$, $c_4 \approx 0.01$, which quickly tend to 0 due to the 'curse of dimensionality'. The plots in [67, Fig. 4] illustrate that the strength $\sigma(A)$ behaves smoothly in the x-coordinate of a vertex and its derivative $|\frac{\partial \sigma}{\partial x}|$ is much smaller than the proved bounds c_n above.* ■

5. Algorithms for complete invariant metrics

For Lemma 5.2, we remind that by Definition 3.2 an Oriented Relative Distribution ORD is a pair $[D(A); M(C;A)]$ of matrices considered up to permutations $\xi \in S_n$ of n ordered points of A. Any column of $M(C;A)$ is a pair (v,s), where $s \in \{\pm 1, 0\}$ and $v \in \mathbb{R}^n$ is a vector of distances from $q \in C - A$ to $p_1,\dots,p_n \in A$.

For simplicity and similar to the case of a general metric space, we assume that a point cloud $C \subset \mathbb{R}^n$ is given by a matrix of pairwise Euclidean distances. If C is given by Euclidean coordinates of points, then any distance requires $O(n)$ computations and we should add the factor n in all complexities below, keeping all times polynomial in m.

The $m-n$ permutable columns of the matrix $M(C;A)$ in ORD from Definition 3.2 can be interpreted as $m-n$ unlabeled points in $\mathbb{R}^n$. Since any isometry is bijective, the simplest metric respecting bijections is the bottleneck distance (also called the Wasserstein distance W_∞).

Definition 5.1 (bottleneck distance W_∞)**.** *For any vector $v = (v_1,\dots,v_n) \in \mathbb{R}^n$, the* Minkowski *norm is $||v||_\infty = \max\limits_{i=1,\dots,n} |v_i|$. For any vectors or matrices N, N' of the same size, the* Minkowski *distance is $L_\infty(N,N') = \max\limits_{i,j} |N_{ij} - N'_{ij}|$. For clouds $C, C' \subset \mathbb{R}^n$ of m unlabeled points, the* bottleneck distance *$W_\infty(C,C') = \inf\limits_{g:C\to C'} \sup\limits_{p\in C} ||p - g(p)||_\infty$ is minimized over all bijections $g: C \to C'$.* ■

Lemma 5.2 (metric on ORDs)**.** *Using the strength σ from Definition 4.1, we consider the bottleneck distance W_∞ on the set of permutable $m-n$ columns of $M(C;A)$ as on the set of $m-n$ unlabelled points $(v, \frac{s}{c_n}\sigma(A\cup\{q\})) \in \mathbb{R}^{n+1}$.*

For another $\mathrm{ORD}' = [D(A'); M(C';A')]$ *and any permutation $\xi \in S_n$ of indices $1,\dots,n$ acting on $D(A)$ and rows of $M(C;A)$, set* $d_o(\xi) = \max\{L_\infty(\xi(D(A)), D(A')), W_\infty(\xi(M(C;A)), M(C';A'))\}$. *Then* $M_\infty(\mathrm{ORD},\mathrm{ORD}') = \min\limits_{\xi\in S_n} d_o(\xi)$ *satisfies all metric axioms on Ordered Relative Distributions (ORDs) and can be computed in time $O(n!(n^2 + m^{1.5}\log^{n+1} m))$.* ■

Proof. The first metric axiom says that $\mathrm{ORD}(C;A), \mathrm{ORD}(C';A')$ are equivalent by Definition 3.2 if and only if $M_\infty(\mathrm{ORD}(C;A), \mathrm{ORD}(C';A')) = 0$ or $d(\xi) = 0$ for some permutation $\xi \in S_n$. Then $d(\xi) = 0$ is equivalent to $\xi(D(A)) = D(A')$ and $\xi(M(C;A)) = M(C';A')$ up to a permutation of columns due to the first axiom for W_∞. The last two conclusions mean that the Oriented Relative Distributions $\mathrm{ORD}(C;A), \mathrm{ORD}(C';A')$ are equivalent by Definition 3.2. The symmetry axiom follows since any permutation ξ is invertible. To prove the triangle inequality
$M_\infty(\mathrm{ORD}(C;A), \mathrm{ORD}(C';A')) +$
$M_\infty(\mathrm{ORD}(C'';A''), \mathrm{ORD}(C';A')) \ge$
$M_\infty(\mathrm{ORD}(C;A), \mathrm{ORD}(C'';A''))$, let $\xi, \xi' \in S_h$ be optimal permutations for the M_∞ values in the left-hand side above. The triangle inequality for L_∞ says that
$L_\infty(\xi(D(A)), D(A')) +$
$L_\infty(\xi'(D(A'')), D(A')) \ge$

$L_\infty(\xi(D(A)),\xi'(D(A''))) =$ $L_\infty(\xi'^{-1}\xi(D(A)),D(A''))$, similarly for the bottleneck distance W_∞ from Definition 5.1. Taking the maximum of L_∞, W_∞ preserves the triangle inequality. Then $M_\infty(\text{RDD}(C;A),\text{RDD}(C'';A'')) = \min\limits_{\xi\in S_n} d(\xi)$ cannot be larger than $d(\xi'^{-1}\xi)$ for the composition of the permutations above, the triangle inequality holds for M_∞.

For a fixed permutation $\xi \in S_{n-1}$, the distance $L_\infty(\xi(D(A)),D(A'))$ requires $O(n^2)$ time. The bottleneck distance $W_\infty(\xi(M(C;A)),M(C';A'))$ on the $(n+1)\times(m-h)$ matrices $\xi(M(C;A))$ and $M(C';A')$ with permutable columns can be considered as the bottleneck distance on clouds of $(m-h)$ unlabeled points in $\mathbb{R}^h$, so $W_\infty(\xi(M(C;A)),M(C';A'))$ needs only $O(m^{1.5}\log^h m)$ time by [27, Theorem 6.5]. The minimization over all permutations $\xi \in S_n$ gives the factor $n!$ in the final time.

