# On Matching Point Configurations 

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#### Abstract

We present an algorithm that verifies if two unlabeled configurations of $N$ points in $\mathbb{R}^{d}$ are or are not an orthogonal transformation of one another, and if applicable, explicitly compute that transformation. We also give a formula for the orthogonal transformation in the case of noisy measurements. AMS subject classification: 65F15, 65F35, 65G99. Key Words: matching point configuration, orthogonal Procrustes problem, perturbation bounds.


## 1 Introduction

In computer vision applications it is often necessary to match an unidentified image to an image from a library of known images such as fingerprints, faces and others. This process is often done by identifying points (landmarks) on the incoming image and checking whether they match the point configuration from an already indexed image in an existing collection. An image does not change under rigid motions (translations, rotations, reflections and compositions of those), which are called isometric affine transformations.

If we denote by $O(d)$ the group of the $d \times d$ orthogonal matrices, and by $\mathcal{S}_{N}$ the group of all permutations of $\{1,2, \ldots, N\}$, a rigid motion $R$ in $\mathbb{R}^{d}$ is defined by

$$
\begin{equation*}
R \mathbf{x}=A \mathbf{x}+\mathbf{b}, \quad \mathbf{x} \in \mathbb{R}^{d}, \tag{1.1}
\end{equation*}
$$

where $A \in O(d)$ is a fixed matrix, and $\mathbf{b} \in \mathbb{R}^{d}$ is a fixed vector . The problem of matching two images can be formulated in the following way: given two collections of $N$ points $\mathcal{P}=$ $\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ in $\mathbb{R}^{d}$, is there an orthogonal matrix $A \in O(d)$, a vector $\mathbf{b} \in \mathbb{R}^{d}$, and a permutation $\pi \in \mathcal{S}_{N}$, such that in the Euclidean norm $\|\cdot\|$, the rigid motion defined by (1.1), satisfies

$$
\begin{equation*}
\left\|R \mathbf{p}_{i}-\mathbf{q}_{\pi(i)}\right\| \leq \varepsilon, \quad i=1, \ldots, N \tag{1.2}
\end{equation*}
$$

[^0]for a sufficiently small $\varepsilon$ ? A positive answer to this question would mean that we have found a match, namely the two images whose representatives are the two collections of points are the same. The presence of $\varepsilon$ in (1.2) reflects the presence of noise due to numerical or measurement errors.

The problem of matching two collections of points has been vastly studied using different approaches. For example, in $[3,4,5]$, the authors investigate a point set via the set of distances between each possible pair of points in the configuration, which is called distance distribution. The main result of this approach, see [3, 4], is that the set of point configurations in $\mathbb{R}^{d}$ that are not uniquely determined from their distance distribution is contained in the zero set of a non-zero polynomial, and thus has Lebesgue measure zero in its respective space. However, the degree of this polynomial grows exponentially in the number of points $N$ which makes its evaluation unfeasible even for moderate values of $N$. In addition, there is no theorem investigating the problem in the presence of noise. On the other hand, even if we have a noiseless distance distribution that uniquely, up to a rigid motion, determines a point configuration, the best known algorithms to match such configurations, according to [4] and the references therein, are of the order $O\left(N^{d^{2}+3 d+1}\right)$.

Other approaches to matching point collections are based on the Gramians of the point configurations. These methods have the advantage that they retain the information about the labeling (indexing) of the points in the configuration. For example, it is a well known fact that given two point configurations $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ in $\mathbb{R}^{d}$, there exists a rigid motion $R$ such that $R \mathbf{p}_{i}=\mathbf{q}_{i}, i=1, \ldots, N$, if and only if the Gramians $P^{T} P=Q^{T} Q$, where $P$ and $Q$ are the matrices with columns $\mathbf{p}_{i}-\overline{\mathbf{p}}$ and $\mathbf{q}_{i}-\overline{\mathbf{q}}$, respectively, with $\overline{\mathbf{q}}=\frac{1}{N} \sum_{i=1}^{N} \mathbf{q}_{i}$ and $\overline{\mathbf{p}}=\frac{1}{N} \sum_{i=1}^{N} \mathbf{p}_{i}$.

In this paper, we first investigate the matching and registration of unlabeled point configuration in the absence of noise using the Gramian approach. We propose and test a new algorithm that verifies whether two unlabeled configurations of $N$ points in $\mathbb{R}^{d}$ are or are not an orthogonal transformation of one another, and if applicable, explicitly compute that transformation. The algorithm is based on ideas used in variable decorrelation, which is routinely solved by principal component analysis (PCA). Compared to the $\binom{N}{2}$ numbers used in the distance distribution approach, our algorithm uses at most $d(1+d+2 N)$ numbers to process a point configuration, which reduces the memory cost and the data access time. Existing algorithms for matching unlabeled point clouds are based on iterative closest point methods, see $[14,17]$, and deal with the registration of unlabeled point clouds of different sizes in the presence of noise. Although quite useful in practice, these methods often assume certain additional information about the point cloud. For example, they assume that the rigid motion $R$ is a small perturbation or it is roughly known, or that the nature of the cloud is such that there is a fast procedure to label a reasonably large subcloud and thus compute the rigid motion based on that labeled subcollection. In contrast to these techniques, our algorithm does not require any information about the geometry of the cloud or the the nature of the rigid motion, but is applicable only to noiseless same size point clouds.

Here, we also present and test a theoretical result, see Theorem 4.2, where we explicitly compute the orthogonal matrix $A$, see (1.1), for labeled point clouds in the presence of noise.

More precisely, we show that if $\varepsilon$ is small enough, and

$$
\begin{equation*}
P^{T} P=Q^{T} Q+\varepsilon M, \tag{1.3}
\end{equation*}
$$

where the entries of the matrix $M$ are bounded, there is an orthogonal matrix $A=A(\varepsilon)$ (which we construct), such that $\|A P-Q\| \leq \varepsilon \tilde{c} N^{2}$, with explicitly computed constant $\tilde{c}$. The converse is not true and we show it by constructing a counterexample.

Our result is closely related to the stability of the orthogonal Procrustes problem for the matrices $P$ and $Q$. The latter is the problem of finding an orthogonal matrix $A$, such that the Frobenius norm $\|A P-Q\|_{F}$ is minimized. In the case when both $P$ and $Q$ have full row rank, the problem was solved in [10]. The solution of the general problem can be found in $[11,15]$, and is given by the matrix $A=U V^{T}$, where $U$ and $V$ come form the singular value decomposition of $Z=Q P^{T}, Q P^{T}=U \Sigma_{Z} V^{T}$. For further details on the problem and its solution, we refer the reader to $[9,12]$ and the references therein.

The stability of $A$ and how noise in the data affects the computed rigid body motion is an important issue in practical applications. In [7], an explicit expression of the error in $A$, to first order, is given in terms of the errors in $P$ and $Q$ when $d=3$. While this result is much more specific than general error bounds that have been established before, it requires the exact values of the matrices $P, Q$ and $A$. Our result from Theorem 4.2 does not require such knowledge and is in the spirit of the work in [16], where supremum bounds for the perturbation error in the solution $A$ of the orthogonal Procrustes problem with the additional restriction that $A$ has a positive determinant, see [11], are derived.

## 2 Preliminaries

This section contains well known facts from linear algebra that will be used throughout the paper, as well as certain Procrustes analysis results, stated for self containment. Some of the proofs are included for clarity, while the basic results are only stated.

