Least-Squares Transformations between Point-Sets

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Abstract. This paper derives formulas for least-squares transformations between point-sets in $\mathbb{R}^d$. We consider affine transformations, with optional constraints for linearity, scaling, and orientation. We base the derivations hierarchically on reductions, and use trace manipulation to achieve short derivations. For the unconstrained problems, we provide a new formula which maximizes the orthogonality of the transform matrix.

Keywords: least-squares, transformation, point-set, rank-deficient.

1 Background

Let $P = [p_1, \ldots, p_m] \in \mathbb{R}^{d \times m}$ and $R = [r_1, \ldots, r_n] \in \mathbb{R}^{d \times n}$. We shall consider affine functions of the form

$$f : \mathbb{R}^d \to \mathbb{R}^d : f(x) = QSx + t, \tag{1}$$

where $Q \in \mathbb{R}^{d \times d}$, $Q^T Q = I_d$, $S \in \mathbb{R}^{d \times d}$, $S^T = S$, and $t \in \mathbb{R}^d$. Given P and R, and possible additional constraints for Q, S, and t, the problem is to find Q, S, and t such that the following least-squares error E is minimized:

$$E(Q, S, t) = \sum_{i=1}^{m} \sum_{j=1}^{n} w_{ij} \left\| QSp_i + t - r_j \right\|^2, \tag{2}$$

where $W \in \mathbb{R}^{m \times n}$, $W_{ij} = w_{ij} \geq 0$, $W \neq 0$, and the norm is induced by the standard inner product $\langle x, y \rangle$. We shall call this problem *unpaired*. Later we will define a simpler paired problem, to which the unpaired problem can be reduced to. Since multiplying E by a positive constant does not change the solution of the minimization problem, it is without loss of generality to assume that $\sum_{i=1}^{m} \sum_{j=1}^{n} w_{ij} = 1$. However, we shall derive the results without using this assumption.

Let $A \in \mathbb{R}^{d \times d}$ be an arbitrary matrix, and $A = UDV^T$ its singular value decomposition. Let $Q = UV^T$ and $S = VDV^T$. Then $Q^T Q = I_d$, $S^T = S$, and $A = QS$. Therefore all matrices can be decomposed as required in the problem description. We will abbreviate $\langle x \rangle = \langle x, x \rangle$, always use the Frobenius norm for matrices and vectors, and denote $\mathbb{1}_n = [1, \ldots, 1]^T \in \mathbb{R}^{n \times 1}$.

J.-K. Kämäräinen and M. Koskela (Eds.): SCIA 2013, LNCS 7944, pp. 501–511, 2013.

1.1 Constraints and Reductions

Let $D \in \mathbb{R}^{d \times d}$ be diagonal, and $s \in \mathbb{R}$. Several variants of the original problem can be devised depending on the chosen constraints:

- Q: orthogonal ($Q^T Q = I_d$), or identity ($Q = I_d$).
- S: scaling ($S^T = S$), conformal scaling ($S = sI_d$), or rigid ($S = I_d$).
- t: affine (t arbitrary), or linear ($t = 0$).
- det(QS): non-oriented ($\det(QS)$ arbitrary), or oriented ($\det(QS) \geq 0$ or $\det(QS) \leq 0$).

Different combinations of these constraints give 24 variants of the problem. Fortunately, many of the variants can be reduced to each other. In particular,

- an affine problem can be reduced to a linear problem,
- an unpaired problem can be reduced to a paired problem,
- a conformal problem can be reduced to a rigid problem, and
- the solution to an oriented problem can be obtained quickly from the solution to the corresponding non-oriented problem.

It can be shown for the linear problem, and for the scaling problem, that if the non-oriented solution has a different orientation than the oriented solution, and a smaller error, then the oriented solution necessarily has $\det(A) = 0$. We leave these oriented problems open.

