UNSUPERVISED ASSET CLUSTER ANALYSIS IMPLEMENTED WITH PARALLEL GENETIC ALGORITHMS ON THE NVIDIA CUDA PLATFORM

by

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Declaration of Authorship

I declare that this dissertation is my own, unaided work. It is being submitted for the Degree of Master of Science in the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination in any other University.

(Signature of candidate)

day of 20
UNIVERSITY OF WITWATERSRAND

Abstract

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During times of stock market turbulence and crises, monitoring the clustering behaviour of financial instruments allows one to better understand the behaviour of the stock market and the associated systemic risks. In the study undertaken, I apply an effective and performant approach to classify data clusters in order to better understand correlations between stocks. The novel methods aim to address the lack of effective algorithms to deal with high-performance cluster analysis in the context of large complex real-time low-latency data-sets. I apply an efficient and novel data clustering approach, namely the Giada and Marsili log-likelihood function derived from the Noh model and use a Parallel Genetic Algorithm in order to isolate residual data clusters. Genetic Algorithms (GAs) are a very versatile methodology for scientific computing, while the application of Parallel Genetic Algorithms (PGAs) further increases the computational efficiency. They are an effective vehicle to mine data sets for information and traits. However, the traditional parallel computing environment can be expensive. I focused on adopting NVIDIA’s Compute Unified Device Architecture (CUDA) programming model in order to develop a PGA framework for my computation solution, where I aim to efficiently filter out residual clusters. The results show that the application of the PGA with the novel clustering function on the CUDA platform is quite effective to improve the computational efficiency of parallel data cluster analysis.
Dedicated to my son Marcel, my parents Waldemar and Urszula
and my brothers Tomasz and Marek
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<td>GPU</td>
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<td>GPGPU</td>
<td>General Purpose Graphics Processing Unit</td>
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<td>CPU</td>
<td>Central Processing Unit</td>
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<td>CUDA</td>
<td>Compute Unified Device Architecture</td>
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<td>Single instruction stream/Single data stream</td>
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<td>MIMD</td>
<td>Multiple instruction stream/Multiple data stream</td>
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<td>MPI</td>
<td>Message passing interface</td>
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<td>API</td>
<td>Application programming interface</td>
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Symbols

\[ R_c \quad \text{random number} \]
\[ P_c f \quad \text{probability (rate) of crossover using a knowledge-based operator} \]
\[ P_m \quad \text{probability (rate) of mutation} \]
\[ P_c \quad \text{probability (rate) of crossover} \]
\[ G_{stall} \quad \text{stall generations} \]
\[ e \quad \text{tolerance value} \]
Chapter 1

Introduction

Cluster analysis is applied to financial time series data in order to identify securities with related returns, so that one can diversify and thus optimise a financial portfolio[2]. Clustering is the process of grouping data into clusters so that objects within a cluster have high similarity in comparison to one another, but are very dissimilar to objects in other clusters[3]. In order to be able to filter through all the noise and isolate structures, one needs to make use of a computational approach, that is well-suited to the traversal of vast search spaces of data and the computation of classifications. Genetic algorithms are such an approach. They are numerical optimisation algorithms inspired by natural selection and genetics[4–6], that intelligently exploit a search space to solve optimisation problems. Although the algorithms must traverse huge spaces, the computationally intensive calculations can be performed independently[4–6]. The application of Parallel Genetic Algorithms (PGAs) increases the computational efficiency and represents an efficient vehicle for the mining of data-sets for information and traits[6]. PGAs paired with a parallel computing environment allows for quick and effective computation[6]. Compute Unified Device Architecture (CUDA) is NVIDIA’s parallel computing platform.
that enables enthusiasts and scientists to dramatically improve computing performance by harnessing the power of the GPU[7–10].

1.1 Objectives

The main objective of this research was to develop a Master-slave Parallel Genetic Algorithm (PGA) framework for unsupervised cluster analysis on the CUDA platform. Master-slave PGAs, also denoted as Global PGAs, involve a single population, but distributed amongst multiple processing units for determination of fitness values and the consequent application of genetic operators[6, 9, 10]. It must be able to isolate residual clusters using the Giada and Marsili likelihood function[11]. The Giada and Marsili’s[11] maximum log-likelihood function is used as a measure of the similarity of objects. It is an unsupervised clustering function, meaning that the optimal number of clusters is unknown a priori and thus not fixed at the beginning of the cluster analysis. Additionally, I investigated and determined the most appropriate genetic operators in order to maximise quality and performance of the proposed cluster analysis approach[11].

1.2 Rationale

This main focus of this research is to investigate the suitability of using the Giada and Marsili log-likelihood function[11] with PGAs in a GPU parallel computing environment. Examining the clustering behaviour of financial instruments, allows me to eliminate any overlap in an investment portfolio by identifying securities with related returns. This approach increases diversification. Diversification strives to smooth out unsystematic risk events in a portfolio so that the positive performance of some investments will
neutralize the negative performance of others and in turn will reduce the inherent risk on the portfolio\[2\].

1.3 Structure

A three-tiered approach was applied to investigate the suitability of using the Giada and Marsili log-likelihood function\[11\] with PGAs in a GPU parallel computing environment. The first tier of the thesis presents an up-to-date literature study on cluster analysis, where the reader is familiarised with a Giada and Marsili log-likelihood function\[11\]. This thesis is the continuation of work done by Mbambiso\[12\], where he utilised a simulated annealing optimisation approach using a maximum likelihood model developed by Noh\[13\] in order to isolate an underlying structure of correlated asset returns, denoted as sectors, and correlated market-wide activities, denoted as states in the SA financial markets. In this research, a similar data clustering approach will be followed by using a Giada and Marsili’s\[11\] log-likelihood function, as a measure of the similarity of objects, and thus clusters, but one will apply a more efficient search heuristic, namely Genetic Algorithms. Artificial Intelligence search heuristic approaches, denoted Genetic Algorithms, are introduced in order to to apply the cluster analysis function in an optimal and efficient manner, thus forming the second tier of the research. The focus then shifts onto Parallel Genetic Algorithms in order to provide a computational approach to push the boundaries of computational performance. The third tier comprises the vehicle for computation: the CUDA platform on General Purpose Graphics Processing Units(GPGPUs). GPGPUs are commodity hardware, which have revolutionised cutting-edge research into Parallel Computing. A closer look is taken at the implementation of Master-Slave Parallel Genetic Algorithm(PGA), with a detailed dissection of all
the approaches taken. The results section depicts the behaviour and intrinsic properties of the algorithm and features a section on algorithm tuning for a training set of four clusters. It includes a section on code execution times obtained, where Gebbie’s serial GA implementation[12, 14] and the newly developed clustering implementation were run on various Operating Systems, justifying the utilisation of GPUs and Parallel Genetic Algorithms with the cluster analysis approach taken. The section is rounded off by the application of the cluster analysis approach to real-world data. It features a clustering analysis of 1780 time units of real-word stock prices taken from the JSE spanning over the time period from 28th September 2012 until 10th of October 2012. A high-level interpretation of trends observed for that specific time period is presented using Multiple Spanning Trees, which depict the correlations of the stock prices of assets under investigation. The conclusion succinctly summarises the findings and presents further prospects which might emanate from this research.
In the research undertaken, I undertake to find an effective and performant approach to classify data clusters in order to better understand correlations between stocks. The novel methods discussed here aim to address the lack of effective algorithms to deal with high-performance cluster analysis in the context of large complex real-time low-latency data-sets. I apply an efficient and novel data clustering approach, namely the Giada and Marsili log-likelihood function\[11\] derived from the Noh model\[13\], to try to classify data clusters. The chapter provides an overview of measures of similarity and dissimilarity to provide a measure for the clusterability of data. I then look at areas of applicability of cluster analysis, list the common types of clustering procedures and then provide an in-depth analysis of the chosen clustering approach, namely the Giada and Marsili log-likelihood function\[11\]. The research will be performed on normalised financial data, meaning that the data will undergo preconditioning in order to remove outliers caused by unusual or one-time influences. The data-set comprises stock returns, which consist of the income and the capital gains relative on an investment in a particular stock asset.
2.1 Introduction

Cluster analysis divides data into groups, or clusters, which are meaningful, useful or both. The goal is that the objects in a group will be similar or related to one other and different from or unrelated to the objects in other groups. The greater the homogeneity within a group, and the greater the heterogeneity between groups, the more pronounced the clustering[3].

2.2 Measures of Similarity and Dissimilarity

There are various measures to express the similarity or dissimilarity between pairs of objects.

2.2.1 Distance measures

The most commonly used proximity measure is the Minkowski metric, which is a generalization of the normal distance between points in Euclidean space[3]. It is defined as

\[ P_{ij} = \left( \sum_{k=1}^{d} \|x_{ik} - x_{jk}\|^r \right)^{\frac{1}{r}} \]  

(2.1)

where, \( r \) is a parameter, \( d \) is the dimensionality of the data object, and \( x_{ik} \) and \( x_{jk} \) are, respectively, the \( k \)th components of the \( i \)th and \( j \)th objects, \( x_i \) and \( x_j \). Literature lists the following Minkowski distances for specific values of \( r \)[3]:

1. \( r = 1 \). City block or Taxicab distance, a common example being the Hamming distance which measures the number of bits that are different in two binary vectors.
2. \( r = 2 \). The most common measure for the distance. This type of distance is referred to as the Euclidean distance and is the most commonly used approach in working with ratio or interval-scaled data.

3. \( r \to \infty \). The supremum distance (\( L_{\text{max norm}}, L_{\infty} \)), which denotes the maximum difference between any component of the vectors.

The dimension \( d \) is combined with the respective Minkowski distance \( r \) to yield an overall distance measure.

### 2.2.2 Correlation measure

The correlation measure is an approach to standardise data by using correlations, in other words the statistical interdependence between data points. The correlation indicates the direction and the degree of the relationship between two data points. The direction of the relationship can either be positive or negative and if positive indicates that the data points are in increasing positive relationship to each other, in other words correlation, whilst if negative, in decreasing relationship to each other, denoted by the term anti-correlation. The degree of the relationship measures the strength of the relationship. The most common correlation coefficient which measures the relationship between data points is the *Pearson correlation coefficient*, which is sensitive only to a linear relationship between them. The Pearson correlation has a value of +1 in the case of a perfect positive linear relationship and a value of −1 in the case of a perfect decreasing linear relationship, and some value between −1 and 1 in all other cases, indicating the degree of linear dependence between the variables. As it approaches zero there is less of a relationship, meaning that there is a diminishing relationship or linear
interdependence between the points and the closer the coefficient is to either $-1$ or $1$, the stronger the correlation between the variables.

### 2.2.3 Ordinal Measures

Another type of proximity measure is derived by ranking the distances between pairs of points from 1 to $m \times (m - 1) / 2$. This type of measure can be used with most types of data and is often used with a number of the hierarchical clustering, which is covered in 2.2.4.