### 2.1 Matrices

Let $\pi \in \mathcal{S}_{N}$ be a permutation of $\{1,2, \ldots, N\}$. Then the $N \times N$ matrix $E_{\pi}$ with columns $\left\{\mathbf{e}_{\pi(1)}, \ldots, \mathbf{e}_{\pi(N)}\right\}$, where $\mathbf{e}_{j}$ is the $j$-th element of the canonical basis of $\mathbb{R}^{N}$ is called the permutation matrix associated to $\pi$. Multiplying a matrix $A$ on the right by $E_{\pi}$ permutes the columns of $A$ by $\pi$.

Lemma 2.1 Let $E_{\pi}$ be the permutation matrix associated to $\pi \in S_{N}$. Let $A$ and $B$ be two positive semidefinite symmetric matrices such that $B=E_{\pi} A E_{\pi}^{T}$. Then the set of eigenvalues of $A$ and $B$ are identical, including their algebraic multiplicity, and there exist eigenvalue decompositions of $A=U_{A} \Lambda U_{A}^{T}$ and $B=U_{B} \Lambda U_{B}^{T}$, such that $E_{\pi}=U_{B} U_{A}^{T}$.

It is important to notice that Lemma 2.1 is an existence result since the eigenvalue decomposition of a matrix is not unique. In general, given arbitrary decompositions $A=$ $\widetilde{U}_{A} \Lambda \widetilde{U}_{A}^{T}$ and $B=\widetilde{U}_{B} \Lambda \widetilde{U}_{B}^{T}$ for the positive semidefinite symmetric matrices $A$ and $B$, the matrix $\widetilde{U}_{B} \widetilde{U}_{A}^{T}$ need not be a permutation matrix.

Lemma 2.2 Let $P$ and $Q$ be two $d \times N$ matrices. Then $P^{T} P=Q^{T} Q$ if and only if there is a $d \times d$ orthogonal matrix $A$ such that $A P=Q$. We call such a matrix $A$ an equivalence matrix.

Proof. If $A P=Q$, where $A$ is orthogonal matrix, we have $Q^{T} Q=(A P)^{T} A P=P^{T}\left(A^{T} A\right) P=$ $P^{T} P$. Conversely, if $P^{T} P=Q^{T} Q$, then $P$ and $Q$ have the same singular values, and the same right singular vectors. Then, by singular value decomposition, there are $d \times d$ orthogonal matrices $U_{P}$ and $U_{Q}$ such that $P=U_{P} \Sigma V^{T}$ and $Q=U_{Q} \Sigma V^{T}$, where $V$ is the $N \times N$ orthogonal matrix containing the eigenvectors of $P^{T} P$. Therefore $Q=U_{Q} \Sigma V^{T}=$ $\left(U_{Q} U_{P}^{T}\right) U_{P} \Sigma V^{T}=A P$, where $A=U_{Q} U_{P}^{T}$.

Finally, in this paper, unless stated otherwise, we use the Euclidean norm of a vector $\mathrm{x} \in \mathbb{R}^{N}$ and the corresponding induced matrix norm of a $d \times N$ matrix $A$,

$$
\|A\|=\max _{\|\mathbf{x}\|=1}\|A \mathbf{x}\|
$$

Note, that the induced matrix Euclidean norm is also the spectral norm of $A$, namely

$$
\|A\|=\sqrt{\lambda_{\max }\left(A^{T} A\right)}=\sqrt{\lambda_{\max }\left(A A^{T}\right)}=\left\|A^{T}\right\|
$$

where $\lambda_{\max }\left(A^{T} A\right)$ is the maximal eigenvalue of $A^{T} A$, and it is submultiplicative, that is $\|A B\| \leq\|A\| \cdot\|B\|$.

### 2.2 Labeled point configurations

We fix a coordinate system in $\mathbb{R}^{d}$ and denote by $\mathcal{P}:=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}:=\left\{\mathbf{q}_{1}, \ldots, \mathbf{p}_{N}\right\}$ two collections of $N$ points in $\mathbb{R}^{d}$, where $\mathbf{p}_{i}$ is the coordinate vector of the $i$-th point from $\mathcal{P}$ with respect to this coordinate system. Let $\overline{\mathbf{p}}=\frac{1}{N}\left(\mathbf{p}_{1}+\cdots+\mathbf{p}_{N}\right)$ and $\overline{\mathbf{q}}=\frac{1}{N}\left(\mathbf{q}_{1}+\cdots+\mathbf{q}_{N}\right)$ be the center of mass of $\mathcal{P}$ and $\mathcal{Q}$, respectively, $\mathcal{P}$ and $\overline{\mathcal{Q}}$ be the new (centered) collections $\overline{\mathcal{P}}:=\left\{\mathbf{p}_{1}-\overline{\mathbf{p}}, \ldots, \mathbf{p}_{N}-\overline{\mathbf{p}}\right\}$ and $\overline{\mathcal{Q}}:=\left\{\mathbf{q}_{1}-\overline{\mathbf{q}}, \ldots, \mathbf{q}_{N}-\overline{\mathbf{q}}\right\}$, and $P$ and $Q$ be the $d \times N$ matrices with columns $\mathbf{p}_{i}-\overline{\mathbf{p}}$ and $\mathbf{q}_{i}-\overline{\mathbf{q}}$, respectively.

If there is a rigid motion $R$ such that $R \mathbf{p}_{i}=\mathbf{q}_{i}, i=1, \ldots, N$, we say that $\mathcal{P}$ and $\mathcal{Q}$ are identically equivalent. The following theorem, based on techniques more extensively discussed in [13], provides a tool to find $R$ if it exists.

Theorem 2.3 The following statements are equivalent.
(i) $\mathcal{P}$ and $\mathcal{Q}$ are identically equivalent.
(ii) $P^{T} P=Q^{T} Q$.
(iii) There is an orthogonal matrix $A$ such that $A P=Q$.

Proof. The equivalence for (ii) and (iii) has been proven in Lemma 2.2.
If there is a rigid motion $R, R \mathbf{x}=A \mathbf{x}+\mathbf{b}$ with an orthogonal matrix $A$ and a vector $\mathbf{b}$, such that $R \mathbf{p}_{i}=\mathbf{q}_{i}, i=1, \ldots, N$, it is easy to verify that $R \overline{\mathbf{p}}=\overline{\mathbf{q}}$. Therefore, $\mathbf{q}_{i}-\overline{\mathbf{q}}=$ $R \mathbf{p}_{i}-R \overline{\mathbf{p}}=A\left(\mathbf{p}_{i}-\overline{\mathbf{p}}\right)$ for every $i=1, \ldots, N$, and thus $A P=Q$. Conversely, if $A P=Q$ for an orthogonal matrix $A$, then $\mathbf{q}_{i}-\overline{\mathbf{q}}=A\left(\mathbf{p}_{i}-\overline{\mathbf{p}}\right)$ and therefore $\mathbf{q}_{i}=A \mathbf{p}_{i}+(\overline{\mathbf{q}}-\overline{\mathbf{p}})=R \mathbf{p}_{i}$, with $\mathbf{b}=\overline{\mathbf{q}}-\overline{\mathbf{p}}, i=1, \ldots, N$. This establishes the equivalence between (i) and (iii).

Note, that given $P^{T} P=Q^{T} Q$, the matrix $A$ can be computed directly if $P$ has rank $d$. In this case $P P^{T}$ is invertible, and it can be shown that $A=Q\left(P P^{T}\right)^{-1} P^{T}$.

