GO-APSR: A Globally Optimal Affine Point Set Registration Method

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ABSTRACT Point set registration under affine transformation is an important problem in computer vision because not only it has many direct applications, but it is also often used as an initial step for non-rigid registration. This problem is challenging when no correspondences between the two point sets are known, and most existing methods start from an initial pose and find a local optimal transformation. This paper presents a deterministic global optimization method for affine point set registration, which is called GO-APSR. We model the two sets to be registered with Gaussian Mixture Models (GMMs) and minimize the L2 distance between the two GMMs under affine transformation. Branch-and-Bound (BnB) is employed to search the transformation parameter space, and we propose a convex quadratic function as the under-estimator of the objective function in each branch. Therefore, calculation of the lower bound in each branch is casted into a bound-constrained convex quadratic programming problem, which can be solved globally and efficiently. Experiment results verify the global optimality of the proposed method and its robustness to noise and outliers. Furthermore, it works very well in the challenging partially-overlap scenarios.

INDEX TERMS Affine registration, Branch-and-bound, Gaussian Mixture Models, Global optimization, Point set registration

I. INTRODUCTION

Point set registration, which finds a spatial transformation to align two point sets, is widely used in computer vision, pattern recognition, and medical image analysis. It can be regarded as solving two inter-locked sub-problems: finding point correspondence and recovering spatial transformation, and when one is known, the other can be easily solved. In literature, many methods have been proposed to solve point set registration under different levels of information about these two sub-problems. In this paper, we focus on solving the problem of aligning two point sets under affine transformation without correspondences. Among all kinds of possible spatial transformation, affine transformation is an important one. It is a generalization of rigid transformation, a good approximation of perspective transformation in many CV applications, and finding an affine transformation to align point sets coarsely can be an important initial step before more complex deformable registration methods are applied.

If exact correspondences between some points are given, closed form solutions exist for finding the optimal rigid transformation between the two point sets [1]. If the spatial transformation between the two point sets is affine, the optimal solution can be easily found by solving a linear equation.

When no correspondence is given, feature matching methods can be applied to establish tentative correspondences [2]. Though there are usually a large proportion of outliers in these correspondences, robust estimation method such as RANSAC [3] and its variants [4], [5] can be used to reject outliers [6]–[8], and find the true correspondences and the optimal rigid or affine transformation at a high probability. However, it is not always easy to establish correspondences between point sets because there is usually no texture and only structural and spatial information of the points can be used. It becomes more challenging when affine transformation is involved, because most of the structure based feature descriptors are not affine invariant.

On the other hand, if an approximate transformation is known in prior, the optimal transformation can be found by local optimization approaches, among which Iterative Closest Point (ICP) [9] is the most widely used method due to its simplicity, intuitive concept and satisfactory performance. ICP starts from an initial spatial transformation and iterate...
between finding correspondences under current transformation and updating spatial transformation under current correspondences. ICP was originally proposed for rigid point set registration, and was later adapted for affine registration [10]. However, there are some inevitable limitations for classical ICP, e.g., its sensitivity to noise and outliers and its tendency to be trapped into a local minimum. A major reason for the above limitations is the assumption of one-to-one correspondence between the points in the two point sets to be registered.

To alleviate the sensitivity to noise and outliers and enlarge the convergence basin of ICP, some researchers have tried to replace the hard one-to-one correspondence in ICP with soft correspondence. For example, in robust point matching [11], the original binary relationship in ICP is relaxed to one in the interval [0, 1]. Furthermore, the idea of soft correspondence exists in new alignment criterions based on the probability distribution constructed from the original point sets, e.g., Kernel Correlation [12] and Gaussian Mixture Models (GMMs) [13], [14]. These probability distribution based alignment criterions are robust to noise and outliers, and can provide a larger convergence basin than ICP, but a good initial transformation is still needed.

Recently there has been a surge of solving point set registration problem globally by using Branch-and-Bound (BnB) optimization framework without prior information on correspondence or transformation. However, most of these approaches focus on rigid registration. To the best of our knowledge, there is only one method [15] that can solve affine point set registration problem globally, which optimizes the one-to-one correspondence between two point sets. However, no exact correspondence exists when there are noise and outliers in the data sets or when the two point sets are only partially overlapped. In these scenarios, optimizing one-to-one correspondence may introduce errors.