### 2.2.4 Hierarchical clustering

[15] describes hierarchical clustering as procedures that are characterised by a tree-like structure, a dendogram, which emerges in the course of the analysis. Clusters are consecutively formed from objects. Initially, this type of procedure starts with each object representing an individual cluster. These clusters are then sequentially merged according to their similarity. First, the two most similar clusters, for example those with the smallest distance between them, are merged to result in a new cluster at the bottom of the hierarchy. This method builds the hierarchy from the individual elements by progressively merging clusters and linking them to a higher level of the hierarchy. This continues until a single, all inclusive cluster at the top and singleton clusters of individual points at the bottom emerge. This allows a hierarchy of clusters to be established from the bottom up. This category of hierarchical clustering is called is agglomerative clustering. A cluster hierarchy can also be generated top-down, where all objects are initially merged into a single cluster, which is then gradually split up as I move down the hierarchy. In hierarchical clustering a cluster on a higher level
of the hierarchy always encompasses all clusters from a lower level. This means that if an object is assigned to a certain cluster, there is no possibility of reassigning this object to another cluster. This category of hierarchical clustering is called *divisive clustering*. The methodology is depicted in Figure 2.1. Hierarchical clustering features a family of methods that differ by the way distances are computed. Apart from the usual choice of distance functions, I also need to decide on the linkage criterion since a cluster consists of multiple objects, and there exist multiple candidates for the computation of the distance[15].

### 2.2.4.1 Nearest-neighbour clustering

The nearest-neighbour method computes the distance between the two closest elements in two respective clusters. The linkage function is described by the following equation:
Chapter 2. Cluster Analysis

\[ D(x, y) = \min_{x \in X, y \in Y} d(x, y) \] where \( X \) and \( Y \) are any two sets of data points considered as clusters, and \( d(x, y) \) denotes the distance between the two elements \( x \) and \( y \).

2.2.4.2 Farthest-neighbour clustering

The farthest-neighbour approach computes the maximum distance between a pair data objects in respective clusters. \[ D(x, y) = \max_{x \in X, y \in Y} (d(x, y)) \] where \( X \) and \( Y \) are any two sets of data points considered as clusters, and \( d(x, y) \) denotes the distance between the two elements \( x \) and \( y \). This approach is an agglomerative procedure.

2.2.4.3 Ward’s Method

For Ward’s method the proximity between two clusters is defined as the increase in the squared error that results when two clusters are merged. Thus, this method uses the same objective function as is used by the K-means clustering. While it may seem that this makes this technique somewhat distinct from other hierarchical techniques, some algebra will show that this technique is very similar to the group average method when the proximity between two points is taken to be the square of the distance between them[15].

2.2.5 Center-Based Partitional Clustering

Another important group of clustering procedures are partitioning methods. As with hierarchical clustering, there is a wide array of different algorithms; of these, the k-means procedure and the k-mediod being the most recognised. The optimization problem itself is known to be NP-hard, and thus the common approach is to search only for approximate solutions. Both techniques are based on the notion that a center point
can represent a cluster. They distinguish themselves by the fact that K-means uses the concept of a centroid, which is the median value of a group of points, which almost never corresponds to an actual data point, whilst the K-medoid clustering approach utilises the idea of determining a medoid, which is the most representative point of a group of points.

### 2.2.5.1 K-means clustering

This algorithm uses the within-cluster variation as a measure of the homogeneity of a cluster. The procedure aims at segmenting data in such a way that the variation of the data points within a cluster is minimised. Prior to analysis, I have to decide on the number of clusters. Based on this information, the algorithm randomly selects a center for each cluster and the clustering process starts by randomly assigning objects to the chosen number of clusters. I proceed then to re-allocate objects to other clusters in order to reduce the within-cluster variation. Given a set of observations \((x_1, x_2, ..., x_n)\), where each observation is a \(d\)-dimensional real vector, \(k\)-means clustering aims to partition the \(n\) observations into \(k\) sets \(S = (S_1, S_2, ..., S_k)\) so as to minimise the Euclidean distance, that being the measure of proximity of the data point to the centroid of the cluster denoted by

\[
\arg \max_S = \sum_{i=1}^{k} \sum_{x_j \in S_i} \|x_j - \mu_i\|^2
\]  

(2.2)

where \(\mu_i\) is the mean of the points in \(S_i\) for every single object. Each object is then assigned to the centroid with the shortest distance to it. I proceed in an iterative manner until pre-defined termination criteria is reached, for example a predetermined number of iterations or there is no change in cluster affiliations, meaning there is no change in centroids.
2.3 Applicability of Cluster Analysis in the finance industry

Conceptually meaningful groups of objects that share common characteristics, play an important role in how people analyse and describe the world. The human mind divides up objects into groups and assigning particular objects to these groups, by the process of classification. In the context of understanding data, clusters are potential classes and cluster analysis is the study of techniques for automatically finding classes.

Analytical models are critical in the Financial Services Industry in every phase of the credit cycle such as Marketing, Acquisitions, Customer Management, Collections, and Recovery. While such models are now commonplace, it is imperative to continuously improve on those models to remain competitive. Customization of the models for each segment of the population is a crucial step towards achieving that end, where cluster analysis is used to segment the data in order to make better modelling decisions. The clusters may be used to drive the model development process, to assign appropriate strategies, or both[15].

In a trading context, cluster analysis is used by Bacidore, Berkow, Polidore and Saraiya[16] to empirically identify the primary strategies used by a trader. They apply k-means to a sample of 'progress charts', representing the portion of the order completed by each point in the day as a measure of a trade’s aggressiveness. Their methodology identifies the primary strategies used by a trader and determines which strategy the trader used for each order in the sample. They also look at ways to exploit this technique to characterize trader behaviour, assess trader performance, and suggest the appropriate benchmarks for each distinct trading strategy.
Da Costa, Cunha, Da Silva[17] employ cluster analysis to show that stocks from selected companies of the Americas can be categorized according to their degree of integration. They show that the stock returns are dependant on geography and macroeconomic features, just to name a few and stock cluster analysis allows them to track those with similar returns but different risks. Cluster analysis allows the informed investor to use the data, which features stock groupings, for identifying same-return stocks and in turn use this information to optimise a financial portfolio.

2.4 Cluster analysis based on the Maximum Likelihood principle

Maximum likelihood estimations is a method of estimating the parameters of a statistical model[11, 18]. Data clustering, on the other hand, deals with the problem of classifying or categorising a set of $N$ objects or clusters, so that the objects within that group or cluster are more similar than objects belonging to different groups. If each object is identified by a number of $D$ observable features, then that object object $i = 1, \ldots, N$ can be represented as a point $\vec{x}_i = (x_i^{(1)}, \ldots, x_i^{(n)})$ in a D dimensional space. Data clustering will try to identify clusters as more densely populated regions in this vector space. Thus, a configuration of clusters is represented by a set $\mathcal{S} = \{s_i, \ldots, s_N\}$ of integer labels, where $s_i$ denotes the cluster that object $i$ belongs to and $N$ is the number of objects[11, 18]. Let’s assumes that $s_i$ takes on values from 1 to $M$ and $M = N$, then each cluster is a singleton cluster constituting one object only. If $s_i = s_j = s$, then object $i$ and object $j$ reside in the same cluster.
2.4.1 Giada and Marsili clustering technique

Giada and Marsili’s[11] stipulate that objects that have something in common; they are either similar to each other or belong to the same grouping. They found that the maximum likelihood function leads naturally to a Hamiltonian of Potts variables, whose low temperature behaviour describes the correlation structure of a data-set[11].

\[
H_q = - \sum_{s_i, s_j \in S} J_{ij} \delta_{s_i, s_j} - \frac{1}{\beta} \sum_{i=1}^{M} h_i^M s_i
\]  

(2.3)

For example, in the Potts’ model of interacting market agents in the trading market, each stock can assume q-states. The state represents a cluster of similar stocks. The model comprises the factor component \( \sum_{s_i, s_j \in S} J_{ij} \delta_{s_i, s_j} \) and a noise component \( \frac{1}{\beta} \sum_{i=1}^{M} h_i^M s_i \). The goal is to specify an objective function, which determines the quality of a classification structure compared to a data-set being sampled. They observed that data-sets belonging to the same cluster share common characteristics. This allowed them to construct an expression for the likelihood of any possible classification structure. It allows for the isolation of residual clusters in correlated data-sets, whilst there will be an absence of clusters uncorrelated data-sets [18]. The essence of Maximum Likelihood data clustering is that objects belonging to the same cluster should share a common component:

\[
\vec{x}_i = g_{s_i} \eta_{s_i} + \sqrt{1 - g_{s_i}^2} \epsilon_i.
\]  

(2.4)

Equation 2.4 \( \vec{x}_i \), represents the features of object \( i \) and \( s_i \) is the label of the cluster that that object belongs to. The data is normalised to have zero mean, and unit variance, as following:

\[
\sum_t \vec{x}_i^{(t)} = 0,
\]  

(2.5)
and
\[ \| \vec{x}_i \|^2 = \sum_t [x_i^{(t)}]^2 = D. \] (2.6)

for all \( i = 1, \ldots, N \). \( \vec{c}_s \) is the vector of features of cluster \( s \) and \( g_s \) is a loading factor that emphasises the similarity or difference between objects in a cluster \( s \). In this research the data-set refers to a set of the objects, denoting \( N \) assets or stocks and their features are prices across \( D \) days in the data-set. The variable \( i \) is an index for stocks or assets, whilst \( d \) represents an index for days.

If \( g_s = 1 \), all objects with \( s_i = s \) are identical, whilst if \( g_s = 0 \) all objects are different. The range of the cluster index is from 1 to \( N \), in order to allow for singleton clusters of one object or asset each. \( \vec{c}_i \) designates the deviation of the features of object \( i \) from the cluster’s features and includes measurement errors. I take equation 2.4 as a statistical hypothesis and assume that both \( \vec{\eta}_s \) and \( \vec{c}_s \), for values of \( i, s = 1, \ldots, N \), are Gaussian vectors and have zero mean and variance:

\[ \mathbb{E} \left[ (\epsilon_s^{(t)})^2 \right] = 1, \] (2.7)

and

\[ \mathbb{E} \left[ (\eta_s^{(t)})^2 \right] = 1. \] (2.8)

Then it is possible to compute the probability density \( P(\{\vec{x}_i\} | G, S) \) for any given set of parameters \( (G, S) = (\{g_s\}, \{s_i\}) \) by observing the data-set \( \{x_i\}, i, s = 1, \ldots, N \) as a realisation of common component Equation 2.4:

\[ P(\{\vec{x}_i\} | G, S) = \prod_{d=1}^{D} \left( \prod_{i=1}^{N} \delta(x_i^{(t)} - g_s \vec{\eta}_i + \sqrt{1 - g_s^2 \vec{c}_i}) \right). \] (2.9)
The variable $\delta$ is the Dirac delta function and $\langle \ldots \rangle$ denotes the mathematical expectation. For a given cluster structure $S$, the likelihood is maximal when the parameter $g_s$ takes the values

$$g_s^* = \frac{c_s - n_s}{n_s^2 - n_s}, n_s > 1. \quad (2.10)$$

If $n_s \leq 1$ then $g_s^* = 0$. $n_s$ in Equation 2.10 denotes the number of objects in cluster $s$

$$n_s = \sum_{i=1}^{N} \delta_{i,s}. \quad (2.11)$$

The variable $c_s$ is the internal correlation of the $s$-th cluster denoted by the following equation:

$$c_s = \sum_{i=1}^{N} \sum_{j=1}^{N} C_{i,j} \delta_{i,s} \delta_{j,s}. \quad (2.12)$$