In some applications, it is often needed to compare point clouds that are captured at different resolutions where the conversion factor is not necessarily available. In this case, in addition to the rigid motion $R$, one has to find the dilation factor $s$, such that $\mathbf{q}_{i}=s R \mathbf{p}_{i}$, or equivalently $R \mathbf{p}_{i}=s^{-1} \mathbf{q}_{i}, i=1, \ldots, N$. By Theorem 2.3, there is an orthogonal matrix $A$ such that $A\left(\mathbf{p}_{i}-\overline{\mathbf{p}}\right)=s^{-1}\left(\mathbf{q}_{i}-\overline{\mathbf{q}}\right)$. Note that since $A$ is an orthogonal matrix, we have $\|A \mathbf{x}\|^{2}=\|\mathbf{x}\|^{2}$ for any $\mathbf{x} \in \mathbb{R}^{d}$, and therefore $s^{2} \sum_{i=1}^{N}\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\|^{2}=\sum_{i=1}^{N}\left\|\mathbf{q}_{i}-\overline{\mathbf{q}}\right\|^{2}$. Hence, $s$ is given by

$$
s=\left(\frac{\sum_{i=1}^{N}\left\|\mathbf{q}_{i}-\overline{\mathbf{q}}\right\|^{2}}{\sum_{i=1}^{N}\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\|^{2}}\right)^{\frac{1}{2}}=\frac{\|Q\|_{F}}{\|P\|_{F}}
$$

where $\|\cdot\|_{F}$ is the Frobenius norm. The choice of computing the dilation factor by the use of the entire point collection, instead of just one of the samples has two goals. First, it can be applied even in the unlabeled case, and second, it provides robustness to noise, as explored in [13].

## 3 Unlabeled point configurations

Often, when landmarks are extracted from an image to generate a point configuration $\mathcal{P}$, it is not possible to a priori enumerate the points in a manner consistent with the enumeration of an existing point collection $\mathcal{Q}$ in our library. In this case, there exist a rigid motion $R$ and a permutation $\pi \in S_{N}$, such that $R \mathbf{p}_{i}=\mathbf{q}_{\pi(i)}, i=1, \ldots, N$, and we call the collections $\mathcal{P}$ and $\mathcal{Q}$ equivalent. This section explores how, given two point configurations, we decide whether they are equivalent.

Theorem 3.1 Let $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ be two collections of $N$ points in $\mathbb{R}^{d}$. The following statements are equivalent.
(i) $\mathcal{P}$ and $\mathcal{Q}$ are equivalent.
(ii) There is a permutation matrix $E_{\pi}$, such that $P^{T} P=E_{\pi}^{T} Q^{T} Q E_{\pi}$.
(iii) There is an orthogonal matrix A, completely determined in Lemma 2.2 and a permutation matrix $E_{\pi}$, such that $A P=Q E_{\pi}$.

Moreover, $E_{\pi}=U_{\mathcal{Q}} U_{\mathcal{P}}^{T}$, where $U_{\mathcal{P}}$ and $U_{\mathcal{Q}}$ are orthogonal matrices from an eigenvalue decomposition of $P^{T} P$ and $Q^{T} Q$, respectively. Note that one does not know which particular eigenvalue decomposition will provide the matrices $U_{\mathcal{P}}$ and $U_{\mathcal{Q}}$.

Proof. Let $\pi \in \mathcal{S}_{N}$ be the permutation from the definition of equivalence of the two collections $\mathcal{P}$ and $\mathcal{Q}$. We consider the permutation matrix $E_{\pi}$, associated with $\pi$. We denote by $\mathcal{Q}_{\pi}$ the re-enumerated collection of points $\mathcal{Q}$ with corresponding matrix $Q_{\pi}$ with columns $\mathbf{q}_{\pi(i)}-\overline{\mathbf{q}}$. Note, that $Q_{\pi}=Q E_{\pi}$. Then, $\mathcal{P}$ and $\mathcal{Q}$ are equivalent if and only if $\mathcal{P}$ and $\mathcal{Q}_{\pi}$ are identically equivalent, which using Theorem 2.3 , is true if and only if $P^{T} P=E_{\pi}^{T} Q^{T} Q E_{\pi}=E_{\pi^{-1}} Q^{T} Q E_{\pi^{-1}}^{-1}$. By Lemma 2.1, there are orthogonal matrices $U_{\mathcal{P}}$ and $U_{\mathcal{Q}}$ such that $P^{T} P=U_{\mathcal{P}} \Lambda U_{\mathcal{P}}^{T}$ and $Q^{T} Q=U_{\mathcal{Q}} \Lambda U_{\mathcal{Q}}^{T}$, such that $E_{\pi^{-1}}=U_{\mathcal{P}} U_{\mathcal{Q}}^{T}$, and therefore $E_{\pi}=U_{\mathcal{Q}} U_{\mathcal{P}}^{T}$.

Relation (ii) can be written as $P^{T} P=\left(Q E_{\pi}\right)^{T} Q E_{\pi}$. By Lemma 2.2 this is true if and only if there is an orthogonal matrix $A$, described in this lemma, such that $A P=Q E_{\pi}$.

Notice, that the matrix $Q Q^{T}$ does not depend on the permutation of the columns of $Q$, since $Q_{\pi} Q_{\pi}^{T}=Q E_{\pi} E_{\pi}^{T} Q^{T}=Q Q^{T}$. The next lemma provides some insight on whether a suitable matrix $A$, related to the rigid motion $R$ exists and if it does, gives another way of its explicit construction.

Lemma 3.2 Let $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ be two equivalent collections of $N$ points in $\mathbb{R}^{d}$. Then the $d \times d$ matrices $P P^{T}$ and $Q Q^{T}$ have the same eigenvalues $0 \leq \lambda_{1} \leq \ldots \leq \lambda_{d}$, including their algebraic multiplicities. Let $\mathbf{v}_{i}$ and $\mathbf{w}_{i}$ be the orthonormal eigenvectors of $P P^{T}$ and $Q Q^{T}$ corresponding to $\lambda_{i}, i=1, \ldots, d$, respectively. Let $V$ and $W$ be the orthogonal matrices with columns $\left\{\mathbf{v}_{i}\right\}$ and $\left\{\mathbf{w}_{i}\right\}$. If the eigenvalues $\left\{\lambda_{i}\right\}$ are distinct, then there are integers $\epsilon_{i}= \pm 1, i=1, \ldots, d$, and a permutation $\pi \in S_{N}$, determined from $Q_{\pi}=A P$, such that

$$
\begin{equation*}
<\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}>=\epsilon_{i}<\mathbf{q}_{\pi(k)}-\overline{\mathbf{q}}, \mathbf{w}_{i}>, \quad k=1, \ldots, N, \quad i=1, \ldots, d . \tag{3.4}
\end{equation*}
$$

Moreover, if $E:=\operatorname{diag}\left(\epsilon_{1}, \ldots, \epsilon_{d}\right)$, then the equivalence matrix $A$ can be written as $A=$ $W E V^{T}$.

Proof. It follows from Theorem 3.1 that if $\mathcal{P}$ and $\mathcal{Q}$ are equivalent, then there is an orthogonal matrix $A$, such that $A P=Q E_{\pi}$ for some permutation $\pi \in S_{N}$, with $\pi=i d$ if the points are identically equivalent. Then we have

$$
Q Q^{T}=A P E_{\pi}^{T} E_{\pi} P^{T} A^{T}=A\left(P P^{T}\right) A^{T}
$$

Since $P P^{T}$ is a real symmetric matrix, and $\mathbf{v}_{i}, i=1, \ldots, d$, are orthonormal eigenvectors of $P P^{T}$ corresponding to the eigenvalues $\lambda_{1} \leq \ldots \leq \lambda_{d}$, we have $P P^{T}=V \Lambda_{P} V^{T}$, with $\Lambda_{P}=\operatorname{diag}\left(\lambda_{1}, \ldots, \lambda_{d}\right)$, and therefore

$$
Q Q^{T}=(A V) \Lambda_{P}(A V)^{T}
$$

Clearly, $A V$ is an orthogonal matrix as a product of two orthogonal matrices. Also, $Q Q^{T}$ and $P P^{T}$ have the same eigenvalues, including their algebraic multiplicities, and $A V$ is a matrix whose columns $\left\{A \mathbf{v}_{i}\right\}$ are eigenvectors of $Q Q^{T}$.

