An Elastic Energy Minimization Framework for Mean Contour Calculation

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Abstract

In this paper we propose a contour mean calculation and interpolation method designed for averaging manual delineations of objects performed by experts and interpolate 3D layer stack images. The proposed method retains all visible information of the input contour set: the relative positions, orientations and size, but allows invisible quantities - parameterization and the centroid - to be changed. The chosen representation space - the position vector rescaled by square root velocity - is a real valued vector space on which the imposed $L^2$ metric is used to define the distance function. With respect to this representation the re-parameterization group acts by isometries and the distance has well defined meaning: the sum of the central second moments of the coordinate functions. To identify the optimal re-parameterization system and proper centroid we use double energy minimization realized in a variational framework.

1 Introduction

A specifically designed mathematical framework for two practical problems: contour averaging and interpolation is proposed and examined in this paper.
Object delineation is an important annotation step to create training data set for the supervised machine learning methods designed for object segmentation. Histopathology images, however rarely provide definite unambiguous object boundaries, often the delineations performed by experts do not agree. One plausible approach to create meaningful annotation samples is to accept the mean of many recommendations excluding some outliers. This approach requires well defined, meaningful metrics on the space of contours.

The resolution of several microscopy techniques in the direction of focusing (direction $Z$) is usually a magnitude less than the resolution of the stack images. Interpolation needs to be carried out in a principled manner to achieve good estimation for the accurate 3D measurements of the object physical quantities, such as surface area or volume. Interpolation can also be useful tool to track the progression of lesions in various diagnostic images.

The proposed method is designed to keep all visible information encoded in the set of the constituent contours including their relative displacement, hence essentially position vector based. The description of the contours by preselected position vector set (landmark points) is the approach of the early shape analysis techniques (with the identification of shape manifolds of $k$-points and the imposed Riemannian metric see for example [4]). On the other hand, the predetermined sampling strategy of the landmark points is related to the fixed parameterization of the contours. In the proposed model this restriction is relaxed and some tools borrowed from the elastic shape analysis [5] are used. The chosen contour representation is the position vector rescaled by square root velocity that - wrt a properly defined centroid - provides covariant description whilst retain all contextual information. It can be considered as the combination of the landmark based and the Square Root Velocity Function (SRVF) representations (for which the analysis of the existence of the optimal reparameterization is found in [1]). The proposed representation and the associated $L^2$ metric are exhaustively examined in this paper mentioning some perspective generalizations. References to the SRVF are also provided wherever informative/relevant.

The structure of the paper is the following. Section 2 presents the framework including numerical methods. Section 3 is dedicated to illustrative interpolation examples, section 4 concludes the paper with discussion and outlook. Appendices contain important proofs and derivations.

## 2 The contour averaging framework

We consider simple, planar contours used to delineate objects to be closed, continuous, one-parameter ($t \in [0, T]$) family objects with winding number one. From now on we simple refer them as 'contours’. The principal representations of contours are often given by position vector wrt some standard basis $i, j$ as $r(t) = x(t)i + y(t)j$, $r(0) = r(T)$ where $x(t), y(t)$ are the coordinate functions. The set of contours used to calculate their mean is referred as contour system.

To develop a framework for efficient contour mean calculation, first we assess
some natural conditions to be fulfilled by any model developed for this purpose:

A) Keep all visible information (relative positions, rotations, size) of the constituents, optimize only for non-visible ones

B) The mean contour derived from the system needs to be invariant for its constituents common translation, rotation, scaling (i.e. the mean of the transformed system is transformed in the same manner as the constituents)

C) The result of the mean determination must be independent of the parameterization of the constituents

The position vector representation obviously satisfies condition A. It also satisfies condition B, if the basis \( i, j \) is determined by the system itself. Condition C however cannot be fulfilled by this representation. One of the possibility to get simple parameterization-invariant representation - known from the shape analysis literature - is the choice of the square root velocity function (SRVF) \[6\]. SRVF however, does not retain the relative translation information. For this reason we use the combination of the position vector and the SRVF: the position, rescaled by square root velocity (Rescaled Position by Square Velocity or RPSV):

\[
q(t) = r(t) \sqrt{|\dot{r}(t)|}.
\]

The points of the position vector \( r(t) \) and its RPSV representation \( q(t) \) lie in the same direction \( u(t) = r(t) / |r(t)| = q(t) / |q(t)| \), hence reproducing the contour (its position vector) requires the determination of its length \( |r(t)| \) at each parameter value \( t \). This can be done iteratively using the Newton–Raphson method (see Appendix C).

2.1 Properties of the representation

Position vector representation \( r: [0, T] \rightarrow \mathbb{R}^2 \) is the vector space of coordinate function duplets, so its reparameterization \( q \)[\(^1\)]Equipped with the inner product

\[
\langle q_1, q_2 \rangle = \int q_1(t) \cdot q_2(t) \, dt
\]

(where \( q_1(t) \cdot q_2(t) \) is the dot product of the position vectors given at parameter value \( t \)) and the distance function based on the \( L^2 \) norm \( ||q||^2 = \langle q, q \rangle \):

\[
d^2(q_1, q_2) = \int (q_1(t) - q_2(t))^2 \, dt
\]

the space of the representations \( q \) becomes Hilbert space, denoted by \( \mathcal{H}_q \). With reference to the Appendix A here we asses the important properties of the chosen representaation:

\(^1\)Representations \( r \) and \( q \) are considered as two parameterization of the underlying space of function duplets.
1. The squared norm \( \|q\|^2 \) of any point in the representation space expresses the sum of the second central moments of the (coordinate functions of) contour \( r(t) \), consequently:

2. The distance function is invariant wrt the common reparameterization of points \( q_1, q_2 \to q_1 \circ \gamma, q_2 \circ \gamma \) and

3. The reparameterization group \( \Gamma = \{ \gamma | \gamma(t) > 0 \} \) acts by isometries wrt the chosen metric and composition, i.e. \( d^2(q_1, q_2) = d^2(q_1 \circ \gamma, q_2 \circ \gamma) \)

The properties above allows us to construct the mean contour in the quotient space \( \mathcal{H}_q/\Gamma \) satisfying the requirements \( A, B, C \) stipulated at the beginning of this section. The mean representation of a system of \( n \) representations \( q_1, q_2, \cdots q_n \) is defined to be:

\[
q(t) = \frac{1}{n} \sum_{i=1}^{n} q_i(t_i), \ t, t_i \in [0,T] \tag{4}
\]

where parameterizations \( t_i = \gamma_i(t) \) are the carefully selected points from the orbit of \( \Gamma \) the for which \( \sum_{i=1}^{n} d^2(q_i(t_i) - q(t)) \) is minimal. Formula (4) can be written directly in position vector ‘coordinates’ of the space \( \mathcal{H}_q \) and takes the form:

\[
r(t) \sqrt{|\dot{r}(t)|} = \frac{1}{n} \sum_{i=1}^{n} r_i(t_i) \sqrt{|\dot{r}_i(t_i)|}. \tag{5}
\]

Later in the paper we use mainly the direct (position vector) coordinates, not forgetting the underlying RPSV representation. We conclude this subsection with the statement: the mean contour is identified as the position vector associated with the mean of the RPSV representations.

