

University of Windsor

Scholarship at UWindor

Electronic Theses and Dissertations

Theses, Dissertations, and Major Papers

2017

Structures from Distances in Two and Three Dimensions using Stochastic Proximity Embedding

Udayamoorthy Navaneetha Krishnan
University of Windsor

Follow this and additional works at: <https://scholar.uwindsor.ca/etd>

Recommended Citation

Navaneetha Krishnan, Udayamoorthy, "Structures from Distances in Two and Three Dimensions using Stochastic Proximity Embedding" (2017). *Electronic Theses and Dissertations*. 7385.
<https://scholar.uwindsor.ca/etd/7385>

This online database contains the full-text of PhD dissertations and Masters' theses of University of Windsor students from 1954 forward. These documents are made available for personal study and research purposes only, in accordance with the Canadian Copyright Act and the Creative Commons license—CC BY-NC-ND (Attribution, Non-Commercial, No Derivative Works). Under this license, works must always be attributed to the copyright holder (original author), cannot be used for any commercial purposes, and may not be altered. Any other use would require the permission of the copyright holder. Students may inquire about withdrawing their dissertation and/or thesis from this database. For additional inquiries, please contact the repository administrator via email (scholarship@uwindsor.ca) or by telephone at 519-253-3000ext. 3208.

Structures from Distances in Two and Three Dimensions using Stochastic Proximity Embedding

By

Udayamoorthy Navaneetha Krishnan

A Thesis

Submitted to the Faculty of Graduate Studies
through the School of Computer Science
in Partial Fulfillment of the Requirements for
the Degree of Master of Science
at the University of Windsor

Windsor, Ontario, Canada

2017

©2017 Udayamoorthy Navaneetha Krishnan

Structures from Distances in Two and Three Dimensions using Stochastic Proximity
Embedding

by

Udayamoorthy Navaneetha Krishnan

APPROVED BY:

M. Hlynka
Department of Mathematics and Statistics

X. Yuan
School of Computer Science

A. Mukhopadhyay, Advisor
School of Computer Science

Y. Aneja, Co-Advisor
Odette School of Business

December 1, 2017

DECLARATION OF ORIGINALITY

I hereby certify that I am the sole author of this thesis and that no part of this thesis has been published or submitted for publication.

I certify that, to the best of my knowledge, my thesis does not infringe upon anyone's copyright nor violate any proprietary rights and that any ideas, techniques, quotations, or any other material from the work of other people included in my thesis, published or otherwise, are fully acknowledged in accordance with the standard referencing practices. Furthermore, to the extent that I have included copyrighted material that surpasses the bounds of fair dealing within the meaning of the Canada Copyright Act, I certify that I have obtained a written permission from the copyright owner(s) to include such material(s) in my thesis and have included copies of such copyright clearances to my appendix.

I declare that this is a true copy of my thesis, including any final revisions, as approved by my thesis committee and the Graduate Studies office, and that this thesis has not been submitted for a higher degree to any other University or Institution.

ABSTRACT

The point placement problem is to determine the locations of a set of distinct points uniquely (up to translation and reflection) by making the fewest possible pairwise distance queries of an adversary. Deterministic and randomized algorithms are available if distances are known exactly.

In this thesis, we discuss a 1-round algorithm for approximate point placement in the plane in an adversarial model. The distance query graph presented to the adversary is chordal. The remaining distances are uniquely determined using the Stochastic Proximity Embedding (SPE) method due to Agrafiotis, and the layout of the points is also generated from SPE. We have also computed the distances uniquely using a distance matrix completion algorithm for chordal graphs, based on a result by Bakonyi and Johnson. The layout of the points is determined using the traditional Young- Householder approach. We compared the layout of both the method and discussed briefly inside.

The modified version of SPE is proposed to overcome the highest translation embedding that the method faces when dealing with higher learning rates.

We also discuss the computation of molecular structures in three-dimensional space, with only a subset of the pairwise atomic distances available. The subset of distances is obtained using the Philips model for creating artificial backbone chain of molecular structures. We have proposed the Degree of Freedom Approach to solve this problem and carried out our implementation using SPE and the Distance matrix completion Approach.

DEDICATION

To my family and my friends

ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to my supervisor Dr. Asish Mukhopadhyay, without him my thesis and my whole Master's is incomplete. I also offer my sincere appreciation to my co-supervisor Dr. Yash P Aneja for his continuous support.

Secondly, I would also like to express my gratitude to my committee members Dr. Myron Hlynka, and Dr. Xiaobu Yuan for their beneficial advice and suggestions for my thesis.

I would also like to thank my research partners Md. Zamilur Rahman and Shalini Bhat-tacharjee for their invaluable help throughout my thesis.

TABLE OF CONTENTS

DECLARATION OF ORIGINALITY	III
ABSTRACT	IV
DEDICATION	V
ACKNOWLEDGEMENTS	VI
LIST OF FIGURES	IX
LIST OF TABLES	XI
1 Introduction	1
1.1 Point Placement Problem in 1D	1
1.2 Point placement problem in 2D	2
1.3 Point placement problem in 3D	3
1.4 Motivation	3
1.5 Preliminaries	4
1.6 Stochastic Proximity Embedding (SPE)	5
1.7 Thesis Organization	7
2 Point Placement Problem on a Plane	9
2.1 Introduction	9
2.2 Motivation	9
2.3 Reductionist Approach	11
2.4 Prior Work	13
2.4.1 Sensor Network Localization Problem	13
2.4.2 Distance Matrix Completion Approach	14
2.5 SPE Approach for Distance matrix completion	18
2.6 Difficulties in SPE	19
2.7 Modified Version of SPE	24
2.8 Comparison and Experiments: DMCA (YH's) Vs. SPE Partial Vs. SPE Complete	27
2.9 Discussions	35
3 Point Placement problem in 3D Space with Degree of Freedom Approach	37
3.1 Molecular Distance Geometry Problem	37
3.2 Prior Work	38
3.2.1 More and Wu's approach	39
3.2.2 Discretizable Distance Geometry Problem	39
3.2.3 Crippen and Havel's Approach	40

3.2.4	Philips Model	42
3.3	Overview of our results	44
3.4	Degree of Freedom Approach	46
3.5	Coordinates computation using SPE	47
3.6	Distance matrix completion approach	48
3.7	Experiments with Philips Model	52
3.8	MD-Jeep With NMR data	53
3.9	Md-Jeep Vs. DMCA + SPE using NMR data	57
3.10	Discussions	58
4	Summary and Discussions	59
4.1	Open Problems	60
	REFERENCES	61
	VITA AUCTORIS	64

LIST OF FIGURES

1	<i>Distance graph for a 1-round algorithm</i>	2
2	<i>Distance graph for a 1-round algorithm</i>	10
3	<i>Points on a two-dimensional integer grid</i>	12
4	<i>Stereographic projection of points on a circle</i>	12
5	<i>A chordal graph on five vertices</i>	15
6	<i>Initial Layout of 20 points with 0.01 as learning rate</i>	20
7	<i>SPE Layout of 20 points with 0.01 as learning rate</i>	21
8	<i>Graph for 30 points with 0.01 as learning rate</i>	22
9	<i>Graph for 50 points with 0.01 as learning rate</i>	23
10	<i>Initial Layout of 20 points with 0.001 as learning rate</i>	25
11	<i>SPE Layout of 20 points with 0.001 as learning rate</i>	26
12	<i>Initial Layout with 22 Vertices</i>	34
13	<i>Initial Layout Versus SPE (Complete distance matrix)</i>	34
14	<i>Initial Layout Versus SPE (Partial distance matrix)</i>	35
15	<i>Initial Layout Versus Young and Householder's approach</i>	35
16	<i>Initial Layout Vs Young and Householder's approach Vs SPE(Partial matrix) Vs SPE(Complete matrix)</i>	36
17	<i>Philips Model</i>	42
18	<i>Protein Chain created using Philips Model</i>	45
19	<i>Initial layout of b</i>	49
20	<i>SPE layout of b</i>	50
21	<i>Chordal Graph Construction</i>	50
22	<i>Protein Chain created using Philips Model</i>	54

23	<i>Original Protein Chain Vs Protein Chain produced by DMCA + SPE</i>	55
24	<i>MD-Jeep Coordinates</i>	56
25	<i>MD-Jeep Coordinates</i>	57
26	<i>Layout produced by DMCA Plus SPE</i>	57

LIST OF TABLES

1	Experimental results using Young Householders	30
2	Experimental results using SPE with Complete distance matrix	31
3	Experimental results using SPE with Partial distance matrix	33

CHAPTER 1

Introduction

A prototypical problem for point placement problem and the graph embedding is given by Saxe [25]. The problem states that: Given an incomplete edge-weighted graph G and a parameter k , map the vertices of the graph G to the points in a Euclidean k -space in such a way for any two vertices connected by an edge, its edge weight is equal to the corresponding points in the k -dimensional space. Deciding if such an embedding exists is strongly NP-complete [25].

Saxe also proved that the problem is NP-complete even when the embedding dimension is 1 and the edge weights are restricted to values in the set $1,2$.

1.1 Point Placement Problem in 1D

The point placement problem on a line is the problem of locating n distinct points on a line up to translation and reflection in adversarial settings. This is a 1-dimensional version of Saxe's problem. The queries can be made in one or more rounds and are modeled as a graph whose nodes represents the points, and there is an edge connecting two points if the distance between the corresponding points is being queried. A prototypical 1-round algorithm uses the line-rigid 3-cycle (or triangle) graph (Fig.1) as the core structure and constructs the distance graph on n points.

Let $P = \{p_1, p_2, \dots, p_n\}$ be n distinct points on a line. A distance graph with n vertices

that has edges joining the pairs of points whose distances are returned by the adversary. The distances returned by the adversary are assumed to be valid if there exists a linear layout consistent with these lengths. The distance graph is said to be line-rigid if a consistent layout exists for all valid adversarial assignments of lengths. [21]

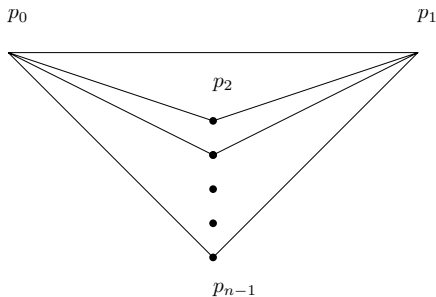


FIGURE 1: *Distance graph for a 1-round algorithm*

The best-known 2-rounds algorithm for point placement on a line is due to Alam and Mukhopadhyay [3] that makes $9n/7$ queries and has a query lower bound of $9n/8$.

1.2 Point placement problem in 2D

The point placement problem on a plane is to determine the location of a linear set of points $\{p_1, p_2, p_3 \dots p_n\}$ up to translation and reflection on the plane by making the fewest possible pairwise distance queries to an adversary. This is a 2-dimensional version of Saxe's problem.

In this thesis, we are proposing an algorithm for the point placement problem on a plane based on Stochastic Proximity Embedding (SPE). A chordal graph is submitted to the adversary as a distance query graph, while the remaining distances in the query graph are uniquely determined using Stochastic Proximity Embedding (SPE). SPE also generates the layout of the points while completing the partial distance matrix.

1.3 Point placement problem in 3D

The Molecular Distance Geometry Problem (MDGP) is defined as the problem of finding the cartesian coordinates of the atoms in a molecule, with only a subset of pairwise interatomic distances available. This is a 3-dimensional version of Saxe's problem. The MDGP arises in NMR experimental techniques that provides a set of inter-atomic distances d_{ij} for certain pairs of atoms (i, j) of a given molecule.

The MDGP can be formulated as follows: A unique three-dimensional structure of a molecule is to be determined when the distances between all pairs of atoms in a molecule are available. However, when there are errors or unavailability of certain distances the unique structure of the molecule may not exist. Here we are approaching the problem, with only a partial set of interatomic distances available.

1.4 Motivation

The abstract version of point placement problem appears in diverse areas of research, such as Wireless Sensor Networks (WSNs), Computational Geometry, Computational Biology and Learning Theory [21].

Localization of sensor nodes has been an active research area in WSNs. Finding the position of nodes is a vital requirement in many WSNs applications including tracking, geometric routing, and monitoring [4]. Distances between the sensors are calculated by measuring the power used between the sensors for two-way communications. Most of the localization techniques are making use of the section of nodes that has prior knowledge of their absolute positions. Such nodes are called anchor nodes. With the position of the anchor nodes known, the localization problem is solved in the Wireless Sensor Networks (WSNs) provided all other unknown distances are determined.

In the area of Computational Geometry, the version of the point placement problem is

known as the turnpike problem. The problem description is as follows. In an expressway from city A to city B, several ONroute exists; the distances between all pairs of ONroute are known. With the know distances between the ONroutes, the geometric location of this route is fixed. This problem was initially studied by Skiena et al. [27] who proposed a practical heuristic for the reconstruction. A polynomial time algorithm was given by Daurat et al. [10].

In the area of Computational Biology, the 3D structure of a molecule can be determined by solving the Molecular Distance Geometry Problem (MDGP) [9]. A molecule is represented in a three-dimensional space by a set X. Each point x_i in the set X is represents an atom in the molecule. Some of the distances between atoms are determined by Nuclear Magnetic Resonance (NMR) spectroscopy. By exploiting such distances, the coordinates of the atoms in a molecule are determined by solving the corresponding Distance Geometry Problem. [13]

1.5 Preliminaries

Let $D = [d_{ij}]$ be a symmetric matrix of size $n \times n$ and $d(p_i, p_j)$ be the Euclidean distance between the points p_i and p_j . The symmetric matrix is said to be Euclidean distance matrix if the points p_1, p_2, \dots, p_n lies in some k-dimensional Euclidean space such that $d_{ij} = d(p_i, p_j)^2$. The diagonal entries in the matrix are zero and the off-diagonal entries are filled with Euclidean distances [23].

Let $G = (V, E)$ be a *graph*, where V is the set of vertices and E is the edges. G consists of a finite set of vertices $\{v_1, v_2, \dots, v_n\}$ and a set of edges $\{\{v_i, v_j\}, i \neq j\}$ joining some pairs of vertices. A *path* in the G is a sequence of vertices v_i, v_{i+1}, \dots, v_k , where $\{v_j, v_{j+1}\}$ for $j = i, i + 1, \dots, k - 1$, is an edge of G . A *cycle* is the closed path in the graph and the size is the number of edges in the path. A chord is an edge joining two non-consecutive vertices in a cycle. A graph G is said to be *chordal* if it has no chordless cycles of size 4 or more. [23]

The *distance graph* of a $n \times n$ distance matrix, is a graph on n vertices with an edge

connecting two vertices v_i and v_j if there is a non-zero entry in the i^{th} row and j^{th} column of the distance matrix. [23]

In a graph G , the *neighbourhood* of a vertex v are those vertices in G that are adjacent to v . If the neighbourhood $N(v)$ of a vertex is clique then the particular vertex is said to be a *simplicial vertex*. A *simplicial ordering* of the vertices of G is a map $\alpha : V \rightarrow \{1, 2, \dots, n\}$ such that v_i is simplicial in the induced graph on the the vertex set $\{v_i, v_{i+1}, \dots, v_n\}$. [23]

1.6 Stochastic Proximity Embedding (SPE)

Stochastic Proximity Embedding (SPE) is the main tool we are using here to solve the point placement problem in 2-dimensional and 3-dimensional spaces.

