Generalized Point Set Registration with the Kent Set Distribution

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Abstract—Point set registration (PSR) is an essential problem in communities of computer vision, medical robotics and biomedical engineering. This paper is motivated by considering the anisotropic characteristics of the error values in estimating both the positional and orientational vectors from the PSs to be registered. To do this, the multi-variate Gaussian and Kent distributions are utilized to model the positional and orientational uncertainties, respectively. Our contributions of this paper are three-folds: (i) the registration problem using the normal vectors is formulated as a maximum likelihood problem, where the anisotropic characteristics in both positional and normal vectors are considered; (ii) the matrix forms of the objective function and its associated gradients with respect to the desired parameters are provided, which can facilitate the computational process; (iii) two approaches of computing the normalizing constant in the Kent distribution are compared. We verify our proposed registration method on various pre-operative and intra-operative PSs (pelvis and femur bones) in computer-assisted surgery (CAS). Extensive experimental results demonstrate that our proposed method outperforms the state-of-the-art methods in terms of the registration accuracy and the robustness.

I. INTRODUCTION

Registration is a common and fundamental problem in computer vision, computer graphics, robotics and biomedical engineering communities [1]–[4], [8]. The objective of registration is to accurately estimate the spatial transformation (rigid or non-rigid) and to recover the point correspondences between two spaces [10]–[15]. The two spaces can be represented with volumetric images or distinctive features (e.g. points). In medical image analysis, registration technique is adopted to align multiple images of the same organs (either from one or two patients) into one common coordinate frame. For example, the pre-operative rigid registration of different imaging modalities, such as Magnetic Resonance Imaging (MRI) and computed tomography (CT), provides the robust fusion of soft tissue information with accurate bone delineation for neurosurgical planning [5]. As indicated in [6], over the past 30 years, we have seen the significant emergence of systems that incorporate imaging, robots, and other technologies to enhance patient care. Computer-assisted interventions (CAIs) or computer-assisted surgery (CAS) provides surgeons with additional information of the patient [7], [8]. Before surgery, the patient usually goes for a CT or MRI scanning to acquire a patient specific 3D model [9]. During surgery, the information together with the pre-operative patient model has to be combined with the intra-operative images, video cameras or robots.

Among the existing various registration methods, iterative closest point (ICP) is perhaps the most well known one. ICP is an iterative algorithm that first finds the best correspondence and then updates the transformation with current updated correspondences. Euclidean distance is used as the measure metrics in both correspondence and registration steps. Notably, in ICP, one-to-one hard correspondence strategy is adopted. The performance of ICP is susceptible to initial transformation and outliers, and easily converges to a local minima while it proves to be accurate and fast in many cases. Built upon the ICP method and the branch and bound (BnB) technique that can search the 3D motion space SE(3) efficiently, Yang et al. have proposed the Go-ICP method that can find the globally optimal solution [16]. On the other hand, to make ICP robust to noise and outliers, different variants of ICP have been developed [17].

In this paper, the positional and orientational error vectors are modelled using multi-variate Gaussian and Kent distributions, respectively. Different from the usual point set registration methods that only utilize the positional information, our proposed method also adopts the orientational information (i.e. normal vectors). Different from the prior registration methods that additionally consider normal vectors, we generalize the noise assumption of the normal vectors to anisotropic cases. Similar to most registration algorithms under the expectation maximization (EM) framework, among the two point sets to be registered, one is considered as model point set while the other as data point set. In the E step, the probability of one specific point in data point set corresponding to one point in model point set is computed. In the M-step, the rigid transformation matrix is updated using posterior probabilities in the E-step. The E and M steps will iterate until convergence.

This paper is organized as follows: Section II reviews the related registration algorithms; Section III describes the motivation and contributions of this paper; Section IV formulates the registration problem; Section V presents the details of the expectation maximization procedures; Section VI introduces the implementation details; Section VII describes the experimental results; Section VIII concludes the paper.

