Computable complete invariants for finite clouds of unlabeled points under Euclidean isometry

Vitaliy Kurlin
Department of Computer Science, University of Liverpool, Liverpool, United Kingdom

Abstract

A finite cloud of unlabeled points is the simplest representation of many real objects such as rigid shapes considered modulo rigid motion or isometry preserving inter-point distances. The distance matrix uniquely determines any finite cloud of labeled (ordered) points under Euclidean isometry but is intractable for comparing clouds of unlabeled points due to a huge number of permutations.

The past work developed approximate algorithms for Hausdorff-like distances minimized over translations, rotations, and general isometries. One big success is the exact algorithm by Paul Chew et al for matching sets in the plane under Euclidean motion with a polynomial complexity of degree five in the number of points. We introduce continuous and complete isometry invariants on the spaces of finite clouds of unlabeled points considered under isometry in any Euclidean space. The continuity under perturbations of points in the bottleneck distance is proved in terms of new metrics that are exactly computable in polynomial time in the number of points for a fixed dimension.

2012 ACM Subject Classification Theory of computation → Computational geometry

Keywords and phrases point cloud, isometry, invariant, classification, metric, continuity

Funding *Vitaliy Kurlin*: EPSRC grant 'Application-driven Topological Data Analysis', EP/R018472/1

1 Motivations, problem statement and overview of new results

A *point cloud* (any finite set of unordered and unlabeled points) in a Euclidean space $\mathbb{R}^n$ is one of the simplest and most fundamental data representations. Since many real-life objects have rigid shapes, the natural equivalence of point clouds is a rigid motion or isometry.

Any isometry of $\mathbb{R}^n$ is a composition of translations, high-dimensional rotations and reflections represented by matrices from the orthogonal group $O(\mathbb{R}^n)$. If reflections are excluded, any orientation-preserving isometry f can be realized by a rigid motion as a continuous family of isometries $f_t : \mathbb{R}^n \to \mathbb{R}^n$, $t \in [0,1]$, where $f_1 = f$ and f_0 is the identity.

Problem 1.1 extends the past efforts in algorithmic detection of isometry between point clouds to a complete classification with a metric that is not only continuous but is also exactly computable in polynomial time. Since any isometry is bijective, a natural metric on isometry classes of point clouds is based on bijections of points as formalized in (1.1d).

▶ **Problem 1.1** (continuous isometry classification of clouds)**.** Find a complete isometry invariant I of finite clouds of unlabeled points in $\mathbb{R}^n$ with a continuous metric d. In detail,

(1.1a) *invariance* : if point clouds $A \cong B$ are *isometric* in $\mathbb{R}^n$ (meaning that $f(A) = B$ for an *isometry* $f : \mathbb{R}^n \to \mathbb{R}^n$ preserving all Euclidean distances $||f(p) - f(q)|| = ||p - q||$ for any points $p, q \in \mathbb{R}^n$), then $I(A) = I(B)$, so the invariant I has *no false negatives*;

(1.1b) *completeness* : if $I(A) = I(B)$, then $A \cong B$ are isometric, so I has *no false positives*;

(1.1c) a *metric* d on invariant values should satisfy all metric axioms below :

(1) *first axiom* : $d(I(A), I(B)) = 0$ if and only if point clouds $A \cong B$ are isometric,

(2) *symmetry* : $d(I(A), I(B)) = d(I(B), I(A))$,

(3) *triangle inequality* : $d(I(A), I(C)) \le d(I(A), I(B)) + d(I(B), I(C))$ for all A, B, C;

(1.1d) *continuity* : for any point cloud $A \subset \mathbb{R}^n$ and $\varepsilon > 0$, there is $\delta > 0$ such that if B is obtained by perturbing every point of A within its δ-neighborhood, then $d(I(A), I(B)) < \varepsilon$.

(1.1e) *computability* : for a fixed dimension n, the invariant $I(A)$ and the metric $d(A, B)$ can be exactly computed in a polynomial time in the number m of points in $A, B \subset \mathbb{R}^n$. ■

A continuous and complete (or injective) invariant I will parameterize the moduli space of all m-point clouds in $\mathbb{R}^n$. In the simplest case of $m = 3$ points, the moduli space of triangles (up to isometry, also called congruence) is parameterized by a triple of unordered edge-lengths [40, section 1.2]. This Euclid's side-side-side theorem from school geometry was extended to plane polygons inscribed into a circle whose moduli space (up to orientation-preserving isometry) is parameterized by a sequence of edge-lengths up to cyclic shifts [39, Chapter 2, Theorem 1.8]. Problem 1.1 remained open for more general cases, see a review in section 2.

Section 3 first introduces the Principal Coordinates Invariant (PCI) to classify generic clouds that allow a unique alignment by principal directions. Section 4 defines a symmetrized metric on PCIs, which is continuous under perturbations in general position and can be computed (for a fixed dimension) faster than in a quadratic time in the number of points.

Section 5 introduces the Weighted Matrices Invariant (WMI) for any point clouds. Section 4 applies the Linear Assignment Cost and Earth Mover's Distance to define metrics on WMIs. For a fixed dimension n, the metric computations need only a polynomial time in the number m of points. For $n = 2$, the time $O(m^{3.5} \log m)$ improves the time $O(m^5 \log m)$ of the *only exact algorithm* [16] for the Hausdorff distance under Euclidean motion. Section 7 discusses the impact on shape recognition in Vision, Graphics, and Materials Science.

2 A review of past work on isometry invariants of finite point sets

The case of labeled point sets in $\mathbb{R}^n$ is easy for isometry classification because the matrix of distances d_{ij} between indexed points p_i, p_j allows us to build a set by using the known distances to the previously constructed points [26, Theorem 9]. For any sets $A, B \subset \mathbb{R}^n$ of the same number m of 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 our points are unlabeled, comparing $m \times m$ matrices requires $m!$ permutations of points, which makes this approach impractical, see the faster order types for labeled points in [12].

Isometry detection refers to a simpler version of Problem 1.1 to algorithmically detect a potential isometry between given sets of m points in $\mathbb{R}^n$. The first solution by Alt et al [2] required $O(m^{n-2} \log m)$ time. The best algorithm by Brass and Knauer [9] takes $O(m^{\lceil n/3 \rceil} \log m)$ time, so $O(m \log m)$ in $\mathbb{R}^3$ [10]. The latest advance is the $O(m \log m)$ algorithm in $\mathbb{R}^4$ [32]. These approaches output a binary answer (yes/no) without quantifying similarity between non-isometric sets by a continuous metric as in Problem 1.1.

The Hausdorff distance [27] 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 further minimize [29, 17, 16, 15] the Hausdorff distance over all isometries f from the full Euclidean group $\mathrm{Iso}(\mathbb{R}^n)$. For $n = 1$, the Hausdorff distance minimized over translations in $\mathbb{R}$ for sets of at most m points can be found in time $O(m \log m)$ [42]. 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. 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 $O(m^{\lceil (n+1)/2 \rceil})$ [49, Chapter 4, Corollary 6]. For more general isometries in higher dimensions $n > 2$, only approximate algorithms [24] tackled minimizations for infinitely many rotations initially in $\mathbb{R}^3$, now extended to any $\mathbb{R}^n$ in [4, Lemma 5.5].

The Gromov-Wasserstein distances can be defined between any metric-measure spaces, not necessarily sitting in a common ambient space. However, even the simplest Gromov-Hausdorff distance cannot be approximated within any factor less than 3 in polynomial time unless P=NP [44, Corollary 3.8]. Polynomial-time algorithms were designed for important partial cases: the exact computation in time $O(m^2)$ for ultrametric spaces [37, Algorithm 1], $\frac{5}{4}$-approximation in time $O(m \log m)$ for sets of at most m points in $\mathbb{R}$ [33, Theorem 3.2].

Diffusion-based signatures are isometry invariant functions for a smooth manifold M [28]. The Heat Kernel Signature $\text{HKS} : \mathbb{R}^+ \times M \to \mathbb{R}$ is a complete isometry invariant of M [47, Theorem 1] when the Laplace-Beltrami operator has distinct eigenvalues. For a manifold sampled by points, the HKS can be discretized and remains continuous [47, section 4] though the completeness of this discretization up to isometry remains unclear. In a similar generic case, Theorem 3.5 will achieve completeness by the Principal Coordinates Invariant (PCI).

Multidimensional scaling (MDS). For a given $m \times m$ distance matrix D of a finite cloud A, the classical MDS [45] finds an embedding $A \subset \mathbb{R}^k$ (if it exists) preserving all distances of M for a minimum dimension $k \le m$. The underlying computation of m eigenvalues the Gram matrix expressed via D needs $O(m^3)$ time. The resulting representation of $A \subset \mathbb{R}^k$ uses orthonormal eigenvectors whose ambiguity up to signs for potential comparisons leads to the time factor 2^k, which can be close to 2^m. The new invariant PCI uses the much smaller $n \times n$ covariance matrix of the cloud A and has the faster time $O(n^2 m + n^3)$ in Lemma 3.6.