SPE is a self-organizing algorithm that attempts to generate the Euclidean embedding that best preserves the similarities from the original embedding. SPE starts with a random initial configuration and refines it by iteratively selecting a random pair of points. This refinement starts adjusting the coordinates so that their distances on the map match more closely with their respective proximities. The adjustment is driven by the learning-rate parameter λ that decreases during simulation to avoid the oscillatory behavior. The main advantage of SPE is SPE scales linearly with respect to sample size and can be applied to the huge data sets unlike the well-known dimensionality reduction techniques like multidimensional scaling(MDS) and nonlinear mapping(NLM). [1]

Converting distances to coordinates is the prevalent theme in Distance Geometry problem. The prototypical example of this problem comes from the field of cartography. Intercity distances are given in the form of a matrix; the aim is to place the cities on a two-dimensional map that reflects their true geographical coordinates. The main idea of this problem is to arrange a set of objects in space to reproduce the observed distances between them.

Let $P = p_1, p_2, \dots, p_n$ be a set of n points in a given plane and $R = [r_{ij}]$ is a symmetric matrix

shows the relationship between these objects. let $P^r = p_1^a, p_2^a, \dots, p_n^a$ be the random initial point set produced by SPE, and the $D = [d_{ij}]$ is a distance matrix showing the relationship between the random point set. The distance matrix R can either be a partial or complete distance matrix. SPE can produce the final embedding even when the distance between the points are not fully available.

Algorithm 1 SPE

Initialize the coordinates of P^r and select an initial learning rate λ
for (C cycles) do
for (S steps) do
Select a pair of points, p_i^a and p_j^a , at random and compute their distance $d_{ij} = \|p_i^a - p_j^a\|$.
if ($d_{ij} \neq r_{ij}$) **then**
 $p_i^a \leftarrow p_i^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_i^a - p_j^a)$, $\epsilon \neq 0$
 $p_j^a \leftarrow p_j^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_j^a - p_i^a)$, $\epsilon \neq 0$
end if
Repeat Step 2 for a prescribed number of steps, S
Decrease the learning rate λ by prescribed decrement $\delta\lambda$
Repeat Steps 2-4 for a prescribed number of cycles, C

Stochastic Proximity Embedding has two cycles, the outer cycle is the learning cycle, and the inner cycle picks up the points randomly from the set P^r and applies the Newton-Raphson Root finding style of correction to the randomly picked points. SPE is controlled by three parameters: number of steps S, the learning rate parameter λ (C Cycles) and the term ϵ . The learning rate parameter λ starts with 1 and decreases over time to a final value 0.

The decrement of the λ value forces the update rule to take more or less the full Newton-Raphson steps at the initial cycles and control the magnitude of the updates for the better embedding; this prevents the oscillation of the updating algorithm. The ϵ value is chosen to be the smaller value and add with d_{ij} to avoid the division by 0 if points i and j happen to coincide.

Iteration steps of the algorithm are $C \cdot S$, where C is the steps for the learning cycle, and

S is the number of times a random point is selected from the point set P^r . The parameter C and S are set so that $CS = o(n^2)$, as the quadratic running times of similar algorithms based on Multi-Dimensional Scaling (MDS), Principal Component Analysis (PCA). The algorithm designers have empirically determined that the algorithm scale linearly with the number of data points. To achieve a practically perfect embedding, it takes 10,000 total pairwise refinements per data point.

The quality of the embedding is measured by the stress function, the stress function is minimized with the course of the refinement:

$$S = \frac{\sum_{i < j} \frac{(d_{ij} - r_{ij})^2}{r_{ij}}}{\sum_{i < j} r_{ij}}$$

1.7 Thesis Organization

This thesis is organized in the following manner, a small description of the content in four chapters that makes up the thesis.

- Chapter 2 gives a brief review of the Point placement on a line problem and discusses the motivation to study the point placement in the plane problem. After the introduction to Sensor Network Localization, 'Distance matrix completion approach' is reviewed, and a detailed description of our algorithm using SPE is discussed. Our modified version of SPE is discussed to overcome the embedding in highest translation that SPE faces during algorithm execution. At last in the experiments section, the comparison between Distance Matrix Completion Approach Vs. SPE with Partial matrix Vs. SPE with complete matrix is analyzed.
- Chapter 3 introduces the Molecular Distance Geometry Problem (MDGP) and our algorithm using SPE and DMCA to solve the MDGP. This chapter discusses the artificial instance creation based on Philips model. We have proposed the Degree of Freedom

approach to reconstruct the chain of a protein molecule with partial distances. Our approach towards solving the MDGP using DMCA and SPE is explained in detail. MD-Jeep software proposed by Lover et al. [19] is reviewed, and the comparison results between MD-Jeep and the DMCA + SPE Approach is also discussed in the experimentation section.

- Chapter 4 summarizes the topics discussed in this thesis and suggests some open problems that can be taken as a research interest in near future.

CHAPTER 2

Point Placement Problem on a Plane

2.1 Introduction

The point placement problem on a plane is to determine the location of a linear set of points, $\{p_1, p_2, p_3 \dots p_n\}$ on the plane by making the fewest possible pairwise distance queries to an adversary. The placement is fixed up to translation and reflection.

The main motivation behind this problem is to fix the sensor network localization. Sensor networks have some nodes with their distances known, and other nodes with the unknown distances. Now the problem is to fix the whole system using the available distances between the nodes and the fixed nodes called anchor nodes [5].

2.2 Motivation

The current approach to the point placement on a line needs testing a large number of distance constraints; these constraints involve the edge lengths of a distance graph. If integer coordinates are used; we can avoid this problem of rounding errors; however for the point placement on a plane this problem is unavoidable even if the coordinates are integral. Thus we are using a distance matrix completion approach to avoid the problem of testing distance constraints.

The main motivation behind the study of the point placement on a plane problem is to

avoid the layer graph construction approach used for the point placement problem on the line. The layer graph concept used in the point placement on a line is discussed below,

A prototypical 1-round algorithm constructs the following distance graph on n points (Fig. 2) by using the line-rigid 3-cycle graph or a triangle as a core structure. As the figure shows that, the graph has $n - 2$ triangles hanging from a common strut. The number of distance queries made is $2n - 3$

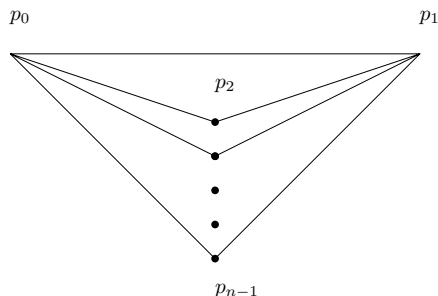


FIGURE 2: *Distance graph for a 1-round algorithm*

The distance graph can be re-drawn orthogonally, such re-drawn graph with satisfying following conditions is called layer graph. The concept of layer graph is first introduced by Chin et al. They also proved that a given distance query graph is not line-rigid iff it has a layer graph drawing in [8]. Layer graph is also used to obtain the rigidity conditions. Conditions to satisfy to be a layer graph:

1. All the edges in the graph G should be parallel to one of the two orthogonal directions x and y
2. The length of an edge e is the distance between the corresponding points on the distance graph L
3. The edges in the graph should not be in a single direction
4. No two vertices coincide if the layer graph is folded onto a line, by a rotation either to the right

Mukhopadhyay et al. [21] showed that the rigidity conditions are easy to verify when exact arithmetic is used in the implementation of the 2-rounds algorithm. Since the adversary is simulated by us, the distances returned are set to be integral. There is a possibility of rounding errors if the pairwise distances are not integral. Checking the rigidity conditions can be difficult because of the rounding errors introduced in finite-precision calculations.

The approach proposed in this thesis is susceptible to generalization in higher dimensions, where there are difficulties in generalizing the current approach to two or three dimensions because of finding the suitable generalization of the layer graph concept and the theorems associated with it.

2.3 Reductionist Approach

Though it is difficult to generalize the layer graph constructions in the point placement on the line problem, reductionist approaches can be used to solve the point placement on a plane problem by solving the point placement on the line problem. We discuss two such reductions below,

Points on a two-dimensional integer grid

Consider the points $p_1, p_2, p_3, \dots, p_n$ lie on an integer grid as shown in the figure below (Fig. 3). Now we can reduce the point placement on a plane problem to the point placement on a line by projecting them on x and y axis. An important assumption is that no two points lie on the small vertical or horizontal line of the grid, to make sure that we have a distinct set of points in a line.

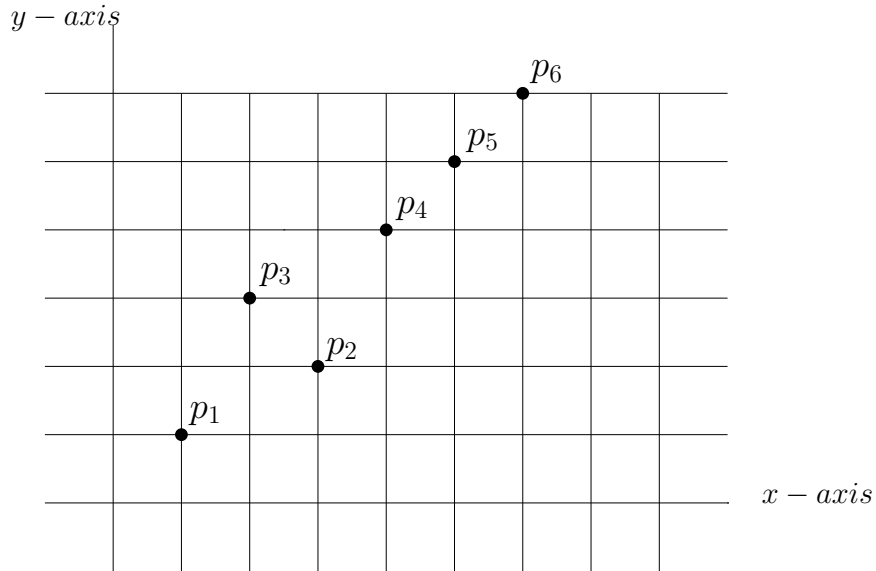


FIGURE 3: *Points on a two-dimensional integer grid*

Stereographic projection of points on a circle

When points $p_1, p_2, p_3, \dots, p_n$ lie on a circle, we can use stereographic projection on the circle and plot the points on the line; now we can solve the problem by applying the 1-Dimensional point placement algorithm to the projected points.

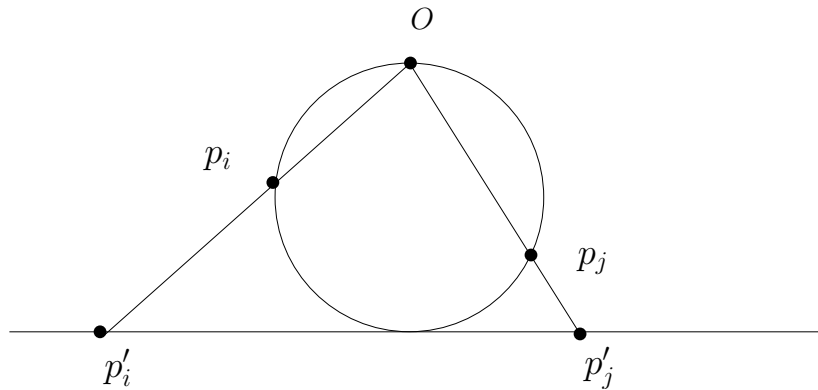


FIGURE 4: *Stereographic projection of points on a circle*

Stereographic projection is a mapping function that projects a sphere onto a plane. The projection is defined on entire sphere except for one point where the projection is defined [29]. In the above figure (Fig. 4), the projection of a sphere is taken place from the point O , which

is the highest point in the sphere.

2.4 Prior Work

2.4.1 Sensor Network Localization Problem

Computing the locations of the nodes in a sensor network is known as the sensor network localization problem. There are existing algorithms proposed to determine the location of the nodes in a network by only knowing the location of fewer nodes. Such fixed nodes are called beacon nodes. When the location of the fewer nodes are fixed, then other nodes try to measure the distance between neighbors and fix their locations. Though algorithms exist to find the location of the nodes, some fundamental questions were not addressed.

The theory of network localization proposed by Aspnes et al. [5] has some theoretical proof to answer the basic questions in network localization. The main underlying idea in this paper is this: grounded graphs are constructed to model the network localization and the rigidity theory for graphs were used to test the conditions for unique localizability. Now the unique networks were constructed using the rigid grounded graph.

The notion of grounded graphs is proposed in this paper [5] to solve the unique network localizability. In grounded graphs, each vertex represents network nodes. If the distance between two nodes is known, or the nodes are beacon nodes, then the corresponding vertices are connected. With the construction of the grounded graphs, the network has a unique localization if and only if its corresponding ground graph is generically globally rigid. To check if a network in the plane is unique localizable, we just need to check if the corresponding grounded graph is redundantly rigid and 3-connected.

The computational complexity of the network localization has been shown as NP-hard when the grounded graph is generically globally rigid via reduction from set-partition.

The trilateration graph is also explored in this paper to study the complexity of network

localization. Aspens et al. [5] showed that the trilateration graphs are uniquely localizable and the node locations are easily be computed. Aspens et al. also showed that the random geometric graphs are trilateration graphs if a node density or the communication radius is reached.

2.4.2 Distance Matrix Completion Approach

A distance matrix completion approach is proposed by Zamilur et al. [23] based on the result of Bakonyi and Johnson. This approach includes the generation of a chordal graph, computing simplicial ordering of the graph, finding the maximal clique and the distance matrix completion. Once the distance matrix is completed the end coordinates are generated by using the traditional Young and Householder’s method.

Computing a chordal graph sequence

Based on the result produced by Grone et al. in [14], chordal graph sequence is generated in this paper. The theorem is as follows,

Theorem 1 [14] *G has no minimal cycles of length exactly 4 if and only if the following holds: For any pair of vertices u and v with $u \neq v$, $\{u, v\} \notin E$, the graph $G + \{u, v\}$ has a unique maximal clique which contains both u and v . (That is: if C and C' are both cliques in $G + \{u, v\}$ which contain u and v , then so is $C \cup C'$.)*

Simplicial ordering computation

The simplicial ordering of a graph, α of G can be found by a breadth-first search of G when the vertices are labeled in the lexicographic order. A well-known LEX-BFS [24] algorithm is used to compute the simplicial ordering of the vertices.

Algorithm 2 Simplicial Ordering

- 1: Empty label list, $()$, is assigned to all the vertex in V
 - 2: **for** $i = n$ to 1 **do**
 - 3: Pick a vertex $v \in V$ with the largest label list in lexicographical order
 - 4: Set $\alpha(v) = i$
 - 5: For each unnumbered vertex w adjacent to v , add i to the label list of w
 - 6: **end for**
 - 7: return α
-

Consider the following chordal graph for the simplicial ordering (Fig. 5) The vertices in the chordal graph are labeled in lexicographical order.

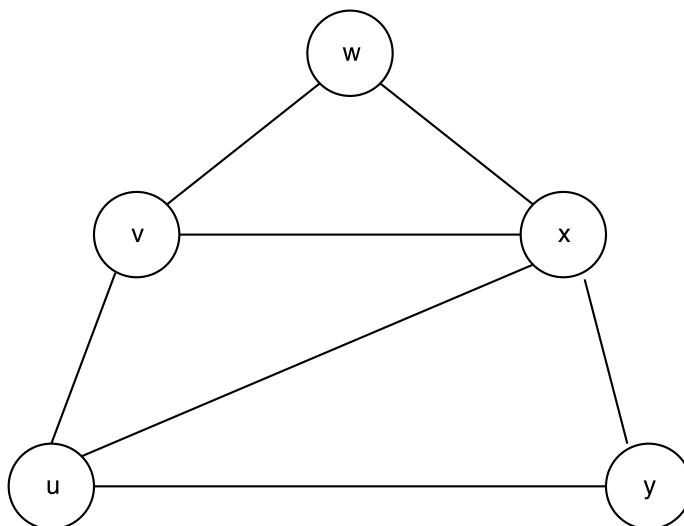


FIGURE 5: A chordal graph on five vertices

By following the algorithm above, the simplicial ordering of the chordal graph is computed and shown in the table below,

	u	v	w	x	y
Step 0	$()$	$()$	$()$	$()$	$()$
Step 1	$()$	(5)	(5)	$()$	$()$
Step 2	$()$	(5)	$(5,4)$	(4)	(4)
Step 3	$()$	(5)	$(5,4)$	(4)	$(4,3)$
Step 4	$()$	(5)	$(5,4)$	$(4,2)$	$(4,3)$

Distance matrix completion of a clique

To find a maximal clique, the algorithm designer is starting with a clique that has two vertices of the given edge, add a vertex to the clique by examining if it is adjacent to every other vertex in the clique; otherwise, discard the current vertex and move on to the next.

Distance matrix completion approach starts with the completion of a clique with one edge missing in [23]; this theorem is formulated as the partial distance matrix completion with one missing entry. The lemma proposed is as follows,

Theorem 2 *This theorem is based on Bakonyi and Johnson's results in [6]*

The partial distance matrix admits at least one completion to a distance matrix F .

$$\begin{pmatrix} 0 & D_{12} & x \\ D_{12}^t & D_{22} & D_{23} \\ x & D_{23}^t & 0 \end{pmatrix}$$

If

$$\begin{pmatrix} 0 & D_{12} \\ D_{12}^t & D_{22} \end{pmatrix}$$

and

$$\begin{pmatrix} D_{22} & D_{23} \\ D_{23}^t & 0 \end{pmatrix}$$

has embedding dimensions as p and q respectively then x can be chosen so that the embedding dimension of F is $s=\max\{p,q\}$.

This result is equivalent to finding the completion of the partial distance matrix:

$$\begin{pmatrix} 0 & 1 & 1 & e^t & 1 \\ 1 & 0 & d_{12} & \bar{D}_{13} & d_{14} \\ 1 & d_{12} & 0 & \bar{D}_{23} & x \\ e & \bar{D}_{13}^t & \bar{D}_{23}^t & \bar{D}_{33} & \bar{D}_{34} \\ 1 & d_{14} & x & \bar{D}_{34}^t & 0 \end{pmatrix}$$

to a matrix in which the Schur complement

$$\begin{pmatrix} a & B & x - d_{12} - d_{14} \\ B^t & C & D \\ x - d_{12} - d_{14} & D^t & f \end{pmatrix}$$

of the upper left 2×2 principal matrix has a positive semidefinite completion of rank s .

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Theorem 3 shows that the solution for x exists. [12]

Let

$$R = \begin{pmatrix} a & B & x \\ B^t & C & D \\ x & D^t & f \end{pmatrix}$$

is a real partial positive semidefinite matrix.

The rank of $\begin{pmatrix} a & B \\ B^t & C \end{pmatrix} = p$ and rank of $\begin{pmatrix} C & D \\ D^t & f \end{pmatrix} = q$

Now the real positive semidefinite completion F of R shows that the rank of F is a maximum of $\{p, q\}$. The completion shown here is unique iff $\text{rank}C = p$ or $\text{rank}C = q$.

Once the distance matrix is completed using the distance matrix completion approach, the completed distance matrix is used as an input to the SPE and compute the coordinates. To compare our results, coordinates are also computed using the Young and Householder's method.

2.5 SPE Approach for Distance matrix completion

The distance query graph presented to the adversary is chordal. Once the chordal graph is computed after the edge lengths returned by the adversary, the remaining distances are uniquely determined using both the distance matrix completion approach proposed by Zamir et al. [23] and the Stochastic Proximity Embedding (SPE) heuristic. The coordinates out of the completed distance matrix are computed using SPE.

Stochastic proximity embedding takes $R = [r_{ij}]$ as a input distance matrix. The R matrix can either be complete or partial distance matrix. In the next step, SPE produces a random number of points equal to the size of the original embedding and computes the distance matrix $D = [d_{ij}]$.

Now SPE starts refining the point by iteratively selecting a random pair; the refinement starts adjusting the coordinates based on the Newton-Raphson method of root-finding so that their respective distances match closely. This adjustment is driven by the learning rate parameter that decreases during simulation to avoid the oscillatory behavior. In our approach, we kept $\epsilon = 0.0001$, and the learning rate parameter goes from 1 to 0 decrementing by 0.001.

Algorithm 3 SPE

```

 $R = [r_{ij}]$  as a input distance matrix, select an initial learning rate  $\lambda$ 
for (C cycles) do
for (S steps) do
Select a pair of points,  $p_i^a$  and  $p_j^a$ , at random and compute their distance  $d_{ij} = \|p_i^a - p_j^a\|$ .
if ( $d_{ij} \neq r_{ij}$ ) then
     $p_i^a \leftarrow p_i^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_i^a - p_j^a)$ ,  $\epsilon \neq 0$ 
     $p_j^a \leftarrow p_j^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_j^a - p_i^a)$ ,  $\epsilon \neq 0$ 
end if
Repeat Step 2 for a prescribed number of steps,  $S$ 
Decrease the learning rate  $\lambda$  by prescribed decrement  $\delta\lambda$ 
Repeat Steps 2-4 for a prescribed number of cycles,  $C$ 

```

At the end of this algorithm, the approximate distance matrix $D = [d_{ij}]$ is completely

refined towards the original distance matrix R ; the respective initial random points are also refined towards the original embedding; thus these points are the final coordinates produced by SPE.

While generating the coordinates using SPE, the values of the coordinates are translated to the highest position. We used the geometric transformation to bring back the layout close to the original layout without altering the structure of the layout. The Geometric transformation is carried out using the Kabsch method.

The summary of the approach used in this problem is this; we are using the using the distance matrix completion approach proposed by Zamilur et al. [23], based on the result produced by Bakonyi et al. [6]. Bakonyi and Johnson showed that if the distance graph corresponding to a partial distance matrix is chordal, then there exists a completion of the partial distance matrix. Once the distance matrix is completed, we are computing the coordinates using SPE. In the original method of completing the graph using Distance matrix completion approach based on a result by Bakonyi and Johnson, coordinates are generated using the traditional Young and Householder’s method [30]. We also approached this problem by skipping the DMCA and input the partial distance matrix into SPE. The result of both SPE with partial distance matrix and the SPE with complete distance matrix and Young and Householder’s method is compared at the end of this problem.

The main difficulty we faced while generating the coordinates using SPE is that the coordinates are transferred to the highest position. We discussed this problem further in this thesis and proposed the solution to overcome this problem.

2.6 Difficulties in SPE

In SPE, the improvisation of the final embedding depends upon the parameters used inside the algorithm. From the study of our experiments, the learning rate parameter λ differs

and improves the points embedding. The decrement we are using here for the λ affects the learning cycle. Some pointsets are tending to learn quickly, and the other needs more steps to learn the original point positions. We have tested our λ decrement from 0.01 to 0.5. The point set with more number of points and huge disparity over the original embedding took more time to learn. While a point set with less number of points and less disparity with the original embedding learned quickly and needed very few steps over λ .

So what happens when the learning cycle is more for a point set that learns quickly. This will overfeed the point set and translate the final structure to highest range. An example showed here will give us the clear picture of what translation and overfeeding do to the point set (See Fig: 7).

The figure below (Fig.7) shows the layout produced by SPE, which represents the original layout (Fig.6) but in the highest range. The structure produced by SPE is same as the original embedding (Needs Rotation), but the range in which SPE produced the embedding is from 94980 to $-1.35e5$. The original embedding lies in the range of 120×120 . This is the result of the more number of learning cycles.

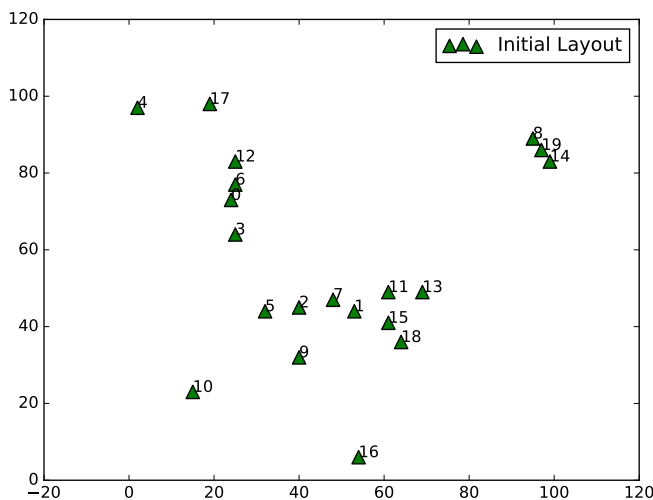


FIGURE 6: *Initial Layout of 20 points with 0.01 as learning rate*

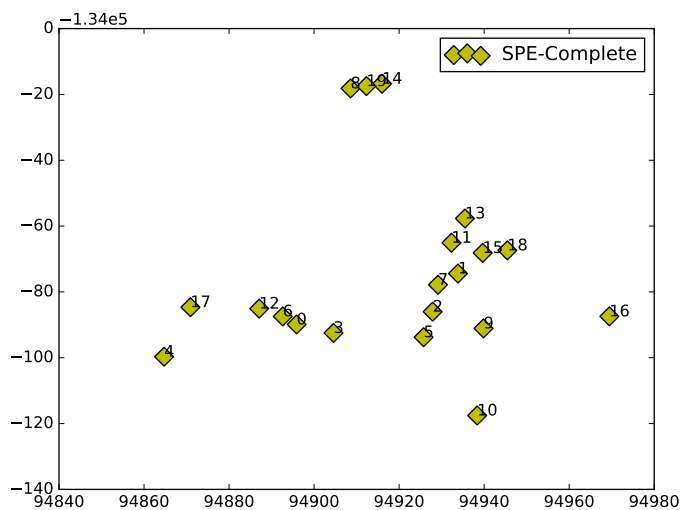


FIGURE 7: *SPE Layout of 20 points with 0.01 as learning rate*

The experiment on the learning rate parameter is discussed here,

Through our series of experiments, we have got the clue that when the learning cycle is more, then the stress function is close to zero. However, when this learning cycle overfeeds the point set, then the translation to the highest position takes place. Below Few charts (See Fig. 8 and 9) shows that the increase in learning cycles, steadily decreasing the stress function.

Learning Rate Vs Stress Function for 30 Points

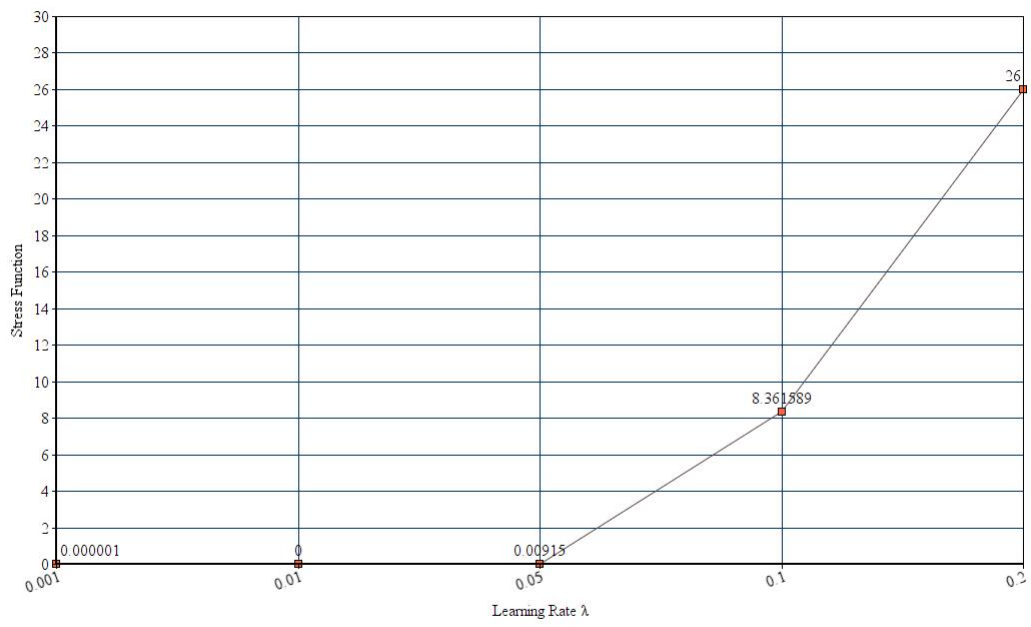


FIGURE 8: Graph for 30 points with 0.01 as learning rate

Learning Rate Vs Stress Function for 50 Points

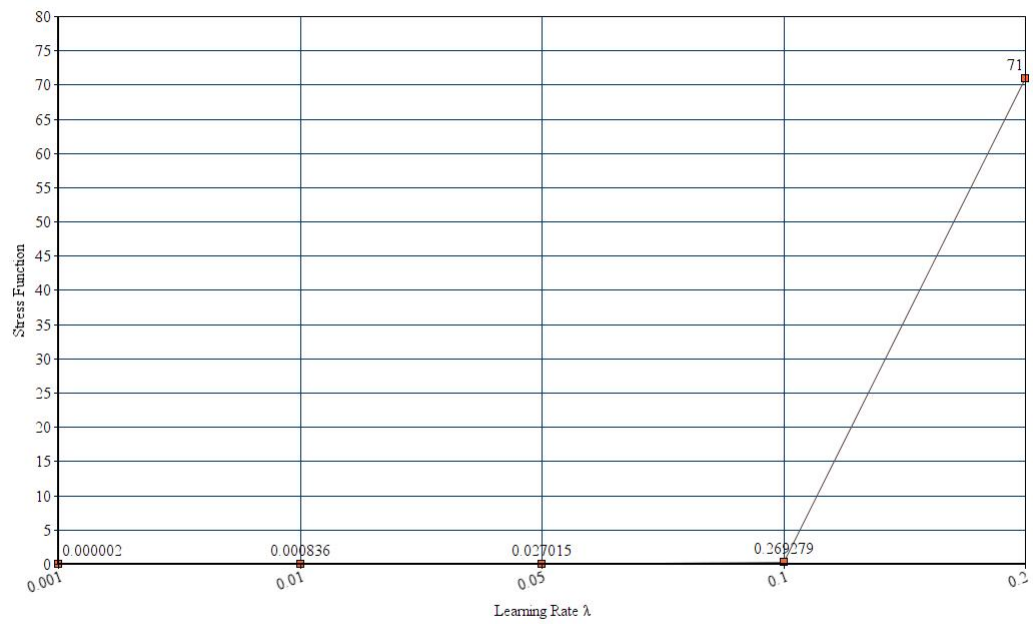


FIGURE 9: Graph for 50 points with 0.01 as learning rate

2.7 Modified Version of SPE

Since the learning rate parameter λ depends upon the number of points, and the disparity between the original and the approximate embedding, λ is hard to control. However, to control the highest translation of the point set, we have proposed the new idea of using anchor nodes. Since the Sensor Network Localization has some nodes fixed, we are taking advantage of such fixed nodes and fixing the remaining tag nodes without altering the positions of the anchor nodes.

The updated SPE algorithm is as follows,

Algorithm 4 Modified SPE

```

Initialize the coordinates of  $P^r$  and select an initial learning rate  $\lambda$ 
for (C cycles) do
for (S steps) do
Select a pair of points,  $p_i^a$  and  $p_j^a$ , at random and compute their distance  $d_{ij} = \|p_i^a - p_j^a\|$ .
if ( $d_{ij} \neq r_{ij}$ ) then
    if  $p_i^a$  is Anchornode but  $p_j^a$  is not then
         $p_j^a \leftarrow p_j^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_i^a - p_j^a)$ ,  $\epsilon \neq 0$ 
    end if
    if  $p_i^a$  is not an Anchornode but  $p_j^a$  is an anchornode then
         $p_i^a \leftarrow p_i^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_i^a - p_j^a)$ ,  $\epsilon \neq 0$ 
    end if
    if Both  $p_i^a$  and  $p_j^a$  is not an Anchor node then
         $p_i^a \leftarrow p_i^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_i^a - p_j^a)$ ,  $\epsilon \neq 0$ 
         $p_j^a \leftarrow p_j^a + \lambda \frac{1}{2} \frac{r_{ij} - d_{ij}}{d_{ij} + \epsilon} (p_j^a - p_i^a)$ ,  $\epsilon \neq 0$ 
    end if
end if
Repeat Step 2 for a prescribed number of steps,  $S$ 
Decrease the learning rate  $\lambda$  by prescribed decrement  $\delta\lambda$ 
Repeat Steps 2-4 for a prescribed number of cycles,  $C$ 

```

Here we are choosing some points as Anchor points and running against the SPE algorithm. Now in SPE, while choosing the i and j at random, we are not updating the anchor nodes if i and j turned out to be one of the anchor nodes. When we get one anchor node

and the other one as the tag node, then we are only updating the tag node.

The figure (Fig. 11) shows the embedding of 20 points with $\lambda = 0.001$, for 20 points. This embedding is reproduced by SPE with learning rate parameter $\lambda = 0.001$ and keeping 2,4,6 as the anchor nodes, for 20 points the learning cycle that goes from 1 to 0.001 is more than what is required. Since we can complete the 20 point structure with the learning rate parameter $\lambda = 0.01$ (Fig. 7) but that translates it to the highest range.

The figure (Fig. 11) shows the SPE embedding with the range same as the original embedding shown above (Fig. 10).

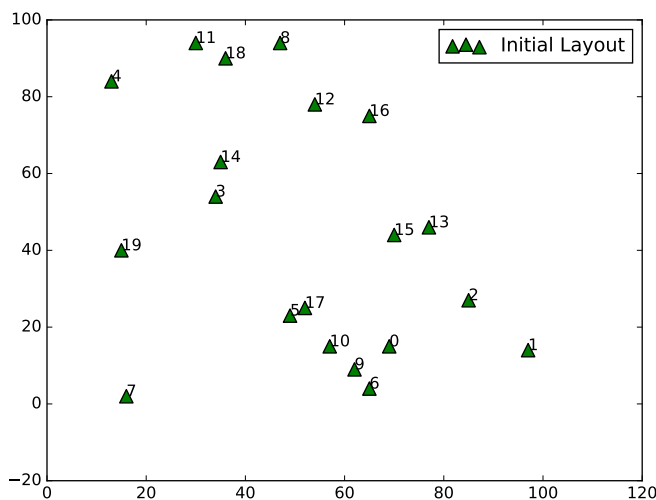


FIGURE 10: *Initial Layout of 20 points with 0.001 as learning rate*

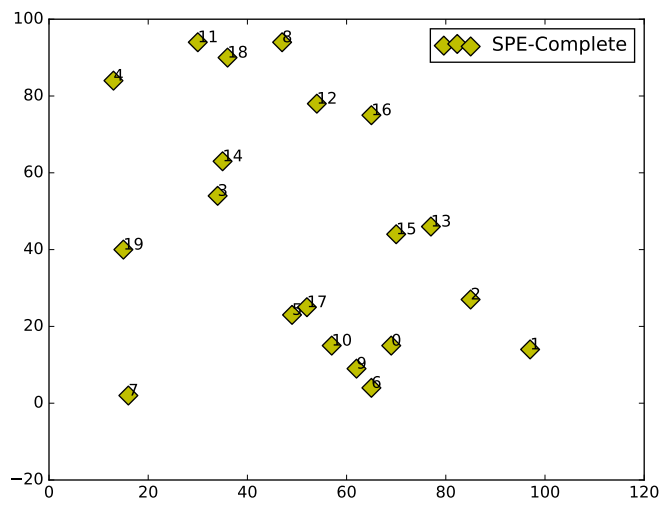


FIGURE 11: *SPE Layout of 20 points with 0.001 as learning rate*

2.8 Comparison and Experiments: DMCA (YH's) Vs. SPE Partial Vs. SPE Complete

The solution to the point placement problem is generated using three different methods as discussed earlier. The first set of coordinates are computed by completing the distance matrix using SPE. To compare our method, we have also computed the coordinates using SPE heuristics and Young Householder's method after completing the distance matrix using distance matrix completion approach due to Zamilur et al. [23].

To match the layout more precisely we carried out the geometric transformation for each method and calculated the error functions for both before and after geometric transformation. Results produced by the experiments showed that the geometric transformation reduced the error function for all three approaches. (See Table 1,2,3)

To measure the difference in the layout produced by three methods, we have computed the RMSD value for the Young Householder's method, SPE method and the SPE with partial distance matrix method. We also calculated the localization error and the stress function for both the SPE approaches. (See Table 1,2,3) All three methods are tested with the vertices number ranging from 4 to 30.

Root Mean Square Deviation (RMSD) measures the difference between the original layout and the computed layout. RMSD is calculated using the following formula,

$$RMSD(p, q) = \sqrt{\frac{1}{n} \sum_{i=1}^n ((p_{ix} - q_{ix})^2 + (p_{iy} - q_{iy})^2)} \quad (1)$$

where,

Stress function is proposed for SPE to measure the quality of the final layout with respect to the original layout. Stress function in SPE is finding the average of the difference between

the initial R matrix and the computed final D matrix. [2]

$$S = \frac{\sum_{i<j} \frac{(d_{ij}-r_{ij})^2}{r_{ij}}}{\sum_{i<j} r_{ij}} \quad (2)$$

Localization error otherwise called as point placement error is similar to the RMSD error calculation. Localization error measures the deviation between original point set and the generated point set in the embedding. [4]

$$PPE(p, q) = \frac{\sum_{i=1}^n ((p_{ix} - q_{ix})^2 + (p_{iy} - q_{iy})^2)}{n} \quad (3)$$

In the figure (12,13,14,15) we displayed the embedding of the final coordinates between all three methods. The embedding shown here is a perfect embedding with all three methods are plotting the same layouts. The initial layout generated in this example is with 22 vertices and 230 edges.

Vertices	edges	YH RMSD Before Rot	YH RMSD After Rot and Trans
4	5	2061.38613755	332.718947801
5	9	2202.6379561	673.471908531
5	8	2184.59522219	424.666372119
5	7	2650.76500519	124.592855294
6	14	1721.47354557	978.613392827
6	13	2315.06013063	5.57342161115E-13
6	12	2347.68434379	4.81494292504E-13
6	11	2601.95709906	128.108823309
7	20	1412.12093121	2.97702022503E-13
7	19	2669.52612392	4.73031519081E-13
7	18	2093.8180598	1393.31680012
7	17	1960.70123927	4.28081464929E-13
7	16	2144.07021047	4.38731885205E-13
7	15	1790.96523847	4.09586882105E-13
7	14	3125.99749455	6.23799407748E-13
8	27	2120.4228321	5.61643470444E-13
8	26	2937.24305761	896.606749692
8	25	2633.56828993	5.55951448917E-13

8	24	1879.95145333	6.16106521486E-13
8	23	2026.02999528	3.34710128792E-13
9	35	1974.59164777	3.70846133555E-13
10	44	3234.44076753	5.58397991437E-13
11	54	2608.67450477	4.89510925586E-13
11	53	3179.822133	5.36396664224E-13
11	52	3239.46433154	5.50984128278E-13
12	65	1889.3397251	8.78311012489E-13
12	64	1973.50863097	3.64950916711E-13
12	63	2995.28074733	1047.95976145
13	77	2005.28703062	5.3937923582E-13
13	76	2443.41425433	9.62375391148E-13
13	75	1855.65567995	1382.31670742
13	74	2883.51031415	5.48291421452E-13
14	90	1919.89125929	1336.18953834
15	104	3283.52995888	857.261738235
15	103	2230.62648667	5.88542166294E-13
17	135	2107.30234718	1172.11118029
17	134	2325.53513206	4.40644345245E-13
17	133	1766.74154046	5.58610690181E-13
18	152	1422.03923007	6.89913864166E-13
19	170	1992.917449	1176.21850955
19	169	1253.8446116	0.0000143580349942
20	189	2713.91084952	1.98613675909E-09
20	184	2002.66972301	1505.67912217
21	209	1255.39526647	9.06812995979E-13
21	208	3145.88993828	1.03290995258E-12
22	230	2339.99609327	4.07399115844E-13
22	228	1821.37130433	1347.60033124
23	252	1827.1580246	1225.90586641
23	251	2184.95489304	6.61271298836E-13
24	275	2639.50660174	1075.60235797
25	299	2778.85977602	6.80704391007E-13
25	298	1861.23667694	1149.65002139
26	324	2476.90641913	7.70174674996E-13
26	323	3345.33431099	1.04990677077E-12
27	350	1492.15551103	4.01073361196E-13

28	377	2021.86398081	1102.61923649
29	405	2676.49811892	0.000000119304199898
30	434	2186.3878422	3.35898384949E-13
33	527	3202.94547	8.61732322337E-13

TABLE 1: Experimental results using Young Householders

Vertices	edges	RMSD Before Rot	RMSD After Rot and Trans	StressFunction	LocalizationError
4	5	18043.260152	67.2144473019	1.07103318596E-27	4517.78192609
5	9	117260452730	673.471904629	2.84983750253E-22	453564.406325
5	8	30401178927.5	0.00000370931260326	1.01424435643E-23	1.37589999887E-11
5	7	1230539981.32	124.592849684	9.49870959458E-24	15523.3781925
6	14	41750608.783	3.22401107721E-09	6.96968329184E-30	1.0394247426E-17
6	13	1880142605.42	0.000000252528984187	3.26540827395E-26	6.37708878544E-14
6	12	1423401766.2	0.000000137402902514	2.64089262974E-26	1.88795576193E-14
6	11	107474288.164	878.660965831	1.58628969938E-25	772045.092875
7	20	1253520759.85	0.000000127021714005	1.07370474862E-26	1.61345158287E-14
7	19	76032392.5475	6.65464511504E-09	2.57579499774E-28	4.42843016072E-17
7	18	8494026.95063	7.50369912643E-10	8.54721111598E-32	5.630550058E-19
7	17	324900589.069	2.66470171063E-08	9.65131375856E-28	7.10063520663E-16
7	16	1220199.0529	1.11842189295E-10	8.32146480343E-32	1.25086753062E-20
7	15	2016199056.8	0.000000249663404461	6.8084183608E-27	6.2331815527E-14
7	14	654977701.028	3.58895384598E-08	1.72752560113E-27	1.28805897086E-15
8	27	12203416.2153	1.12849172436E-09	7.95728107259E-31	1.27349357196E-18
8	26	794572.013269	8.39558702951E-11	1.64224128046E-32	7.04858815701E-21
8	25	2357052.27682	3.70809939166E-10	4.40815551039E-32	1.37500010985E-19
8	24	34043351824.5	0.00000346269968413	1.7891785023E-23	1.19902891025E-11
8	23	9300999.5542	8.12612467333E-09	1.63753302522E-28	6.60339022066E-17
9	35	71155828.5831	4.38971193676E-09	1.00841270257E-28	1.92695708877E-17
10	44	4229986.82734	4.50251440449E-10	2.88406102408E-31	2.02726359626E-19
11	54	1799657.80778	2.08211736013E-10	1.48427659001E-31	4.33521270135E-20
11	53	422169.060493	6.28122502494E-11	9.77056323021E-33	3.9453787814E-21
11	52	3586209.66932	3.70071972899E-10	2.57635145283E-31	1.36953265125E-19
12	65	3132707.81416	2.49125816766E-10	8.06741997844E-32	6.20636725792E-20
12	64	2108317.3026	4.88032892833E-10	4.80715744332E-31	2.38176104487E-19
12	63	1087075.44575	0.000000353280421341	6.85180608122E-25	1.24807056103E-13
13	77	1960694.58685	4.28761937495E-10	1960694.58685	1.83836799044E-19
13	76	799783.187959	2.35417015517E-10	5.71784552333E-32	5.54211711948E-20

13	75	12851169.2444	1.67074435056E-09	2.54649749333E-30	2.79138668493E-18
13	74	48811374.0649	5.58594692648E-09	3.25228216205E-29	3.12028030654E-17
14	90	110840111.478	1336.18953834	1.28168087245E-28	1785402.48236
15	104	4971815.15998	0.000000095807194256	5.65828771036E-27	9.1790184712E-15
15	103	19082002.0952	1.79471706942E-09	3.66420584578E-30	3.22100935925E-18
17	135	1172.11118029	4.86786055487E-11	9.59141279618E-33	2.36960663817E-21
17	134	1239407.41191	1.57878955627E-08	2.69477369691E-28	2.49257646298E-16
17	133	81216598.0597	1.81133827455E-08	7.34479015195E-29	3.28094634486E-16
18	152	108727967.413	108727967.413	0.0000300756802658	46883.853731
19	170	3593977.78682	1.11830982222E-09	1.57337137176E-30	1.25061685847E-18
19	169	37337749.6678	22.4756510155	2.59568875049E-10	505.154888569
20	189	543818.408049	0.000000014400899914	2.47248417024E-27	2.07385918334E-16
20	184	43503204.2272	7.53211266093E-09	9.85438981199E-29	5.6732721137E-17
21	209	765367.835956	683.145241831	0.0007499345183	466687.421436
21	208	4259591.90917	0.47317370069	2.23715854946E-13	0.223893351024
22	230	6026680.76882	0.00147281265794	2.27632990959E-18	0.00000216917712538
22	228	1476638.90224	1347.60033124	7.46458354085E-31	1816026.65275
23	252	13113616.0313	0.000325732698814	1.38788410398E-19	0.000000106101791077
23	251	27549165.3342	6.2121943512E-09	2.52765601352E-29	3.85913586571E-17
24	275	14815753.7909	34.8381020592	1.26328187054E-08	1213.69335509
25	299	185799.642173	0.00369625794304	1.04843704534E-17	0.0000136623227815
25	298	4692133.25034	0.0365003333586	9.39914937104E-16	0.00133227433529
26	324	6309108.56324	1.61851733105	5.24165726042E-12	2.6195983509
26	323	2318986.54327	0.000000969851631606	4.48374916545E-25	9.40612187329E-13
27	350	4009822.91794	4.08266753546	1.3308693632E-11	16.6681742051
28	377	2862562.13634	7.31706445571E-10	3.89183384839E-31	5.3539432249E-19
29	405	21081460.7683	1117.89427484	1.46550922029E-26	1249687.60973
30	434	9701412.68314	0.301698010098	7.3270234131E-14	0.0910216892974
33	527	103497964.83	13.7797668849	1.66105871749E-10	189.881975402

TABLE 2: Experimental results using SPE with Complete distance matrix

Vertices	edges	RMSD Before Rot	RMSD After Rot and Trans	StressFunction	LocalizationError
4	5	151716561583	447.53971618	1.45940642725E-08	200291.797558
5	9	63082137493.9	218.182826821	9.86929916464E-08	47603.7459198
5	8	182076180.074	214.943162064	0.000000825996971301	46200.562918
5	7	1565701696.72	220.033728419	0.0000003495825959	48414.8416419
6	14	1030166048.59	378.914086537	0.000000298807101868	143575.884976

6	13	1990608368.62	713.2369954	0.000000702661662933	508707.011607
6	12	188053348561	903.473784069	0.00000255635079899	816264.878499
6	11	28078410400.1	1092.40333631	0.0000010595213126	1193345.04918
7	20	30011934.6184	318.688834035	0.00000246357429019	101562.572939
7	19	5661286554.02	428.021783801	2.53839638228E-08	183202.647408
7	18	15604812.3723	1392.37641491	4.76273182696E-09	1938712.08079
7	17	1972392.7611	198.050289033	0.000000969798180351	39223.9169859
7	16	181668386.057	965.932099529	0.00000543690190933	933024.820901
7	15	4567403.53195	1344.50969055	2.66752040989E-08	1807706.30799
7	14	48902694.292	1366.51651125	0.00000036027510582	1867367.37553
8	27	3399860.58067	1053.12349407	0.000000028757641283	1109069.09376
8	26	237629108670	444.510525774	7.07463431011E-08	197589.607524
8	25	10151433.3375	1277.71324699	0.000000040292921175	1632551.14154
8	24	18570360.9301	1034.88711306	0.00000175796309786	1070991.33677
8	23	6894762.42834	868.401794764	0.0000236895672642	754121.677149
9	35	89657071.2847	510.622146958	9.89879381772E-09	260734.976964
10	44	5239487.51836	8.2381606773	2.09504908209E-10	67.867291345
11	54	15823092.5722	43.7650979351	1.60225150191E-08	1915.38379727
11	53	14533318.5163	265.699905269	4.70144893691E-08	70596.4396599
11	52	2040373.3106	738.603366932	0.00000244318789575	545534.933643
12	65	523602.748023	1117.1672964	1.33170679218E-09	1248062.76815
12	64	3925140153.81	762.178935519	0.0000131058237785	580916.729749
12	63	799995057.166	1085.62835938	3.11404774542E-08	1178588.9347
13	77	48552227.0725	1048.36217101	3.53973975995E-08	1099063.24161
13	76	27718246.2301	1296.47751865	6.81733894244E-08	1680853.95637
13	75	4255397.55139	248.781245178	0.00000510377354543	61892.1079521
13	74	984654.936116	234.080352689	0.000000731958485155	54793.6115149999
14	90	27809990.0635	16.4468275582	8.0732739609E-10	270.498136731
15	104	4543765.12073	172.855176775	0.000000110988511949	29878.9121379
15	103	1408879155.63	1074.39618261	0.000000809554377008	1154327.15722
17	135	17942836.1809	1.82901048341	1.89048375528E-11	3.34527934843
17	134	12984840.0703	33.738980696	4.90122953996E-09	1138.3188184
17	133	24230435.7011	1250.06200449	0.0000357565881358	1562655.01506
18	152	2560648736.25	455.200692716	0.000000274889950081	207207.67065
19	170	3667301.99917	39.1907401583	6.28887091454E-09	1535.91411415
19	169	611245.401946	95.7337519462	3.49251932534E-08	9164.95126169
20	189	16317030.162	842.813221713	0.0000161423609422	710334.126694

20	184	11246377.5751	98.5656322344	2.97676589802E-08	9715.18385777
21	209	7882585.64085	5.96272819745	1.04865425194E-09	35.5541275567
21	208	1199791.95927	1153.01709326	2.69750872567E-08	1329448.41735
22	230	46268545.4521	0.74031023198	1.25198589858E-12	0.548059239574
22	228	11912594.9573	40.0911446337	1.64296544414E-08	1607.29987804
23	252	10347392.1173	1226.77007179	3.17758913889E-09	1504964.80904
23	251	29324633.4087	48.6902930533	1.10036558529E-08	2370.74463762
24	275	2422208.71519	40.382669602	0.00000030204515818	1630.76000418
25	299	83703247.2669	28.5757352436	1.73490847501E-09	816.572644712
25	298	4992171.22977	76.7177559965	0.000000025162310443	5885.61408514
26	324	418200163.297	10.0017692178	1.11647614028E-09	100.035387487
26	323	2391878098.21	74.1028457574	2.85547736168E-08	5491.23174934
27	350	21718647.8309	1271.83305156	2.60341881589E-09	1617559.31104
28	377	2666430.00197	47.2384964679	5.05523225628E-09	2231.47554855
29	405	1998787.8662	6.52573408417	2.99165833797E-10	42.5852053373
30	434	132581685.649	1222.62243382	0.0000273945141536	1494805.61567
33	527	472414526.944	20.9523650525	2.45922847911E-09	439.001601294

TABLE 3: Experimental results using SPE with Partial distance matrix

To compare the layouts created by three approaches, we have plotted the layouts to check each method, here are the few images to verify the final results.

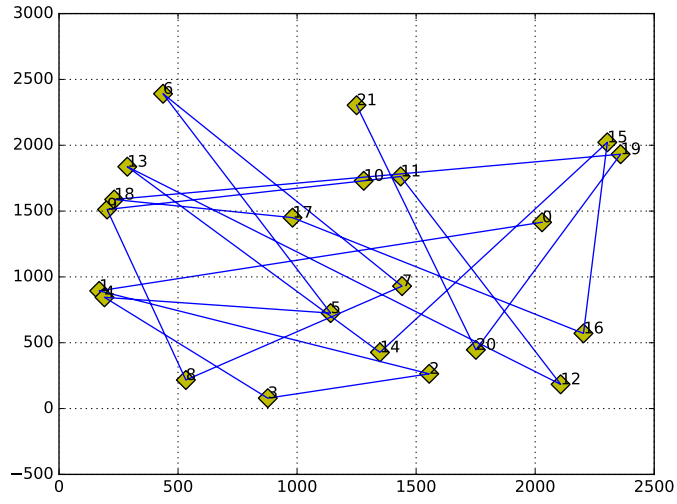


FIGURE 12: *Initial Layout with 22 Vertices*

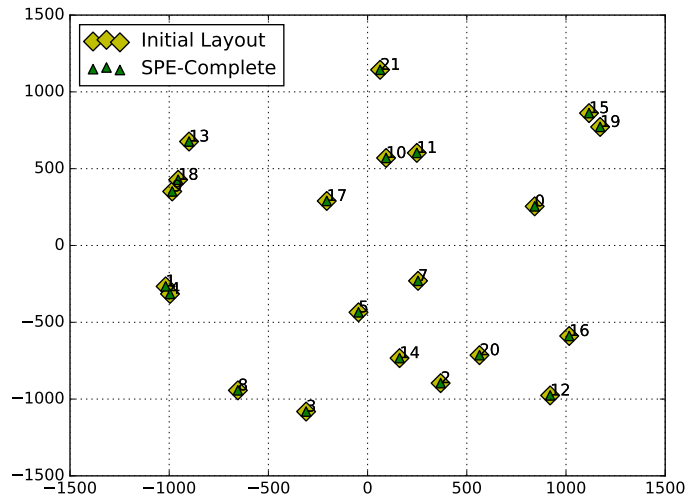


FIGURE 13: *Initial Layout Versus SPE (Complete distance matrix)*

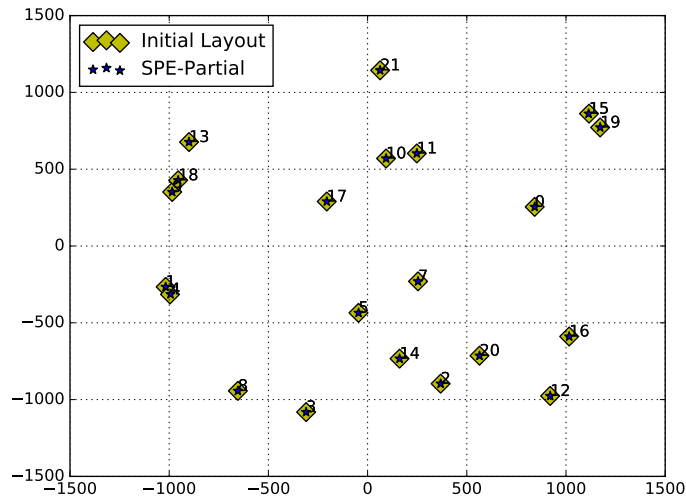


FIGURE 14: *Initial Layout Versus SPE (Partial distance matrix)*

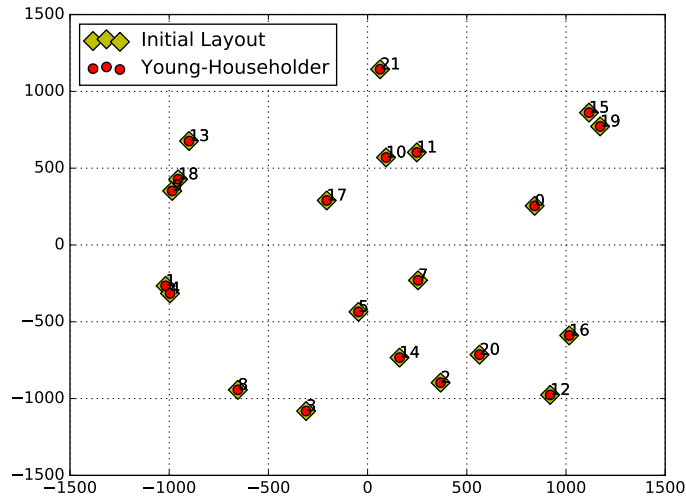


FIGURE 15: *Initial Layout Versus Young and Householder's approach*

2.9 Discussions

Point placement on a plane has thrown up many open problems. While we used chordal graphs in our approach, the extension to other classes of the graph remain open.

We can also use SPE to approach other graphs since SPE is graph independent. There

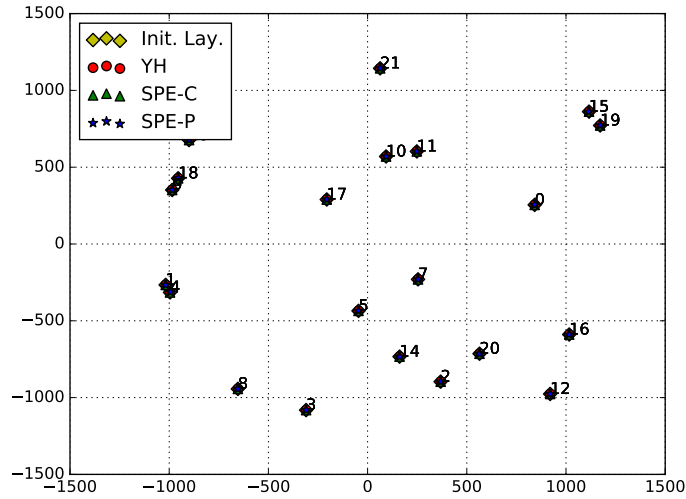


FIGURE 16: *Initial Layout Vs Young and Householder's approach Vs SPE(Partial matrix) Vs SPE(Complete matrix)*

is plenty of potential in Stochastic Proximity Embedding, to explore the point placement problems. The theoretical proof of SPE is still not clear and produces different results time to time. In SPE, the learning rate parameter can be controlled with respect to the number of points and the disparity between the point sets.

CHAPTER 3

Point Placement problem in 3D

Space with Degree of Freedom

Approach

3.1 Molecular Distance Geometry Problem

The Molecular Distance Geometry Problem (MDGP) is defined as the problem of finding cartesian coordinates $x_1 \dots x_N \in R^3$ of the atoms with only a subset of interatomic distances, such that

$$\|x_i - x_j\| = d(i, j); ([i, j] \in S) \quad (1)$$

In equation (1) S is the set of pairs of atoms $[i, j]$ whose Euclidean distances $d(i, j)$ between all the points are known. The problem can be solved in linear time if the distance between all the pair of points is available [7, 11].

The distances are obtained through the NMR experiments or can be produced with our knowledge of bond lengths and bond angles. If all the distances are given, then the problem can be solved by factorizing a distance matrix formed by the given distances. We can use

the eigenvectors to find the coordinates of the points if the distances are consistent and if we can find the three non-zero eigenvalues of the matrix [9]. Also, to get the 3D coordinates, the rank of the distance matrix should be less than or equal to three.

In practice, we cannot usually get the exact distances between all pairs of atoms in the protein. Even NMR experiments can detect only the short-range distances between atoms that are close to protein backbones. Saxe [25] showed that the problem is NP-hard when the exact distances between the pair of points are not known [25]. EMBED algorithm from Crippen and Havel is proposed to solve this problem by estimating the missing distances to build the full set of distances. By estimating the remaining distances, we can now solve the problem with the singular value decomposition [9].

The main motivation behind studying this problem is to determine the structure of the protein molecules. Since NMR experiments can detect the short-range distances between atoms of a protein molecule, we are computing the structure of the whole protein molecule using only the distance between few pairs. Determined structure of a protein molecule will give us a clue about its functionalities.

Determination of the three-dimensional structure of a molecule using a set of distances between pairs of atoms is the goal of the Molecular Distance Geometry Problem (MDGP). To test the algorithms designed to solve MDGP, we have created the artificial backbone chain of a protein molecule using Philips model [17].

3.2 Prior Work

Molecular Distance Geometry Problem (MDGP) has been extensively studied and solved in different forms [26]. More and Wu proposed a continuous approach to solve the MDGP. The discretizable version of the same problem is proposed by Lover et al. [16] is called the Discretizable Molecular Distance Geometry Problem (DMDGP).

3.2.1 More and Wu’s approach

Different approaches have been proposed to solve the Molecular Distance Geometry Problem. More and Wu formulated the DGP as a continuous global optimization problem. The problem is to find the position of the atoms in a molecule with only the distance $d_{i,j}$ between some pairs (i, j) of atoms in a set S of the atom pairs. [18]

$$\|x_i - x_j\| = d(i, j); ([i, j] \in S) \quad (2)$$

The set of constraints in the equation (2) is replaced by the penalty function. The penalty function calculates the disparity between the computed and the known distances. The penalty function is calculated using different approaches, one common method to calculate the penalty function is the Largest Distance Error (LDE): [19]

$$LDE(\{x_1, x_2, \dots, x_n\}) = \frac{1}{m} \sum_{\{u,v\}} \frac{|||x_u - x_v|| - d_{uv}|}{d_{uv}} \quad (3)$$

m is the number of known distances.

In More and Wu’s approach, the global continuation approach is used to determine the global solution to this problem. The continuation approach is shown to find the global solution irrespective of the starting position.

3.2.2 Discretizable Distance Geometry Problem

The DMDGP is inspired by the protein molecules; protein molecules are formed by amino acids and bound together forming a sort of chain. The atoms in the protein backbones which are close in a sequence are also close in the 3D conformation of the protein structure. Since NMR techniques can detect the short-range distances between the atoms, such distances are used to define the whole structure of a protein molecule [19].

To qualify as the DMDGP, the following assumptions needs to be satisfied,

Let $G = (V, E, d)$ be a weighted undirected graph, with total order relation on the vertices. The two important assumptions are,

- Each quadruplet of E is a clique of consecutive vertices
- Triangle inequality must hold between every three vertices

When these assumptions satisfy, there are at least three lower level atoms connected to the current atom. The intersection of this three points can either be a circle, two points or only one point. With the triangle inequality in place, the intersection of three points cannot be a circle. Because the three points cannot be aligned by satisfying the triangle inequality. Since the intersection of three points is rarely one point only, they have taken two possible positions for every atom.

Now with the two possible position, the binary tree is constructed. For every iteration, two new positions are added to the binary tree after passing the feasibility test. Feasibility test is just to test the agreement of the two possible position with the other available distances if any such distance available other than the three distance used to compute the two possible position. When a possible position is not agreeing with the other available distances, then that branch is pruned out of the tree. This pruning phase reduces the binary tree quickly, and the remaining branch is explored through an exhaustive search, which is not too expensive. [19]

3.2.3 Crippen and Havel's Approach

Crippen and Havel [15], proposed a solid algorithm to solve the molecular distance geometry problem using the upper and lower bounds of distances instead of exact distances.

In the first step of the algorithm the given distance bounds are converted to distance limits. This process is termed as bound smoothing. The Floyd's algorithm presented by Dress

and Havel has been used to convert the bounds to limits. The limits that are calculated using Floyd's algorithm should satisfy the triangle inequality. The limits that satisfy the triangle inequality is termed as triangle inequality limits.

For given three points u, v, w the lower bounds and upper bounds are denoted like this, $l_{u,w}, u_{u,v}, u_{u,w}, l_{vw}$

Geometric set of rules are used for the bound smoothing, the upper and lower bounds of the three given points should satisfy the following geometric rules.

$$l_{u,w} = \max(l_{u,w}, l_{u,v} - u_{vw}, l_{vw} - u_{u,v}) \quad (4)$$

$$u_{u,w} = \min(u_{u,w}, u_{u,v} + u_{v,w}) \quad (5)$$

In the next step of the algorithm, the distance limits are converted into distances, this process of converting limits to distances is called Metrization. In this process of metrization, one random distance is selected between the upper and lower bound. Once the random number is selected, the upper and lower limits been set to this number and recompute the triangle inequality limits.

In the next step of the algorithm, the coordinates are computed using the series of steps,

- The distance for each point is calculated from the center of mass.
- Where d_{ij} is the distance between the points i, j
- In the metric matrix A, each elemnt a_{ij} is computed form the origin
- B matrix is calculated like this, $B = W A W$
- where W is the matrix of weights, assumed to be 1 in this case

- Gale and householder showed that if B matrix is semi definite then the coordinate matrix X is obtained like this, $X = \sigma\sqrt{L}$
- Where $L^2 = [\lambda_1^2, \lambda_2^2, \dots, \lambda_r^2, 0, \dots, 0]$

3.2.4 Philips Model

Philips model of instance creation is based on the method proposed by Philips et al. [22]. Philips model considers a molecule as being the chain of N atoms with Cartesian coordinates given by $x_1, \dots, x_N \in R^3$.

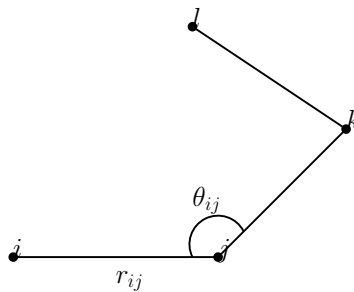


FIGURE 17: *Philips Model*

For every pair of consecutive atoms i, j, k, l :

- $r_{i,j}$ be the bond length which is the Euclidean distance between them.
- $\theta_{i,k}$ be the bond angle corresponding to the relative position of the third atom with respect to the line containing the previous two.
- $\omega_{i,l}$ be the torsion angle between the normals through the planes determined by the atoms i, j, k and j, k, l

In most conformation calculations, all bond lengths and bond angles are assumed to be fixed at their equilibrium values $r_{i,j}^0$ and $\theta_{i,j}^0$, with regarding this we can fix the first three atoms in the chain;

We can always fix the first atom at origin $x_1 = (0, 0, 0)$, and the second atom is positioned at the distance of r_{12} from origin, i.e. $x_2 = (-r_{12}, 0, 0)$, and the third atom is fixed at $x_3 = (r_{23}\cos(\theta_{13}) - r_{12}, r_{23}\sin(\theta_{13}), 0)$. With the torsion angle ω_{14} fourth atom in the chain is determined. With both ω_{14} and ω_{25} the fifth atom in the chain is determined, by fixing another torsion angle ω_{36} the sixth atom in the chain is determined.

In Philips model the bond length and bond angles are set to $r_{ij} = 1.526^\circ$ and $\theta_{ij} = 109.5^\circ$ respectively. The three preferred torsion angles at $60^\circ, 180^\circ$ and 300° are also specified in the Philips model. With these three parameters, torsion angle, bond length, and bond angle we can generate the distance between pairs of atoms and obtain instances for the Molecular Distance Geometry Problem.

The torsion angle values are seen as perturbations of the preferred torsion angle $60^\circ, 180^\circ$ and 300° . Based on the model described in Philips, we are generating the torsion angle by adding the random value from the set $\{\omega + i : i = -15^\circ, \dots, 15^\circ\}$ to the random value out of the three preferred torsion angle.

We are generating the cartesian coordinates to define the set S in (1), (x_{n1}, x_{n2}, x_{n3}) is defined as the cartesian coordinates for each atom in the chain using the following matrices, [22]

$$\begin{pmatrix} x_{n1} \\ x_{n2} \\ x_{n3} \\ x_{n4} \end{pmatrix} = B_1 B_2 \dots B_n \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (n = 1, \dots, N),$$

The matrix to calculate the cartesian coordinates is proposed by Philips et al. [22]

Where

$$B_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, B_2 = \begin{pmatrix} -1 & 0 & 0 & -r_{12} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$B_3 = \begin{pmatrix} -\cos \theta_{13} & -\sin \theta_{13} & 0 & -r_{23} \cos \theta_{13} \\ \sin \theta_{13} & -\cos \theta_{13} & 0 & r_{23} \sin \theta_{13} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$B_i = \begin{pmatrix} -\cos \theta_{(i-2)i} & -\sin \theta_{(i-2)i} & 0 & -r_{(i-1)i} \cos \theta_{(i-2)i} \\ \sin \theta_{(i-3)i} \cos \omega_{(i-3)i} & -\cos \theta_{(i-2)i} \cos \omega_{(i-3)i} & -\sin \omega_{(i-3)i} r_{(i-1)i} & \sin \theta_{(i-2)i} \cos \omega_{(i-3)i} \\ \sin \theta_{(i-2)i} \sin \omega_{(i-3)i} & -\cos \theta_{(i-2)i} \sin \omega_{(i-3)i} & \cos \omega_{(i-3)i} r_{(i-1)i} & \sin \theta_{(i-2)i} \sin \omega_{(i-3)i} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Once the cartesian coordinates for all the atoms are determined, the set S is generated with the cutoff value d , which in terms fetching the atoms i, j if their distance is within the cutoff value d . Cutoff value selection is defined as,

$$S = [i, j] : \|x_i - x_j\| \leq d$$

A sample molecular chain created by the Philips model is shown here, (Fig. 18)

3.3 Overview of our results

We proposed the Degree of freedom (DoF) approach to fetch the partial distances out of a molecular chain and construct the whole chain of a molecule. For each atom, if the distance between the adjacent atom and the next atom is known, then we are completing the layout

by constructing the chordal graph with the partial distances. This gives us the freedom to use DMCA due to Zamilur et al. and the SPE due to Agrafoitis to complete the remaining distances and solve the Molecular Distance Geometry Problem (MDGP).

With the available distances, the partial distance matrix is computed and is completed using both DMCA and SPE. Once the distance matrix is completed then the coordinates are generated using SPE.

We tested our DoF approach with the artificial instance created using the Philips model and obtained good results out of it. In addition to the artificial instances, we have also compared our approach with the Md-Jeep approach due to Carlie Lover et al. [19]. Synthetic NMR datasets available with MD-Jeep are used while comparing the MD-Jeep with our DoF approach.

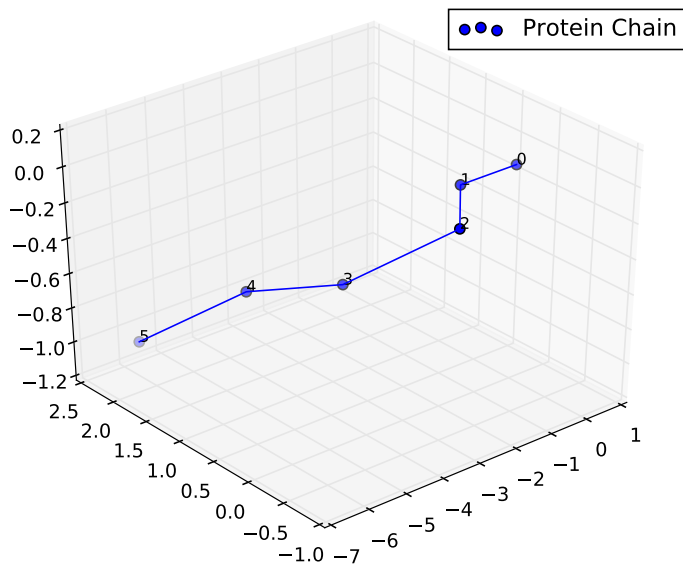


FIGURE 18: *Protein Chain created using Philips Model*

3.4 Degree of Freedom Approach

Our Degree of Freedom (DoF) approach is proposed to complete the backbone chain of a protein molecule by using only the partial set of distances. DoF approach is generated based on the Philips model for instance creation. In Philips model, we are fixing the first three points on a plane with the distances known between all three points. The degree of freedom to fix n points is $3n$ since we are fixing the first point at origin, the DoF is reduced to $3n-3$.

So the degree of freedom to fix n points by fixing the first point at origin is $3n-3$. In our approach we are considering the lost degree of freedom as distance constraints, so out of $3n-3$ DoF, we are choosing $2n-3$ distance constraints to construct the whole chain of the molecule.

The reason behind choosing $2n-3$ distances is explained here,

In Philips model, since the bond length is fixed, we know the distance between the successive atoms this gives us $n-1$ distance constraints. The bond angle for the third atom with respect to the line containing the previous two atoms is also fixed, this gives us additional $n-2$ distance constraints out of n atoms. In total we are taking $2n-3$ distance constraints to fix n atoms that has $3n-3$ degrees of freedom.

In Philips model, the torsion angle is chosen randomly. In our case, we are completing the remaining distances using Distance matrix completion approach and the Stochastic Proximity Embedding.

The algorithm for the degree of freedom approach with the necessary steps is described here,

Algorithm: DEGREE OF FREEDOM APPROACH

Input: Chain of a protein molecule produced by Philips model

Output: Distance matrix with $3n-3$ distances

- 1: Initialize the complete distance matrix with distances between all the atoms
 - 2: **for** all combination of protein pair **do**
 - 3: Pick $n-1$ distances between adjacent atoms
 - 4: Pick $n-2$ distances between the current and the one after the adjacent atom
 - 5: **end for**
 - 6: Generate partial distance matrix with the $2n-3$ distances
 - 7: Use DMCA and SPE to find the structure of the molecule
-

By following the proposed algorithm, we created a sample distance matrix as partial R Matrix and the original matrix as the R Matrix.

$$\text{R Matrix} = \begin{pmatrix} 0 & 2.3286 & 8.8393 & 18.9945 & 32.2019 \\ 2.3286 & 0 & 2.3286 & 8.1887 & 17.3396 \\ 8.8393 & 2.3286 & 0 & 2.3286 & 8.8393 \\ 18.9945 & 8.1887 & 2.3286 & 0 & 2.3286 \\ 32.2019 & 17.3396 & 8.8393 & 2.3286 & 0 \end{pmatrix}$$

Partial R Matrix as follows,

$$\text{Partial R Matrix} = \begin{pmatrix} 0 & 2.3286 & 8.8393 & 0 & 0 \\ 2.3286 & 0 & 2.3286 & 8.1887 & 0 \\ 8.8393 & 2.3286 & 0 & 2.3286 & 8.8393 \\ 0 & 8.1887 & 2.3286 & 0 & 2.3286 \\ 0 & 0 & 8.8393 & 2.3286 & 0 \end{pmatrix}$$

3.5 Coordinates computation using SPE

The degree of Freedom approach takes $n-1$ and $n-2$ distances between the adjacent atoms and the atom next to the adjacent atom respectively. These distances will construct a partial

distance matrix. Since the missing distances can be identified by SPE in the refinement process, our initial idea is to use SPE as a tool to complete the partial distance matrix. However, the layout produced by SPE was not good, which in turn SPE was not able to fix remaining distances with the partial distance matrix produced by our Degree of Freedom approach.

The distance matrix produced by DoF approach looks like this,

$$\text{Partial R Matrix} = \begin{pmatrix} 0 & 2.3286 & 8.8393 & 0 & 0 \\ 2.3286 & 0 & 2.3286 & 8.1887 & 0 \\ 8.8393 & 2.3286 & 0 & 2.3286 & 8.8393 \\ 0 & 8.1887 & 2.3286 & 0 & 2.3286 \\ 0 & 0 & 8.8393 & 2.3286 & 0 \end{pmatrix}$$

The partial distance matrix produced by DoF approach has only distances close to the diagonal, and the other distances are unknown, SPE is very sensitive to the available distance spread. If the available distances are only along the diagonal, the point set takes time to learn and in fact could not get to the position. A simple experimental study has been carried out and the results are as follows,

In the layout shown below (Fig. 20), the points along the straight line are not fixed as the rest of the points were fixed by SPE. From the series of experiments, we studied that if a point lies on a straight line without enough distances and the spread out distances, then the SPE is struggling to learn the relative distances of the point set.

3.6 Distance matrix completion approach

The degree of Freedom approach takes $n-1$ and $n-2$ distances between the adjacent atoms and the atom next to the adjacent atom respectively. These distances represent a chordal

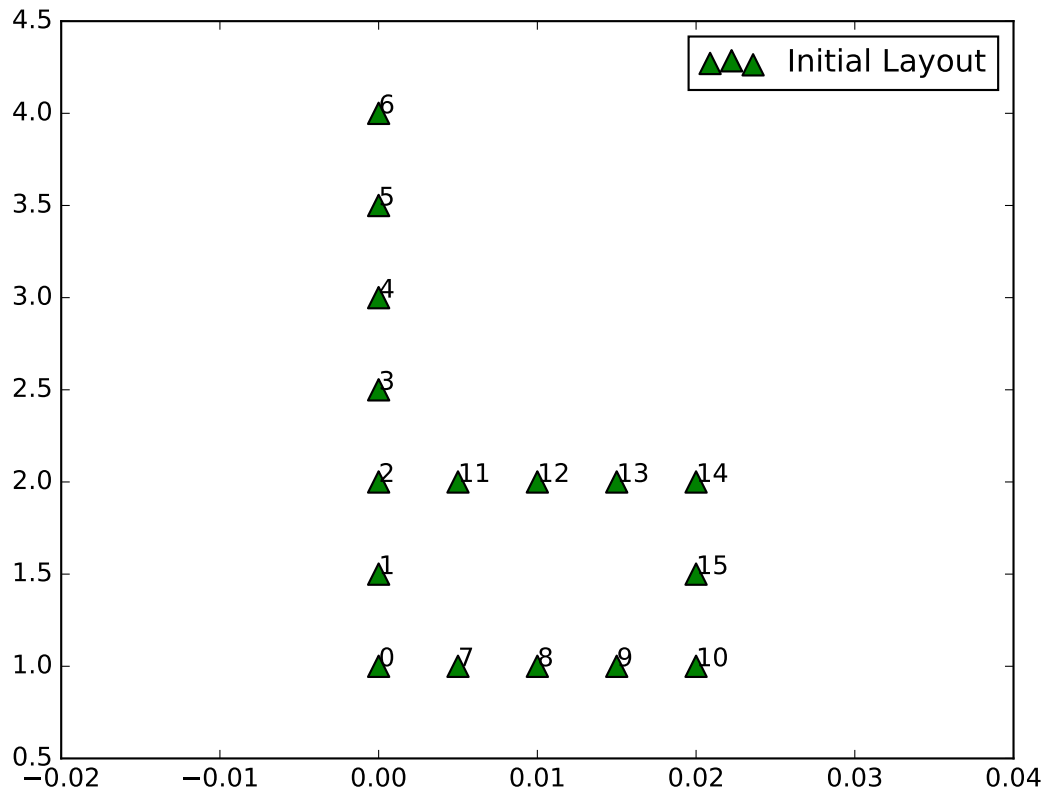


FIGURE 19: *Initial layout of b*

graph. A sample layout is generated using the partial distance matrix, to show the chordal graph is below, (Fig. 21)

In practice, exact distances between all pairs of atoms are not available. Experimental techniques such as NMR can determine the distances between pairs of atoms if they are tightly placed. In general, NMR computes the distance between pairs of atoms which lies close together.

To fix a molecule in 3D space, we need to estimate the remaining distances between pairs of atoms. We considered this problem as a distance matrix completion problem since the layout we are generating is also a chordal graph, we used the DMCA to complete the distance matrix. Once the distance matrix is completed, the 3D coordinates are computed

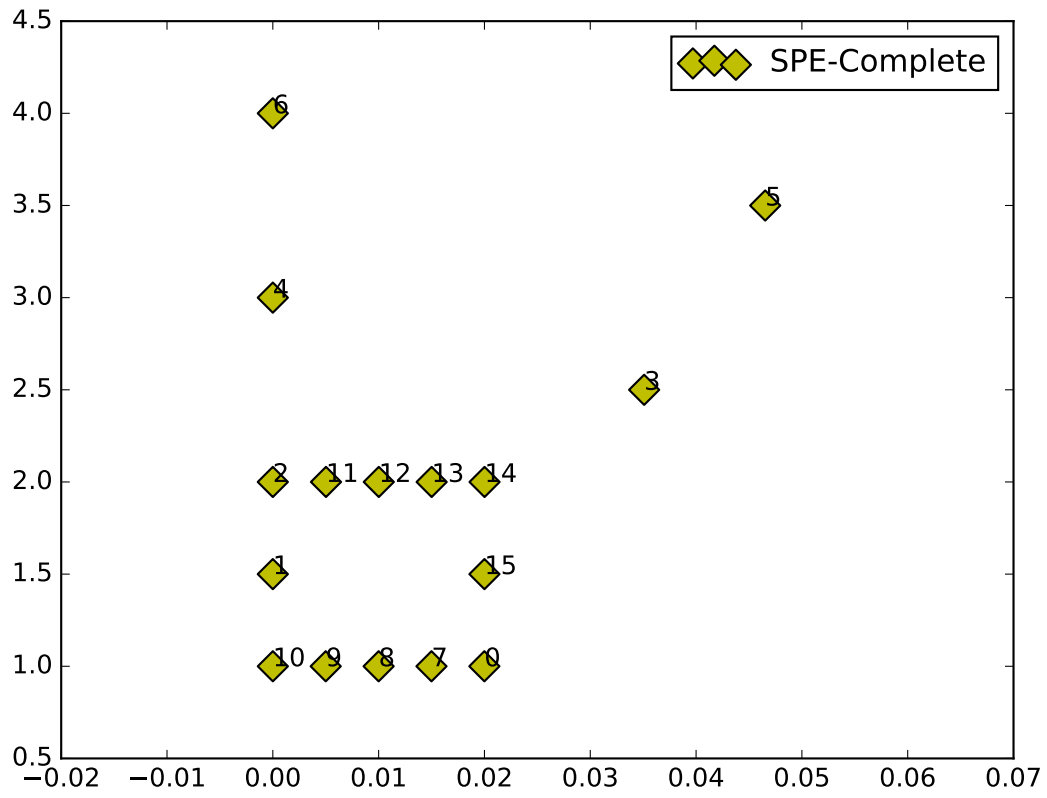


FIGURE 20: *SPE layout of b*

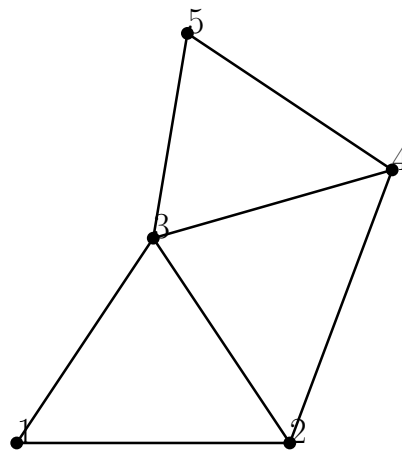


FIGURE 21: *Chordal Graph Construction*

using SPE.

The input to the Distance matrix completion approach is a partial distance matrix that represents a chordal graph. Since the DMCA approach can fill up the edges one by one by completing the clique, we get the final layout with the complete distance matrix.

The output of the Distance matrix completion algorithm is a complete distance matrix. Once the distance matrix is completed, then the coordinates are computed using SPE.

Difficulties With DMCA

The partial distance matrix that represents a chordal graph has been completed by the distance matrix completion algorithm. In rare cases, when the point sets are more, DMCA fails to complete the partial distance matrix because of the numerical errors. The floating point values that add up to the distances and cause the numerical errors.

Completion using SPE

When the numerical errors cause DMCA to stop the distance matrix completion process, then the partial distance matrix with the distances completed using DMCA and the original $2n-3$ distances is transferred to the SPE in runtime and the remaining distances been completed. Since we have extra sparse distances generated through DMCA, and the original $2n-3$ distances, now SPE can able to fill up the remaining distances and produce the coordinates for the output layout.

The Input to the SPE is a distance matrix $R = [r_{ij}]$. R matrix is either a complete or partial distance matrix with distances known between some pairs if it is partial matrix, or all the pairs if it is a complete distance matrix in a set of n atoms $P = p_1, p_2, \dots, p_n$. SPE produces random point set $P^r = p_1^r, p_2, \dots, p_n$ with the same number of points as the original point set. The distance matrix for the random points are calculated as D matrix where

$$D = [d_{ij}].$$

With both the original and the arbitrary embedding, SPE randomly picks up the pair of points and adjust the arbitrary coordinates towards the original coordinates based on the Newton-Raphson method of root finding. This refinement goes through C*S steps, where C is the learning cycle that iterates over the learning rate parameter λ . In our case, λ goes from 1 to 0 decrementing with minimal value. S loop goes for the number of times a random pair is selected.

At the end of C*S steps, all the pairs in the arbitrary embedding are adjusted towards the original embedding. The quality of this refinement is measured using the stress function given by [2]

$$S = \frac{\sum_{i < j} \frac{(d_{ij} - r_{ij})^2}{r_{ij}}}{\sum_{i < j} r_{ij}} \quad (6)$$

3.7 Experiments with Philips Model

Artificial backbone chain of a protein molecule is developed using Philips model and tested with our degree of freedom approach.

By fixing the bond length and the bond angle, but by randomly choosing the torsion angle, we generated the chain of n atoms as a backbone of a protein molecule (Fig. 22) using the model proposed by Philips et al. A sample chain of 6 atoms is produced and the cartesian coordinates of that chain is given here.

Cartesian coordinates = ((0,0,0),(-1.526,0,0),(-2.8962,-0.6716,0),(-3.9072,-0.3790,0.4501),(-5.2984,1.0028,-0.5148),(-6.3070,2.0598,-0.9553))

The protein chain is shown in Fig. 22 is recreated using DMCA + SPE with only $2n-3$ distances.

The completed RMatrix out of Philips model and the Partial RMatrix with $2n-3$ distances

that we used as an input to complete the whole molecular chain is also displayed here.

RMatrix as follows,

$$\text{RMatrix} = \begin{pmatrix} 0 & 2.3286 & 8.8393 & 15.6129 & 29.3441 & 44.9342 \\ 2.3286 & 0 & 2.3286 & 6.0166 & 15.5019 & 28.0139 \\ 8.8393 & 2.3286 & 0 & 2.3286 & 8.8393 & 20.0072 \\ 15.6129 & 6.0166 & 2.3286 & 0 & 2.3286 & 8.8393 \\ 29.3441 & 15.5019 & 8.8393 & 2.3286 & 0 & 2.3286 \\ 44.9342 & 28.0139 & 20.0072 & 8.8393 & 2.3286 & 0 \end{pmatrix}$$

Now the partial distance matrix,

$$\text{RMatrix} = \begin{pmatrix} 0 & 2.3286 & 8.8393 & 0 & 0 & 0 \\ 2.3286 & 0 & 2.3286 & 6.0166 & 0 & 0 \\ 8.8393 & 2.3286 & 0 & 2.3286 & 8.8393 & 0 \\ 0 & 6.0166 & 2.3286 & 0 & 2.3286 & 8.8393 \\ 0 & 0 & 8.8393 & 2.3286 & 0 & 2.3286 \\ 0 & 0 & 0 & 8.8393 & 2.3286 & 0 \end{pmatrix}$$

3.8 MD-Jeep With NMR data

MD-Jeep is a Branch and prune based software proposed by Mucherino et al. [20] to solve the Discretizable Molecular Distance Geometry Problem (DMDGP). DDGP is termed out of Discretizable distance geometry problem, fixing the vertex position in order if the distance between a vertex and the three preceding vertices are known.

An instance to qualify as a DMDGP needs to satisfy this two assumptions,

Let $G = (V,E,d)$ be a weighted undirected graph.

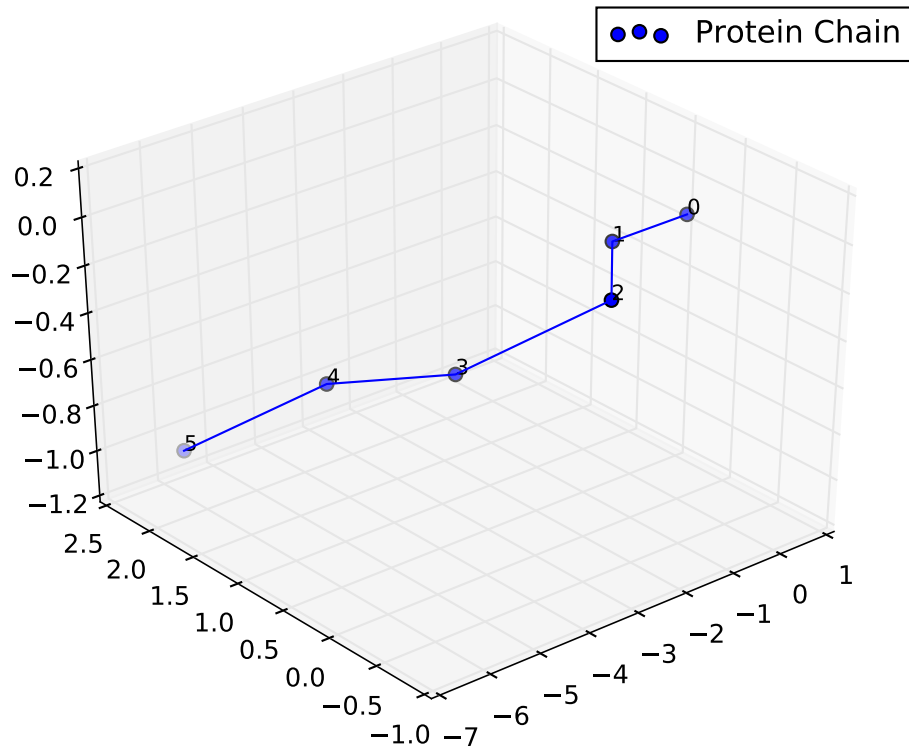


FIGURE 22: *Protein Chain created using Philips Model*

- $1,2,3 \in V$ should be a clique, and for each atom x_i the distance between three preceding and consecutive vertices must be known. i.e. There are edge exists between $(i-1,i)$, $(i-2,i)$ and $(i-3,i)$.
- For each triplet of consecutive atoms, triangle inequality on the corresponding distances must hold.

Now with the position of the three preceding atoms are already known, the intersection of three points can be a circle or two points or one point only. With the triangle inequality condition in place, an intersection of three points cannot be a circle because three points cannot be aligned. So they are assuming it to be two points for the maximum possibility. Now

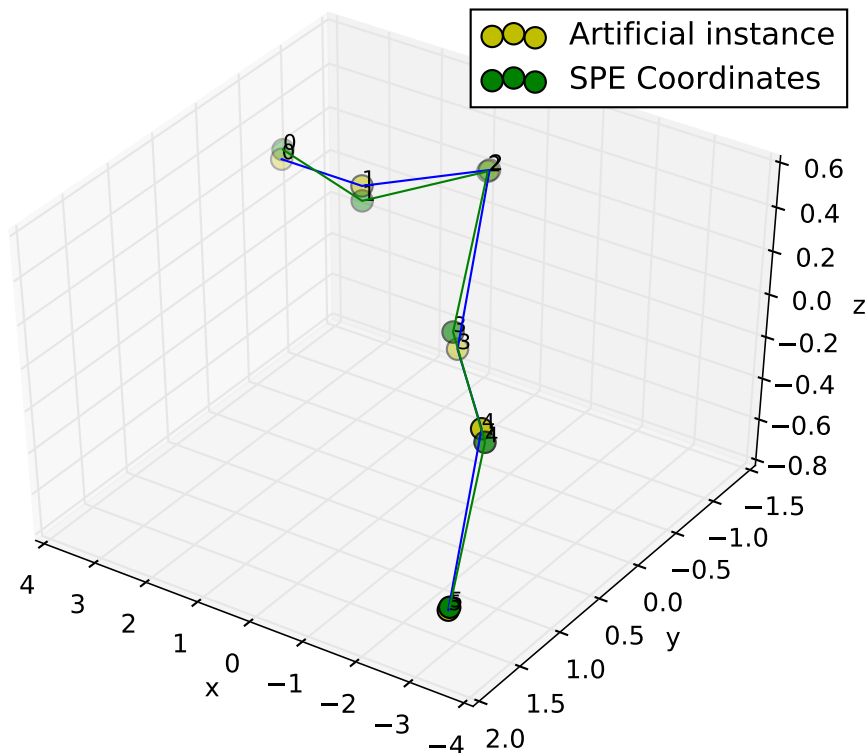


FIGURE 23: *Original Protein Chain Vs Protein Chain produced by DMCA + SPE*

with the possible position for each atom, x_i became two points, a binary tree is constructed with two possible positions. The same procedure is followed for all the atoms in a molecule.

At every iteration, two new positions are added to the binary tree. A Binary tree is built as the search proceeds. Before adding a position to the binary tree, every position should pass a feasibility test; feasibility test is to test the agreement of the two possible position with other available distances. If a position is not agreeing with the other available distances, then that position is not added to the tree and that the whole branch is pruned out of the tree.

The pruning phase in the Branch and Prune algorithm reduces the binary tree quickly, and the remaining branch is explored through an exhaustive search, which is not too expen-

sive.

When all the assumptions are satisfied, the MD-Jeep software with NMR data is producing a good layout. A sample layout out of MD-Jeep is shown in Fig. 24. The MD-Jeep software has some synthetic NMR data's which is created in a way to satisfy the assumptions made in the paper [19].

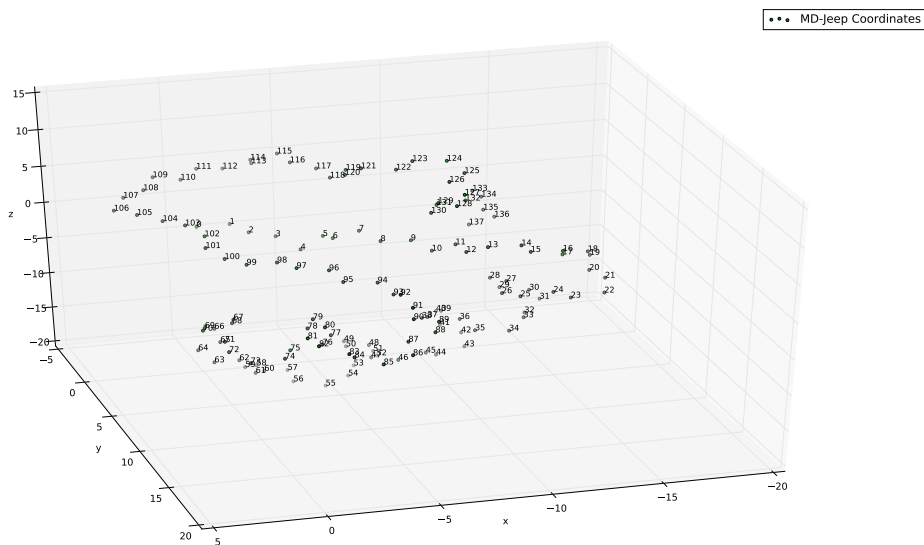


FIGURE 24: *MD-Jeep Coordinates*

3.9 Md-Jeep Vs. DMCA + SPE using NMR data

To compare our method (DMCA + SPE with the degree of freedom approach), we have used the synthetic NMR data found with the MD-Jeep software. Note that the NMR data used here are produced by MD-Jeep authors to satisfy the assumptions made in solving DMDGP.

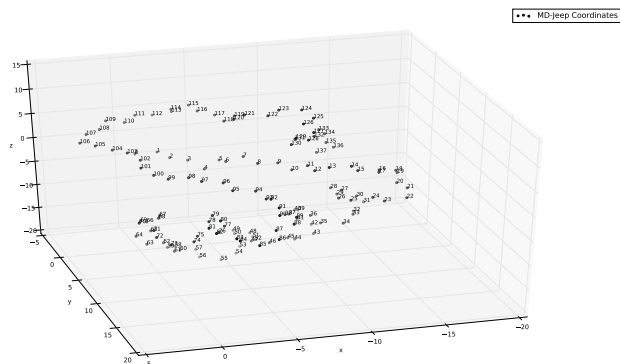


FIGURE 25: *MD-Jeep Coordinates*

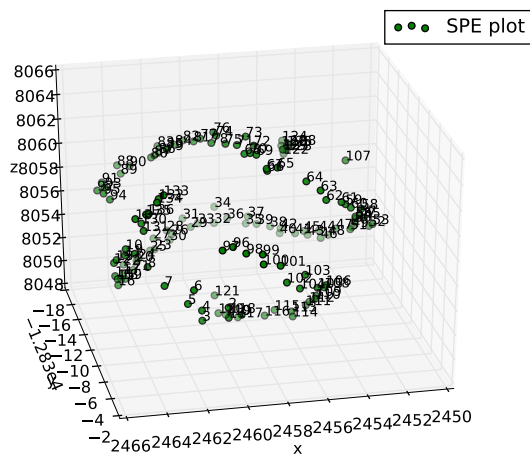


FIGURE 26: *Layout produced by DMCA Plus SPE*

Figure 25 shows the layout produced by MD-Jeep software for the protein Id: 1crn We

used the same NMR file with partial distances and computed the final structure using our proposed approach. Fig. 26 shows the layout produced by DMCA + SPE for the protein Id: 1crn

3.10 Discussions

In this chapter, we proposed an algorithm to solve MDGP using DMCA and SPE. The degree of freedom approach is discussed that gives us the minimum distances to reconstruct the whole chain of a protein molecule. The other algorithm DMDGP proposed by Lover et al. to solve this problem is also reviewed in this chapter. The Philips model to create the artificial backbone chain of a protein molecule is also explained in this chapter. In the end, the results for the degree of freedom approach tested against the chain of n atoms produced by Philips model is discussed, and the corresponding matrix is also displayed in this chapter. Our approach is also tested against the MD-Jeep Software using the synthetic NMR data found with MD-Jeep software.

CHAPTER 4

Summary and Discussions

This thesis mainly contributes towards fixing the sensor network localization problem in 2-dimensional space and computing the structure of a protein molecule in 3-dimensional space.

In chapter 1, we have given an prototypical problem by Saxe. Various versions of the prototypical problem is explained in 2 and 3 dimensions.

In chapter 2, We have discussed the point placement problem in 2D. Our approach towards the point placement problem in 2D is simple and contribute towards fixing the sensor network localization. The nodes of the sensor network are fixed by knowing the position of few nodes called anchor nodes. The idea we proposed here is simple and compatible with very large networks as well. At the end of the second chapter, we also proposed a modified version of SPE approach that uses the anchor nodes to fix the sensor networks. The modified approach is just to avoid the issue of highest translation that SPE faces when we overfeed the point set.

In chapter 3, the point placement problem in 3D is explained, our algorithm contributes towards fixing the structure of a protein molecule. Degree of Freedom approach is proposed to take the partial distances between the atoms and completing the whole structure of a molecule. In Biology, determination of the structure of a protein molecule will give us a clue about the functionality of the molecule. An Artificial backbone chain of a protein molecule

is developed using Philips model. The experiments and results using the Philips model is discussed in the chapter 3.

4.1 Open Problems

- Stochastic proximity embedding can be made more clear theoretically
- A theoretical proof of why and how SPE works would be a great area to explore
- Solving the distance matrix completion approach for other available graphs
- Distance matrix completion approach can be made more robust to handle more number of floating point values
- Proof to show the relationship between Learning rate parameter λ and the points disparity in SPE

REFERENCES

- [1] D. K. Agrafiotis. Stochastic proximity embedding. *Journal of computational chemistry*, 24(10):1215–1221, 2003.
- [2] D. K. Agrafiotis, D. Bandyopadhyay, and E. Yang. Stochastic proximity embedding: a simple, fast and scalable algorithm for solving the distance geometry problem. In *Distance Geometry*, pages 291–311. Springer, 2013.
- [3] M. S. Alam and A. Mukhopadhyay. Three paths to point placement. In *CALDAM*, pages 33–44, 2015.
- [4] G. Aloor and L. Jacob. Distributed wireless sensor network localization using stochastic proximity embedding. *Computer Communications*, 33(6):745–755, 2010.
- [5] J. Aspnes, T. Eren, D. K. Goldenberg, A. S. Morse, W. Whiteley, Y. R. Yang, B. D. Anderson, and P. N. Belhumeur. A theory of network localization. *IEEE Transactions on Mobile Computing*, 5(12):1663–1678, 2006.
- [6] M. Bakonyi and C. R. Johnson. The euclidian distance matrix completion problem. *SIAM Journal on Matrix Analysis and Applications*, 16(2):646–654, 1995.
- [7] R. Biloti, L. T. Santos, and M. Tygel. Multiparametric traveltime inversion. *Studia geophysica et geodaetica*, 46(2):177–192, 2002.
- [8] F. Chin, H. Leung, W. Sung, and S. Yiu. The point placement problem on a line—improved bounds for pairwise distance queries. *Algorithms in Bioinformatics*, pages 372–382, 2007.
- [9] G. M. Crippen, T. F. Havel, et al. *Distance geometry and molecular conformation*, volume 74. Research Studies Press Taunton, UK, 1988.
- [10] A. Daurat, Y. Gérard, and M. Nivat. The chords problem. *Theoretical Computer Science*, 282(2):319–336, 2002.
- [11] Q. Dong and Z. Wu. A linear-time algorithm for solving the molecular distance geometry problem with exact inter-atomic distances. *Journal of Global Optimization*, 22(1-4):365–375, 2002.

- [12] R. L. Ellis and D. C. Lay. Rank-preserving extensions of band matrices. *Linear and Multilinear Algebra*, 26(3):147–179, 1990.
- [13] C. A. Floudas and P. M. Pardalos. *Molecular Distance Geometry Problem, In: Encyclopedia of optimization*. Springer Science & Business Media, 2008.
- [14] R. Grone, C. R. Johnson, E. M. Sá, and H. Wolkowicz. Positive definite completions of partial hermitian matrices. *Linear algebra and its applications*, 58:109–124, 1984.
- [15] T. F. Havel. Distance geometry: Theory, algorithms, and chemical applications. *Encyclopedia of Computational Chemistry*, 120:723–742, 1998.
- [16] C. Lavor, L. Liberti, N. Maculan, and A. Mucherino. The discretizable molecular distance geometry problem. *Computational Optimization and Applications*, 52(1):115–146, 2012.
- [17] L. Liberti and N. Maculan. *Global optimization: from theory to implementation*, volume 84. Springer Science & Business Media, 2006.
- [18] J. J. Moré and Z. Wu. Global continuation for distance geometry problems. *SIAM Journal on Optimization*, 7(3):814–836, 1997.
- [19] A. Mucherino, C. Lavor, and L. Liberti. The discretizable distance geometry problem. *Optimization Letters*, pages 1–16, 2012.
- [20] A. Mucherino, L. Liberti, and C. Lavor. Md-jeep: An implementation of a branch and prune algorithm for distance geometry problems. In *ICMS*, pages 186–197. Springer, 2010.
- [21] A. Mukhopadhyay, P. K. Sarker, and K. K. V. Kannan. Point placement algorithms: an experimental study. *Int. J. Exp. Algorithms*, 6(1):1–13, 2016.
- [22] A. T. Phillips, J. B. Rosen, and V. H. Walke. Molecular structure determination by convex, global underestimation of local energy minima. *Global Minimization of Nonconvex Energy Functions: Molecular Conformation and Protein Folding*, 23:181–198, 1995.
- [23] M. Z. Rahman, A. Mukhopadhyay, Y. P. Aneja, and C. Jean. A distance matrix completion approach to 1-round algorithms for point placement in the plane. In *International Conference on Computational Science and Its Applications*, pages 494–508. Springer, 2017.
- [24] D. J. Rose, R. E. Tarjan, and G. S. Lueker. Algorithmic aspects of vertex elimination on graphs. *SIAM Journal on computing*, 5(2):266–283, 1976.
- [25] J. B. Saxe. *Embeddability of weighted graphs in k-space is strongly NP-hard*. Carnegie-Mellon University, Department of Computer Science, 1980.

- [26] I. S. Sendin, I. B. Vale, and M. A. Batista. An improved stochastic proximity embedding to protein structure determination. In *Proceedings of the International Conference on Bioinformatics & Computational Biology (BIOCOMP)*, page 25. The Steering Committee of The World Congress in Computer Science, Computer Engineering and Applied Computing (WorldComp), 2015.
- [27] S. S. Skiena, W. D. Smith, and P. Lemke. Reconstructing sets from interpoint distances. In *Proceedings of the sixth annual symposium on Computational geometry*, pages 332–339. ACM, 1990.
- [28] Wikipedia. Distance geometry - wikipedia, the free encyclopedia, 2015, 2009.
- [29] Wikipedia. Stereographic projection - wikipedia, the free encyclopedia, 2015, 2009.
- [30] G. Young and A. S. Householder. Discussion of a set of points in terms of their mutual distances. *Psychometrika*, 3(1):19–22, 1938.

VITA AUCTORIS

NAME: Udayamoorthy Navaneetha Krishnan

PLACE OF BIRTH: Aruppukottai, Tamil Nadu, India.

EDUCATION: Bachelor of Engineering in Computer Science, Sriram Engineering College, Chennai, Tamil Nadu, 2013.

Master of Science in Computer Science, University of Windsor, Windsor, Ontario, Canada, 2017.