1.2 Special Cases

The following problems are special cases of this problem:

- Let $n = m$ and $W = I_n$. Then the problem is to minimize

$$\sum_{i=1}^{n} \|QSp_i + t - r_i\|^2 , \tag{3}$$

  i.e. to find a least-squares transformation between paired point-sets. We shall call this problem *paired*.
- Let $n = m$ and W be diagonal. Then the problem is to minimize

$$\sum_{i=1}^{n} w_{ii} \|QSp_i + t - r_i\|^2 , \tag{4}$$

  i.e. to find a weighted least-squares transformation between paired point-sets.
- Let $p : \mathbb{R}^d \to \mathbb{R}$ be defined by $p(x) = \frac{1}{m} \sum_{i=1}^{m} N(x; p_i, \sigma^2)$, where N is the probability density function of a multivariate normal distribution with mean p_i and covariance $\sigma^2 I_d$ (this is called a Gaussian mixture model). Let $w_{ij} = P(i|r_j)$ be the probability of the point r_j being generated by the i:th component of the mixture model. Then minimizing E results in a transformation which maximizes the likelihood of the points in R being generated by the mixture model. In particular, this is used as a component in the Coherent Point Drift algorithm [10].

1.3 Applications

Many algorithms use a least-squares transformation between point-sets as a sub-algorithm. In *point-pattern matching*, see e.g. [17] [16], one is given two unordered point-sets, not necessarily of the same cardinality, and then asked to find a transformation which best matches the point-sets, for some criterion of matching, and some class of transformations. In *point-set registration*, the problem is the same as in point-pattern matching, with the added information that a relatively accurate initial transformation is known so that local optimization suffices to find a global optimum. In both of these fields of study, the least-squares transformations are used either iteratively to get closer to a local optimum, or to improve the transformation between a given candidate matching between the point-sets. The Iterative Closest Point algorithms form a popular family of point-set registration algorithms which use least-squares transformations iteratively [4] [3] [5] [6]. The Coherent Point Drift registration algorithm [10] is a recent point-set registration algorithm which uses the most general form of a least-squares transformation in this paper in its expectation maximization algorithm. While that paper specifically demonstrates the algorithm with non-oriented affine and oriented conformal affine transformations, we note that the underlying family of transformations can be replaced with any of the transformations given in this paper. Point-pattern matching and point-set registration are applied in stereo image matching, content-based image retrieval, image registration, shape recognition, or to reconstruct a representation of an object from multiple overlapping measurements, as when scanning statues from multiple viewpoints by range scanners [7].

1.4 Previous Work

This section reviews previous work done on this problem. Green [2] gives a solution to the paired non-oriented rigid problem in $\mathbb{R}^d$ based on Lagrange multipliers and the inverse square-root of the eigenvalue decomposition of RP^TPR^T. The solution requires RP^TPR^T to be invertible, which is an unnecessary assumption. Arun et al. [13] give a solution to the paired non-oriented rigid problem in $\mathbb{R}^3$ based on the singular value decomposition (SVD). While their interest is actually on the oriented problem, they fail to see how to move forward if the resulting transformation happens to be a reflection. Instead, they accept that the algorithm might sometimes fail, and then give arguments why that should not happen often. It would be trivial to generalize their result to $\mathbb{R}^d$, but for some reason they do not do that. Horn [14] gives a solution to the paired oriented rigid problem in $\mathbb{R}^3$ based on quaternions. Because of the use of quaternions, this solution does not generalize to other dimensions. In another paper, Horn et al. [1] give a solution to the non-oriented conformal problem in $\mathbb{R}^3$ using an inverse square-root of an eigenvalue decomposition which is very similar to what is in the Green paper, but specific to $\mathbb{R}^3$. Walker et al. [9] give a solution to the paired oriented rigid problem in $\mathbb{R}^3$ based on dual quaternions. This algorithm is specific to $\mathbb{R}^3$. Schönemann [11] gives a solution to the paired non-oriented rigid problem in $\mathbb{R}^d$ based on the eigenvalue decomposition. While mathematically correct, the author fails to see that the algorithm actually computes the SVD, but in an inefficient and inaccurate manner; the algorithm diagonalizes S^TS and SS^T to get the right and left singular vectors of S, respectively. Umeyama [15] gives a solution to the paired oriented conformal problem in $\mathbb{R}^d$ using Lagrange multipliers and the SVD. In this case the results correspond to ours, but the derivations are considerably longer than ours. Eggert et al. [12] compare four algorithms for solving the paired non-oriented rigid problem in $\mathbb{R}^3$. These algorithms are the ones above by Arun et al., Horn, Walker et al, and Umeyama. Eggert et al. found that these algorithms behaved very similarly on all measured aspects. The point-set registration algorithm of Myronenko et al. [10] motivates the generalization of the least-squares criterion to the unpaired case. Their results correspond to ours, with a specific matrix of probabilities for W.