When computing the metric M_∞ on ORDs in Lemma 5.2, each of the $m-n$ signs for a point $q \in C-A$ is multiplied by the strength $\sigma(A)$. The strength $\sigma(A)$ in Definition 4.1 is computed from all pairwise distances in $D(A)$ via the Cayley-Menger determinant [57]. One $(n+2)\times(n+2)$ determinant needs time $O(n^3)$ by Gaussian elimination. All $m-n$ strengths need $O(mn^3)$ time, which is smaller than the later time including the factors $m^{1.5}$ and $n!$ Then $m-n$ permutable columns of $M(C;A)$ are considered as $m-n$ unlabelled points in $\mathbb{R}^{n+1}$, which explains the extra factor $\log m$ coming from [27, Theorem 6.5]. □

The coefficient $\frac{1}{c_n}$ in front of the strength $\sigma(A\cup\{q\})$ in Lemmas 5.2 and 5.3 normalizes the Lipschitz constant c_n of σ to 1 in line with changes of distances by at most 2ε when points are perturbed within their ε-neighbourhoods.

Lemma 5.3 (metric on OCDs)**.** *Using the strength σ from Definition 4.1, we consider the bottleneck distance W_∞ on the set of permutable $m-n+1$ columns of $M(C;A\cup\{0\})$ as on the set of $m-n+1$ unlabelled points $\left(v, \dfrac{s}{c_n}\sigma(A\cup\{0,q\})\right) \in \mathbb{R}^{n+1}$. For another* $\text{OCD}' = [D(A'\cup\{0\}); M(C';A'\cup\{0\})]$ *and any permutation $\xi \in S_{n-1}$ of indices $1,\dots,n-1$ acting on $D(A\cup\{0\})$ and the first $n-1$ rows of $M(C;A\cup\{0\})$, set $d_o(\xi)=\max\{L,W\}$,*

$$\text{where } L = L_\infty\Big(\xi(D(A\cup\{0\})), D(A'\cup\{0\})\Big),$$

$$W = W_\infty\Big(\xi(M(C;A\cup\{0\})), M(C';A'\cup\{0\})\Big).$$

Then $M_\infty(\text{OCD},\text{OCD}') = \min\limits_{\xi\in S_{n-1}} d_o(\xi)$ *satisfies all metric axioms on Oriented Centred Distributions (OCDs) and is computed in time $O((n-1)!(n^2+m^{1.5}\log^n m))$.* ■

Proof of Lemma 5.3. All arguments follow the proof of Lemma 5.2 for a subset A consisting of $n-1$ unordered points of C and one central point at the origin. Hence n should be replaced with $n-1$. □

The metrics M_∞ will be used for intermediate costs to get metrics on unordered collections OSDs and SCDs by using standard Definitions 5.4 and 5.5 below.

Definition 5.4 (Linear Assignment Cost LAC [31])**.** *For any $k\times k$ matrix of costs $c(i,j)\geq 0$, $i,j\in\{1,\dots,k\}$, the* Linear Assignment Cost $\text{LAC} = \frac{1}{k}\min\limits_{g}\sum\limits_{i=1}^{k} c(i,g(i))$ *is minimized for all bijections g on the indices $1,\dots,k$.* ■

The normalization factor $\frac{1}{k}$ in LAC makes this metric better comparable with EMD whose weights sum up to 1.

Definition 5.5 (Earth Mover's Distance on distributions)**.** *Let $B=\{B_1,\dots,B_k\}$ be a finite unordered set of objects with weights $w(B_i)$, $i=1,\dots,k$. Consider another set $D=\{D_1,\dots,D_l\}$ with weights $w(D_j)$, $j=1,\dots,l$. Assume that a distance between B_i,D_j is measured by a metric $d(B_i,D_j)$. A* flow *from B to D is a $k\times l$ matrix whose entry $f_{ij}\in[0,1]$ represents a partial* flow *from an object B_i to D_j. The* Earth Mover's Distance *[53] is the minimum of* $\text{EMD}(B,D) = \sum\limits_{i=1}^{k}\sum\limits_{j=1}^{l} f_{ij}d(B_i,D_j)$ *over $f_{ij}\in[0,1]$ subject to $\sum\limits_{j=1}^{l} f_{ij}\leq w(B_i)$ for $i=1,\dots,k$, $\sum\limits_{i=1}^{k} f_{ij}\leq w(D_j)$ for $j=1,\dots,l$, and $\sum\limits_{i=1}^{k}\sum\limits_{j=1}^{l} f_{ij}=1$.* ■

The first condition $\sum\limits_{j=1}^{l} f_{ij}\leq w(B_i)$ means that not more than the weight $w(B_i)$ of the object B_i 'flows' into all D_j via the flows f_{ij}, $j=1,\dots,l$. The second condition $\sum\limits_{i=1}^{k} f_{ij}\leq w(D_j)$ means that all flows f_{ij} from B_i for $i=1,\dots,k$ 'flow' to D_j up to its weight $w(D_j)$. The last condition $\sum\limits_{i=1}^{k}\sum\limits_{j=1}^{l} f_{ij}=1$ forces all B_i to collectively 'flow' into all D_j. LAC [31] and EMD [53] can be computed in a near cubic time in the sizes of given sets of objects.

An equality $\text{OSD}(C)=\text{OSD}(C')$ between unordered collections of ORDs is best detected by checking if the LAC or EMD metric in Theorem 5.6 between these OSDs is 0.

Theorem 5.6 (times for metrics on OSDs)**.** ***(a)*** *For the $k\times k$ matrix of costs computed by the metric M_∞ between* ORDs *from* $\text{OSD}(C)$ *and* $\text{OSD}(C')$, LAC *from Definition 5.4 satisfies all metric axioms on* OSDs *and needs time $O(n!(n^2+m^{1.5}\log^{n+1}m)k^2+k^3\log k)$.*

(b) *Let* OSD*s have a maximum size* $l \leq k$ *after collapsing identical* ORD*s. Then* EMD *from Definition 5.5 satisfies all metric axioms on* OSD*s and can be computed in time* $O(n!(n^2 + m^{1.5}\log^{n+1} m)l^2 + l^3 \log l)$. ■

Proof. The Linear Assignment Cost (LAC) from Definition 5.4 is symmetric because any bijective matching can be reversed. The triangle inequality for LAC follows from the triangle inequality for the metric M_∞ in Lemma 5.2 by using a composition of bijections $\mathrm{OSD}(C; h) \to \mathrm{OSD}(C'; h) \to \mathrm{SDD}(C''; h)$ matching all ORDs similarly to the proof of Lemma 5.2. The first metric axiom for LAC means that LAC $= 0$ if and only if there is a bijection $g : \mathrm{OSD}(C; h) \to \mathrm{OSD}(C'; h)$ so that all matched ORDs are at distance $M_\infty = 0$, so these ORDs are equivalent (hence OSDs are equal) due to the first axiom of $M_\infty = 0$, which was proved in Lemma 5.2.