The variable $C_{i,j}$ is the Pearson’s coefficient of data denoted by the following equation:

$$C_{i,j} = \frac{\bar{x}_i \bar{x}_j}{\sqrt{\|\bar{x}_i^2\| \|\bar{x}_j^2\|}}. \quad (2.13)$$

The maximum likelihood of structure $S$ can be written as $P(G^*, S|\bar{x}_i) \propto e^{\mathcal{L}_c(S)}$, where the resulting likelihood function per feature $\mathcal{L}_c$ is denoted by

$$\mathcal{L}_c(S) = \frac{1}{2} \sum_{s:n_s>1} \left[ \log \frac{n_s}{c_s} + (n_s - 1) \log \frac{n_s^2 - n_s}{n_s^2 - c_s} \right]. \quad (2.14)$$

The maximum likelihood structure maximises $\mathcal{L}_c$. From Equation 2.14, it follows that $\mathcal{L}_c = 0$ for cluster of objects that are uncorrelated, where $g_s^* = 0$ or $c_s = n_s$ or when the objects are grouped in singleton clusters, where $n_s = 1$ for all the cluster indexes. Equation 2.14 illustrates that the resulting maximum likelihood function for $S$ depends
on Pearson’s coefficient $C_{i,j}$ and hence exhibits the following advantages in comparison to conventional clustering methods: it is unsupervised, meaning that the optimal number of clusters is unknown a priori and not fixed at the beginning, and secondly the interpretation of results is transparent in terms of the model, namely Equation 2.4. Unsupervised measures of cluster validity are divided into classes: measures of cluster cohesion denoting the compactness of objects within the cluster and measures of cluster separation measuring how pronounced or well-separated the cluster is from the other clusters. The Giada and Marsili log-likelihood function $L_c$ classifies the objects according to their similarity.

Summa Summarum, Giada and Marsili[11] state that $\max_S L_c(S)$ provides a measure of structure inherent in the cluster configuration represented by the set $S = \{s_1, \ldots, s_n\}$ and the higher the value, the more pronounced the structure of the data-set.

### 2.4.2 Search heuristic approach and rationale

Marsili and Giada[11] made use of the simulated annealing algorithm in order to localise clusters of normalised stock returns in financial data. Simulated annealing is a stochastic metaheuristic utilised in optimization problems of locating a good approximation to the global optimum of a given function in a large search space. It is motivated by an analogy to annealing in solids, simulating the cooling of material in a heat bath. This is a process known as annealing[19]. Marsili and Giada utilised $-L_c$ as the cost function in their application of the log-likelihood function on real-world data-sets to substantiate their approach. The simulated annealing approach makes use of Metropolis algorithm on $s_i$ with progressively decreasing the temperature. They also compared it to other clustering algorithms such as $K$-means as described in Section 2.2.5.1 and other algorithms such as Single Linkage, Centroid Linkage, Average Linkage, Merging and
Deterministic Maximisation[11]. The algorithms simulated annealing and Deterministic Maximisation proved to provide good approximations to the Maximum Likelihood structure, but are inherently computationally expensive. This motivates to utilise a more optimal approach. Parallel Genetic Algorithms are such an approach. $\mathcal{L}_c$ will be used as the fitness function and analogous to Deterministic Maximisation utilise GAs to find the maximum for $\mathcal{L}_c$ in order to efficiently isolate clusters in correlated data of financial data, as explained in subsequent chapters.
Chapter 3

Genetic Algorithms

In order to be able use the Giada and Marsili[11] likelihood function, as described in Chapter 2, to isolate structures and determine optimal cluster configurations, I need to make use of a computational approach, that is well-suited for fast and efficient traversal of vast search spaces. Genetic Algorithms are such a search heuristic and a viable candidate for investigation[20–24]. This chapter reviews the mechanics of Genetic Algorithms, especially Parallel Genetic Algorithms.

3.1 Genetic Algorithms: An Overview

Sivanandam and Deepa[6] state that genetic algorithms, genetic programming and evolutionary computing are terms that can be classified as "Evolutionary Computation". Genetic algorithms are computationally intensive search heuristics, which in contrast to enumerative searches, apply biological evolutionary theory and adapt a population of individuals in successive generations to iteratively hone in on the optimal solution to the problem at hand. A search heuristic, also denoted a metaheuristic, is routinely
used to generate useful solutions to optimisation and search problems. In an evolutionary algorithm, a representation scheme is chosen by the implementer to define the set of solutions, denoted chromosomes, that are contained within the search space for the algorithm. At the outset, a number of individual solutions are created, which will form the initial population or search space. An established steps are then repeated iteratively until a solution is found which satisfies a predefined termination criterion. Each individual is evaluated using a predefined fitness function that is specific to the problem being solved. Based upon their fitness values, a number of individuals are chosen to be parents. Specific genetic operators are applied to the parents, in the process of reproduction, which then give rise to offspring. The genetic operators are: selection, crossover, mutation, elitism and replacement. Figure 3.1 depicts the basic scheme of a Genetic Algorithm.

![Figure 3.1: Basic scheme of the Genetic Algorithm.](image)
3.1.1 Genetic Operators

3.1.1.1 Selection

The selection is the process of selecting two viable individuals, the parents, for crossover. The purpose of selection is to isolate the fitter individuals in the population and allow them to breed so that they can give rise to new offspring which exhibit higher fitness values. It randomly picks chromosomes out of the population according to their fitness function. There are two types of methodologies when it comes to selection schemes: *proportionate selection* and *ordinal-based selection*. Proportionate-based selection picks out individuals based upon their fitness values relative to the fitness of the other individuals in the population. Ordinal-based selection schemes selects individuals upon their rank within the population. Selection has to be maintained in balance with varying crossover and mutation. Too strong selection means highly fit individuals will take over the population, reducing the diversity and converging towards a solution too quickly, which might not be optimal as it might compromise the effort of sampling a diverse search space of candidate solutions; too weak a selection will impede and slow down the process of evolution. The convergence rate of GA is largely determined by selection pressure. Selection pressure gives fitter individuals a higher probability of partaking in the mating process in order to create the next generation so that the GA can focus on promising regions in the search space. Higher selection pressures result in higher convergence rates and lower selection pressures lead to longer search times, though a selection pressure that is too high will lead to convergence towards a local minimum and not the optimal solution to the problem at hand. One needs to find a balance in order to tune the selection process in such a way that on the one hand premature convergence
is avoided but on the other hand the search time for traversal of the search does not spiral out of control[6].

**Roulette Wheel Selection**  In Roulette Wheel Selection an analogy can be drawn between the whole population forming a roulette wheel with the size of of an individual’s slot proportional to it’s fitness. Then a random selection is made analogues to ’spinning’ the wheel and throwing a figurative ’ball’ in. The probability of the ’ball’ coming to rest in any particular slot is proportional to the arc of the slot and thus to the fitness of the respective individual. The probability of the selection of an individual can be computed as follows:

\[
p_i = \frac{f_i}{\sum_{j=1}^{N} f_j}
\]

(3.1)

where \( f_i \) is the fitness of the \( i^{th} \) individual and \( N \) is the number of individuals. The following depicts the approach visually:

![Figure 3.2: Roulette Wheel Selection](image)

**Rank Selection**  Rank Selection ranks the population by the value of their fitness value. The worst has fitness 1 and the best has fitness N. Potential parents are selected
and a tournament is held to decide which of the individuals will be the parent. There are many ways this can be accomplished. Two possible suggestions are:

1. Select a pair of individuals at random. Generate a random number, R, between 0 and 1. If R < r use the first individual as a parent. If the R ≥ r then use the second individual as the parent. This is repeated to select the second parent. The value of r is a parameter to this method.

2. Select two individuals at random. The individual with the highest evaluation becomes the parent. Repeat to find a second parent.

This approach stifles the rate of convergence in slow but keeps up selection pressure when the fitness variance is low, thus preserving diversity and hence leading to a better exploitation of the search space. In effect, potential parents are selected and a random approach is followed to decide which of the individuals will be the parent[6].

**Tournament Selection** Tournament selection involves running several tournaments among a variable size of \( N_u \) individuals chosen at random from the population. The criteria for winning the tournament is having the highest fitness value. The winner is then injected into the mating pool for generating new offspring. The variable tournament size and difference in fitness value of the individuals allows for selection pressure tuning, as a bigger pool will disadvantage weaker individuals, as their chances at selection will be smaller[6].

**Random Selection** This technique randomly picks a parent from the population.

**Stochastic Universal Sampling** In Stochastic Universal Sampling the individuals are mapped to contiguous segments on a selection line. The technique randomly samples
all the solutions by choosing them at uniformly spaced intervals, thus exhibiting zero bias to the selection approach and improves the chances of selection for weaker individuals[6].

The following depicts the approach visually:

![Stochastic Universal Sampling Approach](image)

**Figure 3.3**: Stochastic Universal Sampling Approach

### 3.1.1.2 Crossover

Sivanandam and Deepa[6] state that crossover is the process of mating, involving two individuals, with the expectation that they can produce a fitter individual. The crossover genetic operation involves the selection of a random loci to mark a cross site within the two parent chromosomes and copy the genes to the offspring, thus giving rise to the child that contains both parent’s genetic information and thus a new potential candidate solution that can be interrogated for a fitness value.

**Single Point Crossover** Figure 3.4 visually depicts the process of Single Point Crossover: The technique proceeds by slicing a pair of selected segments at a random location, denoted by the term locus. The locus is selected in a random manner. The segments beyond the locus in either individual are swapped between the two parent individuals.

**Two-Point Crossover** Figure 3.5 visually depicts the process of Two-Point Crossover. Analogous approach to Single-Point Crossover 3.1.1.2, but utilising two loci for exchange
of genetic material.

**Uniform Crossover** The Uniform Crossover Operator randomly decides which genes a parent of a pair of individuals contributes according to a binary crossover mask, with the distinguishing feature that binary value of 1 will signal to copy of the genetic information from the first parent, whilst a 0 will indicate that the information will be sourced from the second parent to yield the offspring\[6\]. The distribution of the binary values is denoted the mixing ratio. Figure 3.6 depicts the technique.
Figure 3.6: Uniform Crossover Approach

**Shuffle Crossover** The Shuffle Crossover approach is analogous to single-point crossover 3.1.1.2, with the distinction that prior to the genetic material being exchanged, the genes are randomly shuffled in both parents. After performing the crossover operation, the genes are 'unshuffled' in reverse order. This removes positional bias as the genes are randomly reassigned each time crossover is performed.

**3.1.1.3 Mutation**

Sivanandam and Deepa[6] state that mutation is the key driver of diversity in the candidate solution set or search space. This is an operator that is applied after crossover with the aim of randomly distributing genetic information and inhibiting the algorithm from being trapped in local minima. It introduces new genetic structures in the population by randomly modifying some of its building blocks and enables the algorithm to traverse the whole search space. It guarantees ergodicity, meaning that near-zero probability of generating any identical solution from any population state.

**Flipping** A parent is chosen which yields an offspring artefact, by taking the chosen binary genome representation and inverting all its bits. The 1’s in the parent become 0’s and vice versa. Figure depicts flipping.
Chapter 3. Genetic Algorithms

Interchanging Two random positions of the string are chosen and the bits corresponding to those positions are interchanged. Figure depicts interchanging.

