Unstructured Point Cloud Matching within Graph-theoretic and Thermodynamic Frameworks

A. Jagannathan and E. L. Miller
Center for Sub-surface Sensing and Imaging Systems, Northeastern University, Boston, MA 02115, USA
{ajaganna,elmiller}@ece.neu.edu

Abstract

In the context of object recognition from point cloud data, we present a thermodynamically-inspired graph theoretic algorithm to address the problem of matching the scene and the model point clouds, when the cardinalities of the two sets are orders of magnitude different. Such an approach determines a subset of points from the model that is structurally and spatially as similar as possible to the set of points in the scene. A new formulation for graph enthalpy characterizes the structural differences between point sets, which together with the existing notions of graph entropy quantifies the Gibbs’ Free Energy. A two-scale approach is proposed, wherein, at the coarse scale, a set of points that comprise the model neighborhood around the scene is identified by minimization of entropy. At the fine scale, the desired correspondence is achieved by a refinement process, aimed at maximizing the Gibbs’ Free Energy. The results demonstrate the robustness and efficiency of the approach.

1. Introduction

The task of recognition of a given partial, unstructured point cloud of the Scene (query data) using a database of stored perceptual representations of the 3D Model point clouds involves (i) classification of the Scene as an instance of one of the stored Models (ii) alignment of the Scene with respect to the identified Model (iii) determination of the location of the Scene within the identified Model. This work addresses the problem of location determination i.e., determination of a set of points in the identified Model that are structurally and spatially as similar as possible to the partial Scene point cloud. A matching algorithm is proposed within the frameworks of classical thermodynamics and graph theory for the determination of the desired correspondence.

There are two fundamental issues that make this problem challenging. First, the number of points in the Model and the Scene point clouds are orders of magnitude different. Secondly, due to sensor inaccuracies or because the Scene points are collected at different times, the two point sets may be non-overlapping i.e., no two points correspond to the exact same location in the 3D coordinate space.

Graph-based structural approaches and spatial location based algorithms have been reported in the literature on point matching. Graph-based algorithms establish the desired correspondence by matching configurations of Scene features to those of a Model [1]. In inexact graph matching, approximate solutions to the problem are obtained based on the minimization of the edit distance [3, 6], probabilistic optimization [17, 18], deterministic annealing [2], bipartite graph matching [5, 20] and spectral graph theory [7, 9, 8, 4]. Most existing graph matching techniques suffer from the inability to match graphs of largely varying sizes. Additionally, their performance severely degrades with small perturbations (positional jitter). Spatial matching approaches determine correspondence solely based on the spatial location of the points [10, 11]. While these algorithms are generally robust, they do not take into account the underlying structural information that exists between the points in a set. With non-overlapping point sets, this could be a problem, since there may be more than one subset of Model points that is spatially close to the Scene.

In this work, a thermodynamically inspired objective function is proposed to capture the structural nuances between a pair of graphs and the spatial differences between the underlying point sets. The desired correspondence is obtained by tackling a sequence of inexact graph matching problems that optimizes the proposed objective function.

We now provide a brief overview of our algorithm, which works in two stages. In the first stage, to facilitate inexact graph matching, the Model space is partitioned into Model Clusters (MCs), such that $|MC| = |Scene|$ (|·| represents the cardinality of a set). The change in entropy, computed for every MC relative to the Scene, identifies the
MC that is spatially the closest to the Scene and the model neighborhood around it. The advantage of such an approach is that the closest MC already provides a fraction of correct correspondences. In the second stage, the maximization of the free energy between the Scene and the closest MC, which is achieved by swapping certain points between the closest MC and the identified Model neighborhood, results in the desired correspondence. The reason for using different objective functions (i.e., based on entropy or free energy) during different processing stages is strongly motivated by the principles of thermodynamics.

Extensive experiments on complex 3D point sets indicate that the thermodynamically inspired cost function efficiently captures the structural and spatial variations, which results in stable matches. Additionally, the proposed algorithm is highly robust in the presence of noise. We contribute to the existing state-of-the-art by:

- defining graph enthalpy to quantify the underlying structural information in the point sets,
- deriving the Gibbs’ free energy for the point sets based on the proposed formulation of graph enthalpy and existing notions of graph entropy,
- optimizing the Free energy-based cost function to obtain the desired correspondence between the Scene and a subset of the Model points.

