New high-performance 3D registration algorithms for 3D medical images

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ABSTRACT

In this presentation a new search method is proposed to improve the speed and accuracy of surface based registration algorithms. Furthermore, a parallel point projection based, multicomponent distance evaluation method is presented. This method offers an elegant solution to the problem of partially overlapping data sets. An adaptive outlier treatment method is also presented. Combination of all these new techniques results in a faster surface based algorithm with better accuracy, but above all with better reliability than existing surface based 3D registration algorithms. In the context of the surface correspondence problem, surface based registration algorithms are compared to feature matching methods.

1. INTRODUCTION

The aim of our applied research is to develop state-of-the-art medical workstations for neuroradiological diagnosis, and for the planning of stereotactic neurosurgery, open neurosurgery, and neuroradiotherapy. These applications often require the use of images obtained from multiple modalities, e.g. for the integrated visualization of anatomical (CT, MR) and functional (PET) information. However, integrated visualization of multimodal images is possible only after solution of the registration problem, i.e. after the determination of the geometric transformation matrix relating the locations of the patient head (or parts of it) in the different images. All registration algorithms use some form of anatomical information obtained by segmentation, e.g. external landmark points, anatomical landmark points, anatomical surfaces, stereotactic frames. In this article we present some new ideas for the enhancement of existing and for the design of new surface based registration algorithms. The ideas logically emerged from the results of a detailed analysis of existing state-of-the-art registration algorithms[6,18,19].

Three different approaches can be pursued for the development of better surface based registration algorithms: (1) existing ones may possibly by improved (see sections 2, 3 and 4), (2) existing ones that have not yet been used for the application at hand may be worth while adapting to the specific application (see section 5), and (3) it may be possible to design entirely new algorithms.

The basic assumptions underlying our definition of surface based 3D registration algorithms are the following. Segmentation of surfaces is assumed to be an independent preprocessing step. Surfaces contain geometric information only, but can have different representations, ranging from simple binary volume images over structured point sets to B-splines. However, if a point based representation is used, it will be assumed to contain sufficient points to allow for interpolation of other surface points. The registration transformation will be taken to be a rigid one with 6 degrees of freedom; i.e. only translations in 3 orthogonal directions and 3 rotations are taken into account. Since in our applications image voxel sizes are accurately known and because patients' heads do not change size, this should not pose any problems.

2. "GROWING HAT" SURFACE BASED 3D REGISTRATION

All surface based 3D registration algorithms iteratively search for registration parameter values that optimize a specific surface based matching criterion. These surface based matching criteria can be divided into two categories: 1) moment based , and 2) point projection based. In this section a method will be described for accelerating iterative search methods used in existing surface based registration algorithms. Because the detailed formulation of the method differs for the different categories of algorithms, it will be explained for algorithms using point projection based distances, and then briefly reformulated for algorithms using moment based criteria.

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Examples of 3D registration algorithms using point projection based distances and currently used for matching brain scans are Pelizzari's[12,13] head-hat algorithm, and Jiang's[9] and Mangin's[11] versions of Borgefors's[4,5] hierarchical chamfer matching algorithm. An example that has not been used in medical practice yet is Besl and McKay's[2,3] free form quaternion based iterative closest point algorithm. Essentially all of them can be described as follows:

- Two collections of corresponding surfaces - two corresponding surfaces in the simplest case - are obtained from segmentation. Let us call them S_1 and S_2. Let us assume that the registration problem at hand is to match S_2 onto S_1; i.e. find the transformation from S_2's image coordinate system into S_1's image coordinate system so that after transformation S_2 will coincide with S_1.

- Both surfaces are preprocessed, but in different ways. Pelizzari gets two surfaces from segmentation in simple surface representations, i.e. as lists of 2D contour coordinates organized by image plane. S_1's point list is transformed into a kind of polar coordinates, called the "head" format. S_2's point list is reduced in size, and in complexity; i.e. a sample of about 250 representative points is selected from the list and put in a new but flat list of 3D image coordinates, called the "hat" format. Borgefors on the other hand calculates the chamfer "distance transform" of S_1, but also uses the "hat" for S_2. Besl and McKay do not prescribe any format for S_1, but they too use a "hat" for S_2.