<table>
<thead>
<tr>
<th>Parent</th>
<th>1 0 1 1 0 1 0 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mutation chromosome</td>
<td>1 0 0 0 1 0 0 1</td>
</tr>
<tr>
<td>Child</td>
<td>0 0 1 1 1 1 0 0</td>
</tr>
</tbody>
</table>

Figure 3.7: Flipping Approach

Reversing A parent is chosen which yields an offspring artefact, by taking the chosen binary genome representation and inverting the bit a specified locus.

<table>
<thead>
<tr>
<th>Parent</th>
<th>1 0 1 1 0 1 0 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Child</td>
<td>1 1 1 1 0 0 0 1</td>
</tr>
</tbody>
</table>

Figure 3.8: Interchanging Approach

Mutation Probability The important parameter in the mutation operation is the mutation probability $P_m$, which determines how often parts of chromosome will be mutated. If the mutation probability is 0%, then the artefacts generated by the crossover operation are the final offspring after mating if mutation probability is 100%, whole chromosome is subjected to the mutation operator[6].

3.1.1.4 Elitism

Sivanandam and Deepa[6] state that elitism is the process of preserving the fittest individuals, by inherent promotion to the next generation, without undergoing any of the
genetic transformations of crossover or mutation. It is purported in literature [4], that fitness-proportional selection does not necessarily favour the selection of any particular individual, even if it is the fittest. This means that the fittest individuals might not survive an evolutionary cycle, which has its advantages and disadvantages. The advantage is that it leads to a more exploration approach of the search space, thus sampling more possible combinations and thereby solutions to the problem in the search space. The disadvantage is that it slows down the process of converging towards the optimal solution and ultimately fails to find the true global optimum, thus not harnessing the full potential of exploitation of discoveries within the search space[4].

3.1.1.5 Replacement

Sivanandam and Deepa[6] state that replacement is the last stage of any evolution cycle, where the algorithms needs to replace old members of the current population and replace them with new ones. There are two replacement schemes: *generational updates and steady-state updates* The basic generational update scheme consists in producing $N/2$ children from a population of $N$ to evolve and create the next generation population, and this new population of children completely replacing the parent selection. This implies that an individual can only reproduce with individuals from the same generation. In a steady state update, new individuals are inserted in the population as soon as they are created, as opposed to the generational update where an entire new generation is produced in each generation. By introducing a new individual one needs to replace an old member, where one can opt for the least fittest one.

**Random Replacement** Random replacement introduces the concept of two offspring artefacts replacing two randomly chosen individuals in the population. The parents are
also candidates for selection. This can be useful for continuing the search in small populations, since weak individuals can be introduced into the population\[4\].

**Weak Parent Replacement**  In Weak Parent Replacement, if two parents mate and yield two offspring, the weaker parent will be replaced by the stronger child and introduced in to evolved population. This introduces bias towards fitter individuals, thus increasing the overall fitness of the population, but reducing the diversity of the mating pool.

**Both Parents Replacement**  In Both Parents Replacement, if two parents mate and yield two offspring, both parents will be replaced by children and introduced in to evolved population, thus each individual gets to breed once in the evolutionary cycle.

### 3.1.1.6 Advantages of Genetic Algorithms

One of the key advantages of genetic algorithms is that they are conceptually simple. As explained in the previous section, Genetic Algorithms (GAs) can be represented by the following steps: *initialise population, evolve individuals, evaluate fitness, select individuals to survive to the next generation*. Genetic Algorithms exhibit the trait of broad applicability\[6\], as it can be applied to any problem whose solution domain can be quantified by a function, that needs to be optimised. GAs find application in the many fields, such as Engineering\[25\], Job scheduling\[26\], Process control, etc. They are adaptive to changing environments, as they use the previously evolved solution to provide a basis that one can tap into to make further improvements to the solution domain\[6\]. Contrary to other optimisation methodologies, GAs do not need to return to the initial state of computation. They can be implemented for all sorts of problem types, as long as one
adheres to the basic guidelines. The evolution process lends itself to parallel processing techniques[21], which opens up new avenues to explore in terms of hybridisation with other optimisation techniques, which can give rise to more efficient ways to solve problems in general. One could for example use a conjugate-gradient minimisation after instituting a primary search with Genetic Algorithms[6].

3.1.2 Non-binary Encodings

By convention, a chromosome is a sequence of symbols and that these symbols are binary in form, thus exhibiting a cardinality of 2. The most effective approach is though when the encoding or the alphabet employed is problem-specific and most fittingly represents the solutions in the search space, as it will be illustrated in this thesis. It shows that higher-cardinality alphabets are more suited to certain type of problems[5, 6]. Empirical studies of high-cardinality alphabets have typically applied chromosomes where each encoding represents an integer[22, 27], or a floating-point number[28]. But those present problems, in terms of the subject matter covered, on how to apply genetic operators such as mutation and crossover to those encodings.[5] defines the following Crossover and Mutation genetic operators for non-binary representations:

1. Crossover:
   - Average : Apply the arithmetic average of the two parent genes.
   - Geometric mean: Apply the square root of the product of the two values.
   - Extension: Take the difference between two values and add to the higher or subtract it from the lower of the two values

2. Mutation:
- Random replacement: Replace the value at specific locus with a random value
- Creep: Add and subtract a small, randomly generated amount.
- Geometric creep: Multiply by random amount close to one.

The random number generator in the above operations might base on a variety of distributions from exponential, uniform within a range to Gaussian or binomial models, Gaussian being the preferred one. [6] states that experiments were conducted with floating point representations and it was determined that floating point representations are faster, more consistent from run to run, and provide higher precision, especially in large domains where binary coding would require unusually long representations. At the same time its performance can be enhanced by the application of special operators to achieve high performance accuracy[28].

### 3.1.3 Knowledge Based Techniques

GA schemes usually apply the traditional crossover and mutation operators, but in certain cases and also in this research undertaken in this thesis, I would rather advocate using a specific type of operators for the task at hand, preferentially that is guided using domain knowledge. This makes the GA less generic and more problem specific, but may improve performance significantly[6, 29]. Where a GA is being designed to tackle a real-world problem, and has to compete with other search and optimization techniques, the incorporation of domain knowledge often is advisable[6, 29]. Domain knowledge may be used to prevent obviously unfit chromosomes or prevent the algorithm from honing in on a sub-optimal solution, or even violate problem constraints, from being produced in the first place[6, 29]. This avoids wasting time evaluating such individuals, and avoids
introducing poor performers into the population. [6] states that areas of utilisation would be:

- Guiding the initialisation of the population at the beginning of the process[6].

- Guiding the crossover operator, so that the crossover operation does in fact yield fitter offspring in order to prevent weaker individuals being introduced into successive matings pools[6].

- Guiding the mutation operator. For example, the application of gradient like bitwise (G-bit) improvement for one or more highly fit chromosomes, allows the change of each bit one at a time to see if the fitness improves. If it does, one would replace the original with the altered chromosome[6].

[6] advise to utilise hybrid GA schemes, combining GAs with other heuristic search algorithms, such as hill climbing or greedy search. The GA would be utilised to locate the solution in the search space or come close to it and then use those optimisation schemes to hone in on the optimal value, thus improving the efficiency and competence of the GA[6].

3.2 Parallel Genetic Algorithms

3.2.1 Discretised Genetic Algorithms

Genetic Algorithms are very effective in solving very complex problems. This positive trait can be unfortunately offset by very long execution times, due to the traversal of the search space. As mentioned in section 3.1.1.6, GAs lend themselves to parallelisation and thus the fitness values can be determined independently for each of the candidate
solutions, utilising one of the parallelisation schemes: \textit{master-slave models, multiple-deme, and fine-grained PGAs}[6]. I will focus on the \textit{master-slave models and the multiple-deme} parallelisation schemes. The \textit{master-slave} parallelisation scheme are relatively easy to implement. On the other hand, the \textit{multiple-deme} parallelisation scheme currently dominates the research on PGAs due its complexity and the fact that its behavior is affected by many parameters[6].

\subsection{3.2.2 Master-slave Parallelisation}

Master-slave GAs, also denoted as Global PGAs, involve a single population, but distributed amongst multiple processing units for determination of fitness values and the consequent application of genetic operators. It lends itself to computation on shared-memory processing entities or to any type of distributed system topology, like for example grid computing [9, 10]. Sivanandam and Deepa[6] have provided the following depiction of the Master-Slave Parallel Genetic Algorithm:

\begin{algorithm}[H]
\caption{Generic Master-Slave Parallel Genetic Algorithm}
\begin{algorithmic}
\State produce an initial population of individuals
\State evaluate the individual's fitness
\ForAll {individuals} \textbf{do in parallel}
\State evaluate the individual's fitness
\End{\textbf{parallel for}}
\While {not termination condition} \textbf{do}
\State select fitter individuals for reproduction
\State produce new individuals
\State mutate some individuals
\ForAll {individuals} \textbf{do in parallel}
\State evaluate the individual's fitness
\End{\textbf{parallel for}}
\State generate a new population by inserting some new good individuals and by discarding some old bad individuals
\End{\textbf{while}}
\end{algorithmic}
\end{algorithm}
Master-slave PGAs are easy to implement and they can be a very efficient method of parallelisation when the evaluation needs considerable computations, thus reducing the execution time of the algorithm. Besides, the method has the advantage of not altering the search behaviour of the GA\cite{6, 30}, so all the theory available for simple GAs can be applied directly without any modifications\cite{6}.

### 3.2.3 Multiple-deme Parallelisation

Multiple-population or Multiple-deme PGAs allow for the populations to be partitioned into disjoint, autonomous sub-populations and undergo subsequent evolution, independently of each other, thus in parallel. The complexity arises when trying to find a balance between the communication cost, trying to constrain it to a minimum, whilst ensuring a diverse mixture of individuals from the respective sub search spaces. I need to establish an optimal segment sizing approach, in order to find the optimal number of demes which will ensure diversity and a comprehensive set of candidate solutions. This will lead to optimal convergence\cite{10}. Multiple-deme parallel GAs are also called ”coarse-grained” or ”distributed” GAs, due to the fact that the communication to computation ratio is low, and they are often implemented on distributed-memory computers\cite{30}. They consist of several sub-populations that undergo evolution independently of each other and at pre-defined intervals, called epochs, exchange individuals with other sub-populations. The arrangement and interconnectivity between the different sub-populations resembles an archipelago, a cluster of islands, thus deeming the Multiple-deme model an ”island model”. These algorithms are quite popular, but very difficult to understand, configure and optimise due to unpredictability of the migration process. Additionally, there exist many parameters that need to be configured that affect their accuracy and efficiency \cite{31}. 
Multiple-deme parallel GAs are also very difficult to configure as they introduce fundamental changes in the operation of the PGA and exhibit a different behaviour to simple GAs[6]. The key drivers are the topology of the different interconnected sub-populations, the deme size, and the migration rate [31]. Migration is geared at introducing diversity and better exploration of the search space compared to other types of GAs.