Let us consider now the case when $P P^{T}$ and $Q Q^{T}$ have $d$ distinct eigenvalues $\lambda_{i}$. Then the dimension of the corresponding eigenspaces $\operatorname{Ker}\left(P P^{T}-\lambda_{i} I\right)$ will be one, and therefore if $\left\{\mathbf{w}_{i}\right\}$ is an orthonormal system of eigenvectors for $Q Q^{T}$, then $\epsilon_{i} \mathbf{w}_{i}=A \mathbf{v}_{i}$ with $\epsilon_{i}= \pm 1$. The latter can be written as $W E=A V$, namely $A=W E V^{T}$. Since $Q_{\pi}=A P$ and $A$ is orthogonal matrix, we have

$$
<\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}>=<A\left(\mathbf{p}_{k}-\overline{\mathbf{p}}\right), A \mathbf{v}_{i}>=\epsilon_{i}<\mathbf{q}_{\pi(k)}-\overline{\mathbf{q}}, \mathbf{w}_{i}>
$$

and the proof is completed.
Note that if $<\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}>=0$, for every $k=1, \ldots, N, \epsilon_{i}$ cannot be determined from (3.4). If this happens, then $P^{T} \mathbf{v}_{i}=\mathbf{0}$, and therefore $P P^{T} \mathbf{v}_{i}=0$. This means that $\mathbf{v}_{i}$ is the eigenvector that corresponds to the eigenvalue 0 , namely $i=1$ and $\lambda_{1}=0$. Thus, if $0<\lambda_{1}<\ldots<\lambda_{d}$, which happens if $\operatorname{rank}(P)=d$, then there is at least one $k$ which may depend on $i$, such that $<\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}>\neq 0$, and we have

$$
\epsilon_{i}=\frac{\left\langle\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}\right\rangle}{\left\langle\mathbf{q}_{\pi(k)}-\overline{\mathbf{q}}, \mathbf{w}_{i}\right\rangle}
$$

In this case the matrix $E=\operatorname{diag}\left(\epsilon_{1}, \ldots, \epsilon_{d}\right)$, and $A=W E V^{T}$ is completely determined if $\pi$ is known.

Since the point collections are not labeled, we do not know $\pi$ and could not use the above formula unless we go through all possible $N$ ! choices for $\pi$. But that would be just an application of the well known PCA for each of the $N$ ! choices of $\pi$, which is not computationally efficient. Our goal is to find $E$, and therefore $A$, without an apriori knowledge of the permutation $\pi$, under the assumption that all eigenvalues of $P P^{T}$ are distinct.

Let $L_{i}^{-}(\mathcal{P}):=\left\{\left|\left\langle\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}\right\rangle\right|: 1 \leq k \leq N,\left\langle\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}\right\rangle<0\right\}, i=1, \ldots, d$, be the collection of the absolute values of all negative scalar products, and $L_{i}^{+}(\mathcal{P}):=\left\{\left\langle\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}\right\rangle: 1 \leq\right.$ $\left.k \leq N,\left\langle\mathbf{p}_{k}-\overline{\mathbf{p}}, \mathbf{v}_{i}\right\rangle>0\right\}$, be the collection of all positive scalar products, including their repetitions. We similarly define $L_{i}^{-}(\mathcal{Q})$ and $L_{i}^{+}(\mathcal{Q})$. If $\operatorname{rank}(P)=d$, at least one of $L_{i}^{-}(\mathcal{P})$ or $L_{i}^{+}(\mathcal{P})$ will have at least one element. The same holds for $L_{i}^{-}(\mathcal{Q})$ and $L_{i}^{+}(\mathcal{Q})$. Let $\mathcal{P}$ be equivalent to $\mathcal{Q}$. Then for any fixed $i=1, \ldots, d$, if $L_{i}^{+}(\mathcal{P}) \neq L_{i}^{-}(\mathcal{P})$, it follows from (3.4) that only one of the two cases happens:

- either $L_{i}^{+}(\mathcal{P})=L_{i}^{+}(\mathcal{Q})$ and $L_{i}^{-}(\mathcal{P})=L_{i}^{-}(\mathcal{Q})$, and thus $\epsilon_{i}=1$, or
- $L_{i}^{+}(\mathcal{P})=L_{i}^{-}(\mathcal{Q})$ and $L_{i}^{-}(\mathcal{P})=L_{i}^{+}(\mathcal{Q})$, and thus $\epsilon_{i}=-1$.

If there is $i_{0}$ such that $L_{i_{0}}^{+}(\mathcal{P})=L_{i_{0}}^{-}(\mathcal{P})$, we cannot make the decision whether $L_{i_{0}}^{+}(\mathcal{P})=$ $L_{i_{0}}^{+}(\mathcal{Q})$ or $L_{i_{0}}^{+}(\mathcal{P})=L_{i_{0}}^{-}(\mathcal{Q})$, and therefore determine whether $\epsilon_{i_{0}}=1$ or $\epsilon_{i_{0}}=-1$. In this case, we should consider both cases. In general, we can have $m \leq d$ indices $i, i_{1}, \ldots, i_{m}$, for which $L_{i_{\ell}}^{+}(\mathcal{P})=L_{i_{\ell}}^{-}(\mathcal{P}), \ell=1, \ldots, m$, and we have to consider $2^{m}$ matrices $E, E_{1}, \ldots, E_{2^{m}}$, corresponding to the various cases of $\pm 1$ located at the positions described by these $m$ indices. If $Q \neq W E_{k} V^{T} P$, for $k=1, \ldots, 2^{m}$, then $\mathcal{Q}$ is not equivalent to $\mathcal{P}$. Otherwise, if there is $k$, such that $Q=W E_{k} V^{T} P$, they are equivalent, and $A=W E_{k} V^{T}$ is the matrix of equivalence.

Let us denote by $\mathcal{L}:=\{\mathcal{P}\}$ a library of collections of $N$ points in $\mathbb{R}^{d}$. Let $\mathcal{R}$ be the subset of $\mathcal{L}$ that contains all collections $\mathcal{P}$ for which the eigenvalues $0 \leq \lambda_{1} \leq \ldots \leq \lambda_{d}$ of $P P^{T}$ are distinct. Let $\mathcal{Q}$ be a configuration of $N$ points in $\mathbb{R}^{d}$ that we need to match to a collection from the library $\mathcal{L}$. The algorithm, described below, is based on the above observations and always determines whether $\mathcal{Q}$ is equivalent to a collection from $\mathcal{R}$ and may or may not determine whether $\mathcal{Q}$ is equivalent to a collection from $\mathcal{L} \backslash \mathcal{R}$.

We have performed several numerical experiments to test our algorithm. In our implementation, as it is usually done in practice, the equality in lines $1,7,9,11$ and 23 in Algorithm 1 has been substituted by $\varepsilon$-distance. For example, $Q=W E V^{T} P$ has been substituted by $\left\|Q-W E V^{T} P\right\| \leq \varepsilon$, with $\varepsilon$ ranging from $10^{-6}$ to $10^{-10}$.

Test 1: For each pair $(d, N), d \in\{2,3,4\}, N \in\left\{2^{n}: 3 \leq n \leq 10\right\}$, we have generated in random a library $\mathcal{L}=\mathcal{L}(d, N)$ of 4000 collections of $N$ points in $\mathbb{R}^{d}$ uniformly distributed inside the unit sphere. We next build a set $\mathcal{T}=\mathcal{T}(d, N)$ of point collections by first choosing (in random) 2000 collections from $\mathcal{L}$, each of which is subsequently shuffled and rotated (in random). For each collection $\mathcal{Q} \in \mathcal{T}$, we apply Algorithm 1 with $\mathcal{P}$ exhausting all elements from $\mathcal{L}$ until a match is found. The algorithm was able to match each $\mathcal{Q}$ from $\mathcal{T}$ to its respective collection in $\mathcal{L}$.

Test 2: For each pair $(d, N), d \in\{2,3,4\}, N \in\left\{2^{n}: 3 \leq n \leq 10\right\}$, we generate in random a library $\mathcal{L}=\mathcal{L}(d, N)$ of 4000 collections of $N$ points in $\mathbb{R}^{d}$ uniformly distributed inside the unit sphere. We next generate the same way a set $\mathcal{T}=\mathcal{T}(d, N)$ of 2000 point collections, and for each collection $\mathcal{Q} \in \mathcal{T}$ apply Algorithm 1 with $\mathcal{P}$ exhausting all elements from $\mathcal{L}$ until a match is found. As expected, the algorithm was not able to find a match.

Note that the eigenvalues of the matrix $P P^{T}$ cannot be computed exactly, as they are roots of a degree $d$ polynomial. However, there are high precision algorithms with complexity $O\left(d^{3}\right)$ to compute the eigenvalue decomposition for Gramians [6]. The proposed algorithm requires the computation of $P P^{T}$, (complexity $O\left(d^{2} N\right)$ ), its eigenvalue decomposition (complexity $O\left(d^{3}\right)$ ), the computation of $d$ sequences ( $\left.<\mathbf{p}_{1}-\overline{\mathbf{p}}, \mathbf{v}_{i}>, \ldots,<\mathbf{p}_{N}-\overline{\mathbf{p}}, \mathbf{v}_{i}>\right)$ and $\left(<\mathbf{q}_{1}-\overline{\mathbf{q}}, \mathbf{w}_{i}>, \ldots,<\mathbf{q}_{N}-\overline{\mathbf{q}}, \mathbf{w}_{i}>\right)$ (complexity $O\left(d N^{2}\right)$ ), the computation of at most $2^{m}$ matrices $A$, each with complexity of at most $O\left(d^{3}\right)$, and the computation of at most $2^{m}$ matrices $A P$, each with complexity $O\left(d^{2} N\right)$. Therefore, for large values of $N \approx d 2^{d}$, our algorithm has complexity of $O\left(d N^{2}\right)$. Note that for every collection $\mathcal{P} \in \mathcal{L}$ the algorithm needs only the $d$ eigenvalues of $P P^{T}$, and when they are distinct, the $d \times N$ matrix $P$, the

```
Algorithm 1 Decision and Orthogonal Matrix Computation
Input:
    \(P,\left\{\lambda_{i}\right\},\left\{\mathbf{v}_{i}\right\},\left\{L_{i}^{+}(\mathcal{P})\right\},\left\{L_{i}^{-}(\mathcal{P})\right\}\).
    \(Q,\left\{\gamma_{i}\right\},\left\{\mathbf{w}_{i}\right\},\left\{L_{i}^{+}(\mathcal{Q})\right\},\left\{L_{i}^{-}(\mathcal{Q})\right\}\).
    \% The eigenvalues should be given in increasing order.
Output:
    res \% Decision value. It may be true, false or inconclusive.
    A \% Orthogonal transformation, if res is true.
    if \(\left\{\lambda_{i}\right\} \neq\left\{\gamma_{i}\right\}\) then
        return res \(\leftarrow\) false
    else if \(\lambda_{1}<\cdots<\lambda_{d}\) then
        \(f \leftarrow 1, i \leftarrow 0\)
        while \(i<d\) and \(f=1\) do
            \(i \leftarrow i+1\)
            if \(\left\{L_{i}^{+}(\mathcal{P})\right\}=\left\{L_{i}^{-}(\mathcal{P})\right\}=\left\{L_{i}^{+}(\mathcal{Q})\right\}=\left\{L_{i}^{-}(\mathcal{Q})\right\}\) then
                \(\epsilon_{i}= \pm 1\)
            else if \(\left\{L_{i}^{+}(\mathcal{P})\right\}=\left\{L_{i}^{+}(\mathcal{Q})\right\}\) and \(\left\{L_{i}^{-}(\mathcal{P})\right\}=\left\{L_{i}^{-}(\mathcal{Q})\right\}\) then
                \(\epsilon_{i}=+1\)
            else if \(\left\{L_{i}^{+}(\mathcal{P})\right\}=\left\{L_{i}^{-}(\mathcal{Q})\right\}\) and \(\left\{L_{i}^{-}(\mathcal{P})\right\}=\left\{L_{i}^{+}(\mathcal{Q})\right\}\) then
                \(\epsilon_{i}=-1\)
            else
                \(f \leftarrow 0\)
            end if
        end while
        if \(f=0\) then
            return res \(\leftarrow\) false
        else
            \(W \leftarrow\left[\mathbf{w}_{1}, \ldots, \mathbf{w}_{d}\right]\)
            \(V \leftarrow\left[\mathbf{v}_{1}, \ldots, \mathbf{v}_{d}\right]\)
            \(E \leftarrow \operatorname{diag}\left(\epsilon_{1}, \ldots, \epsilon_{d}\right)\)
            if \(Q=W E V^{T} P\) then
                return res \(\leftarrow\) true, \(A \leftarrow W E V^{T}\)
            else
                return res \(\leftarrow\) false
            end if
        end if
    else
        return res \(\leftarrow\) inconclusive
    end if
```

$d \times d$ matrix $V$, and the $d$ sequences $\left(<\mathbf{p}_{1}-\overline{\mathbf{p}}, \mathbf{v}_{i}>, \ldots,<\mathbf{p}_{N}-\overline{\mathbf{p}}, \mathbf{v}_{i}>\right)$ which in total is at most $d(1+d+2 N)$ numbers.

## 4 Robustness

In this section, we investigate the problem of matching two labeled point configurations $\mathcal{P}$ and $\mathcal{Q}$ in $\mathbb{R}^{d}$ in the presence of noise. We say that $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ are $\varepsilon$ - identically equivalent, if $\left|\left\|\mathbf{p}_{i}-\mathbf{p}_{j}\right\|^{2}-\left\|\mathbf{q}_{i}-\mathbf{q}_{j}\right\|^{2}\right| \leq \varepsilon$ for all $i, j=1, \ldots, N$. The following statement, whose proof we omit, holds.

## Lemma 4.1

(i) If $\mathcal{P}$ and $\mathcal{Q}$ are $\varepsilon$ - identically equivalent, then

$$
\begin{equation*}
\left|<\mathbf{p}_{i}-\overline{\mathbf{p}}, \mathbf{p}_{j}-\overline{\mathbf{p}}>-<\mathbf{q}_{i}-\overline{\mathbf{q}}, \mathbf{q}_{j}-\overline{\mathbf{q}}>\right| \leq 2 \varepsilon,, \quad \forall 1 \leq i, j \leq N \tag{4.5}
\end{equation*}
$$

(ii) If the Gramians for $\mathcal{P}$ and $\mathcal{Q}$ satisfy

$$
\begin{equation*}
\left|<\mathbf{p}_{i}-\overline{\mathbf{p}}, \mathbf{p}_{j}-\overline{\mathbf{p}}>-<\mathbf{q}_{i}-\overline{\mathbf{q}}, \mathbf{q}_{j}-\overline{\mathbf{q}}>\right| \leq \varepsilon, \quad \forall 1 \leq i, j \leq N \tag{4.6}
\end{equation*}
$$

then $\mathcal{P}$ and $\mathcal{Q}$ are $4 \epsilon$-identically equivalent.