II. RELATED WORK

We briefly review the rigid registration methods based on the Gaussian Mixture Models (GMMs). The main idea of probabilistic methods is to represent one point set by a density function and minimize some ‘distance’ of the densities. The
other key idea of GMM-based registration methods is that the multiply-link correspondence strategy is usually used between two point sets. More specifically, each point in the data point set can be interpreted as being generated by some Gaussian with a specific isotropic covariance. Each point in the mode point set, on the other hand, is considered as the mixture mean. Under the probabilistic framework, the iterations of finding correspondences and updating transformations in the ICP method are reconsidered as a type of EM procedure. In E-step, the expectation over latent correspondence variables is calculated. In M-step, the current correspondences, maximization of complete log-likelihood is conducted over the registration parameters. The two steps iterate until the algorithm converges or a maximum number of iterations is reached.

In the Coherent Point Drift (CPD) algorithm [18], the registration of two point sets is formulated as a probability density estimation problem. With the assumption of isotropic covariance in the data point set, the optimal rotation matrix can be solved in a closed-form solution in M-step. Expectation Conditional Maximization Point Registration (ECMPPR) [19] extends the CPD’s isotropic covariance to anisotropic covariance matrix. In the ECM steps, each M-step in the CPD method is replaced by a sequence of conditional maximization steps or CM-steps. More specifically, during each CM-step, one registration parameter is optimized conditioned by that the other parameters are constants. Estimating the current rigid transformation matrix in CM-steps is reformulated as a quadratic optimization problem and solved using semidefinite relaxation technique. Motivated by enabling mapping and navigation for the robots in dark, complex, unstructured environments such as caves and mines, Tabib et al. have proposed the GMM-based registration method that minimizes the L2-norm between two distributions through an on-manifold parameterization of the objective function [20]. Their results in the cluttered environments demonstrate superior performance compared to the state of the art methods [20].

Joint Registration of Multiple Point Sets (JRMPC) [21] was proposed to eliminate the bias towards one point set in the pair-wise registration problem. In JRMPC, each point set is assumed to be a realization of a common GMM. The joint registration of multiple point sets is formulated as a probabilistic clustering problem. Using the EM scheme, both the GMM parameters and the rigid transformations that relate each individual point set with underlying reference set are estimated. As a by-product, the noise-free underlying reference point cloud (model data) is acquired afterwards. JRMPC algorithm outperforms all the other state-of-the-art registration methods with respect to different percentages of outliers. It should be noted that the covariance matrix is still considered to be isotropic in the JRMPC algorithm. Various registration methods have been proposed to enhance the registration’s robustness to noise and outliers [22]–[24]. For example, Yang et al. have proposed a novel registration method that is very robust to a large amount of outliers in a polynomial time [22].

Deep learning methods first learn to encode PSs with high-dimensional features, and then match keypoints to generate correspondence and optimize over the space of rigid transformations [25]–[28]. PointNetLK uses PointNet to learn feature representation and iteratively align the features representations [29]. DeepGMR leverages a probabilistic registration paradigm, within which a neural network that extracts correspondences between raw PSs and GMM parameters, and two blocks that estimates the optimal parameters from the GMM parameters [30]. However, current deep-learning based methods fail to produce acceptable inlier rates [31].

More recently, we have proposed the normal-assisted rigid point set registration method under the EM framework [32]–[34]. The isotropic error in determining the normal vectors is assumed in [32], [33]. There are also normal-based registration methods under the ICP framework, and thus is not very robust to outliers [35], [36]. In this paper, the normal-assisted registration problem is solved under the EM framework while both the positional error and the orientational error are assumed to be anisotropic in 3D space. In other words, we utilize the multi-variate Gaussian and Kent distribution to model positional and orientational error.