Contributions. 1) Guaranteed global optimality. We propose a new affine point set registration method with guaranteed global optimality, which minimizes the L2 distance between two GMMs constructed from the two point sets to be registered. 2) Robustness. Comparing to APM [15], the proposed method is not based on one-to-one correspondence, so it is more robust to noise and outliers. 3) Novel efficient lower bound. BnB framework is used to minimize the cost function, and we derive a quadratic lower bound function to the cost function in every branch, so that finding the lower bound in each branch is casted into a bound-constrained convex Quadratic Programming (QP) problem, which can be globally optimized quickly.

II. RELATED WORK

This paper deals with point set registration problem without correspondence in prior. For most methods dealing with this problem, being trapped in a local optimum is a major problem, and their probability of reaching the global optimum is low without a good initial transformation. For some applications, it is time-consuming or impossible to find a good enough initial transformation, so a lot of researches have been done to register point sets without prior pose. Initially, some researchers utilize stochastic global optimization methods to increase the probability of reaching the global optimal solution, e.g., [16] and [17]. Random sampling schemes such as RANSAC [3] and 4PCS [4] can also be classified into this category. The main limitation of stochastic methods is that the global optimum cannot be guaranteed and some of them are very computationally expensive.

BnB based deterministic global optimization method has also been explored to register point sets with guaranteed global optimality. The most important ingredient of BnB optimization framework is the upper and lower bounds of the objective function to be optimized, and every new approach involves deriving a novel bound. For example, in [18], a convex under-estimator was obtained by relaxing the rigid rotation transformation. However, some correspondences were required, like point-to-point or point-to-line, to obtain a convex objective function, which is not available in some circumstances. Go-ICP [19] was used to solve the global optimization problem of rigid registration without correspondence for the first time. In that work, ICP was integrated into the BnB framework, and the lower bounds were calculated directly by exploring geometric properties in the \(SE(3)\) space. A similar scheme was used for GMMs based alignment criterions in [20], which led to good scalability and robustness. Different from the L2 distance based objective function in Go-ICP, [21], [22] adopted consensus maximization scheme and searched for the maximum of the objective function using BnB. [23], [24] proposed to decompose the rigid transformation into rotation and translation, reducing the searching space from six dimension to three dimension, and then BnB was applied to search the three-dimension parameter space. However, these works focus on rigid registration, and it is not trivial to extend their bounds to affine registration.

Currently APM [15] has been proposed to solve for point set registration with affine transformation globally. APM optimizes one-to-one correspondences between the two point sets, while the proposed method in this paper optimizes a GMMs based alignment criterion, which is more robust to noise and outliers. [20] also used a GMMs based alignment criterion, but the target problem and the objective function in this paper are different from those in [20], and we derive totally new bounds.

III. GLOBAL OPTIMIZATION

A. OBJECTIVE FUNCTION

Let \(X = \{x_1, \ldots, x_m\}\), \(Y = \{y_1, \ldots, y_n\}\) be the model set and the scene set, respectively, where \(x_i, y_j \in \mathbb{R}^l\), \(l = 2\) are the coordinates of 2D points. The goal is to find an affine transformation \(T\) to align the two point sets. For every point \(x_i\) in the model set, \(T(x_i) = Ax_i + b\), where \(A \in \mathbb{R}^{2 \times 2}\) is the affine matrix and \(b \in \mathbb{R}^2\) is the translation vector. Note that as in [25], an affine matrix \(A\) can be decomposed into four matrices, \(A = (UV^T)(VSV^T) = R(\theta)R(-\phi)SR(\phi)\), where
\( \mathbf{R}(\theta), \mathbf{R}(-\phi) \) and \( \mathbf{R}(\phi) \) are rotation matrices representing three different rotations with three different angles \( \theta, -\phi \) and \( \phi \), and \( \mathbf{S} \) is a diagonal matrix, of which the diagonal entries \( \{s_i\}_{i=1}^{4} \) represent scaling factors. By decomposing, for any point \( \mathbf{x}_i \), \( \mathbf{A}\mathbf{x}_i \) can be considered as \( \mathbf{R}(\theta)\mathbf{R}(-\phi)\mathbf{SR}(\phi)\mathbf{x}_i \), which means that to impose \( \mathbf{A} \), we first rotate the point by \( \phi \), then scale it by \( \{s_i\}_{i=1}^{4} \), and at last rotate it by \( -\phi \) and \( \theta \). This decomposition scheme illustrates the affine transformation clearly and we follow this scheme in this paper. Every point in the two point sets is treated as the center of every point in the two point sets is treated as the center of