Lemma 4.1 shows that if $\mathcal{P}$ and $\mathcal{Q}$ are $C \varepsilon$ - identically equivalent with $C$ being a fixed constant, then their Gramians are close, namely $P^{T} P=Q^{T} Q+\varepsilon M$, where the entries $m_{i j}$ of $M$ are bounded, $\left|m_{i j}\right| \leq c_{0}$, by some positive constant $c_{0}$, and vice versa.

Next, we investigate whether an equivalent of Lemma 2.2 holds in the presence of noise, that is whether two point configurations $\mathcal{P}$ and $\mathcal{Q}$ are $C \varepsilon$-equivalent if and only if there is an orthogonal matrix $A$ for which $A P$ is close to $Q$. The answer to this question is given in Theorem 4.2 and Theorem 4.3.

Theorem 4.2 Let $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ be two collections of $N$ points in $\mathbb{R}^{d}$, such that $\operatorname{rank}(P)=d,\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\| \leq c$ and $\left\|\mathbf{q}_{i}-\overline{\mathbf{q}}\right\| \leq c, i=1, \ldots, N, c=$ const. Let

$$
\begin{equation*}
P^{T} P=Q^{T} Q+\varepsilon M, \tag{4.7}
\end{equation*}
$$

where $M=\left(m_{i j}\right)$ is a matrix with bounded entries, $\left|m_{i j}\right| \leq c_{0}, c_{0}=$ const, and

$$
\begin{equation*}
0<\varepsilon \leq(1-\delta)\left(\left\|\left(P P^{T}\right)^{-1}\right\| N c_{0}\right)^{-1} \tag{4.8}
\end{equation*}
$$

for some $0<\delta<1$. Then, there exists an orthogonal matrix $A=A(\varepsilon)$, such that $\|A P-Q\| \leq$ $\varepsilon \tilde{c} N^{2}$, with a constant $\tilde{c}$,

$$
\tilde{c}=c c_{0}\left\|\left(P P^{T}\right)^{-1}\right\|\left(2+c\left\|\left(P P^{T}\right)^{-1}\right\|^{1 / 2} \delta^{-1 / 2}\right) .
$$

Proof. First, we derive upper bounds for the norms of some matrices that we shall need later in the proof. Let us observe that

$$
\|P\|^{2}=\lambda_{\max }\left(P^{T} P\right) \leq \operatorname{trace}\left(P^{T} P\right)=\sum_{i=1}^{N}\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\|^{2} \leq c^{2} N,
$$

and similarly, $\|Q\| \leq c \sqrt{N}$, where we have used the fact that the trace of any matrix is equal to the sum of its eigenvalues. We also derive a bound for the spectral norm of $M$. For every $\mathrm{x} \in \mathbb{R}^{N}$ with $\|\mathrm{x}\|=1$ we have

$$
\|M \mathbf{x}\|^{2}=\sum_{i=1}^{N}\left(\sum_{j=1}^{N} m_{i j} x_{j}\right)^{2} \leq \sum_{i=1}^{N}\left[\left(\sum_{j=1}^{N} m_{i j}^{2}\right)\left(\sum_{j=1}^{N} x_{j}^{2}\right)\right]=\sum_{i=1}^{N} \sum_{j=1}^{N} m_{i j}^{2} \leq c_{0}^{2} N^{2}
$$

and thus $\|M\| \leq c_{0} N$.
Note, that $P P^{T}$ is invertible since $d=\operatorname{rank}(P)=\operatorname{rank}\left(P P^{T}\right)$, and we can consider the matrices $P^{T}\left(P P^{T}\right)^{-1}$ and $\left(P P^{T}\right)^{-1} P$. We have $\left(P P^{T}\right)^{-1} P=\left(P^{T}\left(P P^{T}\right)^{-1}\right)^{T}$, and thus $\left\|\left(P P^{T}\right)^{-1} P\right\|=\left\|P^{T}\left(P P^{T}\right)^{-1}\right\|$. Clearly, $\left(P^{T}\left(P P^{T}\right)^{-1}\right)^{T}\left(P^{T}\left(P P^{T}\right)^{-1}\right)=\left(P P^{T}\right)^{-1}$, and therefore we have $\left\|P^{T}\left(P P^{T}\right)^{-1}\right\|^{2}=\lambda_{\max }\left[\left(P P^{T}\right)^{-1}\right]$. This result, combined with the fact that

$$
\begin{aligned}
\left\|\left(P P^{T}\right)^{-1}\right\|^{2} & =\lambda_{\max }\left[\left(\left(P P^{T}\right)^{-1}\right)^{T}\left(P P^{T}\right)^{-1}\right]=\lambda_{\max }\left[\left(\left(P P^{T}\right)^{-1}\right)^{2}\right] \\
& =\left(\lambda_{\max }\left[\left(P P^{T}\right)^{-1}\right]\right)^{2}
\end{aligned}
$$

gives

$$
\begin{equation*}
\left\|\left(P P^{T}\right)^{-1} P\right\|=\left\|P^{T}\left(P P^{T}\right)^{-1}\right\|=\sqrt{\left\|\left(P P^{T}\right)^{-1}\right\|} . \tag{4.9}
\end{equation*}
$$

In what follows, we give an explicit construction of the equivalence matrix $A$. We multiply (4.7) on the right by $P$ and on the left by $P^{T}$ to derive

$$
P P^{T} P P^{T}=P Q^{T} Q P^{T}+\varepsilon P M P^{T} .
$$

This equation can be written as

$$
I=\left(P P^{T}\right)^{-1} P Q^{T} Q P^{T}\left(P P^{T}\right)^{-1}+\varepsilon\left(P P^{T}\right)^{-1} P M P^{T}\left(P P^{T}\right)^{-1}
$$

As it was done in Lemma 2.2, we construct the matrix $B:=Q P^{T}\left(P P^{T}\right)^{-1}$, denote

$$
L:=\left(P P^{T}\right)^{-1} P M P^{T}\left(P P^{T}\right)^{-1},
$$

and rewrite the last equation as

$$
\begin{equation*}
I=B^{T} B+\varepsilon L \tag{4.10}
\end{equation*}
$$

Using the bounds for the norms of $Q$ and $M$ and (4.9), we obtain

$$
\begin{equation*}
\|B\| \leq\|Q\| \cdot\left\|P^{T}\left(P P^{T}\right)^{-1}\right\| \leq c \sqrt{N}\left\|\left(P P^{T}\right)^{-1}\right\|^{1 / 2} \tag{4.11}
\end{equation*}
$$

and

$$
\begin{equation*}
\|L\| \leq\left\|P^{T}\left(P P^{T}\right)^{-1}\right\|^{2} \cdot\|M\| \leq c_{0} N\left\|\left(P P^{T}\right)^{-1}\right\| \tag{4.12}
\end{equation*}
$$

Notice, that $B$ is not an orthogonal matrix, and thus cannot be a candidate for an equivalence matrix. However, we can modify $B$ in order to obtain an orthogonal matrix. Let $0 \leq \beta_{1}^{\varepsilon} \leq$ $\ldots \leq \beta_{d}^{\varepsilon}$ be the eigenvalues of $B^{T} B$ and $U_{B}$ be the orthogonal matrix such that

$$
U_{B}^{T} B^{T} B U_{B}=\operatorname{diag}\left(\beta_{1}^{\varepsilon}, \ldots, \beta_{d}^{\varepsilon}\right)
$$

If $\mathbf{x} \in \mathbb{R}^{d},\|\mathbf{x}\|=1$ is the eigenvector, corresponding to $\beta_{i}^{\varepsilon}$, then

$$
\begin{aligned}
\beta_{i}^{\varepsilon} & =\left\|B^{T} B \mathbf{x}\right\|=\|\mathbf{x}-\varepsilon L \mathbf{x}\| \geq\|\mathbf{x}\|-\|\varepsilon L \mathbf{x}\| \geq\|\mathbf{x}\|-\varepsilon\|L\| \cdot\|\mathbf{x}\| \\
& =1-\varepsilon\|L\| \geq 1-(1-\delta)\left(c_{0} N\left\|\left(P P^{T}\right)^{-1}\right\|\right)^{-1} \cdot c_{0} N\left\|\left(P P^{T}\right)^{-1}\right\|=\delta
\end{aligned}
$$

where we have used (4.12) and the inequality for $\varepsilon$. This fact allows us to construct

$$
\Lambda=\Lambda(\varepsilon):=\operatorname{diag}\left(\frac{1}{\sqrt{\beta_{1}^{\varepsilon}}}, \ldots, \frac{1}{\sqrt{\beta_{d}^{\varepsilon}}}\right)
$$

and consider the matrix

$$
\begin{equation*}
A=A(\varepsilon):=B U_{B} \Lambda U_{B}^{T} \tag{4.13}
\end{equation*}
$$

Clearly, $A$ is orthogonal since

$$
A^{T} A=U_{B} \Lambda U_{B}^{T} B^{T} B U_{B} \Lambda U_{B}^{T}=U_{B} \Lambda \operatorname{diag}\left(\beta_{1}^{\varepsilon}, \ldots, \beta_{d}^{\varepsilon}\right) \Lambda U_{B}^{T}=I
$$

Moreover, we will show that $\|A P-Q\| \leq \varepsilon \tilde{c} N^{2}$ for the constant $\tilde{c}$ defined in the theorem. We write

$$
\begin{equation*}
A P-Q=(A-B) P+(B P-Q)=B U_{B}(\Lambda-I) U_{B}^{T} P+(B P-Q) \tag{4.14}
\end{equation*}
$$

and compute the difference $B P-Q$. Multiplication of (4.7) on the right by $P^{T}$ leads to $P^{T} P P^{T}=Q^{T} Q P^{T}+\varepsilon M P^{T}$, which gives $P^{T}=Q^{T} B+\varepsilon M P^{T}\left(P P^{T}\right)^{-1}$, and we have $P=B^{T} Q+\varepsilon\left(P P^{T}\right)^{-1} P M^{T}$. We multiply the last equation on the left by $B$ to derive $B P=B B^{T} Q+\varepsilon B\left(P P^{T}\right)^{-1} P M^{T}$, and therefore

$$
\begin{equation*}
B P-Q=\left(B B^{T}-I\right) Q+\varepsilon B\left(P P^{T}\right)^{-1} P M^{T}=\varepsilon\left(B\left(P P^{T}\right)^{-1} P M^{T}-L Q\right) \tag{4.15}
\end{equation*}
$$

where in the last equality we have used (4.10). It follows from (4.14) and (4.15) that

$$
\begin{equation*}
\|A P-Q\| \leq\left\|B U_{B}(\Lambda-I) U_{B}^{T} P\right\|+\varepsilon\left\|B\left(P P^{T}\right)^{-1} P M^{T}-L Q\right\| . \tag{4.16}
\end{equation*}
$$

We next estimate each of the norms on the right hand side. Using the lower bound for $\beta_{i}^{\varepsilon}$ and (4.12), we have

$$
\begin{aligned}
\|\Lambda-I\| & =\max _{i=1, \ldots, d}\left|\frac{1}{\sqrt{\beta_{i}^{\varepsilon}}}-1\right|=\max _{i=1, \ldots, d} \frac{\left|1-\sqrt{\beta_{i}^{\varepsilon}}\right|}{\sqrt{\beta_{i}^{\varepsilon}}} \leq \frac{1}{\sqrt{\delta}} \max _{i=1, \ldots, d}\left|1-\sqrt{\beta_{i}^{\varepsilon}}\right| \\
& =\frac{1}{\sqrt{\delta}} \cdot \max _{i=1, \ldots, d} \frac{\left|1-\beta_{i}^{\varepsilon}\right|}{1+\sqrt{\beta_{i}^{\varepsilon}}} \leq \frac{1}{\sqrt{\delta}} \cdot \max _{i=1, \ldots, d}\left|1-\beta_{i}^{\varepsilon}\right| \leq \frac{1}{\sqrt{\delta}}\left\|I-B^{T} B\right\| \\
& =\frac{\varepsilon\|L\|}{\sqrt{\delta}} \leq \frac{\varepsilon c_{0} N\left\|\left(P P^{T}\right)^{-1}\right\|}{\sqrt{\delta}}
\end{aligned}
$$

The last inequality, the bounds for the norms of $B$ and $P$ and the fact that $\left\|U_{B}\right\|=\left\|U_{B}^{T}\right\|=1$ give

$$
\begin{align*}
\left\|B U_{B}(\Lambda-I) U_{B}^{T} P\right\| & \leq\|B\|\|\Lambda-I\|\|P\|  \tag{4.17}\\
& \leq c \sqrt{N}\left\|\left(P P^{T}\right)^{-1}\right\|^{1 / 2} c \sqrt{N} \frac{1}{\sqrt{\delta}} \varepsilon c_{0} N\left\|\left(P P^{T}\right)^{-1}\right\| \\
& =\frac{\varepsilon}{\sqrt{\delta}} c_{0} c^{2} N^{2}\left\|\left(P P^{T}\right)^{-1}\right\|^{3 / 2}
\end{align*}
$$

The second norm in (4.16) is evaluated, using (4.9), (4.11), (4.12) and the bounds for the norms of $M$ and $Q$, as follows:

$$
\begin{align*}
\left\|B\left(P P^{T}\right)^{-1} P M^{T}-L Q\right\| & \leq\left\|B\left(P P^{T}\right)^{-1} P M^{T}\right\|+\|L Q\|  \tag{4.18}\\
& \leq\|B\|\left\|\left(P P^{T}\right)^{-1} P\right\|\left\|M^{T}\right\|+\|L\|\|Q\| \\
& \leq 2 c c_{0} N \sqrt{N}\left\|\left(P P^{T}\right)^{-1}\right\| \leq 2 c c_{0} N^{2}\left\|\left(P P^{T}\right)^{-1}\right\|
\end{align*}
$$

Substitution of (4.17) and (4.18) in (4.16) results in

$$
\|A P-Q\| \leq \varepsilon c c_{0}\left\|\left(P P^{T}\right)^{-1}\right\|\left(c \delta^{-1 / 2}\left\|\left(P P^{T}\right)^{-1}\right\|^{1 / 2}+2\right) N^{2}
$$

and the proof is completed.
Unfortunately, the converse of this theorem is in general false, and the following theorem holds.

Theorem 4.3 For any positive constants $c, c_{0}, \tilde{c}$, and for any $0<\varepsilon \leq \frac{1}{2} c^{2} c_{0}^{-1}$, we can find d, $N$, two collections of $N$ points $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ in $\mathbb{R}^{d}$ and an orthogonal matrix $A$, such that $\operatorname{rank}(P)=d,\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\| \leq c$ and $\left\|\mathbf{q}_{i}-\overline{\mathbf{q}}\right\| \leq c, i=1, \ldots, N$, $\|A P-Q\| \leq \varepsilon \tilde{c} N^{2}$, but $P^{T} P=Q^{T} Q+\varepsilon M$, where $M$ is a matrix for which for at least one entry $\left|m_{i j}\right| \geq c_{0}$.