III. MOTIVATIONS AND CONTRIBUTIONS

Our presented work is motivated by improving the registration’s robustness to noise and outliers by (i) incorporating the orientational information (i.e., normal vectors) associated with each point into the registration; (2) considering the anisotropic characteristics in both the positional and normal vectors. Oriental information at each point in both point sets can be readily acquired in various ways at different stages of surgery. Pre-operatively, the normal vector at a certain point can be estimated through Principal Component Analysis (PCA) techniques using surrounding points. Intra-operatively (i.e., during surgery), the normal vectors could also be measured using a tracked probe equipped with a force sensor. Ranging imaging (e.g., stereo-vision based system) typically has relatively higher uncertainty in the depth direction than those in the other two directions. This motivates us to take the anisotropic positional error model into consideration. In addition, in this work, the localization error associated with the normal vectors is generalized to be anisotropic.

Our contributions in this paper can be summarized as follows: (1) The generalized rigid point set registration problem is formulated as a maximum likelihood (ML) problem, where the positional and orientational error values are modelled using multi-variate Gaussian and Kent distributions, respectively. (2) The gradients of the objective function with respect to the desired parameters are computed and provided. In addition, we present the compact matrix form of the objective function to be minimized in the maximization step. (3) We evaluate with extensive experiments the two methods of computing the normalizing constants involved in the Kent distribution, one is the exact form while the other is the approximate one.

IV. PROBLEM FORMULATION

This paper obeys the following notation conventions: Assume \( \mathbf{x}_n, \mathbf{y}_m \in \mathbb{R}^3 \) (\( n, m \in \mathbb{N}^+ \)) are two arbitrary points from the two point sets and the unit vectors \( \mathbf{x}_n, \mathbf{y}_m \in \mathbb{R}^3 \) are the associated normal directions (orientation vectors), where \( |\mathbf{x}_n| = \mathbf{y}_m | \)
values of parameters and then use Bayes’ theorem to compute

The correspondence probability between two generalized KMMs

where \( c(\kappa, \beta) \in \mathbb{R} \) is the normalizing constant of the common Kent distribution \([37]\), \( \Sigma \in \mathbb{S}^3 \) denotes the positional covariance matrix. To account for the noises and outliers existing in the data point set, an additional uniform distribution \( p(\mathbf{d}_n|z_n = M + 1) = \frac{1}{N} \) is added to the original model \( p(\mathbf{d}_n). \) Equal membership probabilities \( P(m) = \frac{1}{N} \) are assumed for all remainder GMM (and KMM) components \( (m = 1, \ldots, M) \). Then the equation of the mixture model is:

where \( 0 \leq w \leq 1 \) denotes the weight of the uniform distribution, the correspondence variable \( z_n \in \mathbb{N}^+ \). To find the optimal estimation of the probability density function of the two-part mixture model is to minimized the accumulative negative log-likelihood function listed as follows,

The correspondence probability between two generalized points \( \left[ y_m^T, \gamma_{1m}^T, \gamma_{2m}^T \right] \) and \( \left[ x_n^T, \hat{x}_n^T, \hat{x}_n^T \right] \) is defined as the posterior probability of the GMMs’ centroid and KMMs’ mean direction given the data PS.

V. EM-BASED REGISTRATION FRAMEWORK

Expectation Maximization (EM) algorithm is adopted to find the parameters \( \Theta = \{ R, t, \kappa, \Sigma, \gamma_{1m}, \gamma_{2m} \} \) iteratively. As indicated in \([18]\), the idea of EM is to first guess the values of parameters and then use Bayes’ theorem to compute a posterior probability distributions \( P^{old}(m|\mathbf{d}_n) \) of mixture components, which is the expectation or E-step of the algorithm. The new parameter values are then found by minimizing the expectation of the total negative log-likelihood function\([38]\):