### 2.2 Mean contour as a minimization problem

Properties 1-3 of RPSV (Properties of the representation) enable to construct the optimal parameterization of the system of contours in a simple way, i.e. choosing one of the constituent contour as ‘reference contour’ and calculate the optimal parameterization of the other contours wrt it, see Lemma A1 in Appendix A.

The minimization problem wrt a fixed origin (will be relaxed later), using direct position vector coordinates can be formulated as:

\[
\min_{\gamma_i} \sum_{i=1}^{n} \int \left(r(t) \sqrt{|\dot{r}(t)|} - r_i(t_i) \sqrt{|\dot{r}_i(t_i)|} \right)^2 dt \tag{6}
\]

where \( r(t) \sqrt{|\dot{r}(t)|} \) stands for the mean contour \( q \), \( t_i = \gamma_i(t) \). As analysed in Appendix A, the solution (system of \( \gamma_i \)) that provides the minimum distances between the constituents \( r_i(t_i) \sqrt{|\dot{r}_i(t_i)|} \) can be determined pairwise wrt
a reference contour (say $r_1$ without loss of generality)

$$
\min_\gamma \int \left( r_1(t) \sqrt{|r_1'(t)|} - r_k(t_k) \sqrt{|r_k'(t_k)|} \right)^2 dt
$$

(7)
as the solution of the Euler-Lagrange equations associated with them:

$$
\dot{r}_1 \cdot r_k - \dot{r}_k \cdot r_1 + \frac{1}{2} (I_k - I_1) = 0
$$

(8)

where the dot over the position vectors stands for the derivatives wrt the parameter $t$, i.e. $\dot{r}_k \equiv \frac{dr_k}{dt} = \gamma_k \frac{dr_k}{d \gamma_k}$, $k = 2, \ldots, n$, (note: since $r_1$ is chosen as reference contour $r_1(\gamma_1(t)) \equiv r_1(t)$ in (6)) and

$$
I_i = \frac{\dot{r}_i \cdot \dot{r}_i}{|\dot{r}_i|^2}, \quad i = 1, \ldots, n,
$$

(9)

are the 'Christoffel divergences' of the parameterization. As expected, the solution for the minimization problem (6) is given by the system $\gamma_k$ determined pairwise, using Euler-Lagrange equation (8), see also Appendix B. Notes:

1. Euler-Lagrange equation (8) retains its form wrt any basis, albeit the resulting system of the optimal parameterization is dependent on the chosen basis; we will address this problem in section Proper centroid

2. (apart from a proportionality factor) Euler-Lagrange equation (8) does not depend explicitly on the reparameterization function $\gamma_k$

3. Christoffel divergences $I = \frac{d \ln |\dot{r}|}{dt}$ can be interpreted as the change of 'elastic stretching' along the contours; indeed the quantity $\ln |\dot{r}|$ has prominent role in definition of elastic shape metrics in [5]

4. assuming $r_1$ is uniformly parameterized in arc length:$I_1 = 0$ and $I_k = 2 (\dot{r}_k \cdot r_1 - \dot{r}_1 \cdot r_k), \quad k = 2, \ldots, n$ determine the elastic stretching/compression

5. from a different point of view, Eq. (7) can be considered as 'dissimilarity measure' between contours

6. as expected, exactly same Euler-Lagrange equations (8) are associated with the similarity maximization $\max \int \dot{r}_1(t) \cdot r_k(t_k) \sqrt{|r_1(t)| \sqrt{|r_k(t_k)|}} dt, \quad k = 2, \ldots, n$ problems

7. note that in the SRVF case, the optimal reparameterization problen can also be formulated as variational problem and its associated Euler-Lagrange equation can be arranged to $\ddot{r}_1 \cdot \dot{r}_k - \ddot{r}_k \cdot \dot{r}_1 + \frac{1}{2} (I_k - I_1) = 0$, having formal similarity to equation (8) with higher-order derivations applied to the first two terms.
2.2.1 Proper centroid

To elaborate a covariant model, the origin of the standard basis $i, j$ wrt the position vectors are expressed must be defined by the contour system itself. Otherwise the mean contour would not be invariant to the common translation of its constituents, violating requirement B stated at the beginning of this section. Now assume, we have our contour system wrt some ad hoc basis and denote the position vector wrt that basis with $R_i(t)$, $i = 1, \ldots, n$. First plausible candidate for the origin would be the usual centroid of the system that minimizes:

$$\min_{R_0} \sum_{i=1}^{n} \int (R_0 - R_i(t))^2 \left| \dot{R}_i \right| dt.$$  \hfill (10)

This candidate provides covariant description, also independent of the parameterization of the constituents (since $\left| \dot{R}_i \right| dt = ds$, the integration is by arc length). From now on we will refer to it as the 'homogeneous' centroid. Problem (10) can be interpreted as simple extreme value problem wrt the centroid coordinates $R_0$ and such the condition:

$$\frac{d}{dR_0} \left( \sum_{i=1}^{n} \int \left( R_0 - R_i(t) \right)^2 \left| \dot{R}_i \right| dt \right) = 0$$  \hfill (11)

provides the following solution:

$$R_0 = \frac{\sum_{i=1}^{n} R_i ds}{\sum_{i=1}^{n} L_i}$$  \hfill (12)

where $L_i$ stands for the length of the $i$-th contour. Adopting the standard basis to be this homogeneous centroid, the position vectors of the contour system wrt this basis would become $r_i(t) = R_i(t) - R_0$ $i = 1, \ldots, n$.

However the question arises naturally: is the choice of the homogeneous centroid 'compatible' with the minimization problem (6)? To decide this question, let’s assume, we displace the basis from the homogeneous centroid position with a vector $\delta d$. The position vectors are then transformed to $r_i(t) \rightarrow r_i(t) - \delta d$. Now check, whether the double minimization problem, generalized from (6):

$$E(\gamma, \delta d) = \min_{\gamma, \delta d} \sum_{i=1}^{n} \int \left( r(t) - \delta d \right) \sqrt{\dot{r}(t)} - (r_i(t_i) - \delta d) \sqrt{\dot{r}_i(t_i)} \right| \dot{r}_i(t_i) dt$$  \hfill (13)

takes its minimum at $\delta d = 0$. From the condition $\frac{\partial E}{\partial \delta d} = 0$, one can derive:

$$\delta d = \frac{\sum_{i=1}^{n} S_i + nS - \left[ \sum_{i=1}^{n} \int \left( r(t) + r_i(t_i) \right) \sqrt{\dot{r}(t) \left| \dot{r}_i(t_i) \right| dt} \right]}{\sum_{i=1}^{n} L_i + nL - \left[ 2 \sum_{i=1}^{n} \int \sqrt{\dot{r}(t) \left| \dot{r}_i(t_i) \right| dt} \right]}$$  \hfill (14)
where notations \( S_i = \int r_i(t_i) \sqrt{\dot{r}_i(t_i)} \, dt \), \( S = \int r(t) \sqrt{\dot{r}(t)} \, dt \) and the lengths of the constituents \( L_i = \int |\dot{r}_i(t_i)| \, dt \) and the mean contour \( L = \int |\dot{r}(t)| \, dt \) are introduced. Now one can notice that in general, the optimal displacement of the homogeneous centroid wrt minimization problem (13) is not zero vector due to the parameterization dependent terms emphasized in brackets in (14). This issue obviously stem from the fact that the optimally parameterized contour system consists of non-uniformly parameterized (in arc length sense) 'inhomogeneous' contours. From now on we refer the centroid that satisfies the double minimization problem (13) as proper centroid.

The optimal centroid and parameterization system are interdependent: wrt a fixed basis a unique optimal reparameterization system can be calculated which in turn determines the location of the proper centroid; on the other hand in general (unless \( \delta d = 0 \) by (14)) the optimal parameterization system is dependent on the choice of the standard basis. This interdependency leads to an iterative solution which is discussed in details in the next section. The optimal reparameterization system and the proper centroid are determined alternately. Using this approach, equation (14) can be simplified as follows. In the first step the optimal reparameterization system is determined wrt the momentary centroid, then the mean contour is calculated (5) and reconstructed. Substituting the mean \( r \sqrt{|\dot{r}|} \) to \( nS \) in (14), two terms are eliminated from the numerator. After some rearrangement (both the numerator and the denominator) we arrive to a simple expression:

\[
\delta d = \frac{\sum_{i=1}^{n} \int \left( r_i \sqrt{|\dot{r}_i|} - r \sqrt{|\dot{r}|} \right) \sqrt{|\dot{r}_i|} \, dt}{2 \sum_{i=1}^{n} \int \frac{|\dot{r}_i| + |\dot{r}|}{2} - \sqrt{|\dot{r}_i| \dot{r}_i} \, dt}.
\]

(15)

In the denominator, the integrand is the sum of the differences of the arithmetic and geometric means of the corresponding elementary arc lengths \( \frac{ds_i + ds}{2} \) and \( \sqrt{ds_i ds} \) respectively (using the \( ds = |\dot{r}| \, dt \) identity). The denominator therefore can be zero only if the lengths of all the corresponding elementary arc segments are identical, the case possible only if the constituent contours are all identical.

2.3 Numerical methods

As in the case of shape analysis, the calculation of the mean contour requires iterative solutions: a double iteration for determination of the optimal reparameterization system and the proper centroid defined by (13), then one for the reconstruction of the contour from its RPSV representation. The components are the following.

1. Reparameterization of the system

2. Mean calculation

3. Reconstruction of the mean contour from its representation
4. Proper centroid calculation

Reparameterization

The identification of the optimal reparameterization system \((13)\) requires the calculation of \(n - 1\) pairwise reparameterization wrt a reference contour. The gradient descent equations are

\[
\frac{\partial \gamma_k}{\partial \tau} = -\dot{r}_1 \cdot r_k + r_1 \cdot \dot{r}_k - \frac{1}{2} r_1 \cdot r_k (\Gamma_1 - \Gamma_k),
\]

where \(\tau\) is the ‘artificial’ time and the Christoffel divergences are defined by \((9)\). These equations are to be solved in the contour space. Two methodologies are possible to determine the optimal parameterization. In the first (recommended) case, after each iteration, the points are redistributed moving them to their new physical position determined by \(\delta \gamma_k^{(i)}\) \((i = 1, \ldots, N\) is the iteration index) along the (static) contours \(r_k\). Derivatives \(\dot{r}_k\) are calculated from the momentary positions of the contour points. Note that in the discrete approximation of contours, uniform distribution wrt parameter value \(t\) can be assumed without loss of generality (that is the parameter values assigned to the neighboring points differ from each other with same \(\Delta t\) everywhere). In this case in the parameter space the parameter values associated with the (moving) points remain constant, albeit their arclength parameters change in general. The final diffeomorphism \(\gamma_k\) is then the composition of the sequence of consecutive approximate diffeomorphisms \(\delta \gamma_k^{(i)}\), that is (assuming overall \(N\) iterations) \(\gamma_k = \delta \gamma_k^{(N)} \circ \cdots \circ \delta \gamma_k^{(2)} \circ \delta \gamma_k^{(1)}\). See Algorithm \([1]\). In the second case \(\gamma_k\) is updated after all iterations with the points physical position retained at their initial position. This approach however, requires the calculations of the derivatives wrt the momentary \(\dot{\gamma}_k^{(i)}\) using explicite formulae for the derivatives \((i.e. \frac{d}{dt} = \dot{\gamma} \frac{d}{d\gamma})\). The first methodology has the advantages a) at each iteration step \(\delta \gamma_k^{(i)}\) needs to be determined wrt the identity diffeomorphism \(\gamma\) \((t) \equiv t\) b) usually, there is no real need for the explicit determination of the final diffeomorphism, only the final point distribution we end up with the first methodology and c) it can be efficiently implemented using a high resolution lookup table for the positions along the contours.

Mean calculation

Given the optimal reparameterization system, the mean is calculated using the closed form equation \([4]\).