Topological Data Analysis studies persistent homology for filtrations of simplicial complexes [20, 13] on a finite point cloud A. If we consider the standard (Vietoris-Rips, Cech, Delaunay) filtrations, then persistent homology is invariant up to isometry of A, not up to more general deformations, and cannot distinguish generic families of inputs [18, 14, 46].

Distance-based invariants. Significant results on matching bounded rigid shapes and registration of finite point sets were obtained in [52, 35, 19]. The total distribution of pairwise distances is complete for point sets in general position [8], though infinitely many counter-examples are known, see the classical counter-example $T \not\cong K$ in Fig. 1 (middle).

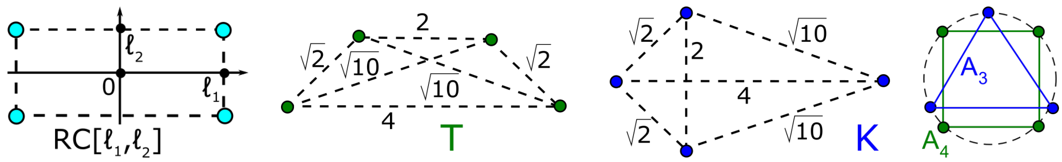

Figure 1 Left: the vertex set $\text{RC}[l_1, l_2]$ of a rectangle. **Middle**: non-isometric sets $T \not\cong K$ of 4 points with the same 6 pairwise distances. **Right**: what is a distance between an equilateral triangle A_3 and a square A_4? See computations of new invariants and metrics in Examples 3.4, 4.5, 6.7.

The stronger *local distributions of distances* [36], also known as *shape distributions* [38, 6, 25, 34, 41, 11] for metric-measure spaces, are similar to the more specialized [50] Pointwise Distance Distributions (PDDs), which can be continuously compared by the Earth Mover's Distance [43], see Fig. 1 (right). Though PDD is conjectured to be complete for discrete point sets in $\mathbb{R}^2$, [50, Fig. 6] provides a counter-example to completeness in $\mathbb{R}^3$. The recent statistical test for isomorphism [11] proposed a faster pseudo-metric based on the distance to measure, but the first metric axiom in Problem (1.1c) remained open.

3 Principal Coordinates Invariant (PCI) is complete in a generic case

We start by recalling the Principal Component Analysis (PCA) whose principal directions [1] are used to build an isometry invariant that is continuous and complete in general position.

▶ **Definition 3.1** (center of mass $\bar{A}$ and radius $\mathrm{rad}(A)$ of a point cloud $A \subset \mathbb{R}^m$)**.** For any cloud $A \subset \mathbb{R}^n$ of m points, the *radius* $\mathrm{rad}(A)$ is the maximum Euclidean distance from any point $p \in A$ to the *center of mass* $\bar{A} = \dfrac{1}{m}\sum\limits_{p\in A} p$. ■

By shifting all m points of a cloud $A \subset \mathbb{R}^n$ by the vector $\bar{A}$ equal to the center of mass $\bar{A} = \dfrac{1}{m}\sum\limits_{p\in A} p$, one can always assume that $\bar{A}$ is the origin 0 of $\mathbb{R}^n$. Then Problem 1.1 reduces to finding continuous invariants of clouds only up to rotations around the origin 0. If we arbitrarily order points $p_1, \dots, p_m$ of a cloud $A \subset \mathbb{R}^n$, we get the sample $n \times m$ matrix (or data table) P, whose i-th column consists of n coordinates of the point $p_i \in A$, $i = 1, \dots, m$.

The *covariance* $n \times n$ matrix $\mathrm{Cov}(A) = \dfrac{PP^T}{n-1}$ is symmetric and positive semi-definite meaning that $v^T \mathrm{Cov}(A) v \geq 0$ for any $v \in \mathbb{R}^n$. Hence $\mathrm{Cov}(A)$ has real *eigenvalues* $\lambda_1 \geq \dots \geq \lambda_n \geq 0$ satisfying $\mathrm{Cov}(A) v_j = \lambda v_j$ for an eigenvector $v_j \in \mathbb{R}^n$, which can be scaled by any real $s \neq 0$. If all eigenvalues are distinct and positive, there is an orthonormal basis of eigenvectors $v_1, \dots, v_n$, which is ordered according to the decreasing eigenvalues $\lambda_1 > \dots > \lambda_n > 0$ and is unique up to reflection $v_j \leftrightarrow -v_j$ of each eigenvector, $j = 1, \dots, n$.

▶ **Definition 3.2** (principally generic cloud)**.** A point cloud $A \subset \mathbb{R}^n$ is called *principally generic* if, after shifting the center of mass $\bar{A}$ to the origin 0, the covariance matrix $\mathrm{Cov}(A)$ has distinct eigenvalues $\lambda_1 > \dots > \lambda_n > 0$. The j-th eigenvalue λ_j defines the j-th *principal direction* parallel to an eigenvector v_j, which is uniquely determined up to scaling. ■

▶ **Definition 3.3** (matrix PCM and invariant PCI)**.** For $n \geq 1$, let $A \subset \mathbb{R}^n$ be a principally generic cloud of points $p_1, \dots, p_m$ with the center of mass at the origin 0. Then A has principal directions along unit length eigenvectors $v_1, \dots, v_n$ well-defined up to a sign.

In the orthonormal basis $V = (v_1, \dots, v_n)^T$, any point $p_i \in A$ has the *principal coordinates* $p_i \cdot v_1, \dots, p_i \cdot v_n$, which can be written as a vertical column $n \times 1$ denoted by Vp_i.

The *Principal Coordinates Matrix* is the $n \times m$ matrix $\mathrm{PCM}(A)$ whose m columns are the *coordinate sequences* $Vp_1, \dots, Vp_m$. Two such matrices are *equivalent* under changing signs of rows due to the ambiguity $v_j \leftrightarrow -v_j$ of unit length eigenvectors in the basis V. The *Principal Coordinates Invariant* $\mathrm{PCI}(A)$ is an equivalence class of matrices $\mathrm{PCM}(A)$. ■

For simplicity, we skip the dependence on a basis V in the notation $\mathrm{PCM}(A)$. The columns of $\mathrm{PCM}(A)$ are unordered, though we can write them according to any order of points in the cloud A considered as the vector $(p_1, \dots, p_m)$. Then $\mathrm{PCM}(A)$ can be viewed as the matrix product VA consisting of m columns $Vp_1, \dots, Vp_m$.

▶ **Example 3.4** (computing PCI)**. (a)** For any $l_1 > l_2 > 0$, let the *rectangular cloud* $\mathrm{RC}[l_1, l_2]$ consist of the four vertices $(\pm l_1, \pm l_2)$ of the rectangle $[-l_1, l_1] \times [-l_2, l_2]$. Then $\mathrm{RC}[l_1, l_2]$ has the center at $0 \in \mathbb{R}^2$ and the sample 2×4 matrix $P = \begin{pmatrix} l_1 & l_1 & -l_1 & -l_1 \\ l_2 & -l_2 & l_2 & -l_2 \end{pmatrix}$. The covariance matrix $\mathrm{Cov}(\mathrm{RC}[l_1, l_2]) = \begin{pmatrix} 4l_1^2 & 0 \\ 0 & 4l_2^2 \end{pmatrix}$ has eigenvalues $\lambda_1 = 4l_1^2 > \lambda_2 = 4l_2^2$. If we choose unit length eigenvectors $v_1 = (1, 0)$ and $v_2 = (0, 1)$, then $\mathrm{PCM}(\mathrm{RC}[l_1, l_2])$ coincides with the sample matrix P above. The invariant $\mathrm{PCI}(\mathrm{RC}[l_1,l_2])$ is the equivalence class of all matrices obtained from P by changing signs of rows and re-ordering columns.

(b) The vertex set T of the trapezium in Fig. 1 consists of four points written in the columns of the sample matrix $P(T) = \begin{pmatrix} 2 & 1 & -1 & -2 \\ -1/2 & 1/2 & 1/2 & -1/2 \end{pmatrix}$ so that the center of mass $\bar{T}$ is the origin 0. Then $\mathrm{Cov}(T) = \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix}$ has eigenvalues 10, 1 with orthonormal eigenvectors $(1,0)$, $(0,1)$, respectively. $\mathrm{PCI}(T)$ is the equivalence class of the matrix $P(T)$ above.

The vertex set K of the kite in Fig. 1 consists of four points written in the columns of the sample matrix $P(K) = \begin{pmatrix} 5/2 & -1/2 & -1/2 & -3/2 \\ 0 & 1 & -1 & 0 \end{pmatrix}$ so that the center of mass $\bar{K}$ is the origin 0. Then $\mathrm{Cov}(K) = \begin{pmatrix} 9 & 0 \\ 0 & 2 \end{pmatrix}$ has eigenvalues 9, 2 with orthonormal eigenvectors $(1,0),(0,1)$, respectively. $\mathrm{PCI}(K)$ is the equivalence class of the matrix $P(K)$ above. ■

▶ **Theorem 3.5** (generic completeness of PCI)**.** Any principally generic clouds $A,B \subset \mathbb{R}^n$ are isometric if and only if the invariants from Definition 3.3 coincide: $\mathrm{PCI}(A) = \mathrm{PCI}(B)$.