- By Pelizzari the distance D_s from S_2 to S_1 is defined as the root mean square average of the distances of all hat points to the head surface along rays through the respective hat points and S_1's centroid. Borgefors and Besl and McKay define D_s to be the root mean square average of the distances from the hat points to the closest points on S_1. So, the main difference between Pelizzari's and both other methods is that they use different projections of S_2's points on S_1. Also Borgefors only approximates the euclidean distance between the points and their projections using the chamfer distance transform, while Pelizzari and Besl and McKay calculate the exact euclidean distances.

- Registration is the minimization of the distance from S_2 to S_1.

  Both Pelizzari and Borgefors reason as follows: "Because the distances defined above do not have analytical expressions general n-dimensional optimization algorithms that do not use derivative information are required to solve the problem. The registration parameters are the optimization variables." In our case there are 6 of them (n=6). In practice the distance function has multiple local minima. Therefore a complete minimization method has two components; i.e. an accurate locally converging algorithm (e.g. Powell's or steepest descent) is used under control of a global optimization algorithm (e.g. simulated annealing, hierarchical optimization).

  Besl and McKay on the other hand reason as follows: "If S_1 and S_2 are in matching locations then S_2's point projections on S_1 coincide with S_2's points. So, in each iteration, let us consider the projections to be the true corresponding points. In that case in each iteration a point based registration problem with point correspondence information has to be solved instead of a surface based registration problem. So, a least squares estimation of the registration parameters can be calculated." Besl and McKay use quaternions for this calculation. But they also mention the calculation based on a singular value decomposition discussed by Faugeras and Hebert[7]. Besl and McKay prove that using a closest point projection their matching distance monotonically converges to a local minimum.

Besl and McKay studied the computational complexity in detail and proposed their own acceleration method based on the prediction of quaternion components by means of a linear and a parabolic extrapolation of D_s in function of the quaternion components' previous values. This acceleration method is meaningful only in case the old quaternion values used for extrapolation are approximately linear in 7D quaternion space, which definitely is not always the case. Each time it is not, the acceleration method does not work in the following steps.

The acceleration presented in this section is inspired upon the fact that optimization steps in distance space are very large in the beginning, and very small at the end when local convergence occurs. This is illustrated in figure 1 for three quaternion registration parameters. Furthermore, the method logically followed from a quality constrained cost analysis of surface based 3D registration algorithms[6]. This analysis shows us that the large computational load of the registration algorithms is mainly due to the number of points selected on S_2 for evaluation of the distance D_s.

Four non-coplanar surface points uniquely determine the position of the surface. So, the following question is a very valid one: "Why should we use 250 points to estimate the direction in which to look for the registration parameters, especially when the last estimate is not even close to the optimal one?".