Proof. Consider any constants $c, c_{0}, \tilde{c}$, $d$ a positive integer, and $N=2 d$. Let $\left\{\mathbf{e}_{1}, \ldots, \mathbf{e}_{d}\right\}$ be the canonical basis for $\mathbb{R}^{d}$, and let $\mathcal{P}=\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right\}$ be the collections of points, where $\mathbf{p}_{2 i-1}=\frac{c}{\sqrt{2}} \mathbf{e}_{i}$ and $\mathbf{p}_{2 i}=-\frac{c}{\sqrt{2}} \mathbf{e}_{i}$ for $i=1, \ldots, d$, and $\mathcal{Q}=\left\{\mathbf{q}_{1}, \ldots, \mathbf{q}_{N}\right\}$ be such that $\mathbf{q}_{1}=$ $\mathbf{q}_{2}=\mathbf{0}$ and $\mathbf{q}_{j}=\mathbf{p}_{j}, j=2, \ldots, N$. A simple computation verifies that $\overline{\mathbf{p}}=\overline{\mathbf{q}}=\mathbf{0}$, and therefore, $\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\|=\left\|\mathbf{p}_{i}\right\|=c / \sqrt{2}<c$. Similarly, $\left\|\mathbf{q}_{i}-\overline{\mathbf{q}}\right\|=\left\|\mathbf{q}_{i}\right\|<c$. If $A=I$, then $A P-Q=P-Q$,

$$
(P-Q)^{T}(P-Q)=\frac{c^{2}}{2}\left(\begin{array}{rrrrr}
1 & -1 & 0 & \cdots & 0 \\
-1 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
& \vdots & & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{array}\right)
$$

| N | $\mathrm{d}=2$ | $\mathrm{~d}=3$ | $\mathrm{~d}=4$ |
| ---: | :---: | :---: | :---: |
| 8 | 0.9468 | 0.7066 | 0.5333 |
| 16 | 0.8403 | 0.6470 | 0.4670 |
| 32 | 0.6114 | 0.5323 | 0.3984 |
| 64 | 0.4622 | 0.4595 | 0.3724 |
| 128 | 0.3829 | 0.3626 | 0.2839 |
| 256 | 0.2709 | 0.2327 | 0.2128 |
| 512 | 0.2002 | 0.1760 | 0.1566 |
| 1024 | 0.1415 | 0.1295 | 0.1182 |

Table 1: Simulation results.
and therefore $\lambda_{\max }\left((P-Q)^{T}(P-Q)\right)=c^{2}$, which gives that $\|P-Q\|=c$. We compute directly that

$$
P^{T} P-Q^{T} Q=\frac{c^{2}}{2}\left(\begin{array}{rrrrc}
1 & -1 & 0 & \cdots & 0 \\
-1 & 1 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
& \vdots & & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 0
\end{array}\right)=\varepsilon M
$$

For any $\varepsilon \leq \frac{1}{2} c^{2} c_{0}^{-1}$, we have that $\left|m_{11}\right|=\frac{c^{2}}{2 \varepsilon} \geq c_{0}$, but if $2 d=N$ is large enough, namely

$$
2 d=N \geq \sqrt{\frac{c}{\varepsilon \tilde{c}}},
$$

we have that $\varepsilon \tilde{c} N^{2} \geq c=\|A P-Q\|$, and the proof is completed.
Finally, we verify the theoretical results from Theorem 4.2 by performing a series of numerical experiments. For each pair $(d, N), d \in\{2,3,4\}, N \in\left\{2^{n}: 3 \leq n \leq 10\right\}$, we choose in random 1000 collections $\mathcal{P}$ of $N$ uniformly distributed points inside the unit sphere and 1000 collections $\mathcal{P}$ of $N$ uniformly distributed points on the unit sphere. We select $\delta=0.9, c_{0}=1, \varepsilon=\frac{1}{2}(1-\delta)\left(\left\|\left(P P^{T}\right)^{-1}\right\| N c_{0}\right)^{-1}=0.05\left(\left\|\left(P P^{T}\right)^{-1}\right\| N\right)^{-1}$. The matrix $Q$ is then generated so that (4.7) holds, $A$ is computed according to (4.13), and $c:=\max _{i=1, \ldots, N}\left\{\left\|\mathbf{p}_{i}-\overline{\mathbf{p}}\right\|,\left\|\mathbf{q}_{i}-\overline{\mathbf{q}}\right\|\right\}$. For each pair $(d, N)$ the biggest ratio $\|A P-Q\| /\left(\varepsilon \tilde{c} N^{2}\right)$ (among the 2000 choices) is recorded in Table 1. It is clearly seen that the empirical results confirm our theoretical bound.

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## References

[1] A. Bekir, S. Golomb, There are no further counterexample to Sophie Piccard's theorem, IEEE Transactions on Information Theory, 53 (2007), 2864-2867.
[2] G. Bloom, A counterexample to a theorem of Sophie Piccard, Journal of Combinatorial Theory, 22 (1977) 378-379.
[3] M. Boutin, G. Kemper, On reconstructing n-point configurations from the distribution of distances or areas, Advances in Applied Mathematics, 32 (2004) 709-735.
[4] M. Boutin, G. Kemper, Which point configurations are determined by the distribution of their pairwise distances?, International Journal of Computational Geometry ${ }^{8}$ Applications, 17 (2007) 31-43.
[5] B. Dekster, J. Wilker, Edge lengths guaranteed to form a simplex, Archiv der Mathematik, 49 (1987) 351-366.
[6] J. Dongarra, D. Sorensen, A fully parallel algorithm for the symmetric eigenvalue problem, SIAM Journal on Scientific and Statistical Computing, 8 (1987), 139-154.
[7] L. Dorst, First order error propagation of the Procrustes method for 3D attitude estimation, IEEE Transactions of Pattern Analysis and Machine Intelligence, 27:2 (2005), 221-229.
[8] J. Gower, Generalized Procrustes analysis, Psychometrika, 40 (1975), 33-51.
[9] J. Gower, G. Dijksterhuis, Procrustes problems, Oxford Statistical Science Series, Oxford University Press, 2004.
[10] B. Green, The orthogonal approximation of an oblique structure in factor analysis, Psychometrika, 17 (1952) 429-440.
[11] R. Hanson, M. Norris, Analysis of measurements based on the singular value decomposition, SIAM J. Sci. Stat. Comput., 2 (1981) 363-373.
[12] N. Higham, Functions of matrices: theory and computation, SIAM, 2008.
[13] B. Horn, H. Hilden, S. Negahdaripour, Closed-form solution of absolute orientation using orthonormal matrices, Journal of the Optical Society of America, 5 (1988), 1127-1135.
[14] S. Rusinkiewicz, M. Levoy, Efficient variants of the ICP algorithm, Proceedings, International Conference on 3-D Digital Imaging and Modeling, 3 (2001), 145-152.
[15] P. Schönemann, A generalized solution of the orthogonal Procrustes problem, Psychometrika, 31 (1966) 1-10.
[16] I. Söderkvist, Perturbation analysis of the orthogonal Procrustes problem, BIT, 33:4 (1993), 687-694.
[17] Z. Zhang, Iterative point matching for registration of free-form curves and surfaces, International Journal of Computer Vision, 13:2 (1994), 119-152.


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