The metric axioms for the Earth Mover's Distance (EMD) are proved in the appendix of [53] assuming the metric axioms for the underlying distance d, which is the metric M_∞ from Lemma 5.2 in our case.

The time complexities for LAC and EMD follow from the time $O(n!(n^2 + m^{1.5}\log^n m))$ for M_∞ in Lemma 5.2, after multiplying by a quadratic factor for the size of cost matrices and adding a near cubic time [31, 32]. □

An equality $\mathrm{SCD}(C) = \mathrm{SCD}(C')$ is interpreted as a bijection between unordered sets $\mathrm{SCD}(C) \to \mathrm{SCD}(C')$ matching all OCDs, which is best detected by checking if metrics in Theorem 5.7 between these SCDs is 0.

Theorem 5.7 (times for metrics on SCDs)**.** ***(a)*** *For the* $k \times k$ *matrix of costs computed by the metric* M_∞ *between* OCD*s in* $\mathrm{SCD}(C)$ *and* $\mathrm{SCD}(C')$*,* LAC *from Definition 5.4 satisfies all metric axioms on* SCD*s and needs time* $O((n-1)!(n^2 + m^{1.5}\log^n m)k^2 + k^3 \log k)$.

(b) *Let* SCD*s have a maximum size* $l \leq k$ *after collapsing identical* OCD*s. Then* EMD *from Definition 5.5 satisfies all metric axioms on* SCD*s and can be computed in time* $O((n-1)!(n^2 + m^{1.5}\log^n m)l^2 + l^3 \log l)$. ■

Proof of Theorem 5.7. All arguments follow the proof of Theorem 5.6 after replacing n with $n-1$. □

If we estimate $l \leq k = \binom{m}{n-1} = m(m-1)\dots(m-n+2)/n!$ as $O(m^{n-1}/n!)$, Theorem 5.7 gives time $O(n(m^{n-1}/n!)^3 \log m)$ for metrics on SCDs, which is $O(m^3 \log m)$ for $n = 2$, and $O(m^6 \log m)$ for $n = 3$.

Though the above time estimates are very rough upper bounds, the time $O(m^3 \log m)$ in $\mathbb{R}^2$ is faster than the only past time $O(m^5 \log m)$ for comparing m-point clouds by the Hausdorff distance minimized over isometries [19].

6. Lipschitz continuity of invariant metrics

Corollary 6.1 (continuity of OSD and SCD)**.** *For a cloud* $C \subset \mathbb{R}^n$ *of* m *unlabelled points, perturbing any point within its* ε*-neighbourhood changes* $\mathrm{OSD}(C)$ *and* $\mathrm{SCD}(C)$ *by at most* 2ε *in the* LAC *and* EMD *metrics.* ■

Proof. If every point is perturbed in its ε-neighbourhood, any distance between points changes by at most 2ε. This upper bound survives under the metrics M_∞, LAC, EMD.

Theorem 4.2 was essential to justify a Lipschitz constant c_n of a strength $\sigma(A)$ so that the last coordinates $\frac{s}{c_n}\sigma(A \cup \{q\})$ change by at most 2ε when the bottleneck distance W_∞ is computed on columns in Lemmas 5.2 and 5.3. □

Definition 6.2 (Oriented Distance Moments ODM)**.** *For any* m*-point cloud* $C \subset \mathbb{R}^n$*, let* $A \subset C$ *be a subset of* n *unordered points. The* Sorted Distance Vector $\mathrm{SDV}(A)$ *is the list of all* $\frac{h(h-1)}{2}$ *pairwise distances between points of* A *written in increasing order. For each column of the* $(n+1) \times (m-n)$ *matrix* $M(C; A)$ *in Definition 3.8, compute the average of the first* n *distances. Write these averages in increasing order and append the vector of increasing values of* $\dfrac{s}{c_n}\sigma(A)$ *taking signs* s *from the* $(n+1)$*-st row of* $M(C; A)$*. Let* $\vec{M}(C; A) \in \mathbb{R}^{2(m-n)}$ *be the final vector.*

The pair $[\mathrm{SDV}(A); \vec{M}(C; A)]$ *is a vector of length* $\frac{n(n-1)}{2} + 2(m-n)$ *called the* Average Oriented Vector $\mathrm{AOV}(C; A)$*. The unordered set of vectors* $\mathrm{AOV}(C; A)$ *for all* $\binom{m}{n}$ *unordered subsets* $A \subset C$ *is the* Average Oriented Distribution $\mathrm{AOD}(C)$*. For* $l \geq 1$*, the* Oriented Distance Moment $\mathrm{ODM}(C; l)$ *is the* l*-th (standardized for* $l \geq 3$*) moment of* $\mathrm{AOD}(C)$ *considered as a probability distribution of* $\binom{m}{n}$ *vectors, separately for each coordinate.* ■

Example 6.3 (ODM for clouds in Fig. 1)**.** *For the non-isometric 4-point clouds* T, K *in Fig. 1, Table 3 summarizes the computations of the Average Oriented Distributions (*AOD*s) from Definition 6.2. The values* $\dfrac{s}{c_2}\sigma(A)$ *involving the strength of a triangle on a 3-point subset* A *use the Lipschitz constant* $c_2 = 2\sqrt{3}$*. We compute the normalized strengths* $\dfrac{\sigma(A)}{c_2}$ *using* $\sigma(A) = \dfrac{V^2(A)}{p^3(A)}$*, see Definition 4.1, where* $V(A)$ *is the area and* $p(A)$ *is the half-perimeter of the triangle on* A*.*

The trapezoid T *has two triangles with sides* $\sqrt{2}, 2, \sqrt{10}$*, area* 1*, half-perimeter* $1 + \dfrac{\sqrt{2}+\sqrt{10}}{2}$*, and normalized strength* $\sigma_1(T) = \dfrac{1}{2\sqrt{3}}\left(\dfrac{2}{\sqrt{2}+2+\sqrt{10}}\right)^3 \approx 0.008$.