\[
gmm(p|\mathbf{T}(\mathbf{X})) = \frac{1}{m} \sum_{i=1}^{m} N(p|\mathbf{x}_i, \mathbf{I}\sigma^2) \tag{1}
\]

\[
gmm(p|\mathbf{Y}) = \frac{1}{n} \sum_{j=1}^{n} N(p|\mathbf{y}_j, \mathbf{I}\sigma^2) \tag{2}
\]

where \( \mathbf{I} \) is the identity matrix and \( \sigma^2 \) is the variance. We use L2 distance to measure the statistical discrepancy between the two GMMs as follows:

\[
D(\mathbf{T}) = \int (gmm(p|\mathbf{T}(\mathbf{X}))-gmm(p|\mathbf{Y}))^2 dp \tag{3}
\]

\[
= \int (gmm(p|\mathbf{T}(\mathbf{X})))^2 dp - 2 \int gmm(p|\mathbf{T}(\mathbf{X}))gmm(p|\mathbf{Y})dp + \int (gmm(p|\mathbf{Y}))^2 dp \tag{4}
\]

where the third term (6) is independent of \( \mathbf{T} \), so that minimizing \( D(\mathbf{T}) \) is equal to minimizing the following objective function:

\[
E(\mathbf{T}) = \int (gmm(p|\mathbf{T}(\mathbf{X})))^2 dp - 2 \int gmm(p|\mathbf{T}(\mathbf{X}))gmm(p|\mathbf{Y})dp \tag{7}
\]

Other than in the rigid case [26], the first term cannot be omitted in affine transformation. According to the identity,

\[
\int N(p|\mu_1, \sigma_1^2)N(p|\mu_2, \sigma_2^2)dp = N(0|\mu_1 - \mu_2, \sigma_1^2 + \sigma_2^2) \tag{9}
\]

we can obtain a closed form solution of \( E(\mathbf{T}) \), that is,

\[
E(\mathbf{T}) = \frac{1}{m^2} \sum_{i=1}^{m} \sum_{j=1}^{m} N(0|\mathbf{Ax}_i - \mathbf{Ax}_j, 2\sigma^2) - 2m \sum_{i=1}^{m} \sum_{j=1}^{m} N(0|\mathbf{Ax}_i + \mathbf{b} - \mathbf{y}_j, 2\sigma^2) \tag{10}
\]

\[
= C_1 \sum_{i=1}^{m} \sum_{j=1}^{m} \exp\left(-\frac{||\mathbf{Ax}_i - \mathbf{Ax}_j||^2}{4\sigma^2}\right) \tag{12}
\]

\[
+ C_2 \sum_{i=1}^{m} \sum_{j=1}^{m} \exp\left(-\frac{||\mathbf{Ax}_i + \mathbf{b} - \mathbf{y}_j||^2}{4\sigma^2}\right) \tag{13}
\]

where \( C_1 \) and \( C_2 \) are constant coefficients.

### B. GLOBAL OPTIMIZATION USING BNB

As mentioned above, we use BnB to search for the global minimum of (12) and (13). As a type of deterministic global optimization method, BnB is a powerful global optimization tool for nonconvex problems. By branching the parameter space and estimating the upper or lower bound in each branch, BnB can prune useless branches without potential for global optimum so that the searching space shrinks gradually, leading to effective global optimization. In our case, the search is conducted directly in the parameter space of affine transformation \( \mathbf{T} \). The key of the proposed method is to obtain the lower bound of the cost function \( E(\mathbf{T}) \) in every branch by solving a bound-constrained convex quadratic programming problem, which is discussed in detail below.

We first give an under-estimator of each of the two terms in (12) and (13). For the first term representing the relationships between points in the model set, let

\[
u_{ij} = \frac{||\mathbf{Ax}_i - \mathbf{x}_j||^2}{4\sigma^2}, \tag{9}
\]

then it can be simplified as

\[
C_1 \sum_{i=1}^{m} \sum_{j=1}^{m} \exp\left[-\frac{||\mathbf{Ax}_i - \mathbf{x}_j||^2}{4\sigma^2}\right] \leq C_1 \sum_{i=1}^{m} \sum_{j=1}^{m} e^{-\nu_{ij}}, \tag{14}
\]

For an arbitrary \( u_{ij} \), the function \( e^{-u_{ij}} \) is illustrated in Fig. 1(a). Given a branch in the parameter space, which corresponds to an interval of each parameter in the matrix \( \mathbf{A} \) and vector \( \mathbf{b} \), the corresponding interval \( [u_{ij}, \pi_{ij}] \) of \( u_{ij} \) can be obtained by interval extensions. Then, a line \( G_{ij}(u_{ij}) = \xi_{ij}u_{ij} + \eta_{ij} \leq e^{-u_{ij}} \) tangent to \( e^{-u_{ij}} \) at \( (0, e^{-\pi_{ij}}) \), can be used as an under-estimator of the first term in \( [u_{ij}, \pi_{ij}] \), as shown in Fig. 1(a), and we have

\[
C_1 \sum_{i=1}^{m} \sum_{j=1}^{m} e^{-u_{ij}} \geq C_1 \sum_{i=1}^{m} \sum_{j=1}^{m} G_{ij} \tag{15}
\]

\[
= C_1 \sum_{i=1}^{m} \sum_{j=1}^{m} (\xi_{ij} ||\mathbf{Ax}_i - \mathbf{x}_j||^2 + \eta_{ij}) \tag{16}
\]

where the gradient \( \xi_{ij} \) and the intercept \( \eta_{ij} \) can be calculated according to \( \pi_{ij} \) and \( e^{-\pi_{ij}}, (16) \) is a quadratic function of the elements of \( \mathbf{A} \) and it is concave because here, \( \xi_{ij} < 0 \).

For the second term in (12) and (13), similarly, let \( v_{ij} = \frac{||\mathbf{Ax}_i + \mathbf{b} - \mathbf{y}_j||^2}{4\sigma^2} \), then it can be simplified as

\[
C_2 \sum_{i=1}^{m} \sum_{j=1}^{m} e^{-v_{ij}} \leq C_2 \sum_{i=1}^{m} \sum_{j=1}^{m} e^{-v_{ij}} \tag{17}
\]

For an arbitrary \( v_{ij} \), the function \( -e^{-v_{ij}} \) is shown in Fig. 1(b). Given a branch in the parameter space, the corresponding interval \( [\bar{v}_{ij}, \bar{v}_{ij}] \) of \( v_{ij} \) can also be calculated by interval extensions. Then, a line \( G_{ij}'(v_{ij}) = \xi_{ij}v_{ij} + \eta_{ij} \leq -e^{-v_{ij}} \) passing through \( (\bar{v}_{ij}, -e^{-\bar{v}_{ij}}) \) and \( (\bar{v}_{ij}, -e^{-\bar{v}_{ij}}) \) can be regarded as
function (12) and (13) can be written as

\[ U = \sum_{i=1}^{m} \sum_{j=1}^{n} e^{-u_{ij}} \]

and its tangent line given an interval of \( u_{ij} \{0.25, 2.25\}\). We have

**Convex function** \( e^{-u_{ij}} \) and its secant line given an interval of \( v_{ij} \{0.25, 2.25\}\). **(c)** Lower bounds of a GMMs with two Gaussians.

\[ C_2 \sum_{i=1}^{m} \sum_{j=1}^{n} - e^{-v_{ij}} \geq C_2 \sum_{i=1}^{m} \sum_{j=1}^{n} G'_{ij} \]

\[ = C_2 \sum_{i=1}^{m} \sum_{j=1}^{n} (\xi_{ij} \| A \xi_i + b - y_j \|^2 + \eta_{ij}') \]

Unlike (17) and (18), (19) and (20) are a convex quadratic function of the elements of \( A \) and \( b \) because here, \( \xi_{ij} > 0 \).