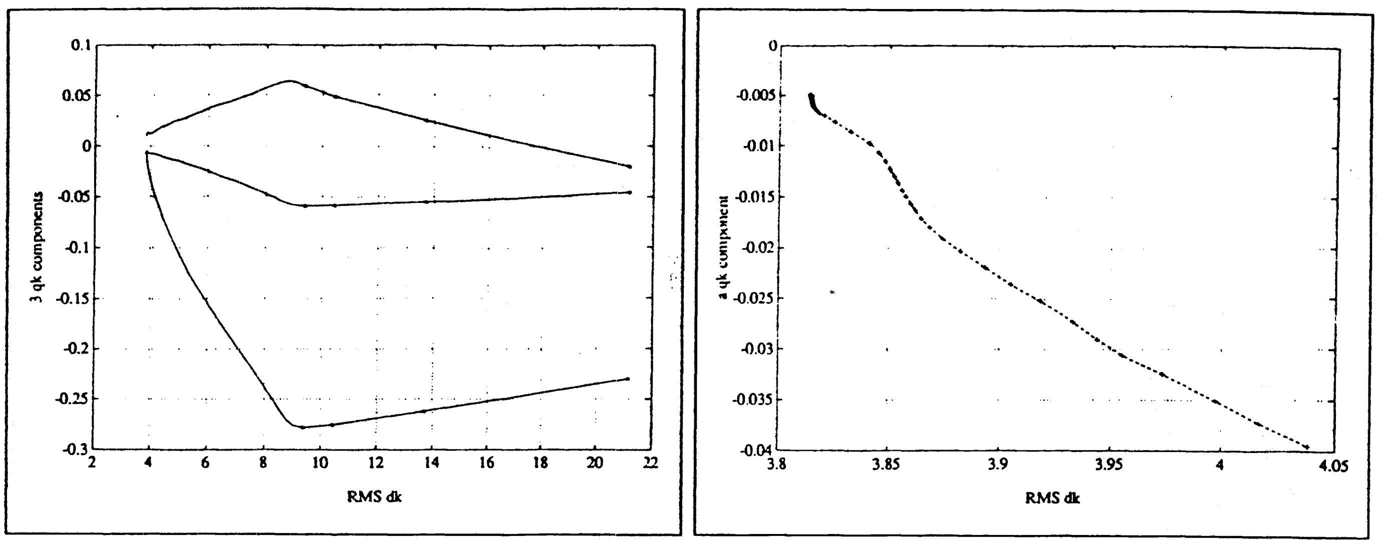

Figure 1: **Left:** The first 3 steps of some of Besl and McKay's quaternion components are very large. **Right:** The following steps are much smaller. This curve shows in detail the last 50 iteration steps (of a total of 100) corresponding to the middle curve on the left.

We have investigated the effect of reducing the number of points in D_s. The results are represented in figure 2. It shows that using few points will cause the function for D_s to have many more bad local minima. The figure also shows that for complete data sets for which a fairly good initial registration position is known beforehand (misregistration less than 25 mm for translations and less than 25 degrees for rotations) the number of points required for evaluation of D_s may be much smaller than 250 as advised by Pelizzari.

We have also investigated the effect of selecting a very small - expressed in number of points - but different hat in each iteration, so that in the end probably more surface points will have been used for distance evaluation than by Pelizzari's or the other algorithms. It is not difficult to understand that in such a search approach not even local convergence can be guaranteed.

The ultimate solution is to select a small set of non-coplanar points on S_2 to start with and let it grow until it comprises all of S_2. So, in the beginning the registration will be much faster than in the algorithms with "fixed hat", while it will be much slower at the end. But the accuracy will be optimal in the sense that all data in S_2 will eventually be used.

The number of points in the hat during the first iteration n_{hat}^0 and the growth factor $g(k)$ of the hat from one iteration k onto the next determine the total calculation time. From the surface based 3D registration algorithms' cost analysis[6] it can be concluded that in each iteration k calculation time is approximately proportional to the number of points n_{hat}^k in the hat. And so, the following approximate expression gives us the total calculation time for "growing hat" surface based registration:

$$T = T_p(n_{hat}^0 + \sum_{k=0}^{k=N-2} g(k) n_{hat}^k) \tag{1}$$

with T_p the time required per point on S_2 and N the number of iterations. Experimentation with this equation rapidly leads us to the conclusion that in order to obtain maximal accuracy using **growing hat** search, speed performance will be worse than with **fixed hat** search assuming that the fixed hat contains 250 points. The best compromise between accuracy and speed performance is obtained with $n_{hat}^0 = 4$ and $g(k) = 2$ until $n_{hat}^{k+1} \geq n_{hat}^{fixed}$ and $g(k) = 1$ thereafter until convergence for speed; then add an extra iteration with $n_{hat}^N = n_{S_2}$ (i.e. all of S_2's points) for accuracy.

An open question is the following: "Does the specific selection of the initial hat influence the search process so that at the end a different local minimum is reached?" Clearly it might in some situations. But of course the answer is irrelevant because of the global optimization algorithm at a higher level.