with respect to the “new” parameters, which is called the maximization or M-step of the algorithm. The Q (i.e. the objective function) is the upper bound of the negative log-likelihood function in (3). The GMM centroids and KMM mean directions are transformed by rotation and translation parameters \( R, t. \) Ignoring the constants independent of \( \Theta = \{ R, t, \kappa, \Sigma, \gamma_{1m}, \gamma_{2m} \} \), we can rewrite \( Q(\Theta) \) in (4) as

\[
Q(R, t, \kappa, \beta, \Sigma, \gamma_{1m}, \gamma_{2m}) =
\sum_{n=1}^{N} \sum_{m=1}^{M} p^{old}(m|\mathbf{d}_n) \log \left( p^{new}(m)p^{new}(\mathbf{d}_n|m) \right)
\]

where \( p^{old}(m|z_n = m|\mathbf{d}_n) \) is defined as the posterior probability of the states \( m \) with \( q \in \mathbb{N} \) is the index of iteration. Afterwards, the sum of the posterior probabilities after the \( q \)-th step is computed as follows,

\[
Q(R, t, \kappa, \beta, \Sigma, \gamma_{1m}, \gamma_{2m}) =
\sum_{n=1}^{N} \sum_{m=1}^{M} p^{old}(m|\mathbf{d}_n) \log \left( p^{new}(m)p^{new}(\mathbf{d}_n|m) \right)
\]

The objective function is further modified by substituting the terms \( R \) with \( dRR^{-1} \), where \( dR \) is \( SO(3) \) denotes the incremental rigid transformation while \( R^{-1} \in SO(3) \) represents the rigid transformation in the last EM step.

\[
Q(dR, dt, \kappa, \beta, \Sigma, \gamma_{1m}, \gamma_{2m}) =
\sum_{n=1}^{N} \sum_{m=1}^{M} p^{old}(m|\mathbf{d}_n) \log \left( p^{new}(m)p^{new}(\mathbf{d}_n|m) \right)
\]

The M Rigid Transformation Step For clarity, we retain the terms

\[
Q(R, t, \kappa, \beta, \Sigma, \gamma_{1m}, \gamma_{2m}) =
\sum_{n=1}^{N} \sum_{m=1}^{M} p^{old}(m|\mathbf{d}_n) \log \left( p^{new}(m)p^{new}(\mathbf{d}_n|m) \right)
\]

where \( z_{mn} = \mathbf{x}_n - dR(R^{-1}x_m + t^{-1}) - dt. \)
that are related with \(dR\) and \(dt\) in (7), which is the following,
\[
Q(dR, dt) = \sum_{n=1}^{N} \sum_{m=1}^{M} \left(C_{P,mn} + C_{O, mn}ight)
\]
(8)

With the Rodrigues formula for representing a rotation matrix, i.e., \(dR = R(x(1 : 3))\) and \(dt = x(4 : 6)\), we can use a six-dimensional vector \(x\) to represent the incremental rigid transformation matrix. The unconstrained optimization problem is presented as the following:
\[
\min \{x\} \sum_{n=1}^{N} \sum_{m=1}^{M} \left(C_{P,mn} + C_{O, mn}\right)
\]
(9)

where \(C_{O, mn} = C_{O, mn1} + C_{O, mn2}\) represents the part that is related with the normal vectors in the objective function. In this way we convert the constrained optimization problem of \((dR, dt)\) into an unconstrained optimization one of \(x\). In what follows, we present the gradients of the objective function \(C\).

The Gradient of the Objective Function Let \(\nabla C\) denote the gradient of \(C\) in (9) with respect to \(x\), i.e., \(\frac{\partial C}{\partial x}\). We can now write \(\nabla C\) as
\[
\nabla C = \sum_{n=1}^{N} \sum_{m=1}^{M} \left(\nabla C_{P,mn} + \nabla C_{O, mn}\right)
\]
(10)

where \(C_{P,mn} = [J_{C_{P,mn}, d\theta} J_{C_{P,mn}, dt}]^{T}\) and \(C_{O, mn} = [J_{C_{O, mn}, d\theta} 0_{1 \times 3}]^{T}\), with which \(J_{C_{P,mn}, d\theta}\) and \(J_{C_{P,mn}, dt}\) denote the Jacobian vector of \(C_{P,mn}\) with respect to \(d\theta\) and \(dt\):

\[
\begin{align*}
J_{C_{P,mn}, d\theta} = & \left[\frac{\partial C_{P,mn}}{\partial d\theta_1}, \frac{\partial C_{P,mn}}{\partial d\theta_2}, \frac{\partial C_{P,mn}}{\partial d\theta_3}\right] \\
J_{C_{P,mn}, dt} = & \left[\frac{\partial C_{P,mn}}{\partial dt_1}, \frac{\partial C_{P,mn}}{\partial dt_2}, \frac{\partial C_{P,mn}}{\partial dt_3}\right]
\end{align*}
\]
(11)

We now derive the expression of \(\frac{\partial C_{P,mn}}{\partial dt_i}\) for \((i = 1, 2, 3)\), where \(\frac{\partial C_{P,mn}}{\partial dt_i}\) is given in the Jacobian style, \(\frac{\partial \nabla C}{\partial x}\) is the operation to compute the trace of a matrix. The readers are noted that the detailed expressions of \(\frac{\partial \nabla C}{\partial x}(i = 1, 2, 3)\) are presented in our prior work [39]. On the other hand, with the chain rule of matrix derivative, we can have:
\[
\frac{\partial C_{P,mn}}{\partial dt_i} = \text{trace}\left(\left(\frac{\partial C_{P,mn}}{\partial dR}\right)\frac{\partial dR}{\partial dt_i}\right).
\]
(13)

Derivation of \(\frac{\partial C_{P,mn}}{\partial dR}\): The expression of \(\frac{\partial C_{P,mn}}{\partial dR}\) is \(\frac{\partial C_{P,mn}}{\partial dR} = -p_{mn}^{T}(\Sigma^{-1})^{-1}\left(x_n(R^{-1}y_m + t^T) + dR(R^{-1}y_m + t^T) - \gamma(R^{-1}y_m + t^T)\right).
\]

Derivation of \(\frac{\partial C_{P,mn}}{\partial dt}\): The expression of \(\frac{\partial C_{P,mn}}{\partial dt}\) is \(\frac{\partial \nabla C_{P,mn}}{\partial dt} = \left(x_n + dt + dR(R^{-1}y_m + t^T)\right).
\]

VI. IMPLEMENTATION DETAILS

The exact formula for calculating the normalizing constant \(c(\kappa, \beta)\) in the Kent distribution is:
\[
c(\kappa, \beta) = 2\pi \int_{\mathbb{R}^2} \frac{\Gamma(\frac{1}{\beta})}{\Gamma(\frac{1}{\beta} + 1)(\kappa + 2)^{\frac{1}{\beta} + \frac{1}{2}}} \left\{\frac{1}{\beta^2} - \gamma^2 - \frac{3}{2}\right\} \frac{1}{\kappa + 2}.
\]

where \(\Gamma(\cdot)\) represents the Gamma function and \(\text{Bessel function of first kind, respectively.}\) In real engineering implementations, people cannot sum the terms with the index from \(j = 0\) to \(99\). The approximate formula of calculating \(c(\kappa, \beta)\) as the following [37]:
\[
c(\kappa, \beta) \approx 2\pi \sum_{j=1}^{9} \left\{\frac{1}{\beta^2} - \gamma^2 - \frac{3}{2}\right\} \frac{1}{\kappa + 2}.
\]

Fig. 1 shows the percentage differences of the normalizing constants using the above two methods. As it is shown in Fig. 1, the percentage differences between the two constants will converge to zero as \(\kappa\) becomes
The percentage differences of the normalizing constants' values computed with the two approaches. Three different cases are tested: $\epsilon = 0.25$, $\epsilon = 0.5$, and $\epsilon = 0.75$.

Fig. 1. The percentage differences of the normalizing constants' values using two methods.

The eccentricity $\epsilon$ becomes smaller. The eccentricity $\epsilon$ takes values on the interval $[0, 1)$ and controls the ellipticity parameter $\beta$ as $\beta = \epsilon^{\frac{3}{2}}$. In this paper, we choose to use the second approximated method of computing $c(\kappa, \beta)$. We initialize the rigid transformation matrix as: $R^0 = I_{3 \times 3}$, $t^0 = 0_{3 \times 1}$, the positional covariance matrices $\Sigma^0$ is initialized to be large (e.g. $\Sigma^0 = \text{diag}([100, 100, 100])$); the concentration parameters $\kappa^0$ to be small (e.g. $\kappa^0 = 10$ which means large variances in normal vectors); the ellipticity parameter $\beta^0$ is initialized to be zero, which means the orientation vectors are considered to be isotropic at the beginning of the algorithm.

larger and $\epsilon$ becomes smaller. The eccentricity $\epsilon$ takes values on the interval $[0, 1)$ and controls the ellipticity parameter $\beta$ as $\beta = \epsilon^{\frac{3}{2}}$. In this paper, we choose to use the second approximated method of computing $c(\kappa, \beta)$. We initialize the rigid transformation matrix as: $R^0 = I_{3 \times 3}$, $t^0 = 0_{3 \times 1}$, the positional covariance matrices $\Sigma^0$ is initialized to be large (e.g. $\Sigma^0 = \text{diag}([100, 100, 100])$); the concentration parameters $\kappa^0$ to be small (e.g. $\kappa^0 = 10$ which means large variances in normal vectors); the ellipticity parameter $\beta^0$ is initialized to be zero, which means the orientation vectors are considered to be isotropic at the beginning of the algorithm.

VII. Experiments

To verify the effectiveness, robustness and accuracy of our proposed algorithm, we validate our algorithm on two data sets: pelvis and femur data sets in the background of computer-assisted orthopedic surgery (CAOS) [32], [33]. In this scenario, the preoperative model acts as the model point set $D_m$ while the intra-operative data acts as the data point set $D_d$. The number of points in $D_m$ is $M = 1568$ while the number of inlier points in $D_d$ is $N_{\text{inliers}} = 100$. In all the experiments, between $D_m$ and $D_d$, the rotational degrees of $R_{\text{true}}$ lie in $[10, 20]^\circ$ and the translation vectors’ magnitudes lie in $[10, 20]$mm as those settings in [33]. We compare several state-of-the-art registration methods with our proposed one: ICP [40], ECMR [19], JRMP [21], HMM(Isotropic) [32], [33]. The first three registration methods utilize only the positional information $X$ and $Y$ while HMM(Isotropic) and our method utilize $D_m$ and $D_d$. In HMM(Isotropic), both the positional and orientational uncertainties are isotropic.

To test and verify the registration method’s robustness to noise and outliers, noise and different percentages of outliers are injected into $D_d$. The covariance matrix is set to be $\Sigma = \text{diag}([\frac{1}{11}, \frac{1}{11}, \frac{1}{11}])$. In each test case with specific noise,
Fig. 4. The registration error results on the pelvis point set, kappa=800. The first column is the rotational error statistics while the second stores the translational error values.

Fig. 5. The registration error results with different registration algorithms on the pelvis point set, kappa = 3200. The first column is the rotational error statistics while the second stores the translational error values.

A novel, robust and accurate probabilistic rigid point set registration algorithm for computer assisted orthopaedic surgery (CAOS) is presented in this paper. The novelty lies in considering the anisotropy in both the positional and orientational error. Experimental results have demonstrated the effectiveness and significantly improved performances of our approach over the state-of-the-art methods.
REFERENCES