Reconstruction

Reconstruction is made by the Newton–Raphson method, solving a sparse linear equation system in each iteration \(A^{(i)}x^{(i+1)} = b^{(i)}\) \((i\) is the iteration index) with coefficient matrix, ray length approximation of the position vector and constant vector all defined in Appendix \(C\) by formulae \([38], [37], [39]\) respectively.
Algorithm 1 Compute pairwise optimal reparameterization

1. Initialize the position vectors $r_k, k = 1\ldots n$ of the contour set wrt the homogeneous centroid (12). Establish the initial discrete point set along the contours with same number of points (can be uniformly distributed in arc length); Set the iteration counter $i = 1$; Set $\delta \gamma_k^{(0)} = t, k = 2\ldots n$ (i.e. $r_1$ is selected as reference)

2. Calculate one step towards $(\delta \gamma_k^{(i)}, k = 2\ldots n)$ the optimal point distribution system using gradient descent equations (16)

3. Update the points along contours $r_k, k = 2\ldots n$, using the calculated valuea $\delta \gamma_k^{(i)}, k = 2\ldots n$

4. Update the diffeomorphism set $\gamma_k^{(i)} = \delta \gamma_k^{(i)} \circ \gamma_k^{(i-1)}$

5. Exit if all $\delta \gamma_k^{(i)}$ (wrt its $\gamma_k^{(i)}$) is small; Otherwise set $\delta \gamma_k^{(i)} = t$, set $i = i + 1$ and repeat from 2

Proper centroid

Proper centroid for the momentary parameterization system is calculated using the closed form formula (15). Once the (better) displacement $\delta d^{(j)}$ is determined all constituent contours have to be updated such as $r_k \rightarrow r_k + \delta d^{(j)}, k = 1\ldots n$ then all previous steps are to be repeated until the minimum of the double minimization problem (13) is reached. The cumulative displacement of the initial (homogeneous) centroid after $M$ iterations is the sum of the preceding (momentary) displacements: $\sum_{j=1}^{M} \delta d^{(j)}$.

The algorithm

Albeit the determination of the optimal reparameterization system and the proper centroid calculation could be incorporated into one iterative method, but the need for the mean contour calculation in (14) after each gradient descent step of (16) would lead to sluggish computing. Therefore a double iteration procedure is recommended: an inner (nested) loop for the optimal reparameterization system under the assumption of centroid constancy, followed by the centroid position updating in the outer (main) loop.

The complete algorithm consists of the steps described above and summarized in Algorithms 1 (nested loop) and 2 (main loop).
Algorithm 2 Solve the double optimization algorithm

1. Initialize the position vectors $\mathbf{r}_k$, $k = 1 \ldots n$ of the contour set wrt the homogeneous centroid (12). Establish the initial discrete point set along the contours with same number of points (can be uniformly distributed in arc length); Set the iteration counter $j = 1$; Set $\delta \mathbf{d}^{(j)} = 0$.

2. In internal loop compute the optimal redistribution system of points pairwise wrt an arbitrarily designated reference contour using gradient descent equation (16) or alternatively compute the optimal reparameterization system $\gamma_i$: Reparameterization; see also Algorithm 1

3. Calculate the mean contour in the representation space RPSV: Mean calculation

4. Reconstruct the mean in contour space: Reconstruction

5. Compute the new momentary proper centroid $\delta \mathbf{d}^{(j)}$: Proper centroid; note that the value for $\delta \mathbf{d}$ according to formula (15) is to be assigned to $\delta \mathbf{d}^{(j)}$

6. Update the position vectors $\mathbf{r}_k \rightarrow \mathbf{r}_k - \delta \mathbf{d}^{(j)}$, $k = 1 \ldots n$ of the contour set

7. Calculate the double energy (13), exit if the change (wrt its previous value) is small; Otherwise set $\delta \mathbf{d}^{(j+1)} = 0$, set $j = j + 1$ and repeat from 2.
3 Illustrative examples

The illustrations show mean of representation $|\mathbf{r}|^m \mathbf{u} \sqrt{|\mathbf{r}|}$ for $m = 1$ Fig. 1a) for one of the simplest circle/ellipse case (notice that the mean contour does not pass the intersection of the constituents), b) the mean of non-trivial contours without and with marking point correspondences Fig. 2.

![Figure 1: Mean contour (green) calculated from the RPSV representations of a circle and an ellipse. The mean contour does not pass the intersection of the constituents.](image)

4 Conclusion

In this paper a contour mean determination method - that designed for averaging manual delineation of objects having non definit boundaries - was presented. The mean contour is calculated from a set of contours in a way that all visible information (relative placement, rotation, scale) are retained. At the same time - borrowed the idea from the state of the art shape analysis methods - the contour parameterization is relaxed. The chosen contour representation (RPSV) and the
imposed $L^2$ metric forms a Hilbert space of the contour representations. The metric is chosen to be invariant wrt the reparameterization, the distance function based on it has well defined meaning, the (sum of) the second moment of the contours. The mean contour calculation is performed in the quotient space of contours modulo reparameterization group and could be formulated as a double optimization problem: a variational for the system of the optimal parameterization and an extreme value problem for the proper centroid identification. Illustrative examples show that the resulted mean contours are intuitive according to human perception sense. Similarities/dissimilarities can be simple measured and the outliers determined in this manner are also coincident with the human perception.

The approach can be generalized in many ways \textit{e.g.} defining various combination of representations and the associated metrics (some of them are partly addressed in the article) that may lead meaningful shape analysis techniques alternative to the current mainstream. Another plausible direction is the generalization of the method to surfaces.

**Appendices**

In the appendices, the important properties of the action of the reparameterization group $t \rightarrow \gamma(t), \ q \rightarrow q \circ \gamma$ \textbf{Appendix A} and the founding theorems of the mean contour calculation \textbf{Appendix B} are examined. The reconstruction
equations are derived in Appendix C.

Notations and terminology used throughout the appendices are as follow. Curves are given by their position vectors wrt some standard basis \( \mathbf{i}, \mathbf{j} \) and denoted as \( \mathbf{r}(t) = x(t) \mathbf{i} + y(t) \mathbf{j} \) where \( x(t), y(t) \) are the coordinate functions; contours are closed curves: \( \mathbf{r}(0) = \mathbf{r}(T) \). The discrete representation of a contour is given by the set of \( M \) points selected at parameter values distributed uniformly; that is: \( \mathbf{r}_1 = \mathbf{r}(t_1), \ldots, \mathbf{r}_M = \mathbf{r}(t_M), t_{i+1} - t_i = \Delta t, t_1 = 0, t_M = T - \Delta t. \)

Vectors are written with bold letters; vector juxtaposition \( \mathbf{a} \cdot \mathbf{b} \) indicates direct (dyadic) product, scalar (contraction of a dyad) and cross products are denoted by dot \( \mathbf{a} \cdot \mathbf{b} \) and cross \( \mathbf{a} \times \mathbf{b} \) respectively. Derivatives wrt contour parameter \( t \) are denoted by dots: \( \ddot{\mathbf{r}} = \frac{d\mathbf{r}}{dt}, \dot{\mathbf{r}} = \frac{d\mathbf{r}}{dt^2} \ldots \) (and dot is reserved to denote the derivatives wrt \( t \)); the derivatives at \( \gamma(t) \) are denoted by primes: \( \mathbf{r}' = \frac{d\mathbf{r}}{d\gamma}, \mathbf{r}'' = \frac{d^2\mathbf{r}}{d\gamma^2} \ldots \). For the line integrals along a contour (along closed curve), symbol \( \oint \) is used. In the case of iterative methods, the identifiers of the iteration ('iteration index') are denoted by upper indices in parentheses e.g. the value of the quantity \( x \) in the \( k \)-th iteration is \( x^{(k)} \).