Along with gathering multiple results together and deriving them in a uniform manner, our original contributions, to the best extent we are aware, are to give a new formula for the linear problem which maximizes the orthogonality of the transform matrix without assuming a full-rank P, and to derive the solution to the linear scaling problem.

2 Reduction from Affine to Linear

We will now derive the reduction from an affine problem to a linear problem. Let $A = QS$. The directional derivative of E with respect to t in direction $\Delta t \in \mathbb{R}^d$ is given by:

$$D_t E(A, t) = 2 \left\langle \sum_{i=1}^{m} \sum_{j=1}^{n} w_{ij} \left(A p_i + t - r_j \right), \Delta t \right\rangle . \tag{5}$$

Setting this to zero, and substituting all standard basis vectors one by one for Δt implies that at an extremum point it necessarily holds that

$$\sum_{i=1}^{m} \sum_{j=1}^{n} w_{ij} \left(A p_i + t - r_j \right) = 0, \tag{6}$$

which in turn is equivalent to

$$A\bar{p} + t = \bar{r}, \tag{7}$$

where

$$\begin{aligned} \bar{p} &= \frac{PW\mathbb{1}_n}{\mathbb{1}_m^T W \mathbb{1}_n}, \text{ and} \\ \bar{r} &= \frac{RW^T\mathbb{1}_m}{\mathbb{1}_m^T W \mathbb{1}_n}. \end{aligned} \tag{8}$$

That is, if t is not restricted, then at an extremum point it holds that the centroid of P should be mapped to the centroid of R. Since it can be shown that $E(A, t)$

is convex in t, the extremum point is a minimum point. This gives us a way to reduce an affine problem to a linear problem. At a minimum point the error is given by

$$E(A) = \sum_{i=1}^{m} \sum_{j=1}^{n} \langle A(p_i - \bar{p}) - (r_j - \bar{r}) \rangle . \tag{9}$$

Thus to solve an affine problem, it is enough to solve a linear problem for the centered point-sets, after which we can compute the optimal t from $t = \bar{r} - A\bar{p}$.

3 Reduction from Unpaired to Paired

We will now derive the reduction from an unpaired problem to a paired problem. Suppose the problem has already been reduced from affine to linear. Let $A = QS$, and $K \in \mathbb{R}^{m \times n}$, where $k_{ij} = \sqrt{w_{ij}}$, and let $K_{i:}$ denote the i:th row of K. We will denote by $\lceil K_{i:} \rfloor$ the diagonal matrix whose diagonal elements are given by $K_{i:}$. Then the reduction is as follows.