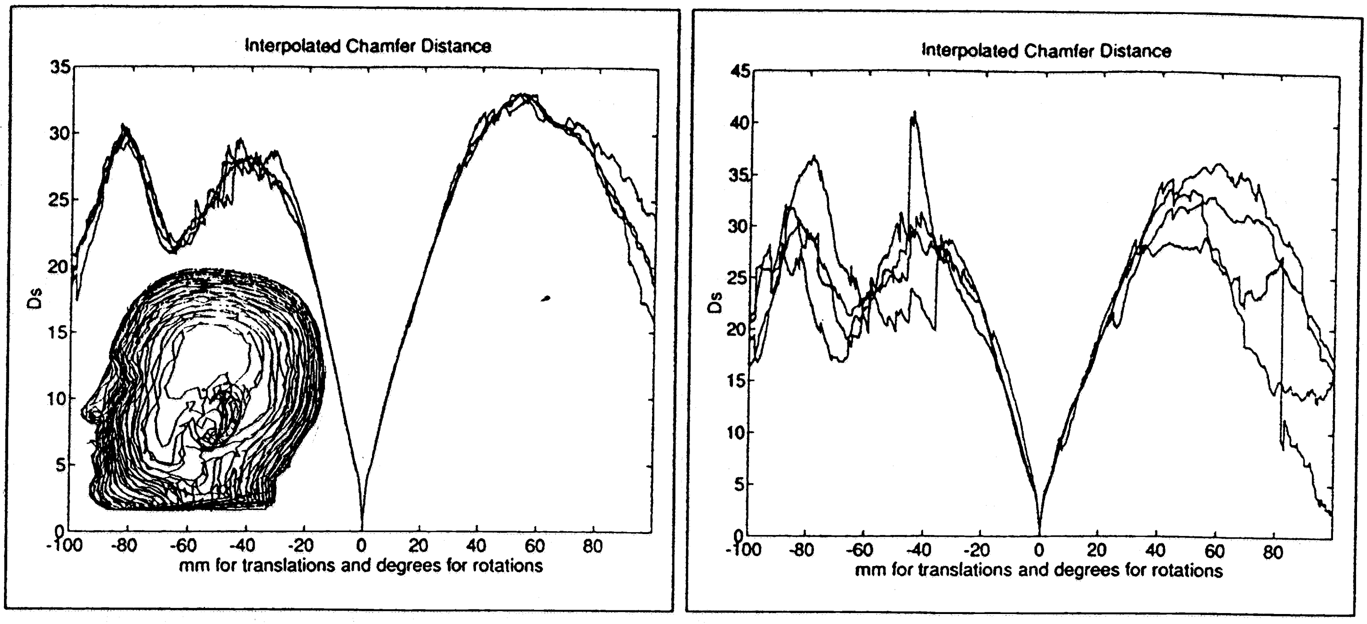

Figure 2: **Left**: For the data set (containing 2543 points) represented at the bottom of the figure D_s-traces are shown in function of simultaneous translations and rotations in all directions. On these traces D_s is the distance of the data set to itself after application of specific misregistration transformations. The number of points involved in the calculation of D_s were 125, 250, 500 and 1000. **Right**: The same traces for 15, 31, 62 and 125 points in D_s.

Note that this entire reasoning was made possible by the fact that D_s is a single number that equals the root mean square average of multiple point distances. It is also assumed that the cost of selecting a growing hat is neglectable. No specific selection algorithms have been proposed. We used the simplest possible; i.e. we selected every i_k-th point from the list of S_2's points where $i_k = n_{S_2}/n_{hat}^k$.

The results of this section can be adapted to surface based 3D registration algorithms using moment based matching criteria by means of a "**field of view box**[1] **with growing resolution**".

3. PARALLEL POINT PROJECTION BASED DISTANCE BETWEEN SURFACES

When trying to adapt the growing hat method to moment based matching criteria the following new method spontaneously emerged. It is based on the combined usage of **3 parallel projections in orthogonal directions** of some of S_2's points on S_1 for calculating 3 ray tracing based distance histograms. The reason why we use the term "ray tracing" in stead of "point projection" here will become clear later on. The root mean square averages from the distance histograms are used as estimates of the registration translation parameters and the histogram spread is used as a measure of matching quality that will be used to search for the optimal rotation parameters.

The algorithm can be summarized as follows (see figure 3):

1. Let us suppose that both S_1 and S_2 are available as chamfer distance transform images. These images are used by Zuiderveld's[21] ray tracing acceleration method. We have selected this method because it is the fastest available for our application.

2. Select three sets A_1, A_2 and A_3 of 2D coordinates in the three orthogonal image planes respectively corresponding to $x = 0, y = 0$ and $z = 0$, where x, y and z are image coordinates in S_2's coordinate system.