Appendix A

Property A1: the reparameterization group \( \mathbf{q} \rightarrow \mathbf{q} \circ \gamma (t \rightarrow \gamma(t)) \) acts by isometries wrt the chosen representation \( \mathbf{q} = \mathbf{r} \sqrt{|\mathbf{F}|} \) \( \dot{\mathbf{r}} = \frac{d\mathbf{r}}{d\gamma} \) and metric \( d^2 \mathbf{q}_1, \mathbf{q}_2 = \oint (\mathbf{r}_1(t) \sqrt{|\mathbf{F}_1(t)|} - \mathbf{r}_2(t) \sqrt{|\mathbf{F}_2(t)|})^2 dt \).

Proof: consider the common reparameterization \( t \rightarrow \gamma(t) \) of the two contours \( \mathbf{q}_1, \mathbf{q}_2 \) involved, then the relation between the operators become \( \frac{d}{dt} = \dot{\gamma} \frac{d}{d\gamma} \) \( (\dot{\gamma} = \frac{d\gamma}{dt}) \). The change squared distance

\[
\| \mathbf{q}_1 \circ \gamma - \mathbf{q}_2 \circ \gamma \|^2 = \oint \left( \mathbf{r}_1(\gamma) \sqrt{\frac{d\mathbf{r}_1(\gamma)}{d\gamma}} \dot{\gamma} - \mathbf{r}_2(\gamma) \sqrt{\frac{d\mathbf{r}_2(\gamma)}{d\gamma}} \right)^2 dt
\]

\[
= \oint \left( \mathbf{r}_1(\gamma) \sqrt{\frac{d\mathbf{r}_1(\gamma)}{d\gamma}} - \mathbf{r}_2(\gamma) \sqrt{\frac{d\mathbf{r}_2(\gamma)}{d\gamma}} \right)^2 \dot{\gamma} dt = \int \left( \mathbf{r}_1(\gamma) \sqrt{\frac{d\mathbf{r}_1(\gamma)}{d\gamma}} - \mathbf{r}_2(\gamma) \sqrt{\frac{d\mathbf{r}_2(\gamma)}{d\gamma}} \right)^2 d\gamma.
\]

The last line is equivalent to the definition with renamed variable of integration, i.e. the common reparameterization of the contours does not influence their distance. This property allows simple strategy to determine the optimal parameterization system of contours, that is Lemma A1: one can designate any constituent of the set of \( n \) contours as the reference contour to determine the optimally parameterized system of contours with pairwise calculation of the optimal (in the sense of minimum distances) reparameterization wrt the reference
we have the optimally reparameterized system: minimizes the squared distances and update $q_\gamma$ be minimized wrt the wish to determine the system of optimal reparameterization Let $q_\gamma \star$.

Appendix B linear path alters linearly. variational problem is solved via its associated Euler-Lagrange equation.

having same parameter range $q_\gamma$ equation determines the minimal distance solution between (any) two endpoints $q_\gamma t$. Where the notation $r_2' = \frac{dr_2}{dt}$ is used (dot is exclusively reserved for $t$). The variational problem is solved via its associated Euler-Lagrange equation. Proof: assume we have the system of $n$ contours $q_1, q_2, \ldots, q_n$ parameterized having same parameter range $[0, T]$ (otherwise arbitrarily). First we determine $\gamma^*_n$ acting between $q_{n-1}, q_n$ such that $d^2 (q_{n-1}, q_n \circ \gamma^*_n)$ admits its minimum, second we repeat with $\gamma^*_{n-1}$ such that $d^2 (q_{n-2}, q_{n-1} \circ \gamma^*_{n-1})$ to be minimal, and update $q_n \circ \gamma^*_n \to q_n \circ \gamma^*_{n-1} \circ \gamma^*_n$. Continuing this procedure, at the end we have the optimally reparameterized system: $q_1, q_2 \circ \gamma^*_2, \ldots, q_n \circ \gamma^*_2 \cdots \circ \gamma^*_n$. However, if the pairwise calculations provide unique solution to the problem $\min d^2 (q_1, q_i \circ \gamma_i), i = 2, \ldots, n$ then the equivalences $\gamma_{1i} \equiv \gamma^*_2 \cdots \circ \gamma^*_i$ must hold. Since the both the reference contour and the order of the contours are arbitrary, the final system is optimally parameterized in the minimum distance sense.

The optimal reparameterization can be uniquely determined, using variational minimization e.g. between contours 1 and 2 it can be formulated as:

$$\min_{\gamma_{12}} \int \left( r_1 \sqrt{|r_1|} - r_2 (\gamma_2) \sqrt{|r_2' (\gamma_2)|} \right)^2 dt,$$

where the notation $r_2' = \frac{dr_2}{dt}$ is used (dot is exclusively reserved for $t$). The variational problem is solved via its associated Euler-Lagrange equation.

Property A2: along a linear path $(1 - \tau) q_1 + \tau q_2$ the same Euler-Lagrange equation determines the minimal distance solution between (any) two endpoints $q_1, q_2$.

Proof: the distance minimizer integral for the point $(1 - \tau) q_1 + \tau q_2$ is:

$$\int \left[ r_1 \sqrt{|r_1|} - (1 - \tau) r_1 \sqrt{|r_1|} + \tau r_2 (\gamma_2) \sqrt{|r_2' (\gamma_2)|} \right]^2 dt = \tau^2 \int \left( r_1 \sqrt{|r_1|} - r_2 (\gamma_2) \sqrt{|r_2' (\gamma_2)|} \right)^2 dt \quad (19)$$

the right side differ from the functional to be minimized (18) only in a constant factor which does not affect the associated Euler-Lagrange equation.

Property A3: also, it is obvious from (18) that the distance $(\sqrt{d^2})$ along a linear path alters linearly.