The kite K *has a triangle with sides* $\sqrt{2}, \sqrt{2}, 2$*, area* 1*, half-perimeter* $1 + \sqrt{2}$*, and normalized strength* $\sigma_1(K) = \dfrac{1}{2\sqrt{3}(1+\sqrt{2})^3} \approx 0.021$.

Average Oriented Vectors in $\mathrm{AOD}(T)$	Average Oriented Vectors in $\mathrm{AOD}(K)$
$\left[\sqrt{2};\ \frac{2+\sqrt{10}}{2}, \frac{4+\sqrt{10}}{2};\ -\sigma_2,\ -\sigma_1(T)\right] \approx$ $[\ 1.414;\ 2.581,\ 3.581;\ -0.015,\ -0.008\ ]$	$\left[\sqrt{2};\ \frac{2+\sqrt{2}}{2}, \frac{4+\sqrt{10}}{2};\ -\sigma_1(K), -\sigma_2\right] \approx$ $[\ 1.414;\ 1.707,\ 3.581;\ -0.021,\ -0.015\ ]$
$\left[\sqrt{2};\ \frac{2+\sqrt{10}}{2}, \frac{4+\sqrt{10}}{2};\ \sigma_1(T), \sigma_2\right] \approx$ $[\ 1.414;\ 2.581,\ 3.581;\ 0.008,\ 0.015\ ]$	$\left[\sqrt{2};\ \frac{2+\sqrt{2}}{2}, \frac{4+\sqrt{10}}{2};\ \sigma_2, \sigma_1(K)\right] \approx$ $[\ 1.414;\ 1.707,\ 3.581;\ 0.015,\ 0.021\ ]$
$\left[2;\ \frac{\sqrt{2}+\sqrt{10}}{2}, \frac{\sqrt{2}+\sqrt{10}}{2};\ -\sigma_1(T), -\sigma_1(T)\right]$ $\approx [\ 2;\ 2.581,\ 2.581;\ -0.008,\ -0.008\ ]$	$\left[2;\ \sqrt{2}, \sqrt{10};\ -\sigma_1(K), \sigma_3\right]$ $\approx [\ 2;\ 1.414,\ 3.162;\ -0.021,\ 0.036\ ]$
$\left[\sqrt{10};\ \frac{2+\sqrt{2}}{2}, \frac{4+\sqrt{2}}{2};\ -\sigma_2, \sigma_1(T)\right] \approx$ $[\ 3.162;\ 1.707,\ 2.707;\ -0.015,\ 0.008\ ]$	$\left[\sqrt{10};\ \frac{2+\sqrt{10}}{2}, \frac{4+\sqrt{2}}{2};\ -\sigma_3, -\sigma_2\right] \approx$ $[\ 3.162;\ 2.581,\ 2.707;\ -0.021,\ -0.015\ ]$
$\left[\sqrt{10};\ \frac{2+\sqrt{2}}{2}, \frac{4+\sqrt{2}}{2};\ -\sigma_1(T), \sigma_2\right] \approx$ $[\ 3.162;\ 1.707,\ 2.707;\ -0.008,\ 0.015\ ]$	$\left[\sqrt{10};\ \frac{2+\sqrt{10}}{2}, \frac{4+\sqrt{2}}{2};\ \sigma_2, \sigma_3\right] \approx$ $[\ 3.162;\ 2.581,\ 2.707;\ 0.015,\ 0.036\ ]$
$\left[4;\ \frac{\sqrt{2}+\sqrt{10}}{2}, \frac{\sqrt{2}+\sqrt{10}}{2};\ \sigma_2, \sigma_2\right] \approx$ $[\ 4;\ 2.288,\ 2.288;\ 0.015,\ 0.015\ ]$	$\left[4;\ \frac{\sqrt{2}+\sqrt{10}}{2}, \frac{\sqrt{2}+\sqrt{10}}{2};\ -\sigma_2, \sigma_2\right] \approx$ $[\ 4;\ 2.288,\ 2.288;\ -0.015,\ 0.015\ ]$

Table 2. The Averaged Oriented Distributions (AODs) from Definition 6.2 for the clouds $T, K \subset \mathbb{R}^2$ in Fig. 1 consist of six vectors in $\mathbb{R}^5$. The coordinate-wise averages of the six vectors in AOD give the Oriented Distance Moment $\mathrm{CDM} \in \mathbb{R}^5$ in Table 3, see Example 6.3.

Both T, K have triangles with sides $\sqrt{2}, \sqrt{10}, 4$, area 2, half-perimeter $2 + \dfrac{\sqrt{2}+\sqrt{10}}{2}$, and normalized strength $\sigma_2 = \dfrac{2}{\sqrt{3}}\left(\dfrac{2}{\sqrt{2}+4+\sqrt{10}}\right)^3 \approx 0.015.$

The kite K has a triangle with sides $2, \sqrt{10}, \sqrt{10}$, area 3, half-perimeter $1+\sqrt{10}$ and normalized strength $\sigma_3 = \dfrac{3^2}{2\sqrt{3}}\left(\dfrac{1}{1+\sqrt{10}}\right)^3 = \dfrac{3\sqrt{3}}{2(1+\sqrt{10})^3} \approx 0.036.$

Every Average Oriented Vector $\mathrm{AOV}(C; A) \in \mathbb{R}^5$ in Table 2 consists of $1+2+2$ coordinates. The first coordinate is the distance between the points of A. The two further coordinates are in increasing order. The two last coordinates are in increasing order, independently of the previous pair.

Table 3 shows the Oriented Distance Moments $\mathrm{ODM}(C; 1)$ obtained by coordinate-wise averaging all vectors in the Average Oriented Distribution $\mathrm{AOD}(C)$.