3. For all coordinates in each set A_i perform a ray tracing calculation perpendicular to the corresponding image plane and so doing construct three lists of S_2's surface points: $L_x = \{(n_x, x_1, \ldots, x_{n_x})\}, L_y = \{(n_y, y_1, \ldots, y_{n_y})\}$ and $L_z = \{(n_z, z_1, \ldots, z_{n_z})\}$. n_x, n_y and n_z are the numbers of surface points on the respective rays and the

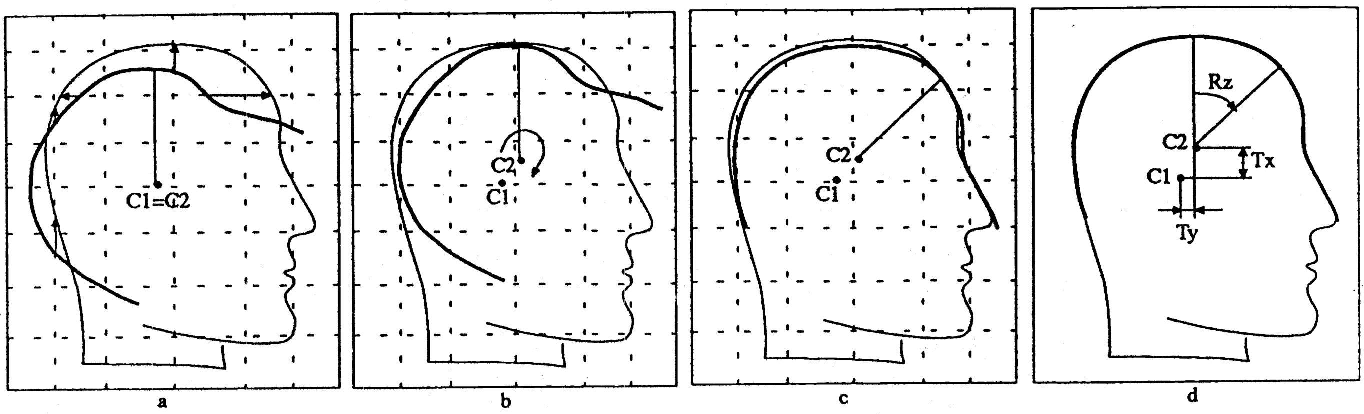

Figure 3: a) The complete head (thin line) represents S_1, while the thick line represents S_2. Distances are determined through parallel ray tracing in 3 orthogonal directions of which two are shown. Note that only the distances selected after application of equation (2) are shown. The selection of the set of rays is not prescribed. b) Averaging the resulting distances for each direction determines the registration translation step. c) Then the rotation angle is determined by minimizing the spread of the global histogram of all point distances. d) Shows the final registration parameters for the 2D case.

other numbers are the coordinates on the rays. This ray tracing step needs to be performed only once. This means that the distance transform image of S_2 does not need to be stored for further calculations.

4. Initialize all translation parameters to values that make both surfaces mass centers coincide and have some estimates for the euler angles initialized by a global optimization algorithm.

5. Transform the selected rays into S_1's coordinate system and perform the same ray tracing operations. In this process 3 more lists $L_{x'}, L_{y'}$ and $L_{z'}$ corresponding to the lists generated in step 3 are constructed.

6. Then three distance histograms H_x, H_y and H_z are constructed by comparing both sets of lists. The following distance calculation rule is used:

$$\forall i \in \{x, y, z\}, \forall k \in L_i : ((n_i^k = n_{i'}^k) \rightarrow \forall i_p \in \{i_1^k, \ldots, i_{n_i^k}^k\} : increment(H_i(i'_p - i_p)) \tag{2}$$

7. Calculate the root mean square average of all histograms: μ_x, μ_y, and μ_z.

8. Adapt the translation parameters as follows:

$$\forall i \in x, y, z : t_i^j = t_i^{j-1} + \mu_i \tag{3}$$

where j is the iteration number.

9. Merge the 3 histograms into one global histogram H_g by simple addition.

10. Calculate a measure of the spread of the new histogram σ^2 and use it as a starting value for the optimizing search for the euler angles in 3D rotation space. For this search any locally converging algorithm can be used. During this optimization phase the intermediate histograms are never calculated.

11. Repeat steps 5 to 10 until the histogram averages and spread do not change anymore (i.e optimize locally). If the histogram spread is too large, start all over again with a new set of values for euler angles (i.e. optimize globally).