Appendix B

Let $q_1, q_2, \ldots, q_n, q_k = r_k \sqrt{r_k}$ a system of representations of $n$ contours. We wish to determine the system of optimal reparameterization $\gamma_k, k = 1..n$ that minimizes the squared distances $d^2 (q_i, q_k), i, k = 1, \ldots, n$ [3] between them. It can be done pairwise wrt a reference contour (see Appendix A). Without loss of generality, let $r_1$ (represented by $q_1$) be chosen as the reference contour (hence $\gamma_1 (t) \equiv t$), then the functionals $\int \left( r_1 \sqrt{|r_1|} - r_k \sqrt{|r_k|} \right)^2 dt, k = 2, \ldots, n$ are to be minimized wrt the $k$-th diffeomorphism $\gamma_k = \gamma_k (t)$.
Using the notations (and dependencies on the different contour parameters) listed below

\[
\begin{align*}
\mathbf{r}_1 &= \mathbf{r}_1(t) \\
\mathbf{r}_k &= \mathbf{r}_k(\gamma_k), \gamma_k = \gamma_k(t) \\
\dot{\mathbf{r}}_1 &= \dot{\mathbf{r}}_1(t) = \frac{d\mathbf{r}_1(t)}{dt} \\
\dot{\mathbf{r}}_k &= \dot{\mathbf{r}}_k(t) = \dot{\gamma}_k(t) \frac{d\mathbf{r}_k(\gamma_k)}{d\gamma_k} = \dot{\gamma}_k \mathbf{r}_k' \\
e_k &= \frac{\dot{\mathbf{r}}_k}{|\dot{\mathbf{r}}_k|} = \frac{\mathbf{r}_k'}{|\mathbf{r}_k'|}
\end{align*}
\]

we first state Lemma B1: The Euler-Lagrange equation associated with the minimization problem \( \min_{\gamma_k} \int \left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k (\gamma_k) \sqrt{|\mathbf{r}_k'| \gamma_k} \right)^2 dt \) is \( \dot{\mathbf{r}}_1 \cdot \mathbf{r}_k - \mathbf{r}_1 \cdot \dot{\mathbf{r}}_k + \frac{1}{2} \mathbf{r}_1 \cdot \dot{\mathbf{r}}_k (I_1 - I_k) \).

Proof: the Lagrangian and its derivatives are:

\[
L(\gamma_k, \dot{\gamma}_k) = \left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right)^2
\]

\[
\frac{\partial L}{\partial \gamma_k} = -2 \left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \left( \mathbf{r}_k' \sqrt{|\mathbf{r}_k'| \gamma_k} + \mathbf{r}_k \frac{\dot{\gamma}_k \mathbf{e}_k \cdot \mathbf{r}_k'}{2 \sqrt{|\mathbf{r}_k'| \gamma_k}} \right)
\]

\[
\frac{\partial L}{\partial \dot{\gamma}_k} = -\left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \mathbf{r}_k \frac{|\mathbf{r}_k'| \gamma_k}{\sqrt{|\mathbf{r}_k'| \gamma_k}}
\]

From the relations between the differential operators

\[
\frac{d}{d\gamma} = \frac{1}{\dot{\gamma}} \frac{d}{dt}
\]

\[
\frac{d^2}{d\gamma^2} = \frac{1}{\dot{\gamma}^2} \left( \frac{d^2}{dt^2} + \frac{d}{dt} \right)
\]

we have

\[
\frac{\partial L}{\partial \gamma_k} = -2 \left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \left[ \frac{1}{\dot{\gamma}_k} \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} + \mathbf{r}_k \frac{\mathbf{e}_k \cdot \left( -\frac{\dot{\gamma}_k}{\dot{\gamma}} \mathbf{r}_k + \frac{1}{\dot{\gamma}} \dot{\mathbf{r}}_k \right)}{2 \sqrt{|\mathbf{r}_k'| \gamma_k}} \right]
\]

\[
= -\left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \frac{\sqrt{|\mathbf{r}_k'| \gamma_k}}{\dot{\gamma}_k} \left( 2 \mathbf{r}_k - \frac{\dot{\gamma}_k}{\dot{\gamma}} \mathbf{r}_k + \mathbf{r}_k \frac{\mathbf{e}_k \cdot \dot{\mathbf{r}}_k}{|\mathbf{r}_k'| \gamma_k} \right)
\]

\[
= -\frac{1}{\dot{\gamma}_k} \left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \mathbf{r}_k \frac{\sqrt{|\mathbf{r}_k'| \gamma_k}}{\dot{\gamma}_k} \left( 2 \mathbf{r}_k - \frac{\dot{\gamma}_k}{\dot{\gamma}} \mathbf{r}_k + \mathbf{r}_k \frac{\mathbf{e}_k \cdot \dot{\mathbf{r}}_k}{|\mathbf{r}_k'| \gamma_k} \right)
\]

\[
\frac{\partial L}{\partial \dot{\gamma}_k} = -\left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k}
\]

\[
= -\frac{1}{\dot{\gamma}_k} \left( \mathbf{r}_1 \sqrt{|\mathbf{r}_1|} - \mathbf{r}_k \sqrt{|\mathbf{r}_k'| \gamma_k} \right) \cdot \mathbf{r}_k,
\]
and
\[
- \frac{d}{dt} \frac{\partial L}{\partial \gamma_k} = \left( r_1 \sqrt{|r_1|} |r_k| - r_k |r_k| \right) \cdot \left( \frac{1}{\gamma_k} \frac{\dot{r}_k}{\gamma_k} - \frac{\dot{\gamma}_k}{\gamma_k} r_k \right) \\
+ \frac{\sqrt{|r_1|}}{\gamma_k} r_k \cdot \left( \dot{r}_1 + \frac{1}{2} r_1 \frac{\dot{r}_1}{|r_1|^2} + \frac{1}{2} r_1 \frac{\dot{r}_1}{|r_1|^2} \right) \\
- \frac{1}{\gamma_k} r_k \cdot \left( \dot{r}_k |r_k| + r_k \frac{\dot{r}_k}{|r_k|^2} \right).
\]

The Euler-Lagrange equation for the k-th diffeomorphism \( \gamma_k = \gamma_k(t) \) is:
\[
\frac{\partial L}{\partial \gamma_k} - \frac{d}{dt} \frac{\partial L}{\partial \gamma_k} = \frac{\sqrt{|r_1|}}{\gamma_k} \left[ \dot{r}_1 \cdot r_k - r_1 \cdot \dot{r}_k + \frac{1}{2} r_1 \cdot r_k \right] \frac{\dot{r}_1 \cdot r_k - \dot{r}_k \cdot \dot{r}_k}{|r_1|^2}.
\]
Assuming \( \frac{\sqrt{|r_1|}}{r_k} \) is not zero at any point, we can divide with it, then the Euler-Lagrange equations to be solved are given with:
\[
\dot{r}_1 \cdot r_k - r_1 \cdot \dot{r}_k + \frac{1}{2} r_1 \cdot r_k (I_1 - I_k) = 0, \quad k = 2, \ldots, n,
\]
where 'Christoffel divergences' \( I_i = \frac{\dot{q}_i}{|q_i|} \), \( i = 1, \ldots, n \) are introduced to simplify the equation.

Note that the optimal contour system can be generalized in many ways, e.g. for the representation \( q = f(r) u \frac{\sqrt{|r|}}{|r|} \) - where \( u = \frac{r}{|r|} \) is the unit vector in the direction of the position vector, \( f \) is appropriately defined scalar valued function. Here we provide equations for the \( q = |r|^m u \frac{\sqrt{|r|}}{|r|} \), \( m \in \mathbb{R} \) cases (the \( m = 1 \rightarrow q = r \frac{\sqrt{|r|}}{|r|} \) is the case examined in this paper in details). For these cases, the pairwise distance minimizers based on the \( L^2 \) metric are formulated as:
\[
\min_{\gamma_k} \int \left( |r_1|^m u_1 \frac{\sqrt{|r_1|}}{|r_1|} - |r_k (\gamma_k)|^m u_k (\gamma_k) \frac{\sqrt{|r_k (\gamma_k)|}}{|r_k (\gamma_k)|} \right)^2 dt,
\]
and the associated Euler-Lagrange equations take the form:
\[
\dot{r}_1 \cdot (m u_1 u_1 + u_1^2 u_1^2) \cdot r_k - r_1 \cdot (m u_k u_k + u_k^2 u_k^2) \cdot \dot{r}_k + \frac{1}{2} r_1 \cdot r_k (I_1 - I_k) = 0
\]
where \( u^2 = k \times u \) is the unit vector perpendicular to the position vector (\( k \) is the unit normal of the plane). There is singularity at \( m = -\frac{1}{2} \) (a uniform scaling \( r \rightarrow \alpha r \) leads to the same representation \( q|_{\alpha r} = q|_r = u \frac{\sqrt{|r|}}{|r|} \)). For this value the reconstruction cannot be made (see also Appendix C).

The important consequence of the Lemma B1:

**Theorem B2:** the solution for the minimization problem \( \min_{\gamma_i} \sum_{i=1}^{n} \int \dot{f} \left( r(t) \frac{\sqrt{|r(t)|}}{|r(t)|} - r_i(t_i) \frac{\sqrt{|r_i(t_i)|}}{|r_i(t_i)|} \right)^2 dt \), where \( r(t) \frac{\sqrt{|r(t)|}}{|r(t)|} = \frac{1}{n} \sum_{i=1}^{n} r_i(t_i) \frac{\sqrt{|r_i(t_i)|}}{|r_i(t_i)|} \)
is the system of optimal reparameterization \( t_i = \gamma_i(t), i = 1, \ldots n \) determined by the pairwise optimizations between the constituents.

Proof: a) repeating the steps of the previous proof, the optimal parameterization system satisfies the set of Euler-Lagrange equations:

\[
\dot{r} \cdot r_k - r \cdot \dot{r}_k \frac{1}{2} \frac{\dot{r} \cdot \ddot{r} - \dot{r}_k \cdot \ddot{r}_k}{|r|^2} = 0, \quad k = 1, \ldots n, \tag{25}
\]

b) taking the derivative wrt \( t \) of the mean expression \( r(t) \sqrt{|F(t)|} = \frac{1}{n} \sum_{i=1}^{n} r_i(t_i) \sqrt{|F_i(t_i)|} \) then the dot product with \( r_k \), we have:

\[
\sqrt{|F|} \left( \dot{r} \cdot r_k + \frac{1}{2} r \cdot \dot{r}_k \frac{\dot{r} \cdot \ddot{r} - \dot{r}_k \cdot \ddot{r}_k}{|r|^2} \right) = \frac{1}{n} \sum_{i=1}^{n} \sqrt{|F_i|} \left( \dot{r}_i \cdot r_k + \frac{1}{2} r_i \cdot \dot{r}_k \frac{\dot{r}_i \cdot \ddot{r}_k}{|r_k|^2} \right) \tag{26}
\]

As assumed \((23)\) equations are satisfied. From this

\[
\dot{r}_i \cdot r_k + \frac{1}{2} r_i \cdot \dot{r}_k = \frac{\dot{r}_i \cdot \ddot{r}_k}{|r_k|^2}. \tag{27}
\]

Substituting \((27)\) to \((26)\), we get:

\[
\sqrt{|F|} \left( \dot{r} \cdot r_k + \frac{1}{2} r \cdot \dot{r}_k \frac{\dot{r} \cdot \ddot{r} - \dot{r}_k \cdot \ddot{r}_k}{|r|^2} \right) = \frac{1}{n} \sum_{i=1}^{n} \sqrt{|F_i|} \left( r_i \cdot \dot{r}_k + \frac{1}{2} r_i \cdot \dot{r}_k \frac{1}{|r_k|^2} \right) = \frac{1}{n} \sum_{i=1}^{n} \sqrt{|F_i|} \left( \dot{r}_i \cdot \ddot{r}_k \right) - \frac{1}{n} \sum_{i=1}^{n} \sqrt{|F_i|} r_i \cdot r_k \cdot \dot{r}_k \sqrt{|F|} \tag{28}
\]

Rearranging, we have:

\[
\sqrt{|F|} \left[ \dot{r} \cdot r_k - \dot{r}_k \cdot r + \frac{1}{2} r \cdot \dot{r}_k \left( \frac{\dot{r} \cdot \ddot{r} - \dot{r}_k \cdot \ddot{r}_k}{|r|^2} \right) \right] = 0,
\]

that is the \( k \)-th equation of \((25)\).

**Appendix C**

In this section we derive the equations used to reconstruct the contours from their RPSV representation \( q(t) \rightarrow r(t) \), where \( q(t) = r(t) \sqrt{|F(t)|} \) is known. Observing that \( \frac{q(t)}{|q(t)|} = \frac{r(t)}{|r(t)|} \), we introduce the notation for the unit vector pointing from the proper centroid to the direction of both points \( q(t), r(t) \):

\[
u(t) = \frac{q(t)}{|q(t)|} = \frac{r(t)}{|r(t)|}. \tag{29}
\]
Having the direction of the position vector, we need to determine only its distance measured from the centroid \(|r(t)|\) then position vector \(r(t) = |r(t)| u(t)\)\(^2\).

(Hereinafter we will also use the notation \(e(t) \equiv \hat{r}(t) / |\hat{r}(t)|\) for the unit tangent vector of the contour.) Now we define the scalar function

\[
f(r, \hat{r}) \equiv |q| - |r| \sqrt{\hat{r}}.
\]

(30)

With this definition, the determination of |\(r|\) becomes root finding problem (at each parameter value \(t\)). In function (30) temporarily we handle the position vector \(r\) and its derivative \(\hat{r}\) as if they were independent variables.