**Algorithm 2** Generic Multiple-deme Parallel Genetic Algorithm

1. initialize P sub-populations of size N each
2. generation number = 1
3. while not termination condition do
4.   for all individuals do in parallel
5.     evaluate and select the individuals by fitness
6.   for all individuals do in parallel
7.     evaluate the individual’s fitness
8.     if generation number mod frequency = 0 then
9.       send K < Nbest individuals to neighbouring population
10.      receive K from neighbouring population
11.      replace K individuals in the sub-population
12.     end if
13.   end parallel for
14. end parallel for
15. generation number ← generation number + 1
16. end while

3.2.3.1 Model Parameters

Multiple-deme PGA key drivers of efficiency are the following parameters[30]:

- The *number of islands* representing separate demes as part of the island cluster configuration.

- The *migration topology* depicting the interconnectivity and arrangement of islands.

- The *migration rate* defining the number of individuals to be exchanged between respective demes.
• The *migration frequency* defining how often a exchange of individuals transpires.

This measure is directly related to the epoch, as the it signifies the period at which the migrations take place.

• The *migration algorithm* specifying all the remaining details.

### 3.2.3.2 Migration Topology

There is a plethora of migration topologies. [1] have explored some of different migration topologies. Figure 3.9 depicts different island cluster configurations. In the past the migration model or topology was largely dependant on the hardware configuration and platform the computations were run on [32]. The *Chain topology* is the simplest of the migration topologies, where the communication can transpire in a uni- or bi-directional manner. The first deme is not partaking in the exchange of individuals at the end of the epoch, as can be deduced from Figure 3.9. A more versatile arrangement would be that of a *Ring topology*. Again, communication may be uni-or bi-directional and is utilised in many traditional GA Islands models [1]. The *Ring + 1 + 2* and *Ring + 1 + 3* archipelago topologies are extensions to the *Ring topology*, which distinguish themselves by increasing the degree of connectivity between the islands. The increase in number of

<table>
<thead>
<tr>
<th>Topology</th>
<th>Number of edges</th>
<th>Valid number of nodes</th>
<th>Diameter</th>
<th>Degree of connectivity</th>
<th>Clustering coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chain (Stepping stone)</td>
<td>n-1</td>
<td>n ∈ N</td>
<td>n-1</td>
<td>0,1</td>
<td>0</td>
</tr>
<tr>
<td>Ring</td>
<td>n</td>
<td>n ≥ 3</td>
<td>n-1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Ring + 1 + 2</td>
<td>2n</td>
<td>n ≥ 5</td>
<td>( \frac{2n}{2} )</td>
<td>4</td>
<td>0.5</td>
</tr>
<tr>
<td>Ring + 1 + 2 + 3</td>
<td>3n</td>
<td>n ≥ 7</td>
<td>( \frac{3n}{3} )</td>
<td>6</td>
<td>0.6</td>
</tr>
<tr>
<td>Lattice</td>
<td>2n(n - ( \sqrt{n} ))</td>
<td>n = k^2</td>
<td>2(( \sqrt{n} - 1 ))</td>
<td>2,3,4</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 3.1: Migration Topology characteristics
Figure 3.9: Schematic representation of migration topologies: A. Chain B. Unidirectional ring C. Ring D. Ring + 1 + 2 E. Ring + 1 + 2 + 3 F. Torus G. Cartwheel H. Lattice [1]
edges is tabulated in 3.1. The topologies also affect the number of nodes that comprise the topology arrangement, which entail a minimum number of nodes to be configured, in order to be able to harness the full potential of the specific migration approach.

### 3.2.3.3 Number of Islands

The number of islands is dependant on the computing platform used, the underlying hardware configuration or the migration topology utilised. PGAs scale very well and with more hardware at my disposal for the goal of computation, I am able to partition the search space into more sub-populations and henceforth improve the overall efficiency of the computations. The migration topology also has a pronounced effect on the number of sub-populations utilised. As tabulated in Section 3.2.3.2, the topology chosen will necessitate a certain number of islands to be declared. In using a specific migration scheme, I need to be cognisant of the fact that the greater the number of edges, the greater the number of exchanges between the respective sub-populations within the archipelago and also the higher the communication overhead. But [32] state, that the higher the number of islands, the better the result of the computation. They also state that this only holds for certain type of problems and algorithms, so quintessentially there is no rule of thumb as to the optimal number of islands. The onus lies with the researcher to apply different migration topologies and investigate the effects of the different parameters on the efficiency of the algorithm.
Chapter 4

Computational Platform

In order to be able to fully harness the capabilities of a Parallel Genetic Algorithm as described in the Chapter 3, I need to make use of a parallel computing platform. CUDA is such a platform. It is a platform and a programming model invented by NVIDIA. This chapter will firstly introduce conventional parallel computing architectures and then acquaint the reader with the CUDA parallel computing platform, specifically chosen for the task of delivering cluster analysis results in an efficient manner. It forms the backbone of the research undertaken and also allows for the proposed clustering analysis approach to be employed.

4.1 Parallel computing

4.1.1 Architectures

There exist several different parallel architectures. They can be grouped into four categories based upon the number of instructions that can be performed concurrently and the number of data streams these instructions can operate upon. The classifications were
first proposed by Flynn[33] in 1966 and are the following: single instruction stream/single data stream (SISD), single instruction stream/multiple data stream (SIMD), multiple instruction stream/single data stream (MISD), and multiple data stream/multiple instruction stream (MIMD)[34]. The MIMD classification has replaced the SIMD as the de facto parallel platform today. The MIMD classification includes shared memory multiprocessor systems and message-passing multi-computers[35]. The architecture of shared memory multiprocessors focuses on the idea of a globally addressable memory location. In shared memory multiprocessor machines, also referred to as symmetric multiprocessors (SMPs), the memory location is physically equidistant or appears physically equidistant from all processors. Variations on the traditional shared memory architecture exist that relax the scalability limitations of traditional shared memory machines, yet still provide the appearance of equidistant memory. These architectures are referred to as distributed shared memory machines and fall under the shared memory category. These include cache coherent non-uniform access (CC-NUMA) machines[34]. In message passing multi-computers, or distributed memory architectures, each processor has its own memory location and the memory is not globally addressable. Parallel architectures in the distributed memory classification do not suffer from the scalability restrictions of the shared memory architectures and hence have gained popularity in the high performance computing segment.

4.1.2 Parallel programming and design paradigms

Programming in parallel environments has been reliant on the use of compiler directives and libraries. Those allow for the integration of parallelism directly into existing code instead of having to use a new language, that is designed specifically for the parallel
environment. This allows the programmer to stay at least somewhat in a familiar environment, where syntax is concerned and allows already written and tested code to be in some cases fairly easily parallelised. Programming in the distributed memory environment has been dominated by message passing interface (MPI) for the last several years. MPI provides a standard for implementations of message passing libraries for many parallel architectures; it is highly portable and can also be used in shared memory environments[36]. Shared memory programming has seen a resurgence of interest with the development of OpenMP, which utilizes compiler directives to easily parallelise sections of code[37]. The following design paradigms are key to programming in a parallel environment and determine the success or failure of an implementation: *data placement, communication latency and synchronisation* [38].

### 4.1.3 Rationale

A proper design of a parallel algorithms along with careful consideration of the chosen platform leads to substantial reductions in execution time. Additionally, new algorithm designs provide benefits in solution quality due to the application of parallelism. However, without careful consideration to design and platform choice, it is also possible to not obtain the full benefit of the parallel computing environment and in the worst case negative results in performance[39].

### 4.2 GPU

Graphics processor units (GPU), traditionally designed for graphics rendering have emerged as massively-parallel ‘co-processors’ to the central processing unit (CPU). According to Flynn’s taxonomy, as stated in 4.1.1, GPUs are classified as SIMDs and belong
to the class of emerging parallel architectures. It has emerged, that small-footprint desktop supercomputers with hundreds of cores can deliver teraflops peak performance at the price of conventional workstations\cite{40}. This can be attributed to the increasing hardware requirements for modern computer games. GPUs offer floating-point calculation much faster than today’s CPU and beyond graphics applications they are well suited to computations which need to be highly parallelised\cite{40}. In order to be able to develop applications to run on the GPU, general purpose high-level languages for GPUs have been developed in order to minimise the complexity of using graphics programming paradigms and apply them to the non-graphics applications realm. One such is NVIDIA’s Compute Unified Device Architecture (CUDA) platform\cite{7}.

### 4.3 NVIDIA CUDA platform

![CUDA Architecture](image)

**Figure 4.1:** Three-Layered CUDA Application Architecture

Compute Unified Device Architecture (CUDA) is NVIDIA’s platform for massively parallel high-performance computing on the NVIDIA GPUs. In order to have hardware cater only for high performance computing, NVIDIA developed the Tesla range of GPU products that caters for the simulations and computations in the high-end market like the oil, gas and computational finance industry. At its core are three key abstractions: a hierarchy of thread groups, shared memories, and barrier synchronisation\cite{7, 8, 41}.
They are provided to the developer as a minimal set of language extensions, which provide a 'platform for fine-grained data parallelism and thread parallelism, nested within coarse-grained data parallelism and task parallelism'[7, 8]. Task parallelism allows for the parallelisation of computer code across multiple processors in parallel computing environments. Task parallelism focuses on distributing execution processes across different parallel computing nodes, whilst data parallelism focuses on distributing the data of a data-set across different parallel computing nodes and the execution of the same process across the elements of the dataset[7].

4.3.1 Execution Environment

The CUDA execution model is based on the primitives of threads, thread blocks, and grids. Code artefacts, denoted by the term kernel, are executed by lightweight individual threads on the device within a thread block and grid. When a kernel function is invoked, the grid’s properties are described by an execution configuration, which has a special syntax in CUDA[8]. The kernel launches are asynchronous, meaning that the GPU will return control to the CPU, even before the invoked kernel completed, which means that successive kernel function invocations will be initiated without waiting for the completion of the previously invoked kernel.

4.3.2 Thread hierarchy

The thread, also known as a stream, is a basic unit of manipulating data in CUDA, which is a 3-component vector, so that threads can be identified using a one-dimensional, two-dimensional, or three-dimensional index, forming a one-dimensional, two-dimensional, or
three-dimensional thread block. Those multi-dimensional blocks are organized into one-dimensional or two-dimensional grids, each block can be identified by one-dimensional or two-dimensional index, and all grids share one global memory [7]. Each thread has a unique local index threadIdx in its block, and each block has a unique index blockIdx in the grid. The dimensions of the thread are accessible through a built-in variable blockDim, the dimensions equivalently stored in the variable gridDim. Figure 4.3 depicts a fine-grained view of the thread hierarchy. The index of a thread executing in a grid
can be uniquely identified as per the mathematical depiction in 4.1.

\[
\text{thread}(x, y, z) = \begin{cases} 
  x &= \text{blockIdx}.x \times \text{blockDim}.x + \text{threadIdx}.x \\
  y &= \text{blockIdx}.y \times \text{blockDim}.y + \text{threadIdx}.y \\
  z &= \text{blockIdx}.z \times \text{blockDim}.z + \text{threadIdx}.z 
\end{cases}
\] (4.1)

For instance, kernels can use these indices to compute array subscripts. Threads in a single block will be executed on a single multiprocessor, using a common data cache, \textit{device memory}, to share data. The kernel execution transpires in groups of 32 threads, denoted by a \textit{warp}. A warp will always be a subset of threads from a single block.