▶ **Lemma 3.6** (complexity of PCI)**.** For a principally generic cloud $A \subset \mathbb{R}^n$ of m points, the asymptotic complexity of computing a matrix $\mathrm{PCM}(A)$ from the class $\mathrm{PCI}(A)$ is $O(n^2m+n^3)$.

Proof. The computational complexity of finding principal directions [5] for the symmetric $n \times n$ covariance matrix $\mathrm{Cov}(A)$ is $O(n^3)$. Each of the nm elements of the matrix $\mathrm{PCM}(A)$ is computed in $O(n)$ time. Hence the total time is $O(n^2m + n^3)$. ◀

4 A continuous and computable metric on principally generic clouds

▶ **Definition 4.1** (bottleneck distance W_∞)**.** For any vector $v = (x_1,\dots,x_n) \in \mathbb{R}^n$, the *Minkowski* norm is $||v||_\infty = \max\limits_{i=1,\dots,n} |x_i|$. For clouds $A,B \subset \mathbb{R}^n$ of m points, the *bottleneck distance* $W_\infty(A,B) = \inf\limits_{g:A\to B} \sup\limits_{p\in A} ||p-g(p)||_\infty$ is minimized over all bijections $g : A \to B$. ■

Below we use the bottleneck distance for a matrix interpreted as a point cloud in $\mathbb{R}^n$.

▶ **Definition 4.2** (m-point cloud $[P] \subset \mathbb{R}^n$ of an $n \times m$ matrix P)**.** For any $n \times m$ matrix P, let $[P]$ denote the unordered set of its m columns considered as vectors in $\mathbb{R}^n$. Then the set $[P]$ of m columns can be interpreted as a cloud of m unordered points in $\mathbb{R}^n$. ■

For any $n \times m$ matrices P,Q, let $g : [P] \to [Q]$ be a bijection of columns indexed by $1,2,\dots,m$. Then the Minkowski distance $M_\infty(v,g(v))$ between columns $v \in [P]$ and $g(v) \in [Q]$ is the maximum absolute difference of corresponding coordinates in $\mathbb{R}^n$. The minimization over all column bijections $g : [P] \to [Q]$ gives the bottleneck distance $W_\infty([P],[Q]) = \min\limits_{g:[P]\to[Q]} \max\limits_{v\in[P]} M_\infty(v,g(v))$ between the sets $[P]$, $[Q]$ considered as m-point clouds in $\mathbb{R}^n$.

An algorithm for detecting an isometry $A \cong B$ will check if $\mathrm{SM}(A,B) = 0$ for the metric SM defined via sign symmetrizations. A change of signs in n rows can be represented by a binary string σ in the product group $\mathbb{Z}_2^n$, where $\mathbb{Z}_2 = \{\pm 1\}$, 1 means no change, -1 means a change. For instance, the binary string $\sigma = (1,-1) \in \mathbb{Z}_2^2$ acts on PCI from Example 3.4:

$$\mathrm{PCM}(\mathrm{RC}[l_1,l_2]) = \begin{pmatrix} l_1 & l_1 & -l_1 & -l_1 \\ l_2 & -l_2 & l_2 & -l_2 \end{pmatrix}, \sigma(\mathrm{PCM}(\mathrm{RC}[l_1,l_2])) = \begin{pmatrix} l_1 & l_1 & -l_1 & -l_1 \\ -l_2 & l_2 & -l_2 & l_2 \end{pmatrix}.$$

▶ **Definition 4.3** (symmetrized metric SM on matrices and clouds)**.** For any $n \times m$ matrices P, Q, the minimization over 2^n changes of signs represented by strings $\sigma \in \mathbb{Z}_2^n$ acting on rows gives the *symmetrized metric* $\mathrm{SM}([P],[Q]) = \min\limits_{\sigma \in \mathbb{Z}_2^n} W_\infty([\sigma(P)],[Q])$. For any principally generic clouds $A, B \subset \mathbb{R}^n$ of m points, the *symmetrized metric* is $\mathrm{SM}(A,B) = \mathrm{SM}([\mathrm{PCM}(A)],[\mathrm{PCM}(B)])$ for any matrices $\mathrm{PCM}(A), \mathrm{PCM}(B)$ from Definition 3.3. ■

If we interpret a column permutation g as the result $g(P)$ of the action on a matrix P, then $\max\limits_{v \in [P]} M_\infty(v, g(v))$ is the Minkowski norm (maximum absolute element) of the matrix difference $g(P) - Q$. The bottleneck distance $W_\infty([P],[Q])$ will be computed by an efficient algorithm for bottleneck matching in Theorem 4.6. All skipped proofs are in Appendix A.

▶ **Lemma 4.4** (metric axioms for SM)**. (a)** The symmetrized metric $\mathrm{SM}(P,Q)$ from Definition 4.3 is well-defined on equivalence classes of $n \times m$ matrices P, Q considered up to changes of signs of rows and permutations of columns, and satisfies all metric axioms.

(b) The symmetrized metric $\mathrm{SM}(A,B)$ from Definition 4.3 is well-defined on isometry classes of any principally generic clouds A, B and satisfies all metric axioms in Problem (1.1c). ■

▶ **Example 4.5** (computing SM)**. (a)** By Example 3.4(a), the vertex set $\mathrm{RC}[l_1, l_2]$ of any rectangle with sides $2l_1 > 2l_2$ in the plane has PCI represented by the matrix $\mathrm{PCM}(\mathrm{RC}[l_1,l_2]) = \begin{pmatrix} l_1 & l_1 & -l_1 & -l_1 \\ l_2 & -l_2 & l_2 & -l_2 \end{pmatrix}$. The vertex set $\mathrm{RC}[l_1', l_2']$ of any other rectangle has a similar matrix whose element-wise subtraction from $\mathrm{PCM}(\mathrm{RC}[l_1,l_2])$ consists of $\pm l_1 \pm l_1'$ and $\pm l_2 \pm l_2'$. Re-ordering columns and changing signs of rows minimizes the maximum absolute value of these elements to $\max\{|l_1 - l_1'|, |l_2 - l_2'|\}$, which should equal $\mathrm{SM}(\mathrm{RC}[l_1,l_2], \mathrm{RC}[l_1',l_2'])$.

(b) The invariants PCI of the vertex sets T and K of the quadrilaterals in Fig. 1 were computed in Example 3.4(b) and represented by the following matrices from Definition 3.3:

$$\mathrm{PCM}(T) = \begin{pmatrix} 2 & 1 & -1 & -2 \\ -1/2 & 1/2 & 1/2 & -1/2 \end{pmatrix}, \quad \mathrm{PCM}(K) = \begin{pmatrix} 5/2 & -1/2 & -1/2 & -3/2 \\ 0 & 1 & -1 & 0 \end{pmatrix}.$$

The maximum absolute value of the element-wise difference of the matrices above is $|1 - (-\frac{1}{2})| = \frac{3}{2}$, which cannot be made smaller by permuting columns and changing signs of rows. Hence the symmetrized metric is $\mathrm{SM}(T,K) = W_\infty(\mathrm{PCM}(T), \mathrm{PCM}(K)) = \frac{3}{2}$. ■

▶ **Theorem 4.6** (complexity of the symmetrized metric SM)**. (a)** Given any $n \times m$ matrices P, Q, the symmetrized metric $\mathrm{SM}(P,Q)$ from Definition 4.3 can be computed in time $O(m^{1.5}(\log^n m)2^n)$ with space $O(m \log^{n-2} m)$. If $n = 2$, the time is $O(m^{1.5} \log m)$.

(b) The above conclusions hold for computing $\mathrm{SM}(A,B)$ of any principally generic m-point clouds $A, B \subset \mathbb{R}^n$ represented by $n \times m$ matrices $\mathrm{PCM}(A), \mathrm{PCM}(B)$ from Definition 3.3. ■

Proof of Theorem 4.6. (a) For a fixed binary string $\sigma \in \mathbb{Z}_2^n$, [21, Theorem 6.5] computes the bottleneck distance $W_\infty(\sigma(P), Q)$ between the clouds $[P]$ and $[Q]$ of unlabeled points in time $O(m^{1.5} \log^n m)$ with space $(m \log^{n-2} m)$. If $n = 2$, the time is $O(m^{1.5} \log m)$ by [21, Theorem 5.10]. The minimization for all $\sigma \in \mathbb{Z}_2^n$ brings the extra factor 2^n in the time.

(b) It follows from part **(a)** for the matrices $P = \mathrm{PCM}(A)$ and $Q = \mathrm{PCM}(B)$. ◀

▶ **Theorem 4.7** (continuity of SM)**.** For any principally generic cloud $A \subset \mathbb{R}^n$ of m points and any $\varepsilon > 0$, there is $\delta > 0$ (depending on A and ε) such that if a principally generic cloud $B \subset \mathbb{R}^n$ of m points has a small bottleneck distance $W_\infty(A,B) < \delta$, then $\mathrm{SM}(A,B) < \varepsilon$. ■

5 The Weighted Matrices Invariant (WMI) is complete for all clouds

If a cloud $A \subset \mathbb{R}^n$ is not principally generic, some of the eigenvalues $\lambda_1 \geq \dots \geq \lambda_n \geq 0$ of the covariance matrix $\mathrm{Cov}(A)$ coincide or vanish. Let us start with the most singular case when all eigenvalues are equal to $\lambda > 0$. The case $\lambda = 0$ means that A is a single point.