The main advantage of this algorithm is that it automatically eliminates points from non-overlapping parts of the surfaces in the evaluation of the matching quality by means of the specific histogram construction rule proposed in equation (2). Other advantages of this method are that:

- If the points on S_2 are whole image coordinates than its distance transform is not required to calculate the ray tracing. It can then be calculated by simply searching through S_2 in head format for example.
- The number of optimization variables to be obtained by search is only 3 (i.e. the rotations), which is much lower than a minimum of 6 for the other algorithms using search based optimisation.
- However all 6 registration parameters can be fixed if their values are known beforehand, unlike some of them in moment based algorithms and unlike the parameters in Besl and McKay's algorithm.
- Using three orthogonal parallel ray tracings automatically results in the selection of a hat that is representative of the surfaces involved. Note that in order to obtain about 250 hat points as proposed by Pelizzari only about 40 rays are required for each orthogonal direction, under the assumption that the surfaces completely overlap and that a ray intersects the surfaces twice.
- The growing hat method presented in the previous section can be applied by changing the number of rays used for ray tracing.
- The surface complexity is not in any way limited by the algorithm.
- The availability of the histogram offers the possibility for easy integration of an outlier treatment algorithm as described in the next section.
- The algorithm can easily be generalized for registration problems of higher dimension.

A disadvantage certainly is the need for a calculation of the distance transform. Therefore the chamfer distance is used. Note that the approximated chamfer distances are not used to evaluate the distance. They are merely used to accelerate the ray tracing. Note also that contrary to what is done by Jiang et al[9], we do not interpolate to obtain an isotropic image coordinate system. In stead we apply a heuristic optimization rule to determine a set of non-isotropic chamfer coefficients. This approach saves a lot of work.

The most important disadvantage is the cost of ray tracing. That is why the availability of the distance transforms is stressed. Zuiderveld's ray tracing algorithm is probably the fastest available for our application.

A problem that is not solved is the problem of local minima in the optimization criterion for the euler angles. So, a global optimization algorithm is still required. But evidently the optimization space is much smaller. If however the orientations of both surfaces are not too different then the first local minimum found will most often also be the global one.

It can be concluded that a new surface based 3D registration algorithm has been designed that offers both some of the speed of moment based direct matching optimization and all of the flexibility of point projection based matching criteria. Its accuracy is of course not worse than that of both categories. Moreover its extension with the use of a "growing ray set" also allows for augmentation of the accuracy.

4. ADAPTIVE OUTLIER TREATMENT

The algorithm presented in the previous section works perfectly if segmentation results are perfect, which is unfortunately never the case in practice. After registration several points on surface S_2 may be at a rather large distance of surface S_1 even though they belong to part of S_2 that does overlap with S_1. Such **outliers** must be eliminated from the calculation of the registration parameters because they would otherwise introduce registration errors. Jiang et al[9]. propose the use of a simple threshold, but they do not say how to select the threshold.

Searching for an adaptive threshold heuristic the following unpublished adaptive outlier treatment algorithm has recently been developed by Géraud et al[8] (see figures 4 and 5):