The distance L_∞ between the vectors $\mathrm{ODM}(T; 1)$ and $\mathrm{ODM}(K; 1)$ in $\mathbb{R}^5$ is $\dfrac{8+5\sqrt{2}+3\sqrt{10}}{12} - \dfrac{6+2\sqrt{2}+4\sqrt{10}}{12} = \dfrac{2+3\sqrt{2}-\sqrt{10}}{12} \approx 0.257.$ ■

Corollary 6.4 (time and lower bound for a metric on ODMs)**.** ***(a)*** *For any cloud $C \subset \mathbb{R}^n$ of m unlabelled points, the Oriented Distance Moment $\mathrm{ODM}(C; l)$ in Definition 6.2 is computed in time $O(m^{n+1}/(n-3)!)$.*

Oriented Distance Moment $\mathrm{ODM}(T;1)$	Oriented Distance Moment $\mathrm{ODM}(K;1)$
$\mathrm{ODM}_1 = \dfrac{3+\sqrt{2}+\sqrt{10}}{3} \approx 2.525$	$\mathrm{ODM}_1 = \dfrac{3+\sqrt{2}+\sqrt{10}}{3} \approx 2.525$
$\mathrm{ODM}_2 = \dfrac{6+2\sqrt{2}+4\sqrt{10}}{12} \approx 1.790$	$\mathrm{ODM}_2 = \dfrac{8+5\sqrt{2}+3\sqrt{10}}{12} \approx 2.046$
$\mathrm{ODM}_3 = \dfrac{16+4\sqrt{2}+4\sqrt{10}}{12} \approx 2.859$	$\mathrm{ODM}_3 = \dfrac{16+3\sqrt{2}+5\sqrt{10}}{12} \approx 3.005$
$\mathrm{ODM}_4 = -\dfrac{\sigma_1(T)+\sigma_2}{6} \approx -0.004$	$\mathrm{ODM}_4 = \dfrac{\sigma_2-\sigma_1(K)}{6} \approx -0.001$
$\mathrm{ODM}_5 = \dfrac{3\sigma_2-\sigma_1(T)}{6} \approx 0.006$	$\mathrm{ODM}_5 = \dfrac{2\sigma_3+\sigma_1(K)-\sigma_2}{6} \approx 0.013$

Table 3. The Oriented Distance Moments (ODMs) from Definition 6.2 for the 4-point clouds $T, K \subset \mathbb{R}^2$ in Fig. 1 are obtained by averaging the six vectors from the Average Oriented Distributions in Table 2.

(b) *The metric L_∞ on* ODMs *needs $O(n^2+m)$ time and provides the lower bound* $\mathrm{EMD}\big(\mathrm{OSD}(C),\mathrm{OSD}(C')\big) \geq |\mathrm{ODM}(C;1)-\mathrm{ODM}(C';1)|_\infty$. ■

Proof. **(a)** For any n-point subset $A \subset C$ and a fixed point $q \in C - A$, the average distance from q to the n points of A written in a column of $M(C;A)$ is computed in time $O(n)$, hence $O(nm)$ for all columns of $M(C;A)$ (or all points $q \in C - A$). Ordering the distance averages and (separately) $m-n$ values $\dfrac{s}{c_n}\sigma(A)$ takes $O(m\log m)$ time.

So the vector $\vec{M}(C;A) \in \mathbb{R}^{2(m-n)}$ from Definition 6.2 takes $O(nm+m\log m)$ time. The list $\mathrm{SDV}(A)$ of Ordered Pairwise Distances is obtained by sorting all pairwise distances from $D(A)$ in time $O(n^2\log n)$. The Average Oriented Vector $\mathrm{AOV}(C;A)$ is obtained by concatenating of the vectors $\mathrm{SDV}(A) \in \mathbb{R}^{\frac{n(n-1)}{2}}$ and $\vec{M}(C;A) \in \mathbb{R}^{2(m-n)}$ and is computed in time $O((n^2+m)\log m)$.

Hence the Average Oriented Distribution $\mathrm{AOD}(C;h)$ for all h-point subsets $A \subset C$ needs $O(m^{n+1}/(n-3)!)$ time including the extra time $O((n^2+m)\log m)$ above, the same as the initial invariant $\mathrm{OSD}(C)$ in Theorem 3.7.

For $l=1$, the first raw moment $\mathrm{ODM}(C;1)$ is the simple average of all $k=\binom{m}{n}$ vectors $\mathrm{AOV}(C;A)$ of length $O(nm)$, hence needs time $O(knm)=O(m^{n+1}/(n-1)!)$. For $l=2$, the standard deviation σ of each coordinate in all vectors $\mathrm{AOV}(C;A)$ requires the same time. Then, for any fixed $l \geq 3$, the l-th standardized moment $\dfrac{1}{k}\sum\limits_{i=1}^{k}\left(\dfrac{a_i-\mu}{\sigma}\right)^l$ needs again the same time $O(m^{n+1}/(n-1)!)$.

(b) For a fixed $l \geq 1$, the vector $\mathrm{ODM}(C;l)$ has the length $\frac{n(n-1)}{2}+2(m-n)$. Computing the metric L_∞ on such vectors needs only $O(n^2+m)$ time. The lower bound of $\mathrm{EMD}\big(\mathrm{OSD}(C),\mathrm{OSD}(C')\big)$ follows from [21, Theorem 1] about averages of distributions. The only extra addition is the $(n+1)$-st row of values $\dfrac{s}{c_n}\sigma(A)$ in the matrices $M(C;A)$. For EMD on OSDs, the bottleneck distance W_∞ on columns of $M(C;A)$ takes the maximum absolute difference of the values for C and its perturbation C'.

The moment $\mathrm{ODM}(C;1)$ involves averaging these values for n-point subsets $A \subset C$. The metric L_∞ on resulting averages cannot be larger than the maximum absolute difference computed by the bottleneck distance W_∞. □

Corollary 6.5 (time and lower bound for a metric on CDMs)**.** ***(a)*** *For any cloud $C \subset \mathbb{R}^n$ of m unlabelled points, the Centred Distance Moment* $\mathrm{CDM}(C;l)$ *in Definition 6.6 is computed in time $O(m^n/(n-4)!)$.*

(b) *The metric L_∞ on* CDMs *needs $O(n^2+m)$ time and* $\mathrm{EMD}\big(\mathrm{SCD}(C),\mathrm{SCD}(C')\big) \geq |\mathrm{CDM}(C;1)-\mathrm{CDM}(C';1)|_\infty$ *holds.* ■

Proof of Corollary 6.5. All arguments follow the proof of Corollary 6.4 after replacing n with $n-1$. □

Corollaries 6.1, 6.4, 6.5 imply that $\mathrm{ODM}(C;1)$ and $\mathrm{CDM}(C;1)$ are continuous under perturbations of a point cloud $C \subset \mathbb{R}^n$ with the Lipschitz constant 2.