Threads in different blocks may be assigned to different multiprocessors concurrently, to the same multiprocessor concurrently, or may be assigned to the same or different multiprocessors at different times, depending on how the blocks are scheduled dynamically.
There is a hard limit on the size of a thread block, this being 512 threads or 16 warps for Tesla, 1024 threads or 32 warps for Fermi. Thread blocks are always created in warp units, so there is no point in trying to create a thread block of size that is not a multiple of 32 threads; all thread blocks in the whole grid will have the same size and shape. A Tesla multiprocessor can have 1024 threads simultaneously active, or 32 warps. These can come from 2 thread blocks of 16 warps, or 3 thread blocks of 10 warps, 4 thread blocks of 8 warps, and so on up to 8 blocks of 4 warps; there is another hard limit of 8 thread blocks simultaneously active on a single multiprocessor. As mentioned, Fermi can have 48 simultaneously active warps, equivalent to 1536 threads, from up to 8 thread blocks.

4.3.3 Memory hierarchy

There are multiple data caches that CUDA threads may access data from during their execution, as illustrated by Figure 4.4 [7].

4.3.3.1 Registers

Registers are the fastest memory units on a GPU, and each multiprocessor on the GPU has a large, but limited, register file which is divided amongst threads residing on that multiprocessor. Registers are private for each thread, and if the threads use more registers than at it’s disposal, a register spillover incurs, with L1 cache and global memory being affected. The more threads utilised, the lower the register availability to each thread [42].
4.3.3.2 Shared memory

The second fastest memory type is shared memory, which exhibits similar access times to registers. It acts a common data cache for all threads belonging to a single thread block, enabling threads to exchange data with each other. Its size is limited to 48 KB, which can impose a limit on threads per block, if a high amount of data needs to be stored or exchanged by threads in a thread block. Shared memory is physically organized into 32 banks that serve one warp with data simultaneously. However, for full speed, each thread must access a distinct bank. Failure to do so leads to more memory requests, one for each bank conflict. A classical way to avoid bank conflicts is to use padding,
where shared memory is padded with an extra element, so that neighbouring elements are stored in different banks thus ensuring singular access to the bank [42].

4.3.3.3 Global memory

Global memory is the main memory of the GPU. It exhibits fast bandwidth, but has a high latency, due to the fact that it takes an order of hundreds of clock cycles to fetch a data value from global memory. This is hidden through rapid switching between threads, but there are still pitfalls. First of all, just as with CPUs, the GPU transfers full cache lines across the bus, called coalesced reads. As a rule of thumb, transferring a single element consumes the same bandwidth as transferring a full cache line. Thus, to achieve full memory bandwidth, I should enforce that warps access continuous regions of memory and the full utilisation of cache lines, which involves address alignment achieved again by padding. To fully occupy the memory bus, the GPU also uses memory parallelism, in which a large number of outstanding memory requests are used to occupy the bandwidth. This is both a reason for high memory latency, and a reason for high bandwidth utilisation [42].

4.3.4 Synchronisation

After performing any type of computation, the need might arise to collate the results. This might be necessary as in the case on performing summation on a data-set with a significant element count. This operation belongs to a categorisation of processes denoted by the technical term reduction, which also involves the operations such as sum, min, max, average, that necessitate the temporary storage of data and in such data communication mechanism between respective threads. This might transpire on
Chapter 4. *Computational Platform*

<table>
<thead>
<tr>
<th>CPUFunction()</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>kernelFunction&lt;&lt;dimGrid, dimBlock&gt;&gt;(...);</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>cudaThreadSynchronise();</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>}</td>
</tr>
</tbody>
</table>

**Figure 4.5:** CPU Explicit Synchronisation

a intra-block and an inter-block level and entails various synchronisation approaches that will allow for consolidation of results and enable further processing in an efficient manner.

### 4.3.4.1 CPU

**CPU Explicit Synchronisation** CPU explicit synchronization is depicted in the code snippet in Figure 4.5, in which kernel `func()` is the kernel function, and the implicit synchronisation barrier is implemented by terminating the current kernel execution and launching the kernel again, thus creating a barrier between the two kernel launches. In addition, in the CPU explicit synchronization, the function `cudaThreadSynchronize()` is utilised. It blocks until all the threads on the device have executed the kernel function.

Once this has been achieved and the control has been passed back to the CPU, a new kernel can be invoked. Thus, in CPU explicit synchronization, the three operations of a kernel’s execution are executed sequentially across different kernel launches. This phenomenon is depicted in Figure 4.5, where `func()` is the kernel function, and the implicit synchronisation barrier is implemented by terminating the current kernel execution and launching the kernel again, thus creating a barrier between the two kernel launches. In addition, in the CPU explicit synchronization, the function `cudaThreadSynchronize()` is utilised. It blocks until all the threads on the device have executed the kernel function.

Once this has been achieved and the control has been passed back to the CPU, a new
kernel can be invoked. In summary, three operations of a kernel’s execution are executed sequentially across different kernel launches.

**CPU Implicit Synchronisation** The code snippet in Figure 4.6 depicts the omission of the synchronisation function `cudaThreadSynchronize()`. As per the discussion in 4.3.1, kernel launches are asynchronous, but the successive kernel launches are pipelined and thus the executions implicitly synchronised with the previous launch, for the exception of the first kernel launch [43][7].

### 4.3.4.2 GPU

CUDA provides a simple and efficient mechanism for thread synchronisation within a block, which forces all threads to wait, until they all reach this point of execution in the code. The thread synchronisation mechanism is especially useful when using shared memory to exchange data between threads in a block. The barrier function `synthreads()` ensures proper communication, the process being referred to as intra-block synchronisation. As stated in Section 4.1.1, CUDA adapts to the Single Program Multiple Data (SPMD) paradigm, where a single kernel or block of code concurrently processes partitioned segments of a collection of data, the same block of instructions processing a different segment of source data. With that in mind, data communication across different blocks might have not being considered by the CUDA developers to be viable with that type of architecture or not considered to be pertinent, which accentuates the fact that inter-block communication is not directly supported during the execution.
of a kernel. The explicit or implicit CPU synchronisation approach covered in 4.3.4.1 try to address the functionality of *inter-block communication*, but in my opinion not effectively. This poses a problem when it comes to the realisation of performant Parallel Genetic Algorithms on the CUDA platform. It is not limited to those type of algorithms, but other algorithms are out of scope of this paper. However, [43] have proposed three strategies namely *GPU simple synchronisation*, *GPU tree-based synchronisation*, *GPU lock-free synchronisation*.

**GPU simple synchronisation**  The algorithm 3 depicts the notion of GPU Simple Synchronisation. It uses a global mutex variable to keep count of all the thread blocks that reach the synchronisation point. This coupled with inter-block synchronisation will ensure that all threads from all the blocks synchronise at the barrier and no thread will proceed until all the threads have reached that execution point. Only one thread, the *leading thread*, from the block will increase the counter and interrogate the state of the mutex, the rest will synchronise via the barrier function. Once the mutex’s value equals a certain value, either being a number of blocks allotted for kernel execution or some pre-defined value, the ‘sluice’ will be opened and the threads are allowed to proceed. The value of the mutex is incremented using and atomic function that prevents dirty reads or read-write conflicts [43].

**Algorithm 3 GPU Simple Synchronisation**

```
Set barrier value $g_{\text{barrier\_value}}$
Initialise mutex variable $g_{\text{mutex}}$

$tid \text{ getThreadId.x * blockDim.y + threadIdx.y}$  \hspace{1cm} ▷ id of thread in block
if $tid = 0$ then  \hspace{1cm} ▷ Is it the leading thread? If yes, then continue
  $g_{\text{mutex getsg_mutex + 1}}$  \hspace{1cm} ▷ Atomic increment
  while $g_{\text{mutex}}! = g_{\text{barrier\_value}}$ do  \hspace{1cm} ▷ Spin until $g_{\text{mutex}} = g_{\text{barrier\_value}}$
    end while
  end if
_syncthreads()
```
**GPU tree-based synchronisation** The GPU tree-based synchronisation is an improvement on the GPU simple synchronisation approach, which reduces the time of the process to update the mutex variable. This can be achieved by increasing the concurrency of the process of updating the mutex. As described in the previous Section 4.3.4.2, the increment operation needs to be atomic and all writes need to be sequential in order to maintain consistency. Figure 4.7 depicts the approach of a 2-level tree-based approach. The thread blocks are subdivided into $m$ thread block groups, each group’s completion state maintained by a group mutex variable $g_{mutex_i}$. Synchronisation transpires on the group level first and proceeds to synchronisation on the block level, so two sets of mutex variables are incremented and queried[43].

![Figure 4.7: GPU tree-based synchronisation](image)

**GPU lock-free synchronisation** The GPU lock-free synchronisation does away with costly atomic operations and aims at maintaining the state without the use of a mutex variable. Synchronization of different thread blocks is controlled by threads in a single block, which can be synchronized by calling the barrier function \texttt{synthreads()}. Algorithm 4 conveys the core aspects of the synchronisation approach. Two array structures are used to realise synchronisation. The indices of these arrays correspond to a block id, meaning that element at index $i$ is mapped to thread $block_i$. The leading thread drives synchronisation. If block $i$ is ready to initiate communication, its leading thread will set the value to a pre-defined value at its mapped \texttt{arrayIn} index location.
and will wait until the same value has been set at its mapped \emph{arrayOut} index location, before it the 'sluice' is opened and the threads within all the blocks can proceed beyond the synchronisation point. Analogous to having a leading thread in block, a leading block is chosen to drive the next stage of synchronisation, namely the first block. Any other block in the grid can be chosen, but in order to maintain consistency and clarity I should revert to using the first block of the grid. All the threads in the leading block will read the value in \emph{arrayIn}, i.e. the $i^{th}$ thread will read the value at index $i$ in the array. Should the value be that of the pre-defined barrier value, then the thread will set the value of the corresponding element at index position $i$ in \emph{arrayOut}. This approach further improves the level of concurrency as all the threads of the leading block are assigned to oversee the state of the blocks in the grid and pull the proverbial lever so that collectively they can open the 'sluice' [43].