2. Definitions and Notations

In this work, a vertex/node $n_i$ (belonging to the Scene or the Model point set) represents the location of a point in 3D space, $n_i = \{x_i, y_i, z_i\}$. In a weighted undirected graph $G(N, E)$, $|N| = u$, an edge $e_{ij} \in E$ has an associated non-negative real weight $w_{ij}$, usually computed as the distance between the corresponding vertices $n_i, n_j \in N$ [12]. For such graphs, the degree $d_i$ of a vertex $n_i \in N$ is given by the sum of weights of all edges incident on $n_i$ i.e., $d_i = \sum_{n_j \in N} w_{ij}$. $A(G) = [w_{ij}]$ denotes a $(u \times u)$ weighted adjacency matrix while $D(G) = \text{diag}(d_i)$ denotes a $(u \times u)$ diagonal matrix [12]. Then, weighted Laplacian $L(G)$ is defined as: $L(G) = D(G) - A(G)$ [12].

Given a complete bipartite graph $G_{CB}((N_1, N_2), E)$, a matching is a set of edges $E_1 \subset E$ such that no two edges of $E_1$ share the same vertex [16]. Let $|N_1| = u_1$ and $|N_2| = u_2$. A matching is perfect, when $|E_1| = |u_1 + u_2|/2$ [16]. In a bipartite graph $G_B((N_1, N_2), E_{N_1,N_2})$, where $|N_1| = |N_2| = u$, $E_{N_1,N_2}$ denotes a minimum weight perfect matching, which is obtained by the implementation of the Hungarian method on $G_{CB}$ [16].

2.1. Notations

$Q$ and $M$ denote the query (Scene) and the identified Model point sets respectively. $|M| \gg |Q|$. $MC$ represents a certain model cluster, obtained by partitioning the Model space such that $|MC| = |Q|$.

As illustrated in Figure 1, the graphs of interest are:

- $G_{MST}(Q, E_Q), G_{MST}(MC, E_{MC})$ represent the minimum spanning tree (MST) constructed over $Q$ and a certain $MC$ respectively.
- $G_B((Q, MC), E_{QMC})$ denotes a bipartite graph constructed over the point sets $Q, MC$, where, $E_{QMC}$ represents the minimum weight perfect matching.
- $G_{U1}((Q, MC), (E_Q, E_{QMC}))$ denotes the union of $G_{MST}(Q, E_Q)$ and $G_B((Q, MC), E_{QMC})$. $G_{U2}((MC, Q), (E_{MC}, E_{QMC}))$ denotes the union of $G_{MST}(MC, E_{MC})$ and $G_B((Q, MC), E_{QMC})$.

The above graphs, denoted by $G_{MST}(Q), G_{MST}(MC)$, $G_B, G_{U1}, G_{U2}$, will be used in Section 3.1 to define graph enthalpy.

3. Point Matching via Classical Thermodynamics- Theory

In chemical thermodynamics, substance conversion results in the Gibbs’ Free Energy $\Delta G$, which quantifies the structural and the spatial differences as:

$$\Delta G = \Delta H - T \Delta S$$  \hspace{1cm} (1)

where $T$ is the temperature and $\Delta H$ is the change in enthalpy, resulting from the structural difference caused by the addition/deletion of chemical bonds between molecules. $\Delta S$ is the change in entropy due to the spatial disorder of the molecules involved [15].

Since graph edges are analogous to chemical bonds [13], a new formulation for graph enthalpy, quantifying the structural differences between a pair of graphs is proposed in Section 3.1. The spatial differences between the point sets are estimated using the existing notions of graph entropy [10]. The Gibbs’s Free energy for the point sets is then derived based on these differences.

3.1. Enthalpy change: Measure of Structural Difference

In classical thermodynamics, at a constant pressure $P$, the enthalpy $H_{s1}$ of a substance $s_1$ is given by:

$$H_{s1} = U_{s1} + PV_{s1}$$  \hspace{1cm} (2)
Theorem 1 [12]: For a graph $G$ on $n$ vertices and the corresponding weighted Laplacian $L$, let the eigenvalues of $L$ be $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ and that $\lambda_2 > 0$. The minimum energy of a balanced orthogonal representation of $G$ in $\mathbb{R}^m$ equals $\sum_{i=2}^{m+1} \lambda_i$.

For our problem, given $Q$ and a $MC$, ($|Q| = |MC|$), the change in graph enthalpy $\Delta H$ is determined by considering $G_{MST}(Q), G_{MST}(MC), G_{UB}$ and $G_{UB1}$. In this regard, two interesting features of $G_B$ need attention. First, the edges in $G_B$ provide a one-to-one correspondence between $MC$ and $Q$. Secondly, these edges are indicative of the extent of structural dissimilarity between $G_{MST}(Q)$ and $G_{UB1}$ or $G_{MST}(MC)$ and $G_{UB2}$. This is because when the lengths of the edges in $G_B$ are all zero i.e., $E_{QMC} = \phi$, then

\[
G_{UB1} = G_{UB1}(Q, MC, E_Q), \\
G_{UB2} = G_{UB2}(MC, Q, E_{MC})
\]

$\Delta H$ quantifies the total structural difference for the two point sets $Q$ and $MC$ as:

\[
\Delta H = \Delta H_1 + \Delta H_2
\]

where, $\Delta H_1 = H(G_{UB1}) - H(G_{MST}(Q))$ and $\Delta H_2 = H(G_{UB2}) - H(G_{MST}(MC))$.

3.2. Entropy Change: Measure of Spatial Difference

Given a set $x_n$, consisting of $n$ points, Ma et.al [10] estimate the entropy by the power weighted length of the MST constructed over the set of vertices as:

\[
\hat{S}(\chi_n) = \frac{1}{1-\alpha} \log \frac{L(\chi_n)}{n^\alpha} - \log \beta
\]

where, $L(\chi_n)$ is the length of the minimum spanning tree, $\beta$ is a constant independent of the underlying density of the points and $\alpha$ is the fractional order of the density.

In this work, the change in entropy $\Delta S$ for the two sets of points $Q$ and $MC$, is computed as

\[
\Delta S = \Delta S_1 + \Delta S_2
\]

where,

\[
\Delta S_1 = \hat{S}(Q \cup MC) - \hat{S}(Q) \\
\Delta S_2 = \hat{S}(Q \cup MC) - \hat{S}(MC)
\]

Using (6), (7), (9), (10) and (1), the Free energy $\Delta G$ is computed for same-sized point sets $Q$ and $MC$. The temperature $T$ measures the degree of desired correspondence. High temperatures imply low degrees of desired correspondence and vice versa. The initialization of $T$ is described in Section 4.4, within the context of the proposed matching algorithm.

3.3. Significance of thermodynamic quantities in the context of the problem

By the laws of thermodynamics,
(a) At very high temperatures, $\Delta G$ is dominated by entropic contributions, and at very low temperatures, it is dominated by enthalpic contributions.

(b) $\Delta H$ and $\Delta S$ decrease with decrease in temperature.

(c) At high temperatures, $\Delta G$ is a large negative number. As the temperature decreases, $\Delta G$ increases toward zero.

Motivated by (a), our matching algorithm uses $\Delta S$ and $\Delta G$ as objective functions for the coarse scale and fine scale processing respectively. Property (b) provides a pruning strategy for minimization of $\Delta S$ during the coarse scale processing. The temperature’s role in the algorithm is influenced by (c), and is described below.

### 3.4. Key Observations

- **Temperature Dependence:**
  
  **Theorem 2** [12]: Let $X$ be a graph with $n$ vertices and let $Y$ be obtained from $X$ by adding an edge joining two distinct vertices of $X$. Then $\lambda_i(X) \leq \lambda_i(Y)$ for all $i$. Theorems 1 and 2 imply that $\Delta H > 0$. Also, $\Delta S > 0$. Therefore, the temperature $T$ decides whether $\Delta G < 0$ or not. In the algorithm, to ensure that $\Delta G < 0$ (property (c), Section 3.3), $T$ is initialized to a large number, which is described in Section 4.4.

- **Correspondence between Point Sets:** At any given $T$, the edges in $G_B$ provide the correspondence between the points in a certain $MC$ and $Q$. The desired correspondence between $Q$ and a subset of the *Model* points is achieved when $\Delta G$ reaches its maximum, at $T = 0$.

### 4. Algorithm

Figure 2 provides an outline of the proposed algorithm. The preprocessing step involves (i) the partitioning of the model space $M$ into model clusters ($MC$s) ($|MC_i| = |Q|$) and, (ii) the construction of a Nearest Neighbor ($NN$) graph over these $MC$s. During the coarse scale processing step, the $MC$ that minimizes $\Delta S$ is identified as the closest $MC$ ($CMC$) and its one-connected neighbors form the neighborhood pool ($NP$). The immediate advantage of identifying the $CMC$ is that it provides a fraction of correct correspondences. However, since the partitioning is in a sense blind, it is very unlikely that the $CMC$ will provide the desired correspondence. This forces a fine scale processing step, wherein, the maximization of $\Delta G$, by swapping certain vertices between the $CMC$ and $NP$, leads to the desired correspondence.

The optimization of the cost functions in both the processing stages is achieved using a Branch and Bound (B&B) approach, wherein a thermodynamically inspired pruning strategy reduces the number of nodes and branches in the search tree that have to be explored. The processing modules are described below.

#### 4.1. Preprocessing

Following [19], the $n$ points that comprise a $MC$ (where $n = |Q|$) are determined by performing a breadth-first search on the delaunay triangulation [14], which is constructed over $M$. The center of a $MC$ is then identified as the vertex with minimum eccentricity. A delaunay triangulation constructed over these centers serves as a $NN$ graph for coarse scale processing.

#### 4.2. Coarse Scale B&B Algorithm

The primary objective here is to identify the $MC$ that minimizes $\Delta S$, i.e., the $CMC$. For this, the $MC$ corresponding to the vertex with the smallest degree (typically on the periphery) in the $NN$ graph is assigned as the root node in the B&B search tree. In the search tree, the connected neighbors of a $MC$ form its children, and at any node ($MC$), using (9) and (10), $\Delta S$ is computed between $Q$ and the corresponding $MC$. While traversing the tree down to the leaves, if $\Delta S_{child} > \Delta S_{parent}$, then the sub-tree is automatically pruned off at such parent nodes. This is because an increase in $\Delta S$, signals an increase in spatial dissimilarity (between a $MC$ and $Q$), which further implies that we are moving away from $Q$ rather than moving in a direction toward it. Such a pruning is consistent with the monotonicity property of the B&B approach [16]. The algorithm’s output
is the CMC, which together with its one connected neighbors i.e., NP, is used for the refinement of correspondences at the finer scale.

### 4.3. Fine Scale B&B Algorithm

The objective here is, to maximize $\Delta G$ by determining the best correspondence for every point $q_i \in Q$ that has not already found its desired match $c_j \in CMC$. The coarse scale CMC forms the root node in the fine scale B&B search tree. With respect to each $q_i$, the set $V_m \subset (NP \cup CMC)$ comprising of $k$ model points of interest, is identified by centering a disc of radius $r$ on $q_i$. At any node in the search tree, $\Delta G_{child}^k$ is computed between $CMC_{child}^k$ and $Q$, where $CMC_{child}^k$ is obtained by swapping out a point $c_i \in CMC$ that was originally associated with $q_i$, and swapping in $V_m(k)$. That is,

$$CMC_{child}^k = (CMC_{parent} \setminus c_i) \cup V_m(k), \ k = 1, \ldots, |V_m|$$  

Swapped out vertices are returned to the NP. Sub trees are pruned off at parent nodes when $\Delta G_{child}^k < \Delta G_{parent}$ (property (c), Section 3.3). Using $G_{MST}(Q)$, a connected neighbor of $q_i$ generates the children in the search tree. Upon termination, the edges in $G_B$, associating the refined CMC and $Q$, provide the desired correspondence. The fine scale processing is illustrated in Figure 3(b)-(e).

### 4.4. Effect of Temperature on $\Delta G$

At the level 0, i.e., at the root of the B&B search tree, the temperature $T$ is initialized as $T = (|Q| - d) \times 10^7$, where $d$ is the number of points in the coarse scale CMC that completely overlap with $Q$. $T = (|Q| - d - i) \times 10^7$ at the tree’s level $i$, $1 \leq i \leq |Q| - d$. Different levels in the tree, along the path leading to maximum $\Delta G$, contribute to different fractions of the desired correspondence (due to the refinement of the CMC). The desired match between $Q$ and CMC is reached at path’s leaf, when $T = 0$.

### 5. Experiments and Discussion

#### 5.1. Point Matching Process: Validation of the Laws of Thermodynamics

The adherence of the graph formulations of $\Delta H$ and $\Delta G$ to the laws of thermodynamics is experimentally proven by considering random 3D point sets where, $|Q| = 100$ points and $|M| = 5000$ points. Using $M$, $Q_1, Q_2, Q_3, Q_4, Q_5$, were generated, corresponding to 100%, 80%, 60% 40%
and 0% overlap respectively. The extent of overlap was decreased by adding white Gaussian noise to a subset of points in $Q_1$.

The graphs in Figure 4(a)-(c), correspond to the fine scale processing stage of $Q_1$, where $T$ was initialized at $70 \times 10^7$, to indicate that 30 vertices from coarse scale CMC overlapped with $Q_1$. For the fine scale processing of $Q_3$ (graphs shown in Figure 4(d)-(f)), $T$ was initialized at $88 \times 10^7$ (since 12 vertices in coarse scale CMC overlapped with $Q_3$). Such temperature initializations to large values ensured that $\Delta G \leq 0$ throughout the correspondence process.

With all the point sets, it is observed that, $\Delta H$ as well as $\Delta S$ decrease with decrease in temperature, while $\Delta G$ increases toward zero. For $Q_1$ and $Q_3$, this is indicated by the direction of the arrows in Figure 4. As shown in Figure 4(a)-(c), for completely overlapping point sets, the desired correspondence is achieved when $\Delta H, \Delta S, \Delta G$ are all zero. For non-overlapping or partially overlapping point sets, the correspondence is recovered when $\Delta G$ reaches its maximum as shown in Figure 4(f). In Figure 4(f), at $T = 0$, the value of $\Delta G$ is dictated only by $\Delta H$, implying that, among the possible matches, all with minimum $\Delta S$, the one that minimizes the structural differences (with the least $\Delta H$) provides the desired correspondence. These results experimentally prove the feasibility of the point matching process based on the laws of thermodynamics.

5.2. Comparison with an existing state-of-the-art

For comparison purposes, we implemented the SVD+EM [8] as well as the basic SVD algorithm [7], since they incorporate spectral graph theoretic ideas as well. An increasing weighted proximity matrix and a gaussian weighted proximity matrix is generated for the SVD+EM [8] and the SVD approaches [7], respectively. These proximity matrices are then used to obtain corresponding modal matrices. In the SVD approach [7], a binary decision on the correspondence is made on the basis of the similarity of different rows of the modal matrices for the two point sets. For the SVD+EM approach [8], using the modal matrices, the probabilities are computed to assess the similarities between the elements of the point sets. The correspondence process is embedded within the EM framework.

Two sets of experiments on random same-sized 3D point sets were conducted to compare the algorithms. In the first series of experiments, we added “extra” Model points, which in [8] are termed as outliers. The outlier to data ratio ranged from 0 to 0.8. Although the performance of the SVD+EM algorithm is better than SVD approach, as Figure 5(a) indicates, it still is quite sensitive to the presence of outliers. Since our algorithm is designed to deal with outliers, a 100% correspondence is always achieved.

In the second series of experiments, our goal was to analyze the algorithms’ tolerance to noise. To begin with, we considered completely overlapping, same-sized
point sets. The scene point cloud was then progressively subjected to varying levels of Gaussian noise (standard deviation ranging from 0 to 0.6). As Figure 5(b) indicates our algorithm provides 100% correspondence while the performance of the spectral correspondence algorithms degrade with increase in noise. As Figure 5(c) indicates, considerable positional jitter (manifested by large standard deviations of noise) is required for the performance of our algorithm to degrade.

5.3. Real Data Sets

We evaluated the performance of our algorithm on 15 real data sets. In Figure 6(a), $|M| = 4370$ points, $|Q| = 200$ and the NP consists of 4 model clusters (as opposed to 22 clusters that characterize the entire model space). Prior to the implementation of the fine scale B&B algorithm, 12% of the CMC points overlap with the scene. The desired correspondence between Q and the CMC is shown in Figure 6(b).

Figure 6(c) shows a more challenging example where the point sets are non-overlapping. The model $M$ is a tank, $|M| = 18,897$. The scene $Q$ consists of 300 points. Of the 63 MCs that describe the entire model space, only 6 MCs constitute the NP. Since none of the coarse scale CMC points exactly overlapped with $Q$, the temperature at the start of fine scale processing was set at $300 \times 10^7$. Figure 6(d) shows the desired correspondence obtained between $Q$ and the refined CMC.

6. Conclusions

Our results indicate that (i) the newly proposed formulation of graph enthalpy efficiently captures the structural differences between non-overlapping point sets (ii) the Gibbs’ free energy based optimization, by combining the spatial and the graph-based structural information, leads to stable and efficient matches, as opposed to simple graph matching. Additionally, the proposed approach is highly robust in the presence of noise. For $|Model| = 5000$ points and $|Scene| = 100$, our algorithm determines the desired correspondence in approximately 1.2 minutes on a Pentium IV, 256MB memory, 1.5 GHz machine (with the code implemented in Matlab). Currently, we are considering alternative optimization algorithms to speed up the matching process. As part of future work, we will apply the proposed thermodynamic formulations for multi-scale object recog- 

References

[1] Y. Keselman, A. Shokoufandeh, M. F. Demirci and S. Dickinson, “Many-to-Many Graph Matching via Metric Embed-