1. Convert the global distance histogram H_g into a new histogram H_a of absolute values of point distances.

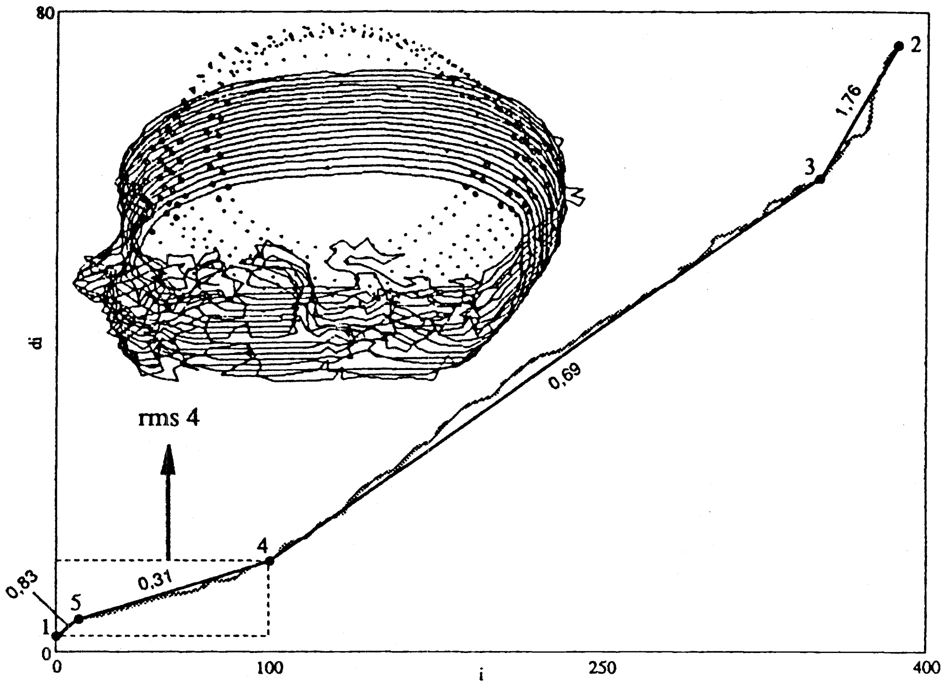

Figure 4: Application of the adaptive outlier treatment method to two surfaces with very small overlap. The resulting root mean square average of the remaining distances is 4 for the desired solution.

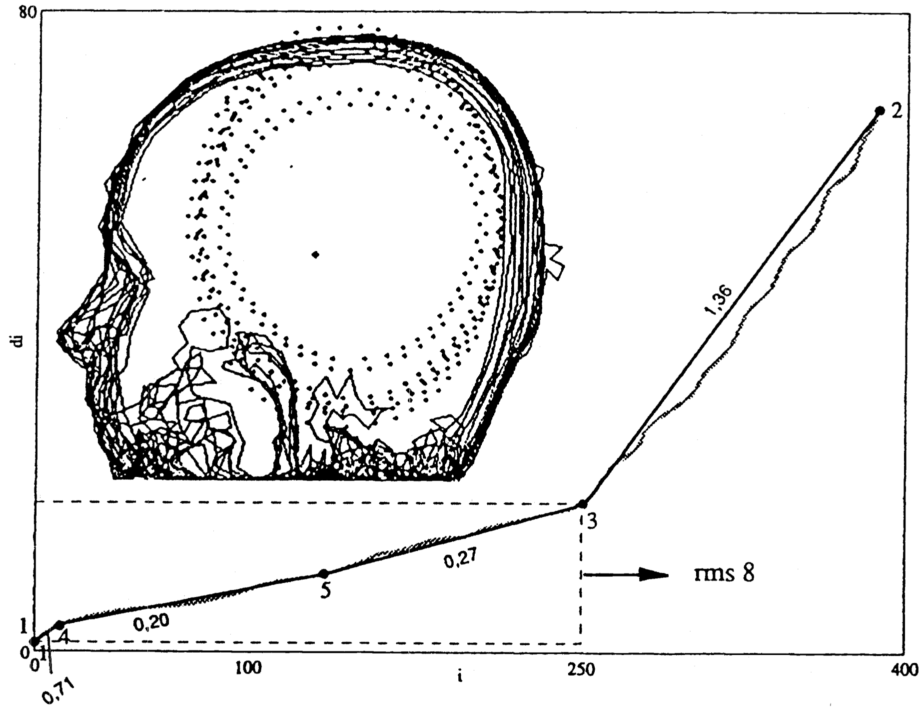

Figure 5: Application of the adaptive outlier treatment method to the same two surfaces as in figure 4. The resulting root mean square average of the distances remaining after application of the adaptive threshold is 8, which is clearly much worse than 4. The 2D projection at the top of the figure shows that the curve corresponds to a bad but locally optimal registration solution.

2. Let the available positive point distances d_i be ordered from small to large, and let the order number be i. The resulting distance-index-function $d_i(i)$ is used then to calculate the threshold above which point distances are no longer meaningful; i.e. the corresponding points are probably outliers and possibly even non-overlapping with the other surface. The function $d_i(i)$ is defined completely by H_a.

3. Inspired on the iterative end point curve approximation method the function $d_i(i)$ is approximated by 5 characteristic points (see points 1 to 5 in the figure). Point 4 and 5 always approximate the segment [1,3]. Point 5 approximates either segment [1,4] or segment [4,3]: the segment with the lowest slope is selected.