Definition 6.6 (Centered Distance Moments CDM)**.** *For any m-point cloud $C \subset \mathbb{R}^n$, let $A \subset C$ be a subset of $n-1$ unordered points. The Sorted Distance Vector* $\mathrm{SDV}(A;0)$ *is the increasing list of all $\frac{(n-1)(n-2)}{2}$ pairwise distances between points of A, followed by $n-1$ increasing distances from A to the origin 0. For each column of the $(n+1)\times(m-n+1)$ matrix $M(C;A\cup\{0\})$ in Definition 3.8, compute the average of the first $n-1$ distances. Write these averages in increasing order, append the list of increasing distances $|q-0|$ from the n-th row of $M(C;A\cup\{0\})$, and also append the vector of increasing values of $\dfrac{s}{c_n}\sigma(A\cup\{0\})$*

taking signs s from the $(n+1)$-st row of $M(C;A\cup\{0\})$. Let $\vec{M}(C;A)\in\mathbb{R}^{3(m-n+1)}$ be the final vector.

The pair $[\mathrm{SDV}(A;0);\vec{M}(C;A)]$ is the Average Centred Vector $\mathrm{ACV}(C;A)$ *considered as a vector of length $\frac{n(n-1)}{2}+3(m-n+1)$. The unordered set of $\mathrm{ACV}(C;A)$ for all $\binom{m}{n-1}$ unordered subsets $A\subset C$ is the Average Centred Distribution $\mathrm{ACD}(C)$. The* Centered Distance Moment $\mathrm{CDM}(C;l)$ *is the l-th (standardized for $l\geq 3$) moment of $\mathrm{ACD}(C)$ considered as a probability distribution of $\binom{m}{n-1}$ vectors, separately for each coordinate.* ■

Example 6.7 (CDM for clouds in Fig. 2)**.** ***(a)*** *For $n=2$ and the cloud $R\subset\mathbb{R}^2$ of $m=3$ vertices $p_1=(0,0)$, $p_2=(4,0)$, $p_3=(0,3)$ of the right-angled triangle in Fig. 2 (middle), we continue Example 3.9(a) and flatten* $\mathrm{OCD}(R;p_1)=[0,\begin{pmatrix}4&3\\4&3\\0&0\end{pmatrix}]$ *into the vector* $\mathrm{ACV}(R;p_1)=[0;3,4;3,4;0,0]$ *of length $\frac{n(n-1)}{2}+3(m-n+1)=7$, whose four parts ($1+2+2+2=7$) are in increasing order, similarly for p_2,p_3. The Average Centred Distribution can be written as a 3×7 matrix with unordered rows:* $\mathrm{ACD}(R)=\left(\begin{array}{c|cc|cc|cc}0&3&4&3&4&0&0\\4&4&5&0&3&0&-6/c_2\\3&3&5&0&4&0&6/c_2\end{array}\right)$. *The area of the triangle on R equals 6 and can be normalized by $c_2=2\sqrt{3}$ (see the appendices) to get $6/c_2=\sqrt{3}$. The 1st moment is* $\mathrm{CDM}(R;1)=\frac{1}{3}(7;10,14;3,11;0)$.

(b) *For $n=2$ and the cloud $S\subset\mathbb{R}^2$ of $m=4$ vertices of the square in Fig. 2 (right), Example 3.9(a) computed* $\mathrm{SCD}(R)$ *as one* $\mathrm{OCD}=[1,\begin{pmatrix}\sqrt{2}&\sqrt{2}&2\\1&1&1\\-&+&0\end{pmatrix}]$, *which flattens to* $\mathrm{ACV}=(1;\sqrt{2},\sqrt{2},2;1,1,1;-\frac{1}{2},\frac{1}{2},0)=\mathrm{ACD}(S)=\mathrm{CDM}(S;1)\in\mathbb{R}^{10}$, *where $\frac{1}{2}$ is the area of the triangle on the vertices* $(0,0),(1,0),(0,1)$. ■

New invariants in Definitions 3.2, 3.8 and main Theorems 3.10, 5.6, and Corollary 6.1 solve Problem 1.1.

Similar and stronger distance-based invariants for more general metric-mesure spaces are explored in [43, 46, 47].

Computations of invariants on atomic clouds from [67, section 5] will be substantially expanded in future work.

This research was supported by the Royal Academy of Engineering fellowship "Data science for next generation engineering of solid crystalline materials" (2021-2023, IF2122/186) and the EPSRC grants "Application-driven Topological Data Analysis" (2018-2023, EP/R018472/1) and "Inverse design of periodic crystals" (2022-2024, EP/X018474/1).

The author thanks all members of the Data Science Theory and Applications group in the Materials Innovation Factory (Liverpool, UK), especially Daniel Widdowson, Matthew Bright, Yury Elkin, Olga Anosova, also Justin Solomon (MIT), Steven Gortler (Harvard), Nadav Dym (Technion) for fruitful discussions, and any reviewers for their valuable time and helpful suggestions.

References

[1] Naveed Akhtar and Ajmal Mian. Threat of adversarial attacks on deep learning in computer vision: A survey. *IEEE Access*, 6:14410–14430, 2018. 2

[2] Olga Anosova and Vitaliy Kurlin. Introduction to periodic geometry and topology. *arXiv:2103.02749*. 2

[3] Olga Anosova and Vitaliy Kurlin. An isometry classification of periodic point sets. In *Proceedings of Discrete Geometry and Mathematical Morphology*, 2021. 2

[4] Olga Anosova and Vitaliy Kurlin. Algorithms for continuous metrics on periodic crystals. *arxiv:2205.15298*, 2022. 2

[5] Olga Anosova and Vitaliy Kurlin. Density functions of periodic sequences. *Lecture Notes in Computer Science (Proceedings of DGMM)*, 2022. 2

[6] O Anosova and V Kurlin. Density functions of periodic sequences of continuous events. *arXiv:2301.05137*, 2023. 2

[7] Jonathan Balasingham, Viktor Zamaraev, and Vitaliy Kurlin. Compact graph representation of crystals using Pointwise Distance Distributions. *arXiv:2212.11246*, 2022. 2

[8] Mireille Boutin and Gregor Kemper. On reconstructing n-point configurations from the distribution of distances or areas. *Adv. Appl. Math.*, 32(4):709–735, 2004. 1