\textbf{Disadvantages of GPU synchronisation} \quad Due to the latency on the call between CPU and GPU, CPU synchronisation incurs a significant overhead and GPU synchronisation is preferred. There is a downside to GPU synchronisation though, that in my mind discredits the whole investigation and methodology. A constraint exits on the number of blocks that can be configures and the number needs to smaller or equal to the Streaming Multiprocessors(SM) on the GPU card. If the number of thread blocks is bigger than the number of SMs on the card, execution will deadlock. This is due to the non-preemptive warp scheduling behaviour of the GPU. If the number is bigger, this will then automatically infer that more than one thread block will be assigned to a SM for execution. The unscheduled thread blocks will not be executed, due to the fact that the active blocks, resident on the SM, are in a state of busy-waiting for the unscheduled thread blocks at the synchronisation point. Further, the published GPU synchronisation approaches just seem not to be a viable option for synchronisation. I am constrained to
Algorithm 4 GPU lock-free synchronisation

Initialise barrier value $g_{\text{barrier\_value}}$

$tid \leftarrow \text{threadIdx.x} \ast \text{blockDim.y} + \text{threadIdx.y}$ \hspace{1cm} \triangleright \text{id of thread in block}$

$numBlocks \leftarrow \text{ blockDim.y} \ast \text{ blockDim.x}$ \hspace{1cm} \triangleright \text{number of blocks executing}$

$\text{blockid} \leftarrow \text{ blockIdx.x} \ast \text{ gridDim.y} + \text{blockIdx.y}$ \hspace{1cm} \triangleright \text{id of block in grid}$

if $tid = 0$ then

\hspace{1cm} $\text{arrayIn}[\text{blockId}] \leftarrow g_{\text{barrier\_value}}$

end if

if $\text{blockid} = 1$ then

\hspace{1cm} if $tid < numBlocks$ then

\hspace{2cm} while $\text{arrayIn}[\text{blockId}]! = g_{\text{barrier\_value}}$ do \hspace{1cm} \triangleright \text{Spin until}$

\hspace{3cm} $gmutex = g_{\text{barrier\_value}}$

\hspace{3cm} Spin

\hspace{3cm} _syncthreads()

\hspace{3cm} if $tid < numBlocks$ then

\hspace{4cm} $\text{arrayOut}[\text{blockId}] \leftarrow g_{\text{barrier\_value}}$

end if

end while

end if

if $tid = 0$ then

\hspace{1cm} while $\text{arrayOut}[\text{blockId}]! = g_{\text{barrier\_value}}$ do \hspace{1cm} \triangleright \text{Spin until}$

\hspace{2cm} $gmutex = g_{\text{barrier\_value}}$

\hspace{2cm} Spin

\hspace{2cm} _syncthreads()

end if

end if

end if

end if

end while

end if

end if

end if

end if

a very limited number of configurations, whilst even with the overhead, GPU synchronisation adds more flexibility and might even allow for improvements in performance due to the same trait. However, it would be premature to settle on a approach and a comprehensive empirical study needs to be conducted, but that is beyond the scope of the research undertaken. Table 4.1 depicts configurations for some of the NVIDIA GPU cards on the market today. It is quite evident I am limited to a maximum of 16 thread blocks per kernel execution. With a maximum thread count of 1024 threads per bock, I would operate on a data-set of 16384 distinct data values, which for some problems might be sufficient, but when dealing with data-sets in cluster analysis utilising PGAs this just might be too constrictive.
### Table 4.1: NVIDIA GPU cards

<table>
<thead>
<tr>
<th>Feature</th>
<th>Tesla S2050</th>
<th>GTX 560Ti</th>
<th>GTX 580</th>
<th>GTX 660Ti</th>
<th>GTX 680</th>
</tr>
</thead>
<tbody>
<tr>
<td>CUDA Cores</td>
<td>448</td>
<td>384</td>
<td>512</td>
<td>1344</td>
<td>1536</td>
</tr>
<tr>
<td>Streaming Multiprocessors (SM)</td>
<td>14</td>
<td>8</td>
<td>16</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Compute Capability</td>
<td>2.0</td>
<td>2.1</td>
<td>3.0</td>
<td>3.0</td>
<td>3.0</td>
</tr>
</tbody>
</table>

#### 4.3.5 Challenges

One fundamental challenge of programming in CUDA is adapting to the data parallelism paradigm, which differs from traditional parallel paradigms in that multiple instances of a single program act on a body of data. Each instance of this program uses unique offsets to manipulate pieces of that data. Data parallelism fits well in this paradigm while task parallelism does not. Once the programming paradigm is understood, there are additional difficulties in using the CUDA language. Since each warp is executed on a single SIMD processor, divergent threads in that warp can severely impact performance. Divergent threads are threads in a warp that follow different execution paths. If this happens, the different execution paths must be serialized, since all of the threads of a warp share a program counter; this increases the total number of instructions executed for this warp. Once all the different execution paths have completed, the threads converge back to the same execution path\[41\]. Hence, all other threads must effectively wait until the divergent thread rejoins them. Thus, divergence forces sequential thread execution, negating a large benefit provided by SIMD processing\[7, 41\]. Another limitation in CUDA is the lack of communication and consequently the lack of synchronization between thread blocks and limited capability of communication between blocks. This creates possible problems of data consistency, typical of parallel modification of singular values and the design and implementation of certain type algorithms on the CUDA platform. However, as described in 4.3.4 \[43\] have proposed efficient methods for inter-block
communication, that does not involve transferring control over to the CPU and thus necessitating the enforcement explicit synchronisation of all the threads on the CPU. But, on the other hand, Section 4.3.4.2 highlights the disadvantages of those inter-block communication mechanisms and until such time as these have being addressed and resolved by the NVIDIA CUDA developers, the implementation of those approaches remains more a theoretical exercise than reality.

### 4.3.6 Performance tuning techniques

"We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil" [44]. Optimising in itself is a difficult task and an even greater task to perform on cutting-edge technology such as GPUs. The CUDA platform features a profiling platform, which provides an invaluable tool for that task. Optimisation is a ongoing exercise, where I will have to isolate one problem area after another, in order to attain a collective improvement in performance. The core bottlenecks for bad performance or degradation in processing throughput on the GPU are the following:

- Kernel might be limited to instruction throughput, memory throughput or latencies.

- CPU-GPU communication[42], which leads to high latency. Please refer to Section 4.3.3.3.

1. The transfer of data between the host and the device should be minimised or if unavoidable I should rather batch small transfers into one large transfer due to the overhead incurred with the process of initialising a CPU-device data exchange.
2. Utilise optimal kernel launch configurations in order to harness as much of the device’s computational capability as possible.

3. Make use of asynchronous data transfers with computations. This is only possible with the utilisation of pinned memory. Pinned memory is memory allocated on the host, that is prevented from being swapped out and which allows for faster transfer times between the host and the device and thus higher throughputs. Figure 4.8 depicts the timeline of execution for two code segments. In the top segment the computation and data transfer occur in a sequential manner. In the bottom segment concurrent copy and kernel execution allows for the overlap of kernel execution on the device with the data transfers between the host and device. This is only a viable option if the results can be segmented into pieces and transferred back to the host as soon as the segment has been computed and prepared for transfer, and I am not reliant on the computational result as a whole.

4. Avoid divergent execution paths within the same warp.

5. Minimise redundant accesses to global memory as possible. It is of paramount importance that accesses to global memory transpire in coalesced manner, so as to minimise the clock cycles for writes and reads as fewer transactions will be needed to serve the thread memory access pattern. The concurrent accesses of the threads of a warp will coalesce into a number of transactions equal to the number of cache lines necessary to service all of the threads of the warp.

6. Optimise instruction usage by avoiding instructions that have low throughput. This equates to trading precision over throughput and utilise single-precision over double-precision operations.
7. The number of threads per block should be a multiple of the warp size. The warp size on the CUDA devices is 32 threads. This will provide optimal computing efficiency and ensures coalescing of the memory accesses, so that memory accesses transpire in an optimal manner and no unnecessary execution time is wasted on sub-optimal fetch operations by the SMs. The minimum size of threads per thread blocks should be 64, only in the case if multiple concurrent blocks execute per thread block.

![Figure 4.8: Asynchronous and Sequential Data Transfers with Computations](image)

### 4.4 PGA implementations on GPUs

As stated in the introduction to this chapter, CUDA allows me to fully harness the capabilities of Parallel Genetic Algorithms. [9, 10] describe the approaches taken to implement PGAs on the CUDA platform.
4.4.1 GAROP: Genetic Algorithms framework for Running On Parallel environments

[45] developed GAROP, a PGA framework which executes in parallel environments. The target parallel processing architectures are multi-core CPUs and GPUs. The purpose of GAROP is to have a user-friendly Application Programming Interface (API), which will increase the user’s productivity by reducing the processing time without the specific knowledge regarding parallel architecture and parallel processing. The target user group of GAROP is presumed to be primarily GA developers. Users utilise a template specific to the parallel execution environment their PGA will execute on, and deploy the templates and the code for evaluation function. The API encapsulates the communication mechanisms and the implementation of scheduling for evaluation tasks. Thus, the users can execute PGAs in parallel environments without needing to have knowledge of communication mechanisms and schedulers, specific to the parallel execution environment.

GAROP introduces the concept of a data store, namely an individual pool, as an interface to link users to parallel environments. The individual pool stores individuals, which are to be evaluated in parallel, automatically. Using this design, any GA model can be executed in parallel. The individual pool has two queues: a ‘throw queue’, which stores individuals tasked for evaluation, and a ‘get queue’, which stores evaluated individuals. As soon as individuals are sent to the ‘throw queue’, they are routed to the calculation resources and evaluated. Evaluated individuals are stored in the get queue. Figure 4.9 depicts GAROP’s conceptual architecture.
GAROP uses a Master-slave parallelisation scheme for computations to be executed on the CUDA platform. The GA runs on the CPU and initiates a sub thread, in order to handle data transfers to and from the GPU. The configuration such as number of blocks and thread, length of an individual, and number of individuals to be processed, are computed on the GPU by a kernel function call. Individuals, that are sent to GPU, are stored in GPU constant memory. Constant memory is accessible to all threads and the CPU, but is limited in size. It is used to store data that will not change over the course of a kernel execution. Each CUDA thread acquires individual information from constant memory and commits data, pertaining to the evaluation of the individual, to GPU global memory. Figure 4.9 depicts GAROP’s conceptual architecture for the GPU.
4.4.2 Hybrid Master-slave and Multiple-deme implementation on the CUDA platform

[10] implemented a hybrid between a Master-slave and Multiple-deme parallelisation approach for the CUDA GPU platform. They ran the genetic operations and fitness evaluations on the GPU, utilising GPU shared memory to store computational data. They divided block shared memory (see Section 4.3.3.2) into $n$ number of parts, which forms a series of continuous addresses. Thus, each block can access or write to each sub-population independently. Due to access to high-speed shared memory in each thread block, the communication cost is being kept to a minimum. They devised a hierarchical PGAs, which is a hybrid of a Multi-deme PGA at a higher level and Master-Slave PGA at lower level. The following steps are followed in the execution of the proposed PGA:

1. Initialise a single large panmictic population in GPU global memory.

2. Distribute each sub-population to the respective shared memory of thread block.

3. Initiate evolution in each thread block; the evolutions run independently of each other.
Figure 4.11 depicts the architecture of the PGA implementation. The pseudo-code in algorithm 5 illustrates the hybrid PGA.

4. After each evolution, initiate block exchanges of best individuals according to the uni-directional ring migration model. See section 3.2.3.2.

5. Commit data, representing the new individual, to GPU global memory.

6. Update global memory with new individuals.

7. If termination criteria not satisfied, proceed with step 2.
Algorithm 5 Hierarchical Master-slave and Multiple-deme hybrid PGA

<table>
<thead>
<tr>
<th>Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initialise thread block.</td>
</tr>
<tr>
<td>Initialise grid.</td>
</tr>
<tr>
<td>Create initial population.</td>
</tr>
<tr>
<td>Distribute the population to block shared memory.</td>
</tr>
<tr>
<td>Invoke GPU kernel A.</td>
</tr>
</tbody>
</table>

**GPU kernel B:**

while termination criteria not met do

   Exchange best individuals with neighbouring blocks (sub-populations).