4. Among the 3 segments between points 1 and 3 select the one with the lowest slope and add the adjacent segments if their slope is not too different ($\leq$ 50% of the highest of the three slopes). The resulting segment extended downto point 1 is the resulting set of distances $d_i(i) < d_{threshold}$. So, $d_{threshold}$ is determined by either point 3, point 4, or point 5.

The example in figures 4 and 5 clearly indicates that even the use of a relative threshold $d_i(i) < f_{threshold}.max(d_i(i))$ would not suffice to distinguish a bad local minimum from the local minimum in D_s that is actually searched for.

Because the introduction of this outlier treatment method is fairly costly we do not advise its use during local registration. Its use is encouraged however to select the correct solution amongst several locally optimal registration solutions. It may also be used to recalculate the registration error in order to obtain a more accuracte value for D_s.

Note that the results in figures 4 and 5 correspond to a set of d_i obtained by Besl and McKay's criterion. The registration criterion presented in the previous section automatically eliminates non-overlapping surface parts. And therefore segment [3,2] in figure 4 will not be present in function $d_i(i)$ in case the results of both this and the previous section are combined. The algorithm needs to be simplified accordingly in that case.

5. FROM SURFACE CORRESPONDENCE TO POINT CORRESPONDENCE

The main difference between point based and surface based registration algorithms is in the availability of point correspondence information. If the information is available outliers can be detected by the criterion proposed by Toennies et al[16]. Points without corresponding points are discarded from the point based registration problem, i.e. non-overlap does not occur. It is exactly the lack of point correspondence information in the surface based registration problem that causes surface based registration algorithms to be iterative search based. It is also the reason why either hat point projections and field of view boxes are used by the point projection and the moment based registration algorithms respectively. In the previous sections several techniques have been proposed on the one hand to accelerate search and on the other hand to eliminate points that have no corresponding points.

A more direct approach for deducing more constraining correspondence information from corresponding surfaces is possible by using features that contain geometric information of a more complicated nature. One such algorithm is described by Shapiro and Brady[14]. Their eigenvector approach to solve the feature-based point correspondence problem can be used to convert surface correspondence information into point correspondence information. This latter form of correspondence information can then be used by a direct point based registration algorithm in order to calculate the registration parameters. In theory this algorithm also is insensitive to non-overlap. Non-overlapping surface parts would correspond to the least significant feature modes with the smallest eigenvalues and they would be truncated from the association or correspondence matrix. Moreover the algorithm is able to cope with small distortions, i.e. outliers in our case. A detailed computational analysis of the algorithm however shows that it does not offer speed advantages over the other surface based registration methods. No accuracy results are available.

Another surface based registration algorithm that solves the correspondence problem before it calculates the registration parameters is the one described by Thirion et al[15]. This algorithm detects crest lines on surfaces and uses them as features to be matched. The advantage is that skull surface crest lines are much more asymmetric than skull surfaces and more interesting even is that they contain a much smaller number of points. This method is very fast. No accuracy results are available yet however.

In general feature based algorithms will use any geometrically invariant feature that can be extracted from the images of all modalities. These general features may not solely be surface based. For example, Van den Elsen et al[17]. propose the use of differential-geometric invariants based on Koenderinck's[10] family of Gaussian differential operators. No accuracy results are available for the 3D case. However Van den Elsen claims accuracy to be better than that of surface based algorithms[20].

While surface based algorithms only require a simple threshold based segmentation algorithm to extract the skin or the skull surface, feature based algorithms using complex features require specific and more complex segmentation algorithms.

6. CONCLUSION

In case of point projection based matching criteria "growing hat search" and in case of moment based matching criteria "growing field of view box search" are proposed to speed up surface based registration algorithms. It is argued that the speed up can be traded for extra accuracy if an adapted hat or field of view box growing scheme is used.

Three orthogonal and parallel ray castings are used to define a multicomponent criterion to evaluate the distance between surfaces. It is shown that this distance function combines advantages of both point projection based and moment based matching criteria. This criterion not only reduces search space; it also offers a simple solution for the problem of partially overlapping surfaces.

Furthermore an adaptive outlier treatment method is proposed that can be used in combination with point projection based matching criteria. It is based on the characterization of the distance-index-function of individual distances between points and their projections. This method is also adapted to the new multicomponent matching criterion. Their combination results in the most reliable surface based registration algorithm known, because it is capable of treating both outliers and partially overlapping surfaces.

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