[9] Matthew J Bright, Andrew I Cooper, and Vitaliy A Kurlin. Welcome to a continuous world of 3-dimensional lattices. *arxiv:2109.11538*, 2021. 2

[10] Matthew J Bright, Andrew I Cooper, and Vitaliy A Kurlin. Geographic-style maps for 2-dimensional lattices. *Acta Crystallographica Section A*, 79(1):1–13, 2023. 2

[11] Michael M Bronstein, Joan Bruna, Taco Cohen, and Petar Veličković. Geometric deep learning: grids, groups, graphs, geodesics, and gauges. *arXiv:2104.13478*, 2021. 2

[12] Michael M Bronstein, Joan Bruna, Yann LeCun, Arthur Szlam, and Pierre Vandergheynst. Geometric deep learning: going beyond Euclidean data. *IEEE Signal Processing Magazine*, 34(4):18–42, 2017. 2

[13] Jean Cardinal, Timothy Chan, John Iacono, Stefan Langerman, and Aurélien Ooms. Subquadratic encodings for point configurations. *J Comp. Geometry*, 10:99–126, 2019. 2

[14] Gunnar Carlsson. Topology and data. *Bulletin of the American Mathematical Society*, 46(2):255–308, 2009. 2

[15] Michael J Catanzaro, Justin M Curry, Brittany Terese Fasy, Jānis Lazovskis, Greg Malen, Hans Riess, Bei Wang, and Matthew Zabka. Moduli spaces of morse functions for persistence. *Journal of Applied and Computational Topology*, 4(3):353–385, 2020. 2

[16] Charalambos A Charalambides. *Enumerative combinatorics*. Chapman and Hall/CRC, 2018. 7

[17] Haiwei Chen, Shichen Liu, Weikai Chen, Hao Li, and Randall Hill. Equivariant point network for 3D point cloud analysis. In *CVPR*, pages 14514–14523, 2021. 2

[18] Paul Chew, Dorit Dor, Alon Efrat, and Klara Kedem. Geometric pattern matching in d-dimensional space. *Discrete & Computational Geometry*, 21(2):257–274, 1999. 2

[19] Paul Chew, Michael Goodrich, Daniel Huttenlocher, Klara Kedem, Jon Kleinberg, and Dina Kravets. Geometric pattern matching under Euclidean motion. *Computational Geometry*, 7(1-2):113–124, 1997. 2, 10

[20] Paul Chew and Klara Kedem. Improvements on geometric pattern matching problems. In *Scandinavian Workshop on Algorithm Theory*, pages 318–325, 1992. 2

[21] Scott Cohen and Leonidas Guibas. The Earth Mover's Distance: lower bounds and invariance under translation. Technical report, Stanford University, 1997. 12

[22] Matthew J Colbrook, Vegard Antun, and Anders C Hansen. The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem. *PNAS*, 119(12):e2107151119, 2022. 2

[23] Justin Curry. The fiber of the persistence map for functions on the interval. *Journal of Applied and Computational Topology*, 2(3):301–321, 2018. 2

[24] Yinpeng Dong, Fangzhou Liao, Tianyu Pang, Hang Su, Jun Zhu, Xiaolin Hu, and Jianguo Li. Boosting adversarial attacks with momentum. In *Computer vision and pattern recognition*, pages 9185–9193, 2018. 2

[25] H Edelsbrunner, T Heiss, V Kurlin, P Smith, and M Wintraecken. The density fingerprint of a periodic point set. In *Proceedings of SoCG*, pages 32:1–32:16, 2021. 2

[26] Herbert Edelsbrunner, David Letscher, and Afra Zomorodian. Topological persistence and simplification. In *Foundations of Computer Science*, pages 454–463, 2000. 2

[27] Alon Efrat, Alon Itai, and Matthew J Katz. Geometry helps in bottleneck matching and related problems. *Algorithmica*, 31(1):1–28, 2001. 9

[28] Y. Elkin and V. Kurlin. The mergegram of a dendrogram and its stability. In *Proceedings of MFCS*, 2020. 2

[29] Y. Elkin and V. Kurlin. Isometry invariant shape recognition of projectively perturbed point clouds by the mergegram extending 0d persistence. *Mathematics*, 9(17), 2021. 2

[30] Peter Elliott. *Probabilistic number theory I*, volume 239. Springer Science & Business Media, 2012. 6, 7

[31] Michael L Fredman and Robert Endre Tarjan. Fibonacci heaps and their uses in improved network optimization algorithms. *Journal ACM*, 34:596–615, 1987. 9, 10

[32] Andrew Goldberg and Robert Tarjan. Solving minimum-cost flow problems by successive approximation. In *Proceedings of STOC*, pages 7–18, 1987. 10

[33] Michael T Goodrich, Joseph SB Mitchell, and Mark W Orletsky. Approximate geometric pattern matching under rigid motions. *Transactions PAMI*, 21:371–379, 1999. 2

[34] Darij Grinberg and Peter J Olver. The n body matrix and its determinant. *SIAM Journal on Applied Algebra and Geometry*, 3(1):67–86, 2019. 2

[35] Chuan Guo, Jacob Gardner, Yurong You, Andrew Gordon Wilson, and Kilian Weinberger. Simple black-box adversarial attacks. In *ICML*, pages 2484–2493, 2019. 2

[36] Felix Hausdorff. Dimension und äuβeres maβ. *Mathematische Annalen*, 79(2):157–179, 1919. 2

[37] Snir Hordan, Tal Amir, Steven J Gortler, and Nadav Dym. Complete neural networks for Euclidean graphs. *arXiv:2301.13821*, 2023. 2

[38] Daniel Huttenlocher, Gregory Klanderman, and William Rucklidge. Comparing images using the Hausdorff distance. *Transactions PAMI*, 15:850–863, 1993. 2

[39] Vitaliy Kurlin. A complete isometry classification of 3-dimensional lattices. *arxiv:2201.10543*, 2022. 2

[40] Vitaliy Kurlin. Computable complete invariants for finite clouds of unlabeled points under Euclidean isometry. *arXiv:2207.08502*, 2022. 2

[41] Vitaliy Kurlin. Exactly computable and continuous metrics on isometry classes of finite and 1-periodic sequences. *arxiv:2205.04388*, 2022. 2