   Update shared memory with new individuals.

end while

**GPU kernel A:**

Access respective sub-population.

Apply genetic operator, i.e. selection, crossover, mutation and evaluation.

Update shared memory with generated children.
Chapter 5

Implementation

This chapter delineates the implementation details and approach taken in implementing a adaptive heuristic search algorithm. As presented in Chapter 2, the Master-slave and Multiple-deme Parallelisation Schemes were chosen to search for the optimal solution to the Giada and Marsili[11] log-likelihood function. A high-level overview of the Master-slave algorithm implementation is presented, the various choices for the genetic operators clearly motivated and, in succession, an overview on the approach taken to implement the kernels and PGA cluster analysis framework on the CUDA platform, provided. A discussion on the execution time trial methodology between the serial Matlab and the parallelised CUDA C implementation closes off the chapter.

A Multiple-deme coarse-grained PGA, leveraging of the CUDA framework, was partially implemented. Implementing the scheme proved to be highly complex. Unfortunately the algorithm crashes once the different code components are assembled. Possible causes are platform drivers and device memory conflicts. This chapter also introduces a novel self-developed knowledge-based genetic operator that allows for highly efficient traversal of the search space.
5.1 Stock correlation taxonomy

A number of authors\cite{46, 47} have focused on graph-theoretical representation and analysis of the financial market. \cite{47} focused on devising hierarchical structures in financial markets, by presenting a topological characterization of the minimal spanning tree (MST), that can be obtained by considering the price return correlations of stocks, traded in a financial market.\cite{46} used correlation matrices devised from stocks in a portfolio, by computing the synchronous time evolution of the logarithm of the difference of the daily stock price. A spanning tree of a graph is a subgraph that contains all the vertices and is a tree. A single graph can have many different spanning trees. A weight is assigned to each edge and used to assign a weight to a spanning tree by computing the sum of the weights of the edges in that spanning tree. Thus, a minimum spanning tree (MST) is then the spanning tree with weight less than or equal to the weight of every other spanning tree. More generally, any undirected graph, which is not necessarily connected, has a minimum spanning forest, which is a union of minimum spanning trees for its connected components. \cite{46} mapped the stocks into the graph nodes and projected the relations between the stocks into the graph edges. The correlations between the pairs of stocks are transformed into metric distances, as depicted by the following equation:

\[
c_{ij} = \sqrt{2(1 - \rho_{ij})}. \tag{5.1}
\]

\(\rho_{ij}\) depicts the correlation value between stock \(i\) and stock \(j\) in the correlation matrix. An application of the MST in the current financial context would denote the sum of all weights of edges, which is minimal among all trees defined on the distance matrix. The MSTs are visual representations of the stock correlation network, which are used for observing, analysing and predicting stock market dynamics.
5.2 Approach

In this research two objectives had to be fulfilled. I investigated and tuned the behaviour of the PGA implementation using a pre-defined training set of 40 simulated stocks, which features 4 distinct disjoint clusters. The second objective was to build a stock correlation network based on stock price correlations, computed from the time series of the respective securities by collecting the real-world ticker data for a pre-defined time period from the Johannesburg Stock Exchange JSE). The approach of using an integer-based encoding was chosen, as motivated in Section 3.1.2. The representation of the individual is as per the Section 2.4 in Chapter 2 and looks as following:

\[ \text{Individual} = \{c_1, c_2, \ldots, c_{i-1}, c_i\}, c = 1, \ldots, K, i = 1, \ldots, N. \] (5.2)

The variable \( c_i \) is the cluster that the object \( i \) belongs to. In terms of the terminology pertaining to Genetic Algorithms, it means that the \( i - th \) gene denotes the cluster that \( i - th \) object or asset belongs to. The numbers of objects or assets is \( N \). This representation was implemented by Gebbie\[12, 14\] in his serial GA algorithm and was also adopted in this research. Section 5.6.7 dissects the type of Genetic Operators used in line with argumentation in Section 3.1.2. The fitness function will be the Giada and Marsili maximum log-likelihood function \( L_c \) as derived in 2.4.1, which is as following:

\[ L_c(S) = \frac{1}{2} \sum_{s: n_s > 1} \left[ \log \frac{n_s}{c_s} + (n_s - 1) \log \frac{n_s^2 - n_s}{n_s^2 - c_s} \right] \] (5.3)

The fitness function will be used as the measure to determine whether the cluster configuration represents the inherent structure of the data set, i.e. the GA will hone in on the fittest individual, which will represent the cluster configuration of distinct residual
clusters of correlated assets or objects in the data set.

The preconditioning and post-processing of the data was performed in MATLAB making use of data pre-processing, post-processing and Minimal Spanning Tree (MST) code libraries supplied by the supervisors for this research [48, 49]. In order to comply with the chosen approach, I had to make modifications to the code libraries. I chose to apply the Batch Sequential Architectural Pattern [50] for the data processing. In a Batch Sequential architecture, the task is subdivided into small processing steps, which are implemented as separate, independent components. Each step runs to completion and then calls the next sequential step until the whole task or job completed. During each step a batch of data is processed and sent as a whole to the next step in form of a batch file. The following steps are executed in order to build the stock correlation network are in adherence with the chosen Architectural Pattern [50].

1. Precondition the data for the cluster analysis algorithm and persist the data to batch file. This is done via the MATLAB function `createRWData.m`.

2. Load the preconditioned data and feed the preconditioned data into the CUDA GA cluster analysis application and persist the data with the calculated cluster configurations to batch file.

3. Load the cluster configurations from the batch file and feed it into the MST generation engine. Plot the generated MSTs and persist the graphical depictions as PNG file type. This is done via the MATLAB function `createMSTs.m`.

4. (Alternative) Collate the plots to an AVI file.
5.3 Pre-processing of data for the Clustering Algorithm

In order to generate the correlation matrices for the relevant stock prices comprising N stocks, the following approach was adopted: the ticker data file, serialised as FTS (Financial Time Series) objects, is read into memory and the data conditioned. Holes in the time series data are plugged using the Matlab function `fillts()` utilising a zero-order hold interpolation approach in order to substitute missing values, denoted by Not A Number (NaN) in the data file. Subsequently, the time series data is extracted out of the FTS format and copied into a 2-columnar matrix, the first column containing the ticker time values and the second column the monetary value of the stock data. The function `average()` is applied to normalise the data and remove the market mode by recursive averaging of the financial data in the matrix. Successively, I remove the Gaussian noise from the generated covariance matrix in order to make the residual clusters more pronounced thus conducting a cleansing of the correlation matrix. Random Matrix Theory is applied in order clean the covariance matrix. The respective matrix is decomposed and re-built via the eigenvector decomposition theorem as per the following equation:

\[
\text{CorrelationMatrix} = \text{eigenvectors} \ast \text{diag(eigenvalues)} \ast \text{eigenvectors}^T
\]  

The sum of the eigenvalues, i.e. the variance of the system is preserved throughout the cleansing process. The derived covariance matrix is converted into a correlation matrix, resulting in a Hermitian matrix. The data is serialised to a text file, which is fed into the cluster analysis PGA algorithm 5.5 for the computation of residual clusters. The cluster configurations are then saved to a flat file for further processing and the rendering of a graphical depiction of the financial data’s clustering characteristics using Minimum
Spanning Trees (MSTs), as discussed in section 5.4.

5.4 Post-processing of data and depiction of residual clusters

Computed cluster configurations are read from the flat file and residual anomalies pruned. Successively, a distance matrix is constructed by using data values from the correlation matrix in conjunction with computed cluster configuration of the respective data set. The distance matrix is now used to construct the Minimum Spanning Tree (MST). The MST exhibits $N-1$ edges, connecting the N stocks of the data set in such a manner such that the sum of the weights of the edges is a minimum. Kruskal’s algorithm was used to generate the MSTs, which depict the linkages between highly correlated stocks, and in such allows me to draw observations and conclusions from it as explained in Section 5.1.

5.5 Implementation of a Parallel Genetic Algorithm: Master-Slave approach

As mentioned in Section 4.3 in Chapter 4, the NVIDIA CUDA platform provides key abstractions, namely thread groups, shared memories, and barrier synchronization, 'for fine-grained task parallelism and thread parallelism, nested within coarse-grained data parallelism'\cite{7}. This means, that I am afforded the capability to subdivide the task that can undergo coarse-grained parallelism, that is tasks in which exchange of data between processing units ensues in an infrequent manner, and most of the execution time is devoted to processing the task or tasks at hand. Those tasks are solved independently in
parallel by blocks of threads, and each sub-problem into even finer units of execution that can be solved cooperatively in parallel by all threads within the block. The primary focus was to leverage of the CUDA’s very scalable programming model in order to parallelise as many of the different operations of the PGA as possible so that computations would ensue in an efficient manner.

The unparallised GA implementation of the likelihood function implemented in MATLAB by Gebbie[12, 14] served as the starting point for this research. In order to maximise the performance of the Genetic Algorithm, the application of genetic operators and evaluation of the fitness function were parallelised. The Master-slave PGA or Global PGAs use a single population, where evaluation of the individuals and successive application of genetic operators are conducted in parallel. The global parallelization model does not predicate anything about the underlying computer architecture, so it can be implemented efficiently on a shared-memory and distributed-memory model platform [6]. I need to outsource as much of the GA execution to the GPU and make use of GPU memory as extensively as possible[10]. This allows for the minimisation of the data transfers between the host and a device, as those transfers have a significantly lower bandwidth than data transfers transpiring between shared or global memory and the kernel executing on the GPU. I need to minimise and even avoid kernel accesses to global memory [51], but this is not a viable option in this case due to the fact that I need to utilise global memory for the storage of the population, which undergoes evolution. The algorithm in 6 was modified in such a manner as to maximise the performance of the Master-slave PGA and have a clear distinction between the master node, the CPU, which controls the evolutionary process, by issuing the commands for the GA operations to be performed on the GPU, the slave nodes or otherwise denoted the worker nodes. In the Master-slave model, as depicted in Figure 5.1, the master, the CPU in this scenario,
Algorithm 6 Master-slave PGA Implementation for residual cluster determination

Initialise ecosystem for evolution
Size the thread blocks and grid to achieve the highest level of parallelisation.

On GPU: Create initial population

for current_generation ≤ MAX_NO_OF_GENERATIONS do

On GPU: Evaluate fitness values of all individuals in current generation
On GPU: Evaluate state and statistics for current generation
On GPU: Determine if termination criteria are met
if Yes then
    Terminate ALGO; Exit While Loop;
else
    Continue
end if
On GPU: Isolate fittest individuals
On GPU: Apply elitism
On GPU: Apply scaling
On GPU: Apply genetic operator : selection
On GPU: Apply genetic operator : crossover
On GPU: Apply genetic operator : mutation
On GPU: Apply replacement ▷ A new generation has been created
end for
Report on Results
Clean-up ▷ Deallocate memory on GPU and CPU; Release Device

Figure 5.1: A schematic depiction of a Master-slave PGA

initiates the population for the Genetic Algorithm and distributes the individuals of a single panmictic population for computation of the fitness function and subsequent application of genetic operators such as selection, crossover, mutation and replacement amongst the slave processing units, this being the Streaming Multiprocessors(SM) of the GPU. A panmictic population is a population with no mