

General Discriminative Optimization for Point Set Registration

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Abstract

Point set registration has been actively studied in computer vision and graphics. Optimization algorithms are at the core of solving registration problems. Traditional optimization approaches are mainly based on the gradient of objective functions. The derivation of objective functions makes it challenging to find optimal solutions for complex optimization models, especially for those applications where accuracy is critical. Learning-based optimization is a novel approach to address this problem, which learns the gradient direction from data sets. However, many learning-based optimization algorithms learn gradient directions via a single feature extracted from the data set, which will cause the updating direction to be vulnerable to perturbations around the data, thus falling into a bad stationary point. This paper proposes the General Discriminative Optimization (GDO) method that updates a gradient path automatically through the trade-off among contributions of different features on updating gradients. We illustrate the benefits of GDO with tasks of 3D point set registrations and show that GDO outperforms the state-of-the-art registration methods in terms of accuracy and robustness to perturbations.

Keywords: Point set registration, Supervised learning, Learning-based

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1. Introduction

Point set registration has been actively studied in computer vision and computer graphics. For shape reconstruction [1] [2], point set registration is used to find the overlaps of point sets reconstructed from images and align them in a global coordinate system. For face recognition [3], point set registration aligns the face descriptors extracted from a face with different facial expressions or different viewpoints. In medical image processing [4], point set registration is the fundamental step to fuse multiple images(e.g., computed tomography (CT), magnetic resonance imaging (MRI), and positron emission tomography (PET)). In intelligent vehicles [5], point set registration is an important step to align the images and extract feature points that will be further used for location and mapping. For shape retrieval [6], point set registration converts unstructured shapes into structured ones to rapidly retrieve 3D shapes that resemble a query object from a database.

The goal of point set registration is to find correspondences and to estimate the transformation between two or more point sets. Various rigid registration methods arise to solve the estimation of transformation parameters, i.e., a map defined as rotation and translation, which is essentially a mathematical optimization task. Gradient-based algorithms are widely used for solving the optimization problems in the applications of registration, such as gradient descent for multi-view reconstruction [7], Gauss-Newton for face alignment [8], Levenberg-Marquardt for surface fitting [9], Conjugate Gradient for surface reconstruction [10].

One of the gradient-based optimization algorithms is Newton's algorithm [11], which is an extremely powerful technique due to quadratic convergence. The computational cost for obtaining the second-order gradient information of the Hessian matrix makes Newton's method not feasible in many cases. Quasi-Newton methods are proposed to generate an estimation of the inverse Hes-

29 sion matrix, which leads to faster computation time. However, Quasi-Newton
 30 methods (such as Broyden–Fletcher–Goldfarb–Shanno algorithm (BFGS)) take
 31 a larger memory space to store the inverse Hessian approximation, thus could
 32 be detrimental for large, complicated tasks. Limited-memory BFGS (LBFGS),
 33 as the variant of the BFGS method, only stores a set of vectors and calculates a
 34 reduced rank approximation to the Hessian approximation, which needs much
 35 less memory to operate. However, the amount of storage required by LBFGS
 36 depends on the parameter setting that determines the number of BFGS correc-
 37 tions saved.

38 The high complexity and the large storage required for inverse Hessian ap-
 39 proximation pose challenges to the applications of gradient-based optimization
 40 methods in computer vision and graphics while limiting the performances of the
 41 traditional registration methods that use gradient-based approaches for param-
 42 eter estimation. In contrast, learning-based registration methods have a higher
 43 performance of registration with less time-consuming. The robustness and the
 44 high efficiency of the learning-based registration are due to that the approach in-
 45 tegrates the traditional optimization (modeling and solution) as a learning-based
 46 optimization process, in which gradient directions are learned without calculat-
 47 ing the Jacobian matrix or Hessian matrix. For example, Supervised Descent
 48 Method (SDM) [12] [13] and Discriminative Optimization (DO) method [14]
 49 learn to update directions from the single feature of the training data set and
 50 mimics gradient descent to estimate transformation parameters without regis-
 51 tration modeling. However, if a single feature lacks robustness, it could make
 52 the learned direction susceptible to perturbations and likely to be trapped in
 53 stationary points rather than optimal solutions.

54 In this paper, we put forward a General Discriminative Optimization (GDO)
 55 method for point clouds registration. GDO, as the learning-based optimization
 56 method, overcomes the limitation of the learning-based registration methods.
 57 Our key insight is that, by balancing the contribution of different extracted fea-
 58 tures on the updating gradient, we can learn a sequence of gradient directions
 59 directly from training data sets while making the gradient path converge to the

60 optimal point as closely as possible. We provide a framework for updating gra-
 61 dient directions via different features and show the proof of GDO’s convergence.
 62 For 3D points registration, GDO learns a sequence of directions through the 3D
 63 coordination and density information of the point sets. The experimental re-
 64 sults show that GDO outperforms the state-of-the-art registered algorithms in
 65 terms of robustness and accuracy on different data sets.

66 In the next section, we review related work on 3D registration and optimiza-
 67 tion. The following sections introduce our framework and theoretical analysis
 68 of GDO. Finally, we evaluate the registration performance of our algorithm.

69 **2. Previous Work**

70 *2.1. 3D point sets registration*

71 Point set registration has been an important problem in computer vision
 72 for the last few decades. The most commonly used method for registration is
 73 based on the iterative closest point (ICP) [15] algorithm, which finds the best
 74 transformation parameters of a group of three-dimensional points through rigid
 75 transformation and continuous iteration to minimize the difference between two
 76 point sets. Due to its conceptual simplicity, high usability, and good perfor-
 77 mance in practice, ICP and its variants are very popular and have been success-
 78 fully applied in numerous real-world tasks. However, ICP is sensitive to outliers
 79 and needs initialization to be close to the optimal solution to avoid a bad local
 80 minimum. ICPMCC [16] combines ICP and the correntropy to improve the ro-
 81 bustness of ICP in terms of the noises and outliers. GO-ICP [17] combines ICP
 82 with a branch-and-bound (BnB) scheme to search the optimal 3D motion space
 83 $SE(3)$ efficiently. RICP [18], as a semantic-based method, avoids ICP trapping
 84 into local minimum due to the non-homogeneous point-set distribution or the
 85 poor initial pose through combining region selection, point matching, and noise
 86 treatment. Iteratively Reweighted Least Squares(IRLS) [19] uses various cost
 87 functions to provide robustness to outliers and avoid bad local minima. Fast
 88 global registration (FGR) [20] searches the correspondences between point sets

89 through 3D feature descriptors and optimizes robust objectives based on those
90 correspondences. Normal Distribution Transformation (NDT) [21] applies a sta-
91 tistical model to match 3D point sets. Coherent Point Drift (CPD) [22] achieves
92 point sets registration based on a Gaussian mixture model, which moves the
93 Gaussian mixture model centroids coherently as a group to preserve the topo-
94 logical structure of the point sets.

95 All the above registration methods cast point set registration as a tradi-
96 tional optimization problem, which can be divided into two stages: registration
97 modeling and searching solutions. And the performances of the traditional reg-
98 istration approaches depend on the robustness of the registration models and
99 searching methods. Learning-based registration methods, such as Supervised
100 Descent Method (SDM) and Discriminative Optimization (DO), integrate the
101 registration modeling and searching solutions as a learning-based optimization
102 process, which leads to the robustness and high efficiency of registration.

103 2.2. Optimization algorithms

A general formula of the objective function of an optimization problem can
be cast as follows:

$$\mathbf{x}_* = \min_{\mathbf{x} \in \mathbf{S}} f(\mathbf{x}). \quad (1)$$

104 $f : \mathbf{S} \rightarrow \mathbf{R}$ models the phenomena of interest and then finds the best solution
105 \mathbf{x}_* through a suitable search method. \mathbf{S} is a set including all possible solutions
106 for the objective function.

107 The least-square regression is the most popular form of objective functions,
108 which is frequently employed in the majority of computer vision and computer
109 graphics [23] [24] [25]. [26] [27] add various regularization terms to improve
110 the robustness of least square regressions and reduce over-fitting. However,
111 the addition of regularization terms increases the complexity of optimization
112 models, which will further make it challenging to get the derivation of objective
113 functions. Gradient descent and its variants, Newton’s methods, and Quasi-
114 Newton methods are commonly used to search optimal solutions of optimization
115 models [28]. The learning rate of gradient descent is not optimal, the gradient

information is not readily available [29], the Hessian matrix may not be positive definite, or the convergence rate is slower.

Several works have proposed to use learning techniques to compute the gradient directions of objective functions. Specifically, this is done by learning a sequence of regressors to replace the gradient directions of objective functions. [30] [31] regard weak learner as a gradient to update the parameter vector. [32] applies cascaded regression into facial landmark tracking system. [33] and [13] all learn a sequence of regressor matrices to update the shape parameters at per iteration. The former learns a set of averaged Jacobian and Hessian matrices from data, and the latter learns a mapping from image features to problem parameters directly.

[34] [35] [14] explore a framework to learn search directions from the feature of data without cost functions. Although this approach avoids the computation of Jacobian and Hessian matrices, it also uses only a *single feature* to learn the update direction. The lack of other features of data increases the risk of perturbations around data on the update of gradient directions. The *cooperation* of multiple features is able to effectively preserve and utilize geometric details of point sets, which is mostly used in semantic segmentation [36].

In view of this, in this paper, our proposed GDO algorithm learns the gradient update directions by combining different features of the point sets, fully utilizing the detailed information of point sets to reduce the impact of perturbations on gradient directions and, as a result, increasing the accuracy of the parameter estimation for registration.

3. General Discriminative Optimization

3.1. Motivation of Discriminative Optimization

Discriminative Optimization (DO) updates gradient directions according to the feature of input data without calculating the Jacobian or Hessian matrix. More specifically, DO splits gradient information as the updating map $\mathbf{D} \in \mathbf{R}^{p \times f}$ and the feature $\mathbf{h} : \mathbf{R}^p \rightarrow \mathbf{R}^f$, and updates the map \mathbf{D} through

approaching the current estimated parameter vector \mathbf{x}_t to ground truth \mathbf{x}_* .

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{D}_{t+1} \mathbf{h}(\mathbf{x}_t) \quad (2)$$

$$\mathbf{D}_{t+1} = \min_{\tilde{\mathbf{D}}} \frac{1}{N} \sum_{i=1}^N \left\| \mathbf{x}_*^i - \mathbf{x}_t^i + \tilde{\mathbf{D}} \mathbf{h}(\mathbf{x}_t^i) \right\|_2^2 + \frac{\lambda}{2} \left\| \tilde{\mathbf{D}} \right\|_F^2. \quad (3)$$

141 Where $\|\cdot\|_F$ is the Frobenius norm, and λ is a hyperparameter.

142 Despite not calculating the Jacobian or Hessian matrix, DO still has several
 143 issues theoretically. One issue is that DO uses a single feature of data to gain a
 144 sequence of updating maps. The lack of other features of data increases the risk
 145 of perturbations around data on the update of gradient directions. In this case,
 146 GDO explores the *collaboration* of different features \mathbf{H}_f to reduce the impact
 147 of perturbations on the gradient direction.

148 Another theoretical issue of DO is that the constraint for the convergence of
 149 DO requires each $\mathbf{D} \mathbf{h}(\mathbf{x})$ to be strictly monotone at ground truth for all samples.
 150 Actually, not all features are able to fulfill this constraint. In other words, the
 151 convergence constraint limits the select of feature function \mathbf{h} . We provide a
 152 weaker constraints for the convergence of the learning-based optimization.

153 3.2. Method

154 The objective function used to derive the feature of GDO can be formulated
 155 as follows:

$$\min_{\mathbf{x}} \Phi(\mathbf{x}) = \sum_{i=1}^I \gamma_i \frac{1}{J_i} \sum_{j_i=1}^{J_i} \varphi_i(\mathbf{g}_{j_i}(\mathbf{x})). \quad (4)$$

156 Where I is the number of categories of the different penalty functions φ_i . J_i is
 157 the number of residual functions \mathbf{g}_{j_i} . γ_i is the weighting coefficient of penalty
 158 function φ_i .

$$\mathbf{h}_i = \frac{1}{J_i} \sum_{j_i=1}^{J_i} \left[\frac{\partial \mathbf{g}_{j_i}}{\partial \mathbf{x}} \right]_{k,l} \delta(\mathbf{v} - \mathbf{g}_{j_i}). \quad (5)$$

$$\gamma_i = \frac{Tr(\mathbf{Cov}(\mathbf{h}_i))}{\sum_{i=1}^I Tr(\mathbf{Cov}(\mathbf{h}_i))}. \quad (6)$$

Where we express $\mathbf{g}_{j_i}(\mathbf{x})$ as \mathbf{g}_{j_i} and $\varphi_i(\mathbf{g}_{j_i}(\mathbf{x}))$ as φ_i to reduce notation clutter. $[\mathbf{Y}]_k$ is the k_{th} row of \mathbf{Y} , and $[\mathbf{y}]_k$ means the k_{th} element of \mathbf{y} . $\delta(\mathbf{x})$ is the Dirac function. $Tr(\mathbf{Cov}(\mathbf{h}_i))$ is the trace of the covariance matrix of \mathbf{h}_i . If $I = 2$, the feature of GDO \mathbf{H}_f can be represented as follows:

$$\mathbf{H}_f = \begin{bmatrix} \gamma_1 \mathbf{h}_1 \\ \gamma_2 \mathbf{h}_2 \end{bmatrix}. \quad (7)$$

The details of the derivation and the summary of notation have been provided in the supplementary material.

3.3. Relation to the original DO

GDO can be seen as the extension of DO. When $I = 1$, the coefficient γ_i is set to 1, which means that DO has a single feature. In this case, GDO and DO are equivalent. When $I \neq 1$, the sum of the coefficients is still equal to 1, and GDO achieves the *cooperation* of multiple features. It is worth noting that the way to combine the features is derived from the function Eq.4, and the coefficients are learned from the features.

4. GDO Framework

4.1. Learning for GDO

Assume that we are given a set of training data $\{(\mathbf{x}_0^i, \mathbf{x}_*^i, \mathbf{H}_f(\mathbf{x}_0^i))\}_{i=1}^N$, including N problem instances, each instance has its ground truth parameter \mathbf{x}_*^i , the initial parameter \mathbf{x}_0^i , and the extracted feature $\mathbf{H}_f(\mathbf{x}_0^i)$. For simplicity, we denote $\mathbf{H}_f(\mathbf{x}_t^i)$ as \mathbf{H}_{ft}^i to represent the feature of the i -th sample at the t -th iteration. GDO aims at learning a sequence of maps \mathbf{D}_{t+1} by approaching \mathbf{x}_t^i to \mathbf{x}_*^i .

$$\mathbf{D}_{t+1} = \min_{\tilde{\mathbf{D}}} \frac{1}{N} \sum_{i=1}^N \left\| \mathbf{x}_*^i - \mathbf{x}_t^i + \tilde{\mathbf{D}} \mathbf{H}_{ft}^i \right\|_2^2 + \frac{\lambda}{2} \left\| \tilde{\mathbf{D}} \right\|_F^2. \quad (8)$$

176 Where $\|\cdot\|_F$ is the Frobenius norm, and λ is a hyperparameter.

177 We can apply the initial training data $\left\{ \left(\mathbf{x}_0^i, \mathbf{x}_*^i, \mathbf{H}_{f0}^i \right) \right\}_{i=1}^N$ to (8) to learn
 178 map \mathbf{D}_1 at first. Then, \mathbf{D}_1 will be applied to (2) to get the current estimation
 179 \mathbf{x}_1 . At each step, a new parameter vector can be created by recursively applying
 180 the update rule in (2). The learning process is repeated until certain termination
 181 criteria are met, for example, until the error is not reduced too much or the
 182 maximum number of iterations T is reached. The pseudocode for training GDO
 183 is shown in Alg.1.

Algorithm 1 Training a sequence of update maps

Require: $\left\{ \left(\mathbf{x}_0^i, \mathbf{x}_*^i, \mathbf{H}_{f0}^i \right) \right\}_{i=1}^N, T, \lambda$

Ensure: $\{\mathbf{D}_t\}_{t=1}^T$

- 1: **for** $t = 0$ to $T - 1$ **do**
 - 2: Compute \mathbf{D}_{t+1} with (8)
 - 3: **for** $i = 1$ to N **do**
 - 4: Update $\mathbf{x}_{t+1}^i := \mathbf{x}_t^i - \mathbf{D}_{t+1} \mathbf{H}_{ft}^i$
 - 5: **end for**
 - 6: **end for**
-

184 4.2. Convergence analysis of GDO

185 **Theorem 4.1 (Convergence of GDO's training error).** Given a training
 186 set $\left\{ \left(\mathbf{x}_0^i, \mathbf{x}_*^i, \mathbf{H}_{f0}^i \right) \right\}_{i=1}^N$, if there exists a linear map $\hat{\mathbf{D}} \in \mathbf{R}^{p \times f}$ where $\hat{\mathbf{D}} \mathbf{H}_f$
 187 meets the condition $\sum_{i=1}^N (\mathbf{x}_*^i - \mathbf{x}_t^i)^\top \hat{\mathbf{D}} \mathbf{H}_{ft}^i > 0$ at \mathbf{x}_*^i for all i , and if there
 188 exists an i where $\mathbf{x}_t^i \neq \mathbf{x}_*^i$, then the update rule:

$$\mathbf{x}_{t+1}^i = \mathbf{x}_t^i - \mathbf{D}_{t+1} \mathbf{H}_{ft}^i. \quad (9)$$

$$\mathbf{D}_{t+1} = \min_{\tilde{\mathbf{D}}} \frac{1}{N} \sum_{i=1}^N \left\| \mathbf{x}_*^i - \mathbf{x}_t^i + \tilde{\mathbf{D}} \mathbf{H}_{ft}^i \right\|_2^2 + \frac{\lambda}{2} \left\| \tilde{\mathbf{D}} \right\|_F^2.$$

189 guarantees that the training error strictly decreases in each iteration:

$$\sum_{i=1}^N \left\| \mathbf{x}_*^i - \mathbf{x}_{t+1}^i \right\|_2^2 < \sum_{i=1}^N \left\| \mathbf{x}_*^i - \mathbf{x}_t^i \right\|_2^2. \quad (10)$$

190 If $\hat{\mathbf{D}}\mathbf{H}_f$ is strongly monotone, and if there exist $H > 0$, $M > 0$ such that
 191 $\left\|\hat{\mathbf{D}}\mathbf{H}_f^i\right\|_2^2 \leq H + M\|\mathbf{x}_*^i - \mathbf{x}^i\|_2^2$ for all i , then the training error converges to
 192 zero.

193 The proof of Thm.4.1 is provided in Supplementary Material. Thm.4.1 says that
 194 for all instances, if $\hat{\mathbf{D}}\mathbf{H}_f$ meets the condition $\sum_{i=1}^N (\mathbf{x}_*^i - \mathbf{x}_t^i)^T \hat{\mathbf{D}}\mathbf{H}_{ft}^i > 0$, then
 195 the average training error will decrease in each iteration; if $\hat{\mathbf{D}}\mathbf{H}_f$ is strongly
 196 monotone at \mathbf{x}_*^i , the average training error will converge to zero. Note that \mathbf{H}_f
 197 can be not only a single function but also a combination of different functions
 198 of \mathbf{x}^i . DO also presents a similar convergence result for a update rule, but it
 199 requires $\hat{\mathbf{D}}\mathbf{H}_{ft}^i$ to be strictly monotone at \mathbf{x}_*^i for all i . Besides, different from
 200 the single feature \mathbf{h} in DO, as the combination composed of several feature
 201 functions, \mathbf{H}_f takes into account more features of data.

202 5. EXPERIMENTATION

203 This section describes how to apply GDO to 3D point set registration with
 204 various perturbations. We compare GDO with other classical registration meth-
 205 ods on various data sets.

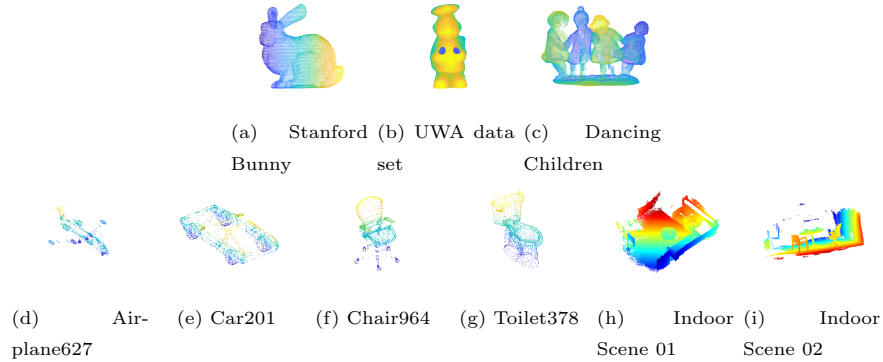


Figure 1: Experimental data sets

206 5.1. 3D Point set Registration

207 Let $\{\mathbf{M}, \mathbf{S}\}$ be two point sets in a finite-dimensional real vector space \mathbf{R}^3 ,
 208 which contains N_m and N_s points, respectively. Our goal is to find a rigid

transformation \mathbf{T} to be applied to scene set \mathbf{S} such that the difference between \mathbf{S} and model set \mathbf{M} is minimized. The transformation matrix \mathbf{T} is posed as the Lie algebra $\mathbf{x} \in \mathbf{R}^6$ in our optimization problem.

Feature for registration

The feature \mathbf{H}_f for registration is combined by two different features: the coordinates-based feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^c$ and the density-based feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$.

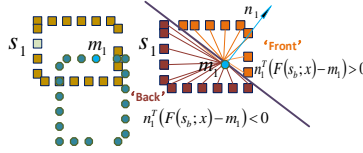


Figure 2: The positional relationship between scene points (square) \mathbf{s}_1 and model point (hexagon) \mathbf{m}_1 .

We use the feature extraction method in [34] to extract the features $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^c$ and $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$, where \mathbf{h} is devised to be a histogram indicating the weights of scene points on the 'front' and the 'back' sides of each model point. As shown in Fig.2.

$$\mathbf{S}_a^+ = \{\mathbf{s}_b : \mathbf{n}_a^T (\mathbf{F}(\mathbf{s}_b; \mathbf{x}) - \mathbf{m}_a) > 0\} \quad (11)$$

\mathbf{S}_a^+ indicates the set of scene points on the 'front' of model point \mathbf{m}_a , and \mathbf{S}_a^- contains the remaining scene points.; $\mathbf{n}_a \in \mathbf{R}^3$ is the normal vector of the model point \mathbf{m}_a ; $\mathbf{F}(\mathbf{s}_b; \mathbf{x})$ is the function that applies rigid transformation with parameter \mathbf{x} to scene point \mathbf{s}_b .

Then the feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^c$ can be calculated through the following formulas:

$$[\mathbf{h}(\mathbf{x}; \mathbf{S})]_{a+}^c = \frac{1}{z} \sum_{\mathbf{s}_b \in \mathbf{S}_a^+} \exp \left(\frac{-1}{\hat{\sigma}^2} \|\mathbf{F}(\mathbf{s}_b; \mathbf{x}) - \mathbf{m}_a\|^2 \right). \quad (12)$$

$$[\mathbf{h}(\mathbf{x}; \mathbf{S})]_{a-}^c = \frac{1}{z} \sum_{\mathbf{s}_b \in \mathbf{S}_a^-} \exp \left(\frac{-1}{\hat{\sigma}^2} \|\mathbf{F}(\mathbf{s}_b; \mathbf{x}) - \mathbf{m}_a\|^2 \right). \quad (13)$$

Where z normalizes \mathbf{h} to sum to 1, and $\hat{\sigma}$ controls the width of the exp function.
The design of the feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$ can be divided into two stages. The first
stage is to calculate the probability of measuring each point of \mathbf{S} in the boxes of
 \mathbf{M} , and the probability of each point of \mathbf{M} in the boxes of \mathbf{S} , as shown in Fig.3.
The second stage is to apply the calculated probability to (12),(13) to extract
the density feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$.

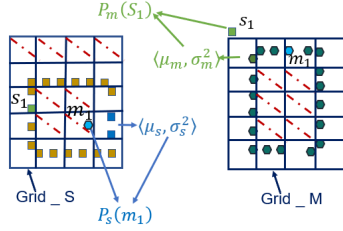


Figure 3: The first stage for designing the density feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$. The Grid.S represents the grids around the model \mathbf{S} . The Grid.M represents the grids around the model \mathbf{M} . The grid marked by the red dotted line represents the grid where is no point, which will be removed when calculating the mean μ and covariance σ^2 .

The probability of measuring each point of \mathbf{S} in the boxes of \mathbf{M} can be
calculated as follows, and the probability of measuring the points of \mathbf{M} in
the boxes of \mathbf{S} can be calculated in a similar way.

1. The 3D space around the point set \mathbf{M} is subdivided regularly into boxes
with constant size (e.g. the Grid_S, Grid_M in Fig.3).
2. For each box, the following is done:
 - Collect all 3D points $\mathbf{m}_{i=1,2,\dots,N_m}$ in \mathbf{M} contained in this box. If
there is no point in a box, the box will be removed (e.g. the grids
marked by the red dotted line in Fig.3).
 - Calculate the mean

$$\mu_m = \frac{1}{N_m} \sum_{i=1}^{N_m} \mathbf{m}_i.$$

- Calculate the covariance matrix

$$\sigma_m^2 = \frac{1}{N_m} \sum_{i=1}^{N_m} (\mathbf{m}_i - \mu_m) (\mathbf{m}_i - \mu_m)^T.$$

240 3. The probability of measuring each point \mathbf{s}_j of \mathbf{S} in this box is now modeled
 241 by the normal distribution $\mathcal{N}(\boldsymbol{\mu}_m, \boldsymbol{\sigma}_m^2)$.

$$\mathbf{P}_m(\mathbf{s}_j) \sim \exp\left(\frac{-(\mathbf{s}_j - \boldsymbol{\mu}_m)^T(\mathbf{s}_j - \boldsymbol{\mu}_m)}{2\boldsymbol{\sigma}}\right).$$

$$[\mathbf{h}(\mathbf{x}; \mathbf{S})]_{a+}^d = \frac{1}{z} \sum_{\mathbf{s}_b \in \mathbf{S}_a^+} \exp\left(\frac{-1}{\hat{\sigma}^2} \|\mathbf{P}_m(\mathbf{F}(\mathbf{s}_b; \mathbf{x})) - \mathbf{P}_s(\mathbf{m}_a)\|^2\right). \quad (14)$$

$$[\mathbf{h}(\mathbf{x}; \mathbf{S})]_{a-}^d = \frac{1}{z} \sum_{\mathbf{s}_b \in \mathbf{S}_a^-} \exp\left(\frac{-1}{\hat{\sigma}^2} \|\mathbf{P}_m(\mathbf{F}(\mathbf{s}_b; \mathbf{x})) - \mathbf{P}_s(\mathbf{m}_a)\|^2\right). \quad (15)$$

242 The final feature \mathbf{H}_f can be posed as:

$$\mathbf{H}_f = \begin{bmatrix} \gamma_1 [\mathbf{h}(\mathbf{x}; \mathbf{S})]^c \\ \gamma_2 [\mathbf{h}(\mathbf{x}; \mathbf{S})]^d \end{bmatrix}. \quad (16)$$

243 We get the coefficients γ_1, γ_2 using (6), which represent the contributions of
 244 features on updating gradient direction.

245 5.2. GDO Training Settings

246 The parameters in the GDO training process are the same as those in the
 247 code provided in the Github of DO [34] for the comparison experiments on
 248 the synthetic data sets. We normalize a given model shape \mathbf{M} to $[-1, 1]^3$ and
 249 uniformly sample from \mathbf{M} with the replacement 400 to 700 points to generate a
 250 scene model. Then we apply the following perturbations to the scene model: (i)
 251 *Rotation and translation*: The rotation is within 60 degrees and the translations
 252 is in $[-0.3, 0.3]^3$, which represents ground truth \mathbf{x}_* ; (ii) *Noise and Outliers*:
 253 Gaussian noise with the standard deviation 0.05 is added to the scene model.
 254 0 to 300 points within $[-1.5, 1.5]^3$ are added as the sparse outliers. Besides, a
 255 Gaussian ball of 0 to 200 points with the standard deviation of 0.1 to 0.25 is
 256 used to simulate the structured outliers; (iii) *incomplete shape*: We remove 40%
 257 to 90% points from scene model to simulate occlusions, the detailed removing
 258 approach can be found in [34]. For all experiments, we generated 30000 training
 259 samples, set up iterations $T = 30$ and set λ as 2×10^{-4} , β^2 as 0.03, and the

260 initial transformation \mathbf{x}_0 is $\mathbf{0}^6$. For the second feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$, we build the
 261 uniform grid in the range $[-2, 2]$ with 81 points in each dimension.

262 For the comparison experiments on Modelnet40 dataset, we design three
 263 modes for GDO training. (i) *mode*₁: The rotation is within 45 degrees and the
 264 translations is in $[-0.5, 0.5]^3$; (ii) *mode*₂: The rotation is within 90 degrees and
 265 the translations is in $[-0.5, 0.5]^3$; (iii) *mode*₃: The rotation is within 90 degrees,
 266 the translations is in $[-0.5, 0.5]^3$ and Gaussian noise with the standard deviation
 267 0.05 is also applied. The first two modes aim to compare the registration of all
 268 methods in terms of varying degrees of rotation, named *single-class training*.
 269 The latter is to compare the performance of different methods on the registration
 270 with multiple perturbations, named *multi-class training*. We generated 30000
 271 training samples for all modes, and the training sample will be normalized to
 272 $[-1, 1]^3$ without downsampling. The number of points of all samples is 5120.

273 5.3. Performance Metrics

274 *Baselines.* We compared GDO with the advanced learning-based approach
 275 DO [34], two point-based approaches (ICP and IRLS), two density-based ap-
 276 proaches (CPD and NDT) and the feature-based approach (FGR).

277 We used the successful registration rate, average MSE and computation time as
 278 performance metrics.

279 *Successful Registration Rate.* A registration is successful when the mean ℓ_2 is
 280 less than 0.05 of the model’s largest dimension.

281 *Average MSE.* It is worth noting that the MSE is the mean ℓ_2 error between
 282 the model and scene sets, and the Average MSE is the average for MSE for all
 283 test sets.

284 In order to make the experimental results more clear, we use \log_{10} MSE and
 285 \log_{10} computing time to describe the accuracy and efficiency of the registration
 286 of all registration methods on ModelNet40 dataset.

287 5.4. Parameters settings

288 The maximum number of iterations of all registration methods were set to
 289 30. For *DO* and *GDO*, we set λ as 2×10^{-4} , β^2 as 0.03. The value of the

290 tolerance of absolute difference between current estimation and ground truth in
 291 iterations is $1e-4$; For *ICP*, the tolerance of absolute difference in translation and
 292 rotation is 0.01 and 0.5 respectively; For *IRLS*, we used *Huber criterion function*
 293 as the regression function, the remaining parameters were set as the same as
 294 the setting of *ICP*. For *CPD*, the type of transformation is set to *rigid*, and
 295 the expected percentage of outliers with respect to a normal distribution is 0.1,
 296 the tolerance value is the same of that in DO. For *NDT*, the value of expected
 297 percentage of outliers is set to 0.55, and the tolerance value is set as the same
 298 of that in *ICP* ; For *FGR*, the value of the division factor used for graduated
 299 non-convexity is 1.4, the maximum correspondence distance is 0.025, the value
 300 of the similarity measure used for tuples of feature points is 0.95, the value of
 301 the maximum tuple numbers for trading off between speed and accuracy is set
 302 to 1000.

303 For *BCPD*, the expected percentage of outliers is set to 0.1, the parameter
 304 in Gaussian kernel is 2.0 and the expected length of displacement vector is 400.
 305 All deep-learning based registration networks are trained on an Nvidia Geforce
 306 2080Ti GPU with 12G memory. For *PCRNNet*, the kernel sizes are 64, 64, 64,
 307 128, 1024, 1024, 512, 512, 256 and 7. The iteration for rotation and translation
 308 is set to 8. Adam optimizer with an initial learning rate of 0.1, 300 epochs
 309 and a batch size of 32 are used for the training process. For *PointnetLK*, the
 310 kernel sizes are 64, 64, 64, 128, 1024. The maximum iteration for rotation and
 311 translation is set to 30. Adam optimizer with an initial learning rate of 0.001,
 312 250 epochs and a batch size of 10 are used for the training process. For *DCP*,
 313 the kernel sizes are 64, 64, 128, 256, 512, 1024, 256, 128, 64, 32 and 7. The
 314 iteration for rotation and translation is set to 1. Adam optimizer with an initial
 315 learning rate of 0.001, 250 epochs and a batch size of 32 are used for the training
 316 process. For *ICPMCC*, the error threshold is set to 10^{-7} , the iteration number
 317 is 30, and the number of nearest points for calculating normal vectors is set to
 318 10.

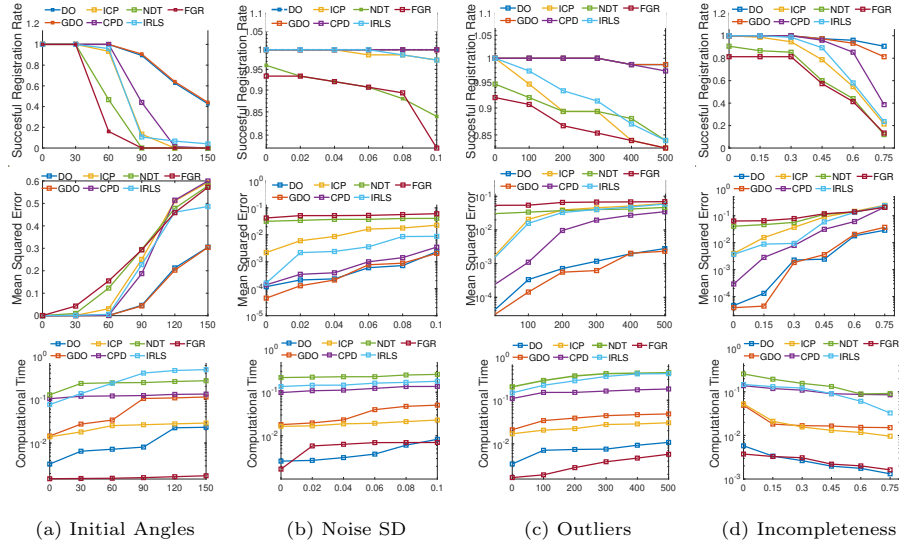


Figure 4: Results of 3D registration with Bunny model under different perturbations;(Top) Examples of scene points with different perturbations. (Second Row) Successful Registration Rate (SRR). (Third row) Average MSE (AMSE). (Bottom) Computation Time. In the presence of noise and outliers, the registration success rates of most algorithms are the same, which is 1, so the number of visualized dash lines is less than the number of algorithms. Learning-based registration algorithms (DO, GDO) can deal with point set registration with more accuracy than traditional registration algorithms (ICP, CPD, NDT, IRLS, and FGR). GDO is more time-consuming than DO, although its performance is slightly better than the performance of DO.

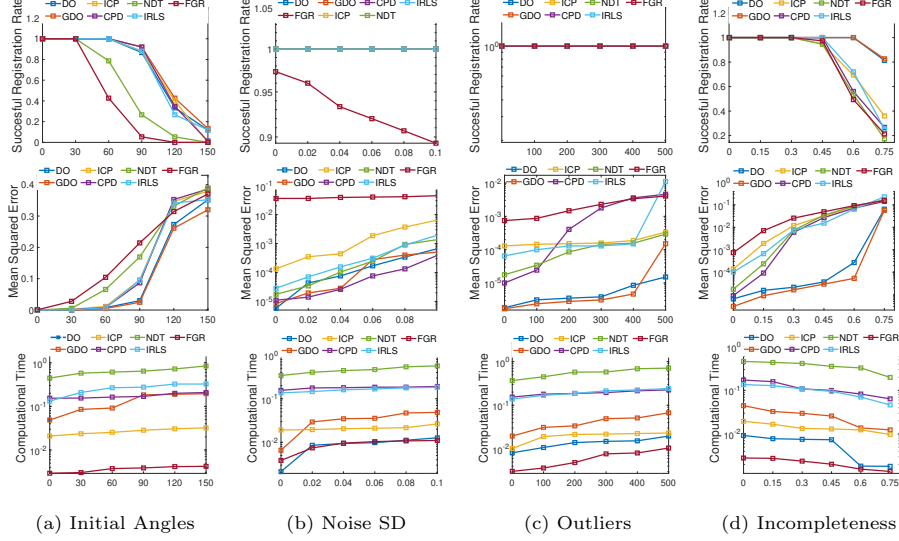


Figure 5: Results of 3D registration with Chef model under different perturbations

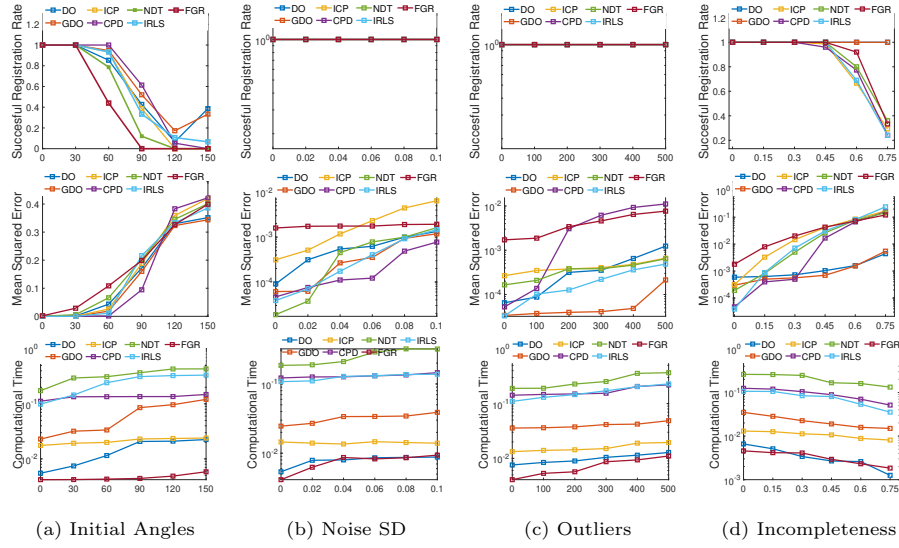


Figure 6: Results of 3D registration with Dancing Children model under different perturbations

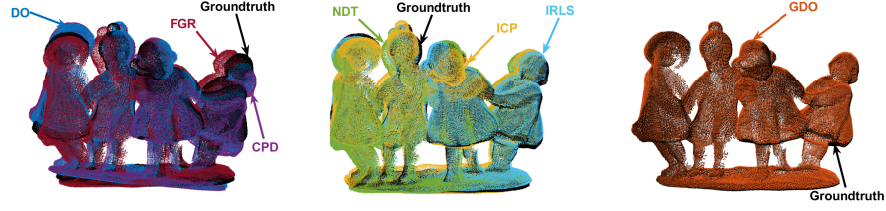


Figure 7: Registration results of Dancing Children model with 500 outliers

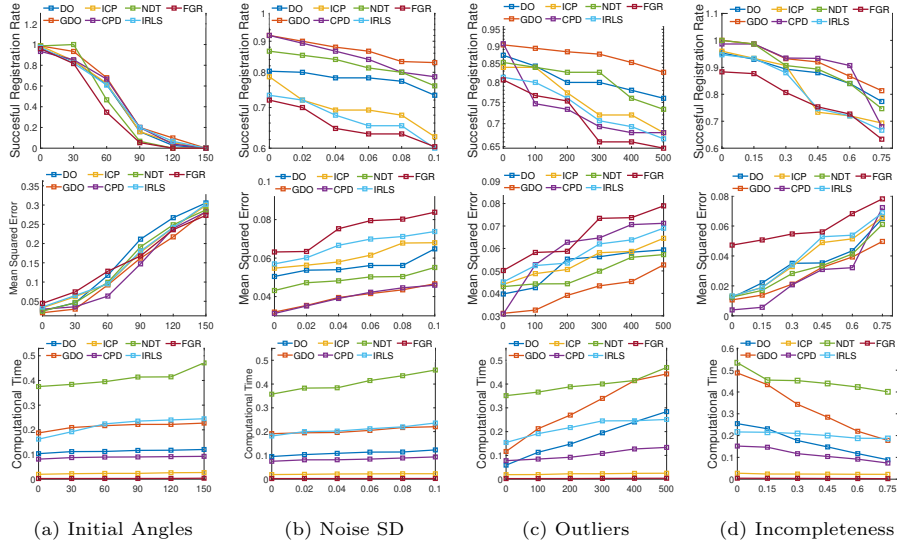


Figure 8: Results of 3D registration with Indoor Scene01 model under different perturbations

5.5. Registration Experiments

We have used the Stanford Bunny model[37], UWA dataset [38], Dancing Children, Indoor Scene[39] as the data sets for experiments Fig.1. Dancing Children are available at the AIM@SHAPE shape repository <http://visionair.ge.imati.cnr.it/ontologies/shapes/>. The model set \mathbf{M} is generated by using the grid average downsample method in MATLAB to select 477 points from the original model. The performance of algorithms are evaluated by comparing the evaluation metrics in the case of various perturbations: (1) *rotation*: We compare the performance metrics when the initial angle is 0° , 30° , 60° , 90° , 120° and 150° [default= 0° to 60°]; (2) *noise*: The standard deviation of the noise

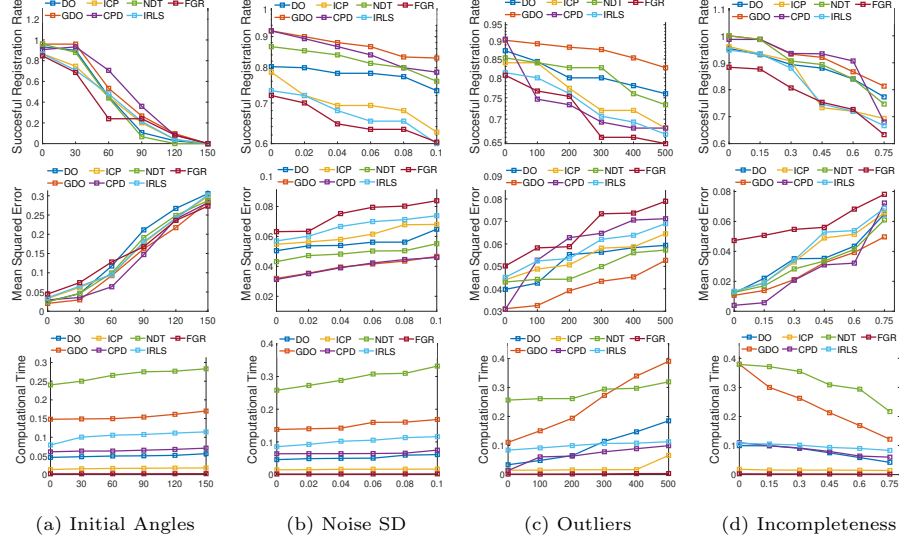


Figure 9: Results of 3D registration with Indoor Scene02 dataset under different perturbations

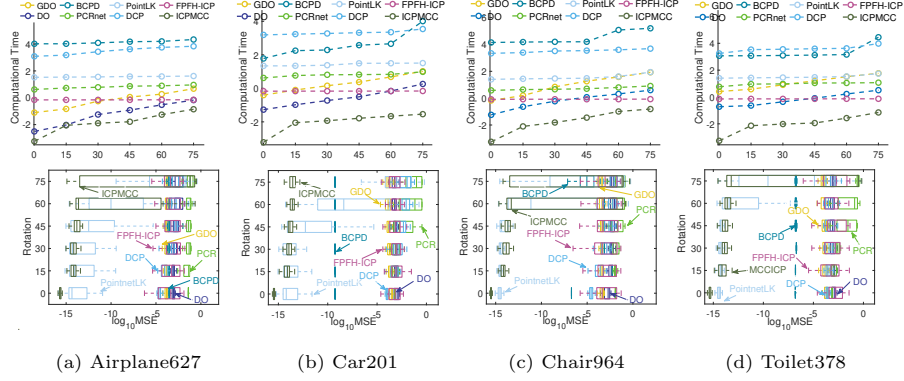


Figure 10: The registration results on Modelnet40 with perturbation setting $mode_1$. (Top) The computational time for registration. (Bottom) the $\log_{10}MSE$ of all the comparison methods. GDO, DO, FPFH-ICP and ICPMCC cost less time to achieve the registration. Although BCPD and PointnetLK register point clouds with more accuracy, the computation time of both is higher, even the time required for BCPD is almost dozens of times the time required for other registration methods. By comparison, GDO represents better registration performance with less computational time. And FPFH-ICP has poor stability. ICPMCC is unable to handle the registration over 60° .

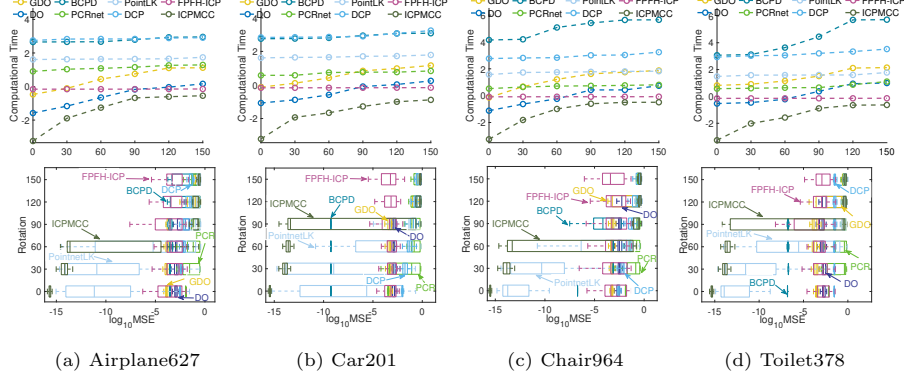


Figure 11: The registration results on Modelnet40 with perturbation setting *mode*₂. (Top) The computational time for registration. (Bottom) the $\log_{10}MSE$ of all the comparison methods. The accuracy of DO, GDO and BCPD has a sharp decrease after the registration over 90° . However, GDO still performs better than other methods in terms of accuracy. The performance of the deep-learning methods (PCR, PointnetLK and DCP) is not good even on the registration with the rotation of 60° . BCPD and DCP are still the most time-consuming.

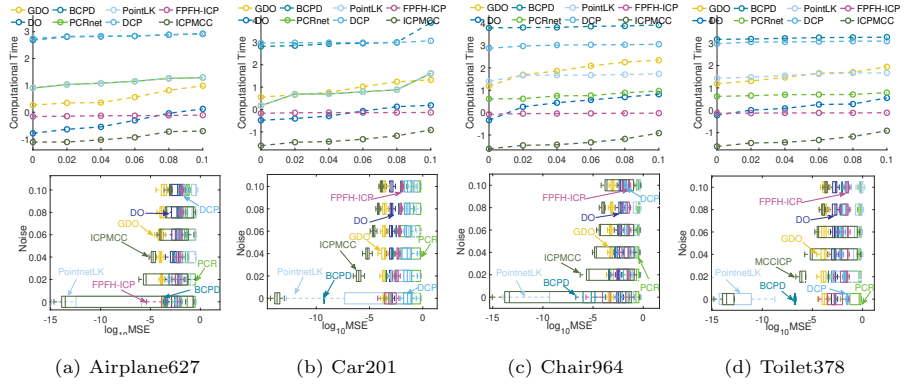


Figure 12: The registration results on Modelnet40 with perturbation setting *mode*₃. (Top) The computational time for registration. (Bottom) the $\log_{10}MSE$ of all the comparison methods. DO and GDO can keep the higher stability and accuracy on the registration with multiple perturbations, compared with other methods. The ability of deep-learning methods to handle the registration with multiple perturbations is poor than that of the traditional methods. The performance of FPFH-ICP is still stable, but the accuracy is not high.

329 is set to 0, 0.02, 0.04, 0.06, 0.08 and 0.1 [default=0]; (3) *outliers*: We set the
 330 number of outliers to 0, 100, 200, 300, 400 and 500 respectively [default=0]; (4)
 331 *incomplete ratio*: The ratio of incomplete scene shape is set to 0, 0.15, 0.3, 0.45,
 332 0.6 and 0.75 [default=0]. The random translation of all generate scenes is within
 333 $[-0.3, 0.3]^3$. When one parameter is changed, the values of other parameters
 334 are fixed to default values. In addition, the scene points are sampled from the
 335 original model, not from \mathbf{M} . We will test 750 testing samples in each variable
 336 setting. It is noteworthy that the training samples are generated by adding
 337 various perturbations to the model \mathbf{M} and assigning random parameters for the
 338 translation and rotation of the model \mathbf{M} . The testing samples are generated
 339 similarly, but the degree of perturbation and the parameters for transformation
 340 are different, and the down-sampled model is the original model instead of the
 341 model \mathbf{M} .

342 We also conduct comparative registration experiments on the ModelNet40
 343 dataset [40] with traditional methods (BCPD [41], FPFH-ICP [42] and ICPMCC [16])
 344 and other advanced deep-learning-based registration methods, such as PCR-
 345 Net [43], PointnetLK [44], and DCP [45] (as shown in (d) ~ (g) of Fig.1). There
 346 are three kinds of comparison settings corresponding to the training modes in
 347 5.2: for *mode*₁: the initial angle is 0°, 15°, 30°, 45°, 60° and 75°; for *mode*₂: the
 348 initial angle is 0°, 30°, 60°, 90°, 120° and 150°; for *mode*₃: the initial angle is 0°,
 349 30°, 60°, 90°, 120° and 150° [default=0° to 90°] and the standard deviation of
 350 Gaussian noise is set to 0, 0.02, 0.04, 0.06, 0.08 and 0.1 [default=0]. It is worth
 351 noting that when we change one parameter, the values of other parameters are
 352 fixed to the default value. We will test 100 test samples in each variable set-
 353 ting. The registration results with the single-class training scheme are shown in
 354 Fig.10 and Fig.11. The registration results with the multi-class training scheme
 355 are shown in Fig.12.

356 *Experimental Results*

357 *Registration results.* Fig.4 and Fig.5 show the 3D registration results on
 358 Bunny model and Chef model with various perturbations. It can be seen that

in the presence of arbitrary perturbation, learning-based registration algorithms (DO, GDO) can achieve more accurate registration results than the traditional registration methods (ICP, CPD, NDT, IRLS, FGR). Compared with DO, the performance of GDO is slightly better than DO. However, GDO is more time-consuming, the reason for which is that the second feature $[\mathbf{h}(\mathbf{x}; \mathbf{S})]^d$ calculates the density probability of each point in point sets, which involves the search of the closest box. Also, the calculation way of the second feature determines that the running time of GDO and the size of the point set are positively correlated.

Fig.6 and Fig.7 show the registration results on Dancing Children model. The trend and distribution of the running time of all algorithms on the Dancing Children model are the same as that on Bunny or Chef models. GDO is more capable when dealing with the complex model than registering simple models (Bunny, Chef), which can be illustrated by the Mean Square Error criteria.

Fig.8 and Fig.9 show the results of 3D registration on Indoor Scenes. The performances of NDT and GDO are prominent when registering real scenes models.

While FGR and ICP required low computation time for all cases, they had low success rates when the perturbations were high. CPD performed well in all cases except when the number of outliers was high. The running time of IRLS was similar to that of CPD when dealing with the registration of simple models (Bunny, Chef); it did not perform well when the model was highly incomplete. NDT achieved more accurate registration of real scenes than other algorithms; it was the most time-consuming for all cases. For the learning-based algorithms, DO and GDO outperformed the baselines when registering simple models. When dealing with the complex model (Dancing Children) and real large scene models, GDO performed better than DO. This is because DO just considers one single feature that does not consider the internal topology or density distribution of points, which makes it lack robustness than GDO.

Fig.10 displays the performance of all methods on registration with *mode*₁. It can be seen that the accuracy of BCPD is higher than other methods, but BCPD takes almost dozens of times as long as other algorithms. DCP takes

about the same time as BCPD, but its accuracy and stability are poor. The poor performance also occurs on the PCRnet method. By contrast, PointnetLK can keep higher stability and accuracy when dealing with the registration not over 60° . Compared with the deep-learning methods, as the traditional learning-based method, DO and GDO can achieve the registration with higher accuracy and stability. FPFH-ICP also performs well. The stability of ICPMCC has a sharp decrease when ICPMCC registers the registration over 60° .

Fig.11 shows the registration results on the perturbation of larger rotations *mode*₂. The stability and accuracy of ICPMCC and PointnetLK are worse when ICPMCC and PointnetLK handle the registration over 60° . The performance of DCP and PCR is unstable as ever. DO, GDO, and BCPD can keep the high accuracy and stability until they register points sets with large rotations (over 120°). Nevertheless, the accuracy of GDO is higher than that of BCPD and DO when dealing with the registration over 120° . FPFH-ICP still keeps its high stability and accuracy, and the performance of ICPMCC is poor once it is used to achieve the registration with larger rotations.

Fig.12 illustrates the registration results on Modelnet40 dataset with multiple perturbations *mode*₃. DO and GDO can keep the higher stability and accuracy on the registration with multiple perturbations, compared with other methods. The ability of deep-learning methods to handle the registration with multiple perturbations is poor than that of the traditional methods. The performance of FPFH-ICP is still stable, but the accuracy is not high.

In summary, the learning-based methods (DO and GDO) have higher stability and robustness compared with deep-learning methods (PCRnet, PointnetLK, and DCP) and other traditional methods. FPFH-ICP performs well even on the registration with larger rotations, but the accuracy of FPFH-ICP is not better, which may be caused by the fewer iterations for FPFH to find correspondences. The ability to achieve more accurate and stable registration on larger rotations or multiple perturbations for the deep-learning methods and ICPMCC is limited.

The benefit of the FPFH-ICP is the ability to handle registration with larger

421 rotations while maintaining higher stability. Comparing the registration results
 422 on $mode_2$ and $mode_3$, it can be seen that the only drawback of the traditional
 423 learning-based methods (DO and GDO) is the less ability to register point clouds
 424 over 120° , which illustrates that the learning-based methods are more vulnera-
 425 ble on rotations, not noises. In addition, the features in GDO can be replaced by
 426 any features extracted by 3D feature descriptors such as Fast Point Feature His-
 427 tograms (FPFH) descriptors, Signature of Histogram of Orientations (SHOT),
 428 and so on. The potential issue of the usage of various descriptors is whether it
 429 will increase the degree of over-fitting of the learning-based methods.

430 *Verify Convergence.* Fig.13 shows the Convergence Criteria and Training
 431 Error of our method on different data sets. We can find that the $\hat{\mathbf{D}}\mathbf{H}_f$ in our
 432 method meets the convergence condition $\sum_{i=1}^N (\mathbf{x}_*^i - \mathbf{x}_t^i)^T \hat{\mathbf{D}}\mathbf{H}_f (\mathbf{x}_t^i) > 0$ for
 all data sets, and the training error of our method decreases in each iteration.

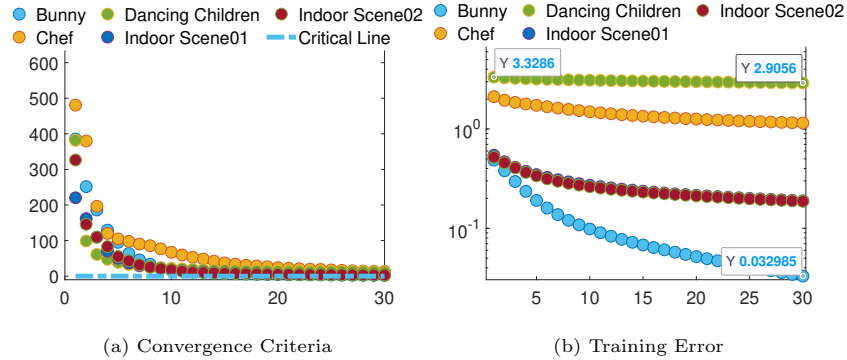


Figure 13: The Convergence Criteria and Training Error of our method on different data sets.
 (a) The value of $\sum_{i=1}^N (\mathbf{x}_*^i - \mathbf{x}_t^i)^T \hat{\mathbf{D}}\mathbf{H}_f (\mathbf{x}_t^i)$ on different data sets. (b) The training error of
 our method on different data sets.

433

434 6. Conclusion and Discussion

435 This paper proposes general discriminative optimization (GDO) method to
 436 solve the transformation parameter estimation in point set registration by learn-
 437 ing update directions from different features of training samples. Specifically,

GDO derives an approach to achieve the *collaboration* of the different extracted features from point sets to reduce the effect of perturbations on updating directions. In this paper, GDO combines a coordinates-based feature and a density-based feature to update the gradient map to improve the accuracy and robustness of transformation estimation. We provided a theoretical result on the convergence of the registration method under mild conditions. We also illustrate GDO outperformed state-of-the-art registration approaches on different data sets. The major advantage of GDO over traditional registration methods and learning-based registration methods include robustness to outliers and other perturbations, which is more prominent when dealing with complex 3D models and real scene models registration. The limitation of GDO is that the training point cloud and the test point cloud are highly relevant, limiting its ability to train many point clouds and achieve multiple point clouds registration like the registration methods based on deep learning. In addition, the feature extraction approach of GDO takes longer as the number of points increases. Future works of interest are to design a feature function that is more robust to perturbations and more efficient, and to design a registration framework to enable GDO to achieve multiple point clouds registration. The strong theoretical foundation and good registration performance of GDO suggest its usefulness as a general-purpose registration technique.

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