From (17), (18), (19) and (20), in an arbitrary interval of the elements of \( A \) and \( b \), an under-estimator of the objective function (12) and (13) can be written as

\[ B_L(A, b) = C_1 \sum_{i=1}^{m} \sum_{j=1}^{n} (\xi_{ij} \| A x_i - x_j \|^2 + \eta_{ij}) \]

\[ + C_2 \sum_{i=1}^{m} \sum_{j=1}^{n} (\xi_{ij} \| A x_i + b - y_j \|^2 + \eta_{ij}') \]

Therefore, in each branch of the parameter space, the original objective function of the sum of exponentials in (12) and (13) is lower bounded by the sum of quadratic functions in (21) and (22), which is much easier to deal with because the result of the summation is a quadratic function. This is the key of the proposed method. In every branch, calculating the minima of \( B_L(A, b) \) is a bound-constrained QP problem.

However, we cannot guarantee that the QP is convex. Enlightened by [27], [28], we add a non-negative term to \( B_L(A, b) \) to make the Hessian matrix of the new quadratic problem positive semi-definite, and we obtain

\[ B'_L(\theta) = B_L(\theta) + \alpha \sum_{i=1}^{d} (\theta_i - \theta_i^*)(\theta_i - \theta_i^*) \]

where the parameters of affine transformation, which are the elements of \( A \) and \( b \), are stacked into vector \( \theta \), and \( d \) is the dimension of the parameter space. Therefore, \( d \) equals 6 for 2D affine transformations. \( \alpha \) is a positive value that needs to be determined to make the Hessian matrix of \( B'_L(\theta) \) positive semi-definite, and it can be calculated using the method in [29]. Therefore, \( B'_L(\theta) \) is a convex under-estimator of the objective function in each branch, and calculating its minimum is a bound-constrained convex QP problem, which can be solved globally and efficiently.

We summarize the proposed method as in Algorithm 1.

**Algorithm 1 GO-APSR: An algorithm for deterministic global optimization of GMM-based affine point set registration**

**Require:** mixture models \( G_x \) and \( G_y \), parameterized by means \( X \) and \( Y \) respectively, variance \( \sigma^2 \); threshold \( \epsilon \); initial \( \theta_0 \); initial hypercube \( C \) in parameter space.

1: Put \( C \) into priority queue \( \mathcal{Q} \).
2: \( E^* \leftarrow \) local optimal solution.
3: while \( \mathcal{Q} \) is not empty do
4: Remove \( C^l \) with lowest lower-bound \( E \) from \( \mathcal{Q} \).
5: \( \epsilon \leftarrow \) local optimal solution in \( C^l \).
6: if \( E^* \leq E^* \) then
7: \( E^* \leftarrow E^* \).
8: end if
9: if \( E^* - E \leq \epsilon \) then
10: Quit the loop.
11: end if
12: Divide \( C^l \) into sub-cubes.
13: for each sub-cube \( C_i \) do
14: Compute \( E_i \) for \( C_i \).
15: if \( E < E^* \) then
16: Add \( C_i \) to \( \mathcal{Q} \).
17: end if
18: if \( E > E^* \) then
19: Discard \( C_i \) and continue the loop.
20: end if
21: end for
22: end while
23: return \( \epsilon \)-optimal value \( E^* \) and corresponding \( \theta^* \).

**IV. EXPERIMENT RESULTS**

In this section, we evaluate the performance of the proposed algorithm GO-APSR and compare it against state-of-the-art methods.
affine point set registration methods APM [15] and CPD [28] on both synthetic and real data. Fig. 2 illustrates some of the data used in the experiments. The algorithm GO-APSR was implemented with MATLAB, the code of APM is from http://www4.comp.polyu.edu.hk/ cslzhang/APM.html, and the code of CPD is from www.pudn.com. All experiments were conducted on a workstation with one 3.2GHz XEON CPU and 32GB RAM. To generate a random affine transformation, we follow the decomposition in [25], which is $\mathbf{A} = (\mathbf{UV}^T)(\mathbf{VSV}^T) = \mathbf{R}(\theta)\mathbf{R}(-\phi)\mathbf{SR}(\phi)$, and set the rotation angle $\theta$ and $\phi$ random numbers in the range of $[0, \pi]$. The scaling factors, which are diagonal entries in the diagonal matrix $\mathbf{S}$, were set as random numbers in the range of $[0.8, 1.2]$.

A. GLOBAL OPTIMALITY

In this section, several experiments were performed to verify the global optimality of the proposed approach, which is the first advantage of GO-APSR. In the first experiment, we tested the convergence range of GO-APSR against GMMReg [14], [14] and CPD [28] in rigid registration. The contour, fish and the Chinese character Fu in Fig. 2 were used in this experiment. Each point set was rotated from $-\pi$ to $\pi$ to test if it can be aligned back to the original one. The convergence ranges of the three approaches are listed in Table 1, where the convergence ranges of GMMReg and CPD are as reported in [14]. Our approach can converge in the entire rotation range for all three point sets, while the other two algorithms can only converge in a subset of the rotation range.

The second experiment was used to test if GO-APSR can recover an arbitrary affine transformation. For the point set fish and Chinese character Fu, 200 random affine transformations were used on them to generate scene point sets, and the original point sets were registered to the scene point sets by GO-APSR. In all of the experiments, the randomly generated affine transformations were recovered. The average distance between corresponding points after registration is $6.3324e-7$ for Fish and $8.7659e-7$ for Chinese character.

Another experiment was conducted to demonstrate the evolution of the global lower bound $E$ in the registration of point set of Chinese character Fu, and the results is illustrated in Fig. 3 (a). As the time increases, the gap $\epsilon$ between the lower bound and the optimal value of the objective function becomes smaller and smaller. In this experiment, $\epsilon$ was set to $0.1$ and $\sigma$ was $0.35$.

We notice that GO-APSR can find the global optimum after tens of iterations while the rest of the running time is taken to decrease the gap $\epsilon$ between the upper and lower bounds. This phenomenon is illustrated in Figure 3 (b). Random affine transformations were conducted to fish and GO-APSR was applied with different $\sigma$ to align the sets. Instead of setting a gap $\epsilon$, the algorithm was terminated after some given iterations. When the average Target Registration Error (TRE) was less than $10^{-5}$, the registration was considered to be successful. Then we calculated the success rate among 100 registrations. The figure demonstrates that the success rate approaches $100\%$ with the growth of number of iterations. Larger $\sigma$ leads to higher success rate with fewer iterations due to the fact that larger $\sigma$ makes the objective function smoother and bears less local minima, which reduces the time of finding the global optimum comparing to small $\sigma$. This fact is also mentioned in [14]. However, if it is too large, some bias will be introduced to the global optimum, which is the reason why the success rate of $\sigma = 0.5$ is a little bit lower than that of $\sigma = 0.1$, as shown in Fig 3 (b). With this heuristic experimental result, we can terminate the algorithm after some iterations in practice so that the desirable registration accuracy can be obtained within a relatively short time. Note that the following experiments are all conducted based on this thought except for special clarification.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>GO-APSR</th>
<th>GMMReg</th>
<th>CPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>contour</td>
<td>$[-\pi, \pi]$</td>
<td>$[-1.8, 1.8]$</td>
<td>$[-1.53, 1.53]$</td>
</tr>
<tr>
<td>fish</td>
<td>$[-\pi, \pi]$</td>
<td>$[-2.0, 2.0]$</td>
<td>$[-1.25, 1.24]$</td>
</tr>
<tr>
<td>Chinese character</td>
<td>$[-\pi, \pi]$</td>
<td>$[-2.2, 2.2]$</td>
<td>$[-1.51, 1.54]$</td>
</tr>
</tbody>
</table>

B. REGISTRATION OF DEGENERATE POINT SETS

In this section, we evaluate the performance of GO-APSR for registering point sets contaminated with different kinds of degeneration, such as outlier, noise and occlusion, and compare it against state-of-the-art methods. We made comparison to a newly proposed globally optimal affine point set registration method APM [15] and a typical local method CPD [28]. It should be pointed out that there are not many methods to compare to, because APM [15] is the only method currently available to perform global affine point set registration. Please note that, via [15], this experiment provides an indirect comparison with several global rigid
registration methods, including GO-ICP, in the capability of recovering affine transformation. We chose CPD [28] as the representative of local optimization methods that can deal with affine transformations. Local approaches usually have a lower computational cost than global ones like GO-APSR. However, it is not our goal to compete with local approaches in terms of computational cost. On the contrary, we show that GO-APSR can find the globally optimal affine transformation while local methods need a good initial transformation to start with.

For each experimental condition, to generate fair Monte Carlo simulations, we run each algorithm 20 times with random affine transformation between the model and the scene point sets. As analyzed in Section IV.A, we can terminate the algorithm after some iterations to avoid excessive runtime and choose an appropriate \( \sigma \) to make the algorithm efficiently and accurately. Considering the degeneration added to the point sets (e.g., outlier, noise or occlusion), the \( \sigma \) was set as 0.05, and we terminated the algorithms after 60 iterations. The average TRE between corresponding points is reported in Fig. 4.

**Outlier.** In the first experiment, the model point set was obtained by transforming the fish and the Chinese character with a random affine transformation and adding different numbers of randomly distributed outlier points. The model point set was registered back to the scene point set with GO-APSR, APM and CPD. The average TRE with respect to the number of outlier points is shown in the first column of Fig. 4. We can see that the average TRE of GO-APSR is always very small, which means that GO-APSR restores the true affine transformation between the two point sets in all cases. As mentioned in Section II, the results demonstrate APM cannot handle outliers very well because the correspondence based approach may result in mismatches when there are outlier points.

**Noise.** In the second experiment, the scene point sets were generated by applying random affine transformations and adding Gaussian white noise with different levels of standard deviation. Additionally, there are 10 points missing in every scene set. The results are shown in the second column of Fig. 4, and we can see that GO-APSR and APM significantly outperform CPD. APM also performs fairly well because there are no outliers, and the probability of mismatching is low.

**Partial-to-whole.** When occlusion happens, some points in one set may not have counterparts in the other set, and the problem becomes tough. Partial-to-whole registration represents the situation that one of the point set is occluded. In this experiment, we took 2 to 20 points off from the original data to get the model sets, and the original data were transformed by random affine transformations to get scene sets. The results are shown in the third column of Fig. 4. GO-APSR aligned the two point sets in every case perfectly, while the error of APM tends to increase with the growth of the number of missing points. Again, CPD cannot converge in some cases and the average TRE of CPD is very large.

**Partially-overlap.** Partially-overlap is another case when occlusion happens, in which both point sets have missing points. This is a more challenging problem. One pair of partially-overlap point sets were generated by deleting some points from the head and the tail of the fish and the character separately. Random affine transformations are used to generate the scene sets as in previous experiments. The results in the fourth column of Fig. 4 show that GO-APSR can register partially-overlap point sets accurately and APM cannot handle this situation correctly when the two sets are both occluded.

Note that the two point sets used in this section are of different levels of symmetry. The fish is more symmetric than the character, and this may be the reason that the results of the character are better than the results of fish for APM. The average TRE of CPD are all very large, and the reason is that there are always some cases where CPD cannot converge in every experimental condition.

**C. CONVERGENCE TIME**

To terminate the algorithm with theoretically guaranteed global optimality, we need to set a convergence threshold \( \epsilon \), which is the gap between the current optimum of the objective function and the current lower bound. \( \epsilon \) has a direct influence on the convergence time, and a longer time is needed to achieve a smaller \( \epsilon \). Experiments were conducted in registering a randomly generated point set containing 90 points with two different \( \sigma \), and the results are plotted in Fig. 5 (a). The smaller the \( \epsilon \) is, the \( \epsilon \)-optimal result found by the algorithm gets more closely to the global optimum, but on the other hand, the longer time the algorithm needs to converge.

In addition, convergence time increases with the growth of the number of Gaussian components. The part of time complexity directly related to the number of Gaussian components is the division of a branch and calculating the lower bounds of all sub-branches using convex QP, which corresponds to the line 12 to line 21 in Algorithm 1. The time needed in this inner loop of our algorithm against the number of points is tested with registration of randomly

FIGURE 5: (a) Convergence time against gap $\epsilon$. Red line: $\sigma = 0.3$; green line: $\sigma = 0.25$. (b) Time needed in the inner loop (line 12 to line 21) of the GO-APSR algorithm against the number of points.

In this paper, one Gaussian component was placed on every point. In real application with very large number of points, preprocessing can be used to cluster the points into small number of Gaussian components before registration, as in [20].

**D. DEAL WITH THE LARGE-SCALE DATA**

In this section, GO-APSR is used to deal with some large-scale data sets containing thousands of points. In Fig. 2, we show an example shape from part B of CE-Shape-1 of MPEG database. We extracted points from the edge of the shape and obtained a point set containing 2245 points.

When dealing with large-scale data, we can simply downsample the data to make the problem easier, but the downsampled point sets cannot be too sparse to maintain the shape. Due to being based on GMMs, GO-APSR can alternatively take advantages of some methods that construct GMMs with fewer number of Gaussian components. Here we use SVGM [26] to build up GMMs with tens of components. Compared with naive down-sampling, SVGM can use fewer points to represent the original data set and it is robust to occlusion or missing points according to [31].

The model sets were obtained by taking 5% to 30% points off from the original data and the scene sets were generated by applying random affine transformation. For GO-APSR, SVGM was applied first to both sets to build up GMMs with tens of components and then GO-APSR was used to align the two GMMs. For APM, which can only use down-sampling to get smaller set, the two sets were randomly down-sampled to the same size as the point sets generated by SVGM. Then APM was used to register the two down-sampled point sets. The results are shown in Fig. 6, and we can see that GO-APSR can handle large-scale data set fairly well with the help of SVGM.

**E. INITIALIZING DEFORMABLE REGISTRATION**

As mentioned in Section I, affine registration can be used as an initial step for more complicated deformable registration. In this section, we will study the performance of GO-APSR in initializing and approximating deformable registration between MRI images of human brain.

As show in Fig. 7, we chose 2 slices of brain MRI images from BrainWeb [32], and generated the deformed images by applying B-spline deformation. We detected interest points on both the original and the deformed images by Harris corner detector, and get corresponding pairs by extracting and matching feature descriptors on these interest points. Before registration, the interest points in the deformed images are...
rotated with a random angle from 0 to π, and then GO-APSR was used to register the two point sets. The experiment was conducted 100 times on each pair of images, and GO-APSR did not only restore the gross rotation but also decrease the average distance between corresponding points caused by deformation transformation (from 0.0052 to 0.0049 for the first case and from 0.0129 to 0.0108 for the second case). In practice, when there is gross rotation between two images before, sole deformable registration method cannot align them very well, and GO-APSR can be applied as a preprocessing step to align them coarsely.

V. DISCUSSION AND CONCLUSION

In this paper, we introduce a novel deterministic global optimization method, GO-APSR, for affine registration of point sets. The method uses the L2 distance between the Gaussian Mixture Models generated from the two point sets as the objective function. We employ the BnB framework to optimize the objective function, and to do so, we propose a convex quadratic function as the under-estimator of the objective function in each branch. We conducted experiments on four 2D point sets, and the method performed very well in terms of global optimality and robustness to noise and outlier. In particular, the algorithm achieved good results in the challenging partially-overlap registration experiment. The results of the experiments demonstrate the advantages of the proposed method GO-APSR, which is 1) providing guarantee for the global optimality, 2) robust to different kinds of degenerations and 3) capable of realizing efficiently convergence due to the proposed novel lower bound.

The convergence threshold $\epsilon$ and the standard deviation of the Gaussian kernel $\sigma$ are two important parameters in the GO-APSR algorithm. As also noted in [14], a larger $\sigma$ results in a smoother objective function, but a smaller $\sigma$ is needed in some challenging scenarios, such as in the experiments in Section IV.B. The convergence threshold $\epsilon$ has a direct influence on the convergence time of the algorithm and how close the solution is to the true global optimum. If a small enough $\epsilon$ is used, the algorithm can find the $\epsilon$-optimal solution very close to the true global optimum, but the smaller the $\epsilon$ is, the longer time the algorithm needs to converge. To deal with large-scale data, GO-APSR can take advantages of SVGM to generate some Gaussian components to obtain the GMMS, which is more robust than directly down-sampling the point sets. At last, we show that GO-APSR can be applied as an initial step for deformable registration and it can help to reduce the error caused by deformation, which is important in medical image analysis.

![Before registration](image1.png) ![After registration](image2.png)

FIGURE 6: Registration results of large-scale data set. The left and middle column shows qualitative illustration of registration results of GO-APSR: before and after registration, respectively. The right column is average TRE of partial-to-whole registration using the set.

![Before deformation](image3.png) ![After deformation](image4.png)

FIGURE 7: Data used in the experiment of using GO-ASPR for initializing deformable registration.
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