▶ **Definition 5.1** (Weighted Matrices Invariant for $A \subset \mathbb{R}^2$)**.** Let a cloud A of m points $p_1, \dots, p_m$ in $\mathbb{R}^2$ have the center of mass at the origin 0. For any point $p_i \in A - \{0\}$, let v_1 be the unit length vector parallel to $p_i \neq 0$. Let v_2 be the unit length vector orthogonal to v_1 whose anti-clockwise angle from v_1 to v_2 is $+\frac{\pi}{2}$. The $2 \times m$ matrix $M(p_i)$ consists of the m pairs of coordinates of all points $p \in A$ written in the orthonormal basis v_1, v_2, for example, $p_i = \begin{pmatrix} ||p_i||_2 \\ 0 \end{pmatrix}$. Each matrix $M(p_i)$ is considered up to re-ordering of columns. If one point p of A is the origin 0, there is no basis defined by $p = 0$, let $M(p)$ be the zero matrix in this centered case. If $k > 1$ of the matrices $M(p_i)$ are *equivalent* up to re-ordering of columns, we collapse them into one matrix with the weight $\frac{k}{m}$. The unordered collection of equivalence classes of $M(p)$ with weights for all $p \in A$ is the *Weighted Matrices Invariant* $\mathrm{WMI}(A)$. ■

In comparison with the generic case in Definition 3.3, for any fixed $i = 1, \dots, m$, if $p_i \neq 0$, then the orthonormal basis v_1, v_2 is uniquely defined without the ambiguity of signs, which will re-emerge for higher dimensions $n > 2$ in Definition 5.3 later.

▶ **Example 5.2** (regular clouds $A_m \subset \mathbb{R}^2$)**.** Let A_m be the vertex set of a regular m-sided polygon inscribed into a circle of a radius r. Due to the m-fold rotational symmetry of A_m, the invariant $\mathrm{WMI}(A_m)$ consists of a single matrix (with weight 1) whose columns are the vectors $\begin{pmatrix} r\cos\frac{2\pi i}{m} \\ r\sin\frac{2\pi i}{m} \end{pmatrix}$, $i = 1, \dots, m$. For instance, the vertex set A_3 of the equilateral triangle has $\mathrm{WMI}(A_3) = \left\{ \begin{pmatrix} r & -r/2 & -r/2 \\ 0 & r\sqrt{3}/2 & -r\sqrt{3}/2 \end{pmatrix} \right\}$. The vertex set A_4 of the square has $\mathrm{WMI}(A_4) = \left\{ \begin{pmatrix} r & 0 & 0 & -r \\ 0 & r & -r & 0 \end{pmatrix} \right\}$. Let B_m be obtained from A_m by adding the origin $0 \in \mathbb{R}^2$. Then $\mathrm{WMI}(B_m)$ has the matrix from $\mathrm{WMI}(A_m)$ with the weight $\frac{m}{m+1}$ and the zero 2×4 matrix with the weight $\frac{1}{m+1}$ representing the added point at the origin 0. ■

Definition 5.3 below applies to all clouds $A \subset \mathbb{R}^n$ including the most singular case when all eigenvalues of $\mathrm{Cov}(A)$ are equal, so we have no preferred directions at all.

▶ **Definition 5.3** (Weighted Matrices Invariant $\mathrm{WMI}(A)$ for any cloud $A \subset \mathbb{R}^n$)**.** Let a cloud $A \subset \mathbb{R}^n$ of m points $p_1, \dots, p_m$ have the center of mass at the origin 0. For any ordered sequence of points $p_1, \dots, p_{n-1} \in A$, build an orthonormal basis $v_1, \dots, v_n$ as follows.

The first unit length vector v_1 is p_1 normalized by its length. For $j = 2, \dots, n-1$, the unit length vector v_j is $p_j - \sum\limits_{k=1}^{j-1} (p_j \cdot v_k) v_k$ normalized by its length. Then every v_j is orthogonal to all previous vectors $v_1, \dots, v_{j-1}$ and belongs to the j-dimensional subspace spanned by $p_1, \dots, p_j$. Define the last unit length vector v_n by its orthogonality to $v_1, \dots, v_{n-1}$ and the positive sign of the determinant $\det(v_1, \dots, v_n)$ of the matrix with the columns $v_1, \dots, v_n$.

The $n \times m$ matrix $M(p_1, \dots, p_{n-1})$ consists of column vectors of all points $p \in A$ in the basis $v_1, \dots, v_n$, for example, $p_1 = (||p_1||_2, 0, \dots, 0)^T$. If the points $p_1, \dots, p_{n-1} \in A$ are affinely dependent, let $M(p_1, \dots, p_{n-1})$ be the $n \times m$ matrix of zeros in this centered case.

If $k > 1$ of all these matrices are *equivalent* up to re-ordering of columns, we collapse them into a single matrix with the weight $\dfrac{k}{N}$, where $N = m(m-1)\dots(m-n+1)$.

The *Weighted Matrices Invariant* $\mathrm{WMI}(A)$ is the unordered set of equivalence classes of matrices $M(p_1,\dots,p_{n-1})$ with weights for all sequences of points $p_1,\dots,p_{n-1} \in A$. ■

If $\mathrm{Cov}(A)$ has unequal eigenvalues, $\mathrm{WMI}(A)$ can be made smaller by choosing bases depending on points of A only for subspaces of eigenvectors that have the same eigenvalue.

▶ **Theorem 5.4** (completeness of WMI for all clouds)**.** Any clouds $A, B \subset \mathbb{R}^n$ are related by orientation-preserving isometry if and only if one of the equivalent conditions below holds:

(a) there is a bijection $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$ of these unordered sets preserving all weights;

(b) there are matrices $P \in \mathrm{WMI}(A)$ and $Q \in \mathrm{WMI}(B)$ related by re-ordering of columns.

So $\mathrm{WMI}(A)$ is a complete invariant of a cloud A up to orientation-preserving isometry or rigid motion, which is a composition of translations and rotations from the group $\mathrm{SO}(\mathbb{R}^n)$.

(c) Any mirror reflection $f : A \to B$ induces a bijection of matrices $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$ respecting their weights and changing the sign of the last row in every matrix. This pair $\mathrm{WMI}(A), \mathrm{WMI}(B)$ is a complete invariant of A up to isometry including reflections. ■

In practice, one can keep in memory only one matrix $M(p_1,\dots,p_{n-1})$ from $\mathrm{WMI}(A)$. Any such matrix suffices to reconstruct a point cloud A up to orientation-preserving isometry of $\mathbb{R}^n$ by Theorem 3.5. The full $\mathrm{WMI}(A)$ can be computed from the reconstructed $A \subset \mathbb{R}^n$.

▶ **Lemma 5.5** (complexity of WMI)**.** For any cloud $A \subset \mathbb{R}^n$ of m points and any sequence $p_1,\dots,p_{n-1} \in A$, the matrix $M(p_1,\dots,p_{n-1})$ from Definition 5.3 can be computed in time $O(nm+n^3)$. All $N = m(m-1)\dots(m-n+1) = O(m^{n-1})$ matrices in the Weighted Matrices Invariant $\mathrm{WMI}(A)$ can be computed in time $O((nm+n^3)N) = O(nm^n + n^3m^{n-1})$. ■

Proof. For a fixed sequence $p_1,\dots,p_{n-1} \in A$, the vectors $v_1,\dots,v_{n-1}$ are computed by the formulae in Definition 5.3 in time $O(n^2)$. The last vector v_n might need the $O(n^3)$ computation of the determinant $\det(v_1,\dots,v_n)$. Every point $p \in A$ can be re-written in this basis as $p = \sum\limits_{j=1}^{n}(p \cdot v_j)v_j$ in time $O(n)$. Hence the matrix $M(p_1,\dots,p_{n-1})$ is computed in time $O(nm+n^3)$. Since there are $N = m(m-1)\dots(m-n+1)$ ordered sequences of points $p_1,\dots,p_{n-1} \in A$, all matrices in $\mathrm{WMI}(A)$ are computed in time $O((nm+n^3)N)$. ◀

6 Exactly computable metrics for isometry classes of all point clouds

Since any isometry $f : A \to B$ induces a bijection $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$, we will use a linear assignment cost [30] based on permutations within a Weighted Matrices Invariant.

▶ **Definition 6.1** (linear assignment cost)**.** Recall that Definition 4.3 introduced the bottleneck distance W_∞ on matrices considered up to re-ordering of columns. For any clouds $A, B \subset \mathbb{R}^n$ of m points, consider the *Linear Assignment Cost* $\mathrm{LAC}(A,B) = \min\limits_{g} \sum\limits_{P \in \mathrm{WMI}(A)} W_\infty(P, g(P))$ minimized [30] over all bijections $g : \mathrm{WMI}(A) \to \mathrm{WMI}(B)$ of full Weighted Matrices Invariants consisting of all $N = m(m-1)\dots(m-n+1)$ equivalence classes of matrices. ■

▶ **Lemma 6.2** (LAC metric on clouds)**.** **(a)** The Linear Assignment Cost $\mathrm{LAC}(A,B)$ from Definition 6.1 satisfies all metric axioms on clouds up to orientation-preserving isometry.

(b) Let A' denote any mirror image of A. Then $\min\{\mathrm{LAC}(A,B), \mathrm{LAC}(A',B)\}$ is a metric on classes of point clouds A, B up to general isometry including reflections. ■

Proof. **(a)** The only non-trivial first axiom follows from Theorem 5.4 and the first axiom of the bottleneck distance W_∞: any point clouds A, B are isometric if and only if there is a bijection $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$ matching all matrices up to a permutation of columns.

(b) All axioms for the minimum follow from the corresponding axioms for $\mathrm{LAC}(A, B)$. ◀

▶ **Theorem 6.3** (complexity of LAC on WMI)**.** For any clouds $A, B \subset \mathbb{R}^n$ of m points, the invariants $\mathrm{WMI}(A), \mathrm{WMI}(B)$ have a maximum size $N = m(m-1)\dots(m-n+1) = O(m^{n-1})$. Then the metric $\mathrm{LAC}(A, B)$ from Definition 6.1 can be computed in time $O(m^{1.5}(\log^n m)N^2 + N^3) = O(m^{2n-0.5}\log^n m + m^{3n-3})$. If $n = 2$, the time is $O(m^{3.5}\log m)$. ■

Proof. By [21, Theorem 6.5], for any matrices $P \in \mathrm{WMI}(A)$ and $Q \in \mathrm{WMI}(B)$, the bottleneck distance $W_\infty([P],[Q])$ can be computed in time $O(m^{1.5}\log^n m)$. For $N \times N$ pairs of such matrices, computing all costs $c(P, Q) = W_\infty([P],[Q])$ takes $O(m^{1.5}(\log^n m)N^2)$ time. If $n = 2$, [21, Theorem 5.10] reduces the time of all costs $W_\infty([P],[Q])$ to $O(m^{1.5}(\log m)N^2)$. Finally, with all N^2 costs $c(P, Q)$ ready, the algorithm by Jonker and Volgenant [30] computes the Linear Assignment Cost $\mathrm{LAC}(A, B)$ in the extra time $O(N^3)$. ◀

The worst-case estimate $N = O(m^{n-1})$ of the size (number of matrices in) $\mathrm{WMI}(A)$ is very conservative. If the covariance matrix $\mathrm{Cov}(A)$ has equal eigenvalues, then $\mathrm{WMI}(A)$ is often smaller due to extra symmetries of A. However, for the dimension $n = 2$, even the rough estimate of the LAC time $O(m^{3.5}\log m)$ improves the time $O(m^5\log m)$ for computing the exact Hausdorff distance between m-point clouds under Euclidean motion in $\mathbb{R}^2$.

Because of inevitable noise including erroneous points, it is practically important to continuously quantify the similarity between close clouds consisting of different numbers of points. The weights of matrices allow us to match them more flexibly via the Earth Mover's Distance [43] than via strict bijections $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$ in Definition 6.1.

The Weighted Matrices Invariant $\mathrm{WMI}(A)$ can be considered as a finite distribution $C = \{C_1, \dots, C_k\}$ of matrices (equivalent up to re-ordering columns) with weights.

▶ **Definition 6.4** (Earth Mover's Distance on weighted distributions)**.** Let $C = \{C_1, \dots, C_k\}$ be a finite unordered set of objects with weights $w(C_i)$, $i = 1, \dots, k$. Consider another set $D = \{D_1, \dots, D_l\}$ with weights $w(D_j)$, $j = 1, \dots, l$. Assume that a distance between any objects C_i, D_j is measured by a metric $d(C_i, D_j)$. A *flow* from C to D is a $k \times l$ matrix whose entry $f_{ij} \in [0, 1]$ represents a partial *flow* from an object C_i to D_j. The *Earth Mover's Distance* is the minimum *cost* $\mathrm{EMD}(C, D) = \sum\limits_{i=1}^{k}\sum\limits_{j=1}^{l} f_{ij} d(C_i, D_j)$ over $f_{ij} \in [0, 1]$ subject to $\sum\limits_{j=1}^{l} f_{ij} \le w(C_i)$ for $i = 1, \dots, k$, $\sum\limits_{i=1}^{k} f_{ij} \le w(D_j)$ for $j = 1, \dots, l$, and $\sum\limits_{i=1}^{k}\sum\limits_{j=1}^{l} f_{ij} = 1$. ■

The first condition $\sum\limits_{j=1}^{l} f_{ij} \le w(C_i)$ means that not more than the weight $w(C_i)$ of the object C_i 'flows' into all objects D_j via the flows f_{ij}, $j = 1, \dots, l$. Similarly, the second condition $\sum\limits_{i=1}^{k} f_{ij} \le w(D_j)$ means that all flows f_{ij} from C_i for $i = 1, \dots, k$ 'flow' into 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 to 'flow' all C_i to all D_j.

The EMD is a partial case of more general Wasserstein metrics [48] in transportation theory [31]. In the case of finite weighted distributions as in Definition 6.4, the metric axioms for EMD were proved in [43, appendix]. Also, EMD can compare any weighted distributions of different sizes. Hence, instead of the bottleneck distance W_∞ on columns on PCM matrices, one can consider EMD on the distributions of columns (with equal weights) in PCMs.

▶ **Lemma 6.5** (complexity of EMD on distributions of columns)**.** Any matrix P of a size $n \times m(P)$ can be considered as a distribution of $m(P)$ columns with equal weights $\frac{1}{m(P)}$. For two such matrices P, Q having the same number n of rows but potentially different numbers $m(P), m(Q)$ of columns, measure the distance between any columns by the Minkowski metric M_∞ in $\mathbb{R}^n$. For the matrices P, Q considered as weighted distributions of columns, $\text{EMD}(P, Q)$ can be computed in time $O(m^3 \log m)$, where $m = \max\{m(P), m(Q)\}$. ■

Proof. For weighted distributions of sizes at most m, EMD needs $O(m^3 \log m)$ time [23]. ◀

▶ **Theorem 6.6** (complexity of EMD on clouds)**.** Let clouds $A, B \subset \mathbb{R}^n$ of up to m points have pre-computed invariants $\text{WMI}(A), \text{WMI}(B)$ of sizes at most $N \leq m(m-1)\dots(m-n+1) = O(m^{n-1})$. Measure the distance between any matrices $P \in \text{WMI}(A)$ and $Q \in \text{WMI}(B)$ as $\text{EMD}(P, Q)$ from Lemma 6.5. Then $\text{EMD}(\text{WMI}(A), \text{WMI}(B))$ from Definition 6.4 can be computed in time $O(m^3(\log m)N^2 + N^3 \log N) = O((m^{2n+1} + nm^{3n-3}) \log m)$. ■

Proof. By Lemma 6.5, the metric $\text{EMD}(P, Q)$ can be computed in time $O(m^3 \log m)$. For $N \times N$ pairs of such matrices, computing all costs $c(P, Q) = \text{EMD}(P, Q)$ takes $O(m^3(\log m)N^2)$ time. The algorithm from [23] computes $\text{EMD}(A, B)$ in the extra time $O(N^3 \log N)$. ◀

▶ **Example 6.7** (EMD for a square and equilateral triangle)**.** Let A_4 and A_3 be the vertex sets of a square and equilateral triangle inscribed into the same circle of a radius r in Example 5.2. $\text{PCM}(A_3) = \begin{pmatrix} r & -r/2 & -r/2 \\ 0 & r\sqrt{3}/2 & -r\sqrt{3}/2 \end{pmatrix}$ and $\text{PCM}(A_4) = \begin{pmatrix} r & 0 & 0 & -r \\ 0 & r & -r & 0 \end{pmatrix}$. Notice that switching the signs of the 2nd row keeps the PCI matrices the same up to permutation of columns. The weights of the three columns in $\text{PCM}(A_3)$ are $\frac{1}{3}$. The weights of the four columns in $\text{PCM}(A_4)$ are $\frac{1}{4}$. The EMD optimally matches the identical first columns of $\text{PCM}(A_3)$ and $\text{PCM}(A_4)$ with weight $\frac{1}{4}$ contributing the cost 0. The remaining weight $\frac{1}{3} - \frac{1}{4} = \frac{1}{12}$ of the first column $\begin{pmatrix} r \\ 0 \end{pmatrix}$ in $\text{PCM}(A_3)$ can be equally distributed between the closest (in the M_∞ distance) columns $\begin{pmatrix} 0 \\ \pm r \end{pmatrix}$ contributing the cost $\frac{r}{12}$. The column $\begin{pmatrix} -r \\ 0 \end{pmatrix}$ in $\text{PCM}(A_4)$ has equal distances $M_\infty = \frac{r}{2}$ to the last columns $\begin{pmatrix} -r/2 \\ \pm r\sqrt{3}/2 \end{pmatrix}$ in $\text{PCM}(A_3)$ contributing the cost $\frac{r}{8}$. Finally, the distance $M_\infty = \frac{r}{2}$ between the columns $\begin{pmatrix} 0 \\ \pm r \end{pmatrix}$ and $\begin{pmatrix} -r/2 \\ \pm r\sqrt{3}/2 \end{pmatrix}$ with the common signs is counted with the weight $\frac{5}{24}$ and contributes the cost $\frac{5r}{48}$. The final optimal flow (f_{jk}) matrix $\begin{pmatrix} 1/4 & 1/24 & 1/24 & 0 \\ 0 & 5/24 & 0 & 1/8 \\ 0 & 0 & 5/24 & 1/8 \end{pmatrix}$ gives $\text{EMD}(\text{PCM}(A_3), \text{PCM}(A_4)) = \frac{r}{12} + \frac{r}{8} + \frac{5r}{48} = \frac{5r}{16}$. ■

7 Discussion: conclusions and impact on rigid shape recognition

Problem 1.1 was stated in the hard settings for clouds of unlabeled points in any $\mathbb{R}^n$ because real rigid shapes are much easier given by unlabeled points through scans or salient point detection. Indeed, point labeling often involves manual work and unavoidable bias.

The Principal Coordinates Invariant (PCI) should suffice for object retrieval [43, 47] and other applications in Vision and Graphics due to inevitable noise in measurements, which makes real data generic. Then, for a fixed dimension n, Theorem 4.6 computes the symmetrized metric SM on PCIs faster than in a quadratic time in the number m of points.

The key insight was the realization that Principal Component Analysis (PCA) belongs not only to classical statistics but also provides easily compitables invariants of point clouds under isometry. Though sensitivity of PCA under perturbations was studied for many years, Theorem 4.7 required more work and recent advances to guarantee the continuity of PCI.

The Weighted Matrices Invariant (WMI) completely parameterizes the moduli space of m-point clouds under isometry. The complete classification in Theorem 5.4 goes far beyond the state-of-the-art parameterizations, which are available for moduli spaces of point clouds only in dimension 2 [39]. For proteins and other molecules in $\mathbb{R}^3$, the moduli space was described only under continuous deformations not respecting distances [40]. Any real molecule remains well-defined as long as inter-atomic bonds keep the molecule connected. Hence certain inter-atomic distances should be preserved, at least within short ranges.

This paper focused on foundations. Experiments will appear in a future paper. The exactly computable metric on WMIs will be adapted to the complete isometry invariants of periodic crystals [3] based on local neighborhoods of atoms. The earlier invariants [51, 50] detected geometric duplicates, which had wrong atomic types but were deposited in the well-curated (mostly by experienced eyes) largest database of crystals. The new metrics on molecules and crystals will stop paper mills producing such fakes on the industrial scale [7].

Another forthcoming work will prove the continuity of WMIs under perturbations of point clouds whose subsets are linearly independent. In comparison with equal eigenvalues for symmetric clouds, the linear independence is much easier to satisfy by removing points whose positions are uniquely determined by their neighbors. Indeed, any point inside a simplex is reconstructed from its barycentric coordinates relative to the vertices of this simplex.

We thank all reviewers in advance for their valuable time and helpful suggestions.

A Detailed proofs of all auxiliary results

Proof of Theorem 3.5. Any isometry $f:\mathbb{R}^n\to\mathbb{R}^n$ is a linear map, which sends the center of mass $\bar A$ to the center of mass $\bar B$. Hence one can assume that both centers of mass coincide with the origin $0\in\mathbb{R}^n$, which is preserved by f. Any isometry f preserving the origin can be represented by an orthogonal matrix $O_f\in \mathrm{O}(\mathbb{R}^n)$. In a fixed orthonormal basis of $\mathbb{R}^n$, let P_A be the sample matrix of the point cloud A. In the same basis, the point cloud B has the sample matrix $P_B=O_fP_A$ and the covariance matrix $\mathrm{Cov}(B)=\dfrac{P_BP_B^T}{n-1}=\dfrac{O_f(P_AP_A^T)O_f^T}{n-1}$. Any orthogonal matrix $O_f\in \mathrm{O}(\mathbb{R}^n)$ has the transpose $O_f^T=O_f^{-1}$. Then $\mathrm{Cov}(B)$ is conjugated to $\mathrm{Cov}(A)=\dfrac{P_AP_A^T}{n-1}$ and has the same eigenvalues as $\mathrm{Cov}(A)$, while eigenvectors are related by O_f realizing the change of basis. If we fix an orthonormal basis of eigenvectors $v_1,\dots,v_m$ for A, any point $p\in A$ and its image $f(p)\in B$ have the same coordinates in the bases $v_1,\dots,v_m$ and $f(v_1),\dots,f(v_m)$, respectively. Hence $\mathrm{PCM}(A),\mathrm{PCM}(B)$ are related by re-ordering of columns (equivalently, points of A,B) and by changing signs of rows (equivalently, signs of unit length eigenvectors). So the equivalence classes coincide: $\mathrm{PCI}(A)=\mathrm{PCI}(B)$.

Conversely, any $n \times m$ matrix PCM(A) from the class PCI(A) contains the coordinates $p_i \cdot v_j$ of points $p_1, \dots, p_m \in A$ in an orthonormal basis $v_1, \dots, v_n$. Hence all points $p_1, \dots, p_m$ are uniquely determined up to a choice of an orthonormal basis or up to isometry of $\mathbb{R}^n$. ◀

Proof of Lemma 4.4. **(a)** The first axiom follows from Definition 4.3: $\text{SM}([P],[Q]) = 0$ means that there is a binary string $\sigma \in \mathbb{Z}_2^n$ changing signs of rows such that $W_\infty([\sigma(P)],[Q]) = 0$. By the first axiom for W_∞, the point clouds $[\sigma(P)],[Q] \subset \mathbb{R}^n$ should coincide, hence $[Q]$ is obtained from $[P]$ by a compositions of reflections in the axes x_i with $\sigma_i = -1$.

The symmetry $\text{SM}([P],[Q]) = \min\limits_{\sigma \in \mathbb{Z}_2^n} W_\infty([\sigma(P)],[Q]) = \min\limits_{\sigma^{-1} \in \mathbb{Z}_2^n} W_\infty([P],[\sigma^{-1}(Q)]) = \text{SM}([Q],[P])$ follows due to inversibility of $\sigma \in \mathbb{Z}_2^n$ and the symmetry of W_∞.

To prove the triangle inequality $\text{SM}(P,M) + \text{SM}(Q,M) \geq \text{SM}(P,Q)$, let binary strings $\sigma_P, \sigma_Q \in \mathbb{Z}_2^n$ be optimal for the distances $\text{SM}(P,M)$ and $\text{SM}(Q,M)$, respectively, in Definition 4.3. The triangle inequality for the bottleneck distance W_∞ implies that

$$\text{SM}(P,M) + \text{SM}(Q,M) = W_\infty([\sigma_P(P)],[M]) + W_\infty([\sigma_Q(Q)],[M]) \geq W_\infty([\sigma_P(P)],[\sigma_Q(Q)]).$$

Since applying the same change σ_Q^{-1} of signs in both matrices $\sigma_P(P)$ and $\sigma_Q(Q)$ does not affect the minimization for all changes of signs, the final expression equals $W_\infty([\sigma_Q^{-1} \circ \sigma_P(P)],[Q])$, which has the lower bound $\text{SM}(P,Q) = \min\limits_{\sigma \in \mathbb{Z}_2^n} W_\infty([\sigma(P)],[Q])$ due to the minimization over all binary strings $\sigma \in \mathbb{Z}_2^n$ replacing one coordinate-wise product $\sigma_Q^{-1} \circ \sigma_P$ in $\mathbb{Z}_2^n$.

(b) The first axiom follows from Theorem 3.5: $A \cong B$ are isometric if and only if $\text{PCI}(A) = \text{PCI}(B)$ meaning that any matrices PCM(A), PCM(B) representing the equivalence classes PCI(A), PCI(B), respectively, become identical after a column permutation $g : [\text{PCM}(A)] \to [\text{PCM}(B)]$ and the change of signs of rows by a binary string $\sigma \in \mathbb{Z}_2^n$. Indeed, $M_\infty(v, g(v)) = 0$ for all columns v in the matrix $\sigma(\text{PCM}(A))$ means that the matrices $\sigma(\text{PCM}(A))$ and PCM(B) become identical after the column permutation g. The symmetry and triangle axioms for $\text{SM}(A,B)$ follow from part **(a)** for the matrices $P = \text{PCM}(A)$ and $Q = \text{PCM}(B)$. ◀

Lemmas A.1 and A.2 will help prove the continuity of SM in Theorem 4.7. Recall that any $n \times n$ matrix E has the *2-norm* $||E||_2 = \sup\limits_{||v||_2 = 1} ||Ev||_2$ and $||E||_\infty = \max\limits_{j=1,\dots,n} \sum\limits_{k=1}^{n} |E_{jk}|$. If the center of mass $\bar{A}$ is the origin, rad(A) is an upper bound for any coordinate of $p \in A$.

▶ **Lemma A.1** (upper bounds for matrix norms). Let $A, B \subset \mathbb{R}^n$ be principally generic clouds of n points with covariance matrices Cov(A), Cov(B). Then $||\text{Cov}(A) - \text{Cov}(B)||_2 \leq n\sqrt{n}w$ and $||\text{Cov}(A) - \text{Cov}(B)||_\infty \leq nw$, where $w = mW_\infty(A,B)(\text{rad}(A) + \text{rad}(B))$. ■

Proof of Lemma A.1. Assume that A, B have centers of mass at the origin 0. Let $\beta : A \to B$ be a bijection minimizing the bottleneck distance $W_\infty(A,B)$. Let A consist of m points $p_1, \dots, p_m$. Set $\tilde{p}_i = \beta(p_i)$ for $i = 1, \dots, m$. Let $x_j(p)$ denote the j-th coordinate of a point $p \in \mathbb{R}^n$, $j = 1, \dots, n$. Then $\text{Cov}(A)_{jk} = \sum\limits_{i=1}^{m} x_j(p_i)x_k(p_i)$ and $\text{Cov}(B)_{jk} = \sum\limits_{i=1}^{m} x_j(\tilde{p}_i)x_k(\tilde{p}_i)$.

Since the Minkowski distance $M_\infty(p_i, \tilde{p}_i) \leq W_\infty(A,B)$, the upper bounds $|x_j(p_i) - x_j(\tilde{p}_i)| \leq W_\infty(A,B)$ hold for all $i = 1, \dots, m$ and $j = 1, \dots, n$, and will be used below to estimate each element of the difference matrix $E = \text{Cov}(A) - \text{Cov}(B)$ as follows: $|E_{jk}| \leq$

$$\sum_{i=1}^{m} |x_j(p_i)x_k(p_i) - x_j(\tilde{p}_i)x_k(\tilde{p}_i)| = \sum_{i=1}^{m} \Big| x_j(p_i)\big(x_k(p_i) - x_k(\tilde{p}_i)\big) + x_k(\tilde{p}_i)\big(x_j(p_i) - x_j(\tilde{p}_i)\big) \Big| \leq$$

$$\leq \sum_{i=1}^{m} \Big(|x_j(p_i)| \cdot \big|x_k(p_i) - x_k(\tilde{p}_i)\big| + |x_k(\tilde{p}_i)| \cdot \big|(x_j(p_i) - x_j(\tilde{p}_i)\big| \Big)$$

$$\leq W_\infty(A,B) \sum_{i=1}^{m} \Big(|x_j(p_i)| + |x_k(\tilde{p}_i)| \Big) \leq mW_\infty(A,B)(\text{rad}(A)+\text{rad}(B)) = w \text{ (upper bound).}$$

Let $E_1,\dots,E_n \in \mathbb{R}^n$ be the rows of the $n\times n$ matrix $E = \text{Cov}(A) - \text{Cov}(B)$. Then

$$||E||_2 = \sup_{||v||_2=1} ||Ev||_2 \leq \sup_{||v||_2=1} || \sqrt{\sum_{j=1}^{m} (E_j \cdot v)^2} \leq \sum_{j=1}^{n} ||E_j||_2 \leq m\sqrt{m \max_{k=1,\dots,n} E_{jk}^2} \leq n\sqrt{n}u,$$

and $||E||_\infty = \max_{j=1,\dots,n} \sum_{k=1}^{n} |E_{jk}| \leq nw$ as required. ◀

The following recent result is quoted in a slightly simplified form for the PCA case.

▶ **Lemma A.2** (eigenvector perturbation [22, Theorem 3]). Let C be a symmetric $n\times n$ matrix whose eigenvalues $\lambda_1 > \dots > \lambda_n > 0$ have a minimum $\text{gap}(C) = \min_{j=1,\dots,n} \lambda_j - \lambda_{j+1} > 0$, where $\lambda_{n+1} = 0$. Let $v_i, \tilde{v}_i$ be unit length eigenvectors of C and its symmetric perturbation $\tilde{C}$ such that $E = C - \tilde{C}$ has the 2-norm $||E||_2 < \text{gap}(C)/2$. Then $\max_{j=1,\dots,n} ||v_j - \tilde{v}_j||_2 = O\left(\frac{n^{3.5}\mu^2||E||_\infty + n\sqrt{\mu}||E||_2}{\text{gap}(C)}\right)$, where the *incoherence* μ is the maximum sum of squared j-th coordinates of $v_1,\dots,v_n$ for $j = 1,\dots,n$, which has the rough upper bound n. ■

Proof of Theorem 4.7. Let $g : A \to B$ be a bijection minimizing the distance $W_\infty(A,B)$ so that the Minkowski distance between $p \in A, g(p) \in B$ is $M_\infty(p, g(p)) \leq W_\infty(A,B)$.

By Lemma A.1 the difference of covariance matrices $E = \text{Cov}(A) - \text{Cov}(B)$ has matrix norms bounded in terms of $w = mW_\infty(A,B)(\text{rad}(A)+\text{rad}(B))$. By Lemma A.2 the maximum difference of eigenvectors of $C = \text{Cov}(A)$ and $\text{Cov}(B)$ has the maximum Euclidean norm

$$\max_{j=1,\dots,n} ||v_j - \tilde{v}_j||_2 \leq U(A,B) := O\left(\frac{n^{6.5}}{\text{gap}(C)}\right) nW_\infty(A,B)\big(\text{rad}(A) + \text{rad}(B)\big).$$

The bijection $g : A \to B$ induces a bijection between the columns of $\text{PCM}(A), \text{PCM}(B)$ so that the column of every point $p_i \in A$ maps to the column of $\tilde{p}_i = g(p_i) \in B$. We can permute the columns of $\text{PCM}(B)$ so that the columns of $p_i, \tilde{p}_i$ have the same index i. Let $v_1,\dots,v_n$ and $\tilde{v}_1,\dots,\tilde{v}_n$ be unit length eigenvectors of $\text{Cov}(A), \text{Cov}(B)$, respectively.

Estimate the difference of j-th elements in the i-th columns of $\text{PCM}(A), \text{PCM}(B)$.

$$|p_i \cdot v_j - \tilde{p}_i \cdot \tilde{v}_j| = |(p_i - \tilde{p}_i)\cdot v_j + \tilde{p}_i \cdot (v_j - \tilde{v}_j)| \leq ||p_i - \tilde{p}_i||_2 ||v_j||_2 + ||\tilde{p}_i||_2 ||v_j - \tilde{v}_j||_2 \leq$$

$$\leq ||p_i - \tilde{p}_i||_2 + \text{rad}(B)U(A,B) \leq W_\infty(A,B)\left(1 + \text{rad}(B) O\Big(\frac{m^{6.5}}{\text{gap}(C)}\Big) n\big(\text{rad}(A) + \text{rad}(B)\big)\right).$$

For any $\varepsilon > 0$, one can choose a small $\delta > 0$ (depending on A, B) such that $W_\infty(A,B) < \delta$ guarantees that $|p_i \cdot v_j - \tilde{p}_i \cdot \tilde{v}_j| < \varepsilon$ for any $i = 1,\dots,m$ and $j = 1,\dots,n$.

Then the i-th columns $u_i \in [\text{PCM}(A)]$ and $u'_i \in [\text{PCM}(B)]$ have the Minkowski distance $M_\infty(u_i, u'_i) < \varepsilon$ for all $i = 1,\dots,m$. Hence $\text{SM}(A,B) < \varepsilon$ by Definition 4.3. ◀

Proof of Theorem 5.4. **(a,b)** As in the proof of Theorem 3.5, assume that the centers $\bar{A}, \bar{B}$ coincide with the origin 0. Given an orientation-preserving isometry $f : \mathbb{R}^n \to \mathbb{R}^n$ mapping A to B, any ordered sequence $p_1, \dots, p_{n-1} \in A$ maps to $f(p_1), \dots, f(p_{n-1}) \in B$. Since f is a linear map preserving all scalar products and lengths of vectors, we conclude that

$$f(p_j - \sum_{k=1}^{j-1}(p_j \cdot v_k)v_k) = f(p_j) - \sum_{k=1}^{j-1}(f(p_j) \cdot f(v_k))f(v_k).$$

By Definition 5.3 the isometry f maps the orthonormal basis $v_1, \dots, v_n$ of the sequence $p_1, \dots, p_{n-1} \in A$ to the orthonormal basis $f(v_1), \dots, f(v_n)$ of the sequence $f(p_1), \dots, f(p_{n-1}) \in B$. Then any point $p \in A$ has the same coordinates $p \cdot v_j = f(p) \cdot f(v_j)$, $j = 1, \dots, n$, in the basis $v_1, \dots, v_n$ as its image $f(p) \in B$ in the basis $f(v_1), \dots, f(v_n)$. Hence the matrices $M(p_1, \dots, p_{n-1}) \in \mathrm{WMI}(A)$ and $M(f(p_1), \dots, f(p_{n-1})) \in \mathrm{WMI}(B)$ coincide when their columns (equivalently, points of A, B) are matched by the given isometry f. By choosing any sequence $p_1, \dots, p_n \in A$, the isometry $f : A \to B$ induces the bijection $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$ respecting the weights of matrices (equivalent up to re-ordering of columns). So condition **(a)** holds and implies **(b)** saying that some $P \in \mathrm{WMI}(A)$ and $Q \in \mathrm{WMI}(B)$ are equivalent.