[42] Vitaliy Kurlin. Mathematics of 2-dimensional lattices. *Found. Comp. Mathematics*, pages Dec 7: 1–59, 2022. 2

[43] Vitaliy Kurlin. Simplexwise distance distributions for finite spaces with metrics and measures. *arXiv:2303.14161*, 2023. 13

[44] Cassidy Laidlaw and Soheil Feizi. Functional adversarial attacks. *Adv. Neural Inform. Proc. Systems*, 32, 2019. 2

[45] Sushovan Majhi, Jeffrey Vitter, and Carola Wenk. Approximating Gromov-Hausdorff distance in Euclidean space. *arXiv:1912.13008*, 2019. 2

[46] Facundo Mémoli. Gromov–Wasserstein distances and the metric approach to object matching. *Foundations of Computational Mathematics*, 11(4):417–487, 2011. 13

[47] Facundo Mémoli and Tom Needham. Distance distributions and inverse problems for metric measure spaces. *Studies in Applied Mathematics*, 149(4):943–1001, 2022. 13

[48] Facundo Mémoli, Zane Smith, and Zhengchao Wan. The Gromov-Hausdorff distance between ultrametric spaces: its structure and computation. *arXiv:2110.03136*, 2021. 2

[49] Marco M Mosca and Vitaliy Kurlin. Voronoi-based similarity distances between arbitrary crystal lattices. *Crystal Research and Technology*, 55(5):1900197, 2020. 2

[50] Jigyasa Nigam, Michael J Willatt, and Michele Ceriotti. Equivariant representations for molecular hamiltonians and n-center atomic-scale properties. *Journal of Chemical Physics*, 156(1):014115, 2022. 2

[51] Blaine Rister, Mark A Horowitz, and Daniel L Rubin. Volumetric image registration from invariant keypoints. *Transactions on Image Processing*, 26(10):4900–4910, 2017. 2

[52] Jakob Ropers, Marco M Mosca, Olga D Anosova, Vitaliy A Kurlin, and Andrew I Cooper. Fast predictions of lattice energies by continuous isometry invariants of crystal structures. In *International Conference on Data Analytics and Management in Data Intensive Domains*, pages 178–192, 2022. 2

[53] Y. Rubner, C. Tomasi, and L. Guibas. The earth mover's distance as a metric for image retrieval. *Intern. Journal of Computer Vision*, 40(2):99–121, 2000. 9, 10

[54] Felix Schmiedl. Computational aspects of the Gromov–Hausdorff distance and its application in non-rigid shape matching. *Discrete Comp. Geometry*, 57:854–880, 2017. 2

[55] Isaac Schoenberg. Remarks to Maurice Frechet's article "Sur la definition axiomatique d'une classe d'espace distances vectoriellement applicable sur l'espace de Hilbert. *Annals of Mathematics*, pages 724–732, 1935. 2

[56] Anthony Simeonov, Yilun Du, Andrea Tagliasacchi, Joshua B Tenenbaum, Alberto Rodriguez, Pulkit Agrawal, and Vincent Sitzmann. Neural descriptor fields: SE(3)-equivariant object representations for manipulation. In *ICRA*, pages 6394–6400, 2022. 2

[57] Manfred Sippl and Harold Scheraga. Cayley-Menger coordinates. *PNAS*, 83:2283–2287, 1986. 6, 7, 9

[58] Philip Smith and Vitaliy Kurlin. Families of point sets with identical 1d persistence,. *arxiv:2202.00577*, 2022. 2

[59] Phil Smith and Vitaliy Kurlin. A practical algorithm for degree-k voronoi domains of three-dimensional periodic point sets. In *Lecture Notes in Computer Science (Proceedings of ISVC)*, volume 13599, pages 377–391, 2022. 2

[60] Riccardo Spezialetti, Samuele Salti, and Luigi Di Stefano. Learning an effective equivariant 3d descriptor without supervision. In *ICCV*, pages 6401–6410, 2019. 2

[61] Matthew Toews and William M Wells III. Efficient and robust model-to-image alignment using 3d scale-invariant features. *Medical image analysis*, 17(3):271–282, 2013. 2

[62] Aikaterini Vriza, Ioana Sovago, Daniel Widdowson, Peter Wood, Vitaliy Kurlin, and Matthew Dyer. Molecular set transformer: Attending to the co-crystals in the cambridge structural database. *Digital Discovery*, 1:834–850, 2022. 2

[63] E Weisstein. Triangle. *https://mathworld. wolfram. com*. 1

[64] Carola Wenk. Shape matching in higher dimensions. *PhD thesis, FU Berlin*, 2003. 2

[65] D Widdowson and V Kurlin. Pointwise distance distributions of periodic point sets. *arxiv:2108.04798*, 2021. 2

[66] Daniel Widdowson and Vitaliy Kurlin. Resolving the data ambiguity for periodic crystals. *Advances in Neural Information Processing Systems (NeurIPS)*, 35, 2022. 2

[67] Daniel Widdowson and Vitaliy Kurlin. Recognizing rigid patterns of unlabeled point clouds by complete and continuous isometry invariants with no false negatives and no false positives. In *Proceedings of CVPR*, 2023. 2, 8, 13

[68] Daniel Widdowson, Marco M Mosca, Angeles Pulido, Andrew I Cooper, and Vitaliy Kurlin. Average minimum distances of periodic point sets - foundational invariants for mapping all periodic crystals. *MATCH Comm. in Math. and in Computer Chemistry*, 87:529–559, 2022. 2

[69] N Zava. The Gromov-Hausdorff space isn't coarsely embeddable into any Hilbert space. *arXiv:2303.04730*, 2023. 2

[70] Q Zhu, J Johal, D Widdowson, Z Pang, B Li, C Kane, V Kurlin, G Day, M Little, and A Cooper. Analogy powered by prediction and structural invariants: Computationally-led discovery of a mesoporous hydrogen-bonded organic cage crystal. *J Amer. Chem. Soc.*, 144:9893–9901, 2022. 2

[71] Wen Zhu, Lingchao Chen, Beiping Hou, Weihan Li, Tianliang Chen, and Shixiong Liang. Point cloud registration of arrester based on scale-invariant points feature histogram. *Scientific Reports*, 12(1):1–13, 2022. 2