$$\begin{aligned}
E(A) &= \sum_{i=1}^{m} \sum_{j=1}^{n} w_{ij} \left\| Ap_i - r_j \right\|^2 \\
&= \sum_{i=1}^{m} \sum_{j=1}^{n} \left\| Ak_{ij}p_i - k_{ij}r_j \right\|^2 \\
&= \sum_{i=1}^{m} \left\| [Ak_{i1}p_i - k_{i1}r_1, \cdots, Ak_{in}p_i - k_{in}r_n] \right\|^2 \\
&= \sum_{i=1}^{m} \left\| A[k_{i1}p_i, \cdots, k_{in}p_i] - [k_{i1}r_1, \cdots, k_{in}r_n] \right\|^2 \\
&= \sum_{i=1}^{m} \left\| Ap_iK_{i:} - R\lceil K_{i:} \rfloor \right\|^2 \\
&= \sum_{i=1}^{m} \left\| APe_iK_{i:} - R\lceil K_{i:} \rfloor \right\|^2 \\
&= \left\| [APe_1K_{1:} - R\lceil K_{1:} \rfloor, \ldots, APe_mK_{m:} - R\lceil K_{m:} \rfloor] \right\|^2 \\
&= \left\| AP\,[e_1K_{1:}, \ldots, e_mK_{m:}] - R\,[\lceil K_{1:} \rfloor, \ldots, \lceil K_{m:} \rfloor] \right\|^2 \\
&= \sum_{i=1}^{mn} \left\| A\widehat{p}_i - \widehat{r}_i \right\|^2 ,
\end{aligned} \tag{10}$$

where

$$\begin{aligned}
\widehat{P} &= P[e_1K_{1:}, \ldots, e_mK_{m:}] \in \mathbb{R}^{d \times (mn)}, \\
\widehat{R} &= R\,[\lceil K_{1:} \rfloor, \ldots, \lceil K_{m:} \rfloor] \in \mathbb{R}^{d \times (mn)}, \\
[e_1, \ldots, e_m] &= I_m .
\end{aligned} \tag{11}$$

The problem with this reduction is that these matrices are too big to be practically useful. However, this problem can be avoided by noticing that the matrices that are of actual interest are $\widehat{R}\widehat{P}^T$ and $\widehat{P}\widehat{P}^T$. They are given by

$$\begin{aligned} \widehat{P}\widehat{P}^T &= P \lceil W\mathbb{1}_n \rfloor P^T, \text{ and} \\ \widehat{R}\widehat{P}^T &= RW^T P^T. \end{aligned} \tag{12}$$

4 Linear Problem

We will now derive the solution to the unconstrained linear problem. Let $A = QS$. Suppose the problem has already been reduced from affine to linear, and from unpaired to paired. Then the error is given by

$$\|AP - R\|^2 = \text{tr}\left(A^T APP^T\right) - 2\text{tr}\left(A^T RP^T\right) + \text{tr}\left(RR^T\right). \tag{13}$$

The directional derivative of $\|AP - R\|^2$ with respect to A in direction ΔA is given by

$$D_A \|AP - R\|^2 = 2\text{tr}\left(\Delta A^T (APP^T - RP^T)\right). \tag{14}$$

Substituting $\Delta A = e_i {e_j}^T$ for all $i, j \in [1, d]$ shows that at an extremum point it necessarily holds that

$$APP^T = RP^T. \tag{15}$$

Since it can be shown that $\|AP - R\|$ is convex with respect to A, this is a necessary and sufficient condition for a minimum point. Let

$$\begin{aligned} PP^T &= U_P D_P [X, 0] V^T, \text{ and} \\ RP^T &= U_R D_R [X, 0] V^T \end{aligned} \tag{16}$$

be the generalized singular value decomposition [18] between PP^T and RP^T, where $U_P, U_R \in \mathbb{R}^{d\times d}$ are orthogonal, $D_P, D_R \in \mathbb{R}^{d\times r}$, $X \in \mathbb{R}^{r\times r}$ is non-singular, $V \in \mathbb{R}^{d\times d}$ is orthogonal, $0 \in \mathbb{R}^{r\times(d-r)}$ is the zero matrix, and

$$r = \text{rank}(P) = \text{rank}\left(\begin{bmatrix} PP^T \\ RP^T \end{bmatrix}\right). \tag{17}$$

It holds that D_P is diagonal, and that both ${D_P}^T D_P$ and ${D_R}^T D_R$ are diagonal, with ${D_P}^T D_P + {D_R}^T D_R = I_r$. The D_R is block-diagonal with diagonal blocks; it is not diagonal unless $r = d$. Precisely, let $U_P = [U_{P_1}, U_{P_2}]$, $U_R = [U_{R_1}, U_{R_2}]$, $D_P = \begin{bmatrix} D_{P_1} \\ 0 \end{bmatrix}$, and $D_R = \begin{bmatrix} 0 \\ D_{R_2} \end{bmatrix}$, where $U_{P_1}, U_{R_2} \in \mathbb{R}^{d\times r}$, $U_{P_2}, U_{R_1} \in \mathbb{R}^{d\times(d-r)}$, and $D_{P_1}, D_{R_2} \in \mathbb{R}^{r\times r}$ are diagonal, with D_{P_1} non-singular. Then the minimum condition is equivalent to

$$A = U_{R_2} D_{R_2} D_{P_1}^{-1} U_{P_1}^T + M{U_{P_2}}^T, \tag{18}$$

where $M \in \mathbb{R}^{d\times(d-r)}$ is arbitrary. We can use this freedom to select additional properties for the optimal A. For example, setting $M = 0$ minimizes $\|A\|$ (then $A = RP^{+}$, where $+$ is the Moore-Penrose pseudo-inverse). Since this would lead to a singular A, we propose instead to minimize the orthogonality error

$$\left\|A^T A - I_d\right\| = \left\|A_1 {A_1}^T - I_d + MM^T\right\|, \tag{19}$$

where $A_1 = U_{R_2} D_{R_2} D_{P_1}^{-1} U_{P_1}^T$. The directional derivative of $\left\|A^T A - I_d\right\|^2$ with respect to M in direction ΔM is given by

$$D_M \left\|A^T A - I_d\right\|^2 = 4\mathrm{tr}\left(\Delta M M^T (MM^T + A_1 {A_1}^T - I_d)\right). \tag{20}$$

Therefore at a point of minimum orthogonality error it necessarily holds that

$$(MM^T + A_1 {A_1}^T - I_d)M = 0. \tag{21}$$

Let $M = U_M D_M {V_M}^T$ be the *thin* singular value decomposition of M, where $U_M \in \mathbb{R}^{d\times(d-r)}$, $D_M \in \mathbb{R}^{(d-r)\times(d-r)}$, and $V_M \in \mathbb{R}^{(d-r)\times(d-r)}$. The necessary condition is then equivalent to

$$D_{Mii} = 0 \text{ or } A_1 {A_1}^T U_{M:i} = (1 - D_{Mii}^2) U_{M:i}. \tag{22}$$

for all $i \in [1, d-r]$. The necessary condition states that either $D_{Mii} = 0$, or $U_{M:i}$ and $(1 - D_{Mii}^2)$ are an eigen-vector and its eigen-value, respectively, of $A_1 {A_1}^T$. Fortunately, an eigen-value decomposition of $A_1 {A_1}^T$ is readily available as

$$A_1 {A_1}^T = U_R \begin{bmatrix} 0 & 0 \\ 0 & D_{R_2}^2 D_{P_1}^{-2} \end{bmatrix} U_R^T. \tag{23}$$

Since V_M cancels in MM^T, we may arbitrarily choose $V_M = I_{d-r}$. If we set $D_{Mii} = 0$, then the choice of $U_{M:i}$ does not affect the matrix M, and we may as well choose an eigen-vector of $A_1 {A_1}^T$. Therefore, M can be written in the form

$$M = U_R J \begin{bmatrix} D_M \\ 0 \end{bmatrix}, \tag{24}$$

where $J \in \mathbb{R}^{d\times d}$ is a permutation matrix. Now

$$\left\|A^T A - I_d\right\|^2 = \left\|\begin{bmatrix} -I_{d-r} & 0 \\ 0 & D_{R_2}^2 D_{P_1}^{-2} - I_r \end{bmatrix} + J \begin{bmatrix} {D_M}^2 & 0 \\ 0 & 0 \end{bmatrix} J^T \right\|^2, \tag{25}$$

which is minimized by $J = I_d$, and $D_M = I_{d-r}$. The minimum orthogonality error is then given by

$$\left\|A^T A - I_d\right\|^2 = \left\|D_{R_2}^2 D_{P_1}^{-2} - I_r\right\|^2. \tag{26}$$

The matrix A which minimizes the orthogonality error subject to minimizing the error is given by

$$A = U_R \begin{bmatrix} 0 & I_{d-r} \\ D_{R_2} D_{P_1}^{-1} & 0 \end{bmatrix} {U_P}^T. \tag{27}$$

5 Linear Rigid Problem

We will now derive the solution to the linear rigid problem. Suppose the problem has already been reduced from affine to linear, and from unpaired to paired. Let $Q \in \mathbb{R}^{d \times d}$ be an orthogonal matrix and $M \in \mathbb{R}^{d \times d}$ be an arbitrary matrix. Since

$$\|Q - M\|^2 = \operatorname{tr}(I_d) - 2tr(Q^T M) + \operatorname{tr}\left(M^T M\right), \tag{28}$$

minimizing $\|Q - M\|$ is equivalent to maximizing $\operatorname{tr}\left(Q^T M\right)$. Let $M = UDV^T$ be the singular value decomposition of M, where $U, V \in \mathbb{R}^{d \times d}$ are orthogonal and $D \in \mathbb{R}^{d \times d}$ is diagonal. Now

$$\begin{aligned} \operatorname{tr}\left(Q^T M\right) &= \operatorname{tr}\left(Q^T UDV^T\right) \\ &= \operatorname{tr}\left(V^T Q^T UD\right) \\ &= \operatorname{tr}(XD), \end{aligned} \tag{29}$$

where $X = V^T Q^T U$ is an arbitrary orthogonal matrix. Furthermore,

$$\operatorname{tr}(XD) = \sum_{i=1}^{d} X_{ii} D_{ii}, \tag{30}$$

since D is diagonal. Now, $|X_{ii}|^2 \leq \sum_{k=1}^{d} |X_{ki}|^2 \leq 1$, since the columns of X are unit vectors. Over arbitrary matrices X, without the orthogonality constraint, but with the diagonal constraint, $\forall i : X_{ii} = 1$ maximizes $\operatorname{tr}(XD)$, since the diagonal elements of D are non-negative. However, the identity matrix I_d is an orthogonal matrix with this property. Thus $X = V^T Q^T U = I_d$, from which it follows that

$$Q = UV^T. \tag{31}$$

Similarly, $Q = -UV^T$ maximizes the error. Now

$$\|QP - R\|^2 = \operatorname{tr}\left(PP^T\right) - 2\operatorname{tr}\left(Q^T RP^T\right) + \operatorname{tr}\left(RR^T\right), \tag{32}$$

which minimizes (maximizes) when $\operatorname{tr}\left(Q^T RP^T\right)$ maximizes (minimizes). Therefore, the optimal Q is given by the previous result, where $M = RP^T$. That is, if UDV^T is the singular value decomposition of RP^T, then the optimal Q is given by $Q = UV^T$.

5.1 Orientation

The corresponding oriented solution is obtained from the non-oriented solution as follows. If Q is required to have $\det(Q) = \pm 1$, then define $D = \lceil 1, \ldots, 1, \pm \det(UV^T) \rfloor$, and compute

$$Q = UDV^T. \tag{33}$$

Here we have assumed that in the singular value decomposition the singular values are sorted from greatest to smallest downwards. Thus replacing the smallest singular value incurs the smallest error.

6 Varying S

Suppose the problem has already been reduced from affine to linear, and from unpaired to paired. Then the error E can be written as

$$E(Q,S) = \mathrm{tr}\left(S^2PP^T\right) - 2\mathrm{tr}\left(SQ^TRP^T\right) + \mathrm{tr}\left(RR^T\right). \tag{34}$$

The directional derivative of E with respect to S in direction $\Delta S \in \mathbb{R}^{d\times d}$, where $\Delta S^T = \Delta S$, is given by

$$D_S E(Q,S) = \mathrm{tr}\left(\Delta S(PP^TS + SPP^T - 2Q^TRP^T)\right). \tag{35}$$

Therefore, at an extremum point it necessarily holds that

$$\mathrm{tr}\left(\Delta S(PP^TS + SPP^T - 2Q^TRP^T)\right) = 0, \tag{36}$$

for all valid variations ΔS.

7 Reduction from Conformal to Rigid

We will now derive the reduction from a conformal problem to a rigid problem. Suppose the problem has already been reduced from affine to linear, and from unpaired to paired. For the conformal problem, $S = sI_d$. Then the variation ΔS must also satisfy $\Delta S = \Delta s I_d$. Substituting this into Equation 36, the necessary condition for an extremum is then given by

$$\mathrm{tr}\left(\Delta s(2sPP^T - 2Q^TRP^T)\right) = 0. \tag{37}$$

Since this holds for all Δs,

$$s = \frac{\mathrm{tr}\left(Q^TRP^T\right)}{\mathrm{tr}\left(PP^T\right)}. \tag{38}$$

If Q is constrained to I_d, we are done. Otherwise, substituting s back into Equation 34, we get

$$E(Q) = -\frac{\mathrm{tr}\left(Q^TRP^T\right)^2}{\mathrm{tr}\left(PP^T\right)} + \mathrm{tr}\left(RR^T\right).$$

We are thus interested in either minimizing or maximizing $\mathrm{tr}\left(Q^TRP^T\right)$, which ever gives a greater absolute value. Substituting $S = I_d$ in Equation 34 shows that maximizing (minimizing) $\mathrm{tr}\left(Q^TRP^T\right)$ is equivalent to minimizing (maximizing) $\|QP - R\|^2$. Therefore, the minimizer Q for the conformal problem is either the maximizer or the minimizer Q for the rigid problem. In the solution for the linear rigid problem we showed that if UDV^T is the singular value decomposition of RP^T, then $\mathrm{tr}\left(Q^TRP^T\right)$ is maximized by UV^T, and minimized by $-UV^T$. Since both of these solutions give the same $\mathrm{tr}\left(Q^TRP^T\right)^2$, either one can be used. We choose $Q = UV^T$, since this results in $s \geq 0$. Now

$$s = \frac{\mathrm{tr}\left(D\right)}{\mathrm{tr}\left(PP^T\right)}. \tag{39}$$

7.1 Orientation

The determinant of QS is given by $\det(QS) = \det(Q)\det(S)$. If Q is constrained to I_d, and $\det(QS) = \det(S)$ is of the wrong sign, then the previous derivation can be repeated with s^2 instead of s to show that the optimal oriented transformation has $s = 0$. Therefore $S = 0$. Assume Q is not constrained to I_d. Since we chose $s \geq 0$, $\det(QS) \geq 0$ is equivalent to $\det(Q) \geq 0$. Therefore the optimal Q can be obtained by solving the oriented linear rigid problem.

8 Linear Scaling Problem

We will now derive the solution to the linear scaling problem. Suppose the problem has already been reduced from affine to linear, and from unpaired to paired. Now $Q = I_d$, and S is a symmetric matrix. We have already shown that at an extremum point it must hold that

$$\operatorname{tr}\left(\Delta S(PP^T S + SPP^T - 2RP^T)\right) = 0, \tag{40}$$

for all symmetric variations ΔS. By substituting $\Delta S = e_i {e_j}^T + e_j {e_i}^T$ for all $i, j \in [1, d]$, it can be seen that this is equivalent to $PP^T S + SPP^T - 2RP^T$ being skew-symmetric. Thus

$$PP^T S + SPP^T = RP^T + PR^T. \tag{41}$$

These types of equations are known as continuous Lyapunov equations, or more generally as Sylvester equations. It can be shown that S has a unique solution if and only if PP^T is invertible. A classic algorithm for solving Sylvester equations is given in [8]. In Matlab, continuous Lyapunov equations can be solved by the lyap function.

9 Conclusions

We derived formulas for finding constrained and unconstrained least-squares transformations between point-sets. These formulas work whether the point-sets are rank-deficient or not, and in any dimension. Using the generalized singular value decomposition, we derived a new formula for the unconstrained problem which maximizes the orthogonality of the transform matrix.

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