Conversely, if a matrix $P \in \mathrm{WMI}(A)$ coincides with a matrix $Q \in \mathrm{WMI}(B)$, let $v_1, \dots, v_n$ and $u_1, \dots, u_n$ be the orthonormal bases used for writing these matrices in Definition 5.3. The isometry f mapping $v_1, \dots, v_n$ to $u_1, \dots, u_n$ maps A to B because any $p \in A$ in the basis $v_1, \dots, v_n$ has the same coordinates as $f(p) \in B$ in the basis $f(v_1), \dots, f(v_n)$.

(c) Let $f : \mathbb{R}^n \to \mathbb{R}^n$ be any orientation-reversing isometry such as a mirror reflection. For any ordered sequence of affinely independent points $p_1, \dots, p_{n-1} \in A$, the matrix $M_A(p_1, \dots, p_{n-1})$ from Definition 5.3 describes A in the basis defined by $p_1, \dots, p_{n-1}$ with a fixed orientation of $\mathbb{R}^n$. Composing f with an orientation-preserving isometry moving $f(p_1), ..., f(p_{n-1})$ back to $p_1, \dots, p_{n-1}$, respectively, we can assume that f fixes each of $p_1, \dots, p_{n-1}$, while WMI is preserved by the proved condition **(b)**. Then f is the mirror reflection $A \to B$ in the hyperspace spanned by the fixed points $p_1, \dots, p_{n-1}$. Since the basis vector v_n is uniquely defined by $p_1, \dots, p_{n-1}$ for a fixed orientation of $\mathbb{R}^n$, any other point $p \in A$ maps to its mirror image $f(p) \in B$, so p and $f(p)$ have opposite projections to v_n. Then the matrix $M_B(p_1, \dots, p_{n-1})$ describing $f(A) = B$ in the basis $v_1, \dots, v_n$ differs from $M_A(p_1, \dots, p_{n-1})$ by the change of sign in the last row. Hence f induces a bijection $\mathrm{WMI}(A) \to \mathrm{WMI}(B)$, where each matrix changes the sign of its last row and is still considered up to permutation of columns. Conversely, any matrix from $\mathrm{WMI}(A)$ whose last row is considered up to a change of sign is enough to reconstruct a point cloud A up to isometry. ◀

References

1. Hervé Abdi and Lynne J Williams. Principal component analysis. *Wiley interdisciplinary reviews: computational statistics*, 2(4):433–459, 2010.
2. Helmut Alt, Kurt Mehlhorn, Hubert Wagener, and Emo Welzl. Congruence, similarity, and symmetries of geometric objects. *Discrete and Computational Geometry*, 3:237–256, 1988.
3. O Anosova and V Kurlin. An isometry classification of periodic point sets. In *Proceedings of Discrete Geometry and Mathematical Morphology*, 2021.
4. Olga Anosova and Vitaliy Kurlin. Algorithms for continuous metrics on periodic crystals. *arXiv:2205.15298*, 2022.
5. Peter Arbenz. Divide and conquer algorithms for the bandsymmetric eigenvalue problem. *Parallel computing*, 18(10):1105–1128, 1992.
6. Serge Belongie, Jitendra Malik, and Jan Puzicha. Shape matching and object recognition using shape contexts. *Trans. Pattern Analysis and Machine Intelligence*, 24(4):509–522, 2002.

7 David Bimler. Better living through coordination chemistry: A descriptive study of a prolific papermill that combines crystallography and medicine. 2022. URL: `https://doi.org/10.21203/rs.3.rs-1537438/v1`, `https://www.chemistryworld.com/news/800-crystallography-related-papers-appear-to-stem-from-one-paper-mill/4015589.article`.

8 Mireille Boutin and Gregor Kemper. On reconstructing n-point configurations from the distribution of distances or areas. *Advances in Applied Mathematics*, 32(4):709–735, 2004.

9 Peter Brass and Christian Knauer. Testing the congruence of d-dimensional point sets. In *Proceedings of SoCG*, pages 310–314, 2000.

10 Peter Brass and Christian Knauer. Testing congruence and symmetry for general 3-dimensional objects. *Computational Geometry*, 27(1):3–11, 2004.

11 Claire Brécheteau. A statistical test of isomorphism between metric-measure spaces using the distance-to-a-measure signature. *Electronic Journal of Statistics*, 13(1):795–849, 2019.

12 Jean Cardinal, Timothy Chan, John Iacono, Stefan Langerman, and Aurélien Ooms. Subquadratic encodings for point configurations. *J Computational Geometry*, 10(2):99–126, 2019.

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

14 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.

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

16 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.

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

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

19 N Dym and S Kovalsky. Linearly converging quasi branch and bound algorithms for global rigid registration. In *Proceedings ICCV*, pages 1628–1636, 2019.

20 Herbert Edelsbrunner and John Harer. Persistent homology-a survey. *Contemporary mathematics*, 453:257–282, 2008.

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

22 Jianqing Fan, Weichen Wang, and Yiqiao Zhong. An eigenvector perturbation bound and its application to robust covariance estimation. *Journal of Machine Learning Research*, 18(207):1–42, 2018.

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

24 Michael T Goodrich, Joseph SB Mitchell, and Mark W Orletsky. Approximate geometric pattern matching under rigid motions. *Transactions on Pattern Analysis and Machine Intelligence*, 21(4):371–379, 1999.

25 Cosmin Grigorescu and Nicolai Petkov. Distance sets for shape filters and shape recognition. *IEEE transactions on image processing*, 12(10):1274–1286, 2003.

26 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.

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

28 Elton Hsu. *Stochastic analysis on manifolds*. Number 38 in Graduate Studies in Mathematics. American Mathematical Society, 2002.

29 Daniel P Huttenlocher, Gregory A. Klanderman, and William J Rucklidge. Comparing images using the Hausdorff distance. *Transactions on pattern analysis and machine intelligence*, 15(9):850–863, 1993.

30 Roy Jonker and Anton Volgenant. A shortest augmenting path algorithm for dense and sparse linear assignment problems. *Computing*, 38(4):325–340, 1987.

31 Leonid Kantorovich. Mathematical methods of organizing and planning production. *Management science*, 6(4):366–422, 1960.

32 Heuna Kim and Günter Rote. Congruence testing of point sets in 4 dimensions. *arXiv:1603.07269*, 2016.

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

34 Siddharth Manay, Daniel Cremers, Byung-Woo Hong, Anthony Yezzi, and Stefan Soatto. Integral invariants for shape matching. *Transactions on Pattern Analysis and Machine Intelligence*, 28(10):1602–1618, 2006.

35 Haggai Maron, Nadav Dym, Itay Kezurer, Shahar Kovalsky, and Yaron Lipman. Point registration via efficient convex relaxation. *ACM Transactions on Graphics*, 35(4):1–12, 2016.

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

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

38 Robert Osada, Thomas Funkhouser, Bernard Chazelle, and David Dobkin. Shape distributions. *ACM Transactions on Graphics (TOG)*, 21(4):807–832, 2002.

39 R Penner. *Decorated Teichmüller theory*, volume 1. European Mathematical Society, 2012.

40 R Penner. Moduli spaces and macromolecules. *Bull. Amer. Math. Soc*, 53(2):217–268, 2016.

41 Helmut Pottmann, Johannes Wallner, Qi-Xing Huang, and Yong-Liang Yang. Integral invariants for robust geometry processing. *Computer Aided Geometric Design*, 26(1):37–60, 2009.

42 Günter Rote. Computing the minimum Hausdorff distance between two point sets on a line under translation. *Information Processing Letters*, 38(3):123–127, 1991.

43 Yossi Rubner, Carlo Tomasi, and Leonidas Guibas. The earth mover's distance as a metric for image retrieval. *International Journal of Computer Vision*, 40(2):99–121, 2000.

44 Felix Schmiedl. Computational aspects of the Gromov–Hausdorff distance and its application in non-rigid shape matching. *Discrete and Computational Geometry*, 57(4):854–880, 2017.

45 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.

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

47 Jian Sun, Maks Ovsjanikov, and Leonidas Guibas. A concise and provably informative multi-scale signature based on heat diffusion. In *Computer Graphics Forum*, volume 28, pages 1383–1392, 2009.

48 Leonid Vaserstein. Markov processes over denumerable products of spaces, describing large systems of automata. *Problemy Peredachi Informatsii*, 5(3):64–72, 1969.

49 Carola Wenk. Shape matching in higher dimensions. *PhD thesis, FU Berlin*, 2003.

50 Daniel Widdowson and Vitaliy Kurlin. Pointwise distance distributions of periodic sets. *arXiv:2108.04798*, 2021.

51 Daniel Widdowson, Marco M Mosca, Angeles Pulido, Andrew I Cooper, and Vitaliy Kurlin. Average minimum distances of periodic point sets. *MATCH Communications in Math. Comp. Chemistry*, 87:529–559, 2022.

52 Jiaolong Yang, Hongdong Li, Dylan Campbell, and Yunde Jia. Go-ICP: A globally optimal solution to 3D ICP point-set registration. *Transactions on Pattern Analysis and Machine Intelligence*, 38:2241–2254, 2015.