Assume we know the value of \(f\) at some initial guess point \(r^{(k)}, \hat{r}^{(k)}\) close to its root, its linear approximation around can be written as

\[
y(r, \hat{r}) = f + \frac{\partial f}{\partial r} \cdot (r - r^{(k)}) + \frac{\partial f}{\partial \hat{r}} \cdot (\hat{r} - \hat{r}^{(k)})
\]

(31)

where function \(f\) and its gradients \(\frac{\partial f}{\partial r}\) and \(\frac{\partial f}{\partial \hat{r}}\) are all evaluated at \(r^{(k)}, \hat{r}^{(k)}\). The gradients are:

\[
\frac{\partial f}{\partial r} = -\sqrt{\hat{r}} u
\]

\[
\frac{\partial f}{\partial \hat{r}} = -\frac{1}{2} \frac{|r|}{\sqrt{\hat{r}}} e.
\]

(32)

Substituting the gradient expressions into (31) at point \(r^{(k)}, \hat{r}^{(k)}\), we have the the equation for the root \((y = 0)\) of the linear approximation (31):

\[
|q| - |r^{(k)}| \sqrt{\hat{r}^{(k)}} = 0
\]

(33)

This assumption is taken throughout the paper.

2This also means that the unit direction vector remains always constant (i.e. does not change during the iteration described in this appendix).

3This assumption is taken throughout the paper.
Solution (34) can be approximated using the simple finite central differences scheme \( \dot{r} \approx \frac{r_x - r_x}{2 \Delta t}, \quad r_x = |r| \frac{u_x}{|\dot{r}|} \) as:

\[
|r| + \left\{ \frac{1}{4 \Delta t} \left| \frac{r^{(k)}}{\hat{r}^{(k)}} \right| \mathbf{e}^{(k)} \cdot \mathbf{u}_+ \right\} |r_+| - \left\{ \frac{1}{4 \Delta t} \left| \frac{r^{(k)}}{\hat{r}^{(k)}} \right| \mathbf{e}^{(k)} \cdot \mathbf{u}_- \right\} |r_-| = \frac{|q|}{\sqrt{|\dot{r}^{(k)}|}} + \frac{1}{2} |r^{(k)}|.
\]

(36)

On the right side all quantities are known; on the left side the known coefficients are emphasized by putting them into braces. For the whole point set this constitutes a linear equation system with sparse matrix three-diagonal almost everywhere except the first and last line. The derivation above follows the steps of the derivation of Newton–Raphson method. This method is widely used to determine the root of the nonlinear equations iteratively. Starting from an intermediate result (approximation of the root of (30)) \( \hat{r}^{(k)} \), the next (expectably more accurate) approximation \( r^{(k+1)} \) is given as the solution of (36). With the substitution \( |r| \rightarrow |r^{(k+1)}| \), the linear equation system \( A^{(k)} \mathbf{x}^{(k+1)} = \mathbf{b}^{(k)} \) needs to be solved for the next \( (k+1)-\text{th} \) root vector \( \mathbf{x}^{(k+1)} \) with the sought components

\[
\mathbf{x}^{(k+1)} = \left[ \begin{array}{c} |r_1^{(k+1)}| \\ \vdots \\ |r_M^{(k+1)}| \\ \vdots \\ |r_M^{(k+1)}| \end{array} \right]^T
\]

(37)

using the matrix

\[
A^{(k)} = \begin{bmatrix}
1 & a_{1,2}^{(k)} & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 1 & a_{i-1,i}^{(k)} & 0 \\
a_{M,1}^{(k)} & 0 & \cdots & 0 & a_{M,M-1}^{(k)}
\end{bmatrix}
\]

(38)

\[
a_{i,i-1}^{(k)} = -\frac{1}{4 \Delta t} \left| \frac{r_i^{(k)}}{\hat{r}_i^{(k)}} \right| \mathbf{e}_i^{(k)} \cdot \mathbf{u}_{i-1},
\]

\[
a_{i,i+1}^{(k)} = \frac{1}{4 \Delta t} \left| \frac{r_i^{(k)}}{\hat{r}_i^{(k)}} \right| \mathbf{e}_i^{(k)} \cdot \mathbf{u}_{i+1},
\]

\[
a_{1,2}^{(k)} = -\frac{1}{4 \Delta t} \left| \frac{r_1^{(k)}}{\hat{r}_1^{(k)}} \right| \mathbf{e}_1^{(k)} \cdot \mathbf{u}_1,
\]

\[
a_{M,1}^{(k)} = \frac{1}{4 \Delta t} \left| \frac{r_M^{(k)}}{\hat{r}_M^{(k)}} \right| \mathbf{e}_M \cdot \mathbf{u}_1
\]

and the vector

\[
\mathbf{b}^{(k+1)} = \left[ \begin{array}{c} b_1^{(k+1)} \\ \vdots \\ b_M^{(k+1)} \end{array} \right]^T,
\]

(39)

\[
b_i^{(k+1)} = \frac{|u_i|}{\sqrt{|\dot{r}_i^{(k)}|}} + \frac{1}{2} |r_i^{(k)}|, \quad i = 1 \ldots M
\]
calculable from the \( k \)-th iteration.

Note that for the generalized representation \( q = |r|^m \frac{u}{\sqrt{|\dot{r}|}} \) the reconstruc-
tion equations \((36)\) (with the substitution \(|r| \rightarrow |r^{(k+1)}|\)) take the form:

\[
\begin{align*}
|r^{(k+1)}| + & \left\{ \frac{1}{4m \Delta t} \frac{|r^{(k)}|}{|\dot{r}^{(k)}|} (e^{(k)} \cdot u_+) \right\} |r_+^{(k+1)}| - \left\{ \frac{1}{4m \Delta t} \frac{|r^{(k)}|}{|\dot{r}^{(k)}|} (e^{(k)} \cdot u_-) \right\} |r_-^{(k+1)}| \\
= & \frac{|q|}{m |\dot{r}^{(k)}|^{m-1} \sqrt{|r^{(k)}|}} + \left( 1 - \frac{1}{2m} \right) |r^{(k)}| .
\end{align*}
\]

(40)

Cases of special interest are: a) \(m = 0, \ q = u \sqrt{|\dot{r}|} \), in this case the \(L^2\) metric expresses the length of the contour, the reconstruction equations can be deduced from (40) by multiplying both sides with \(m\):

\[
\left\{ e^{(k)} \cdot u_+ \right\} |r_+^{(k+1)}| - \left\{ e^{(k)} \cdot u_- \right\} |r_-^{(k+1)}| = 4 \Delta t \left( |q| \sqrt{|\dot{r}|} - \frac{1}{2} |\dot{r}^{(k)}| \right) \quad (41)
\]

the coefficient matrix has special structure: the lack of diagonal elements; b) \(m = -\frac{1}{2}, \ q = u \sqrt{|\dot{r}|} \), in this case the right hand side of (36) is proportional to

\[
1 - |q| \sqrt{|\dot{r}^{(k)}|/|r^{(k)}|}, \quad (42)
\]

so at the solution this value becomes zero leading to homogeneous equation system with the solution of identically zero \(|r(t)|\), an obvious contradiction. The latter case is inherently singular as already pointed out in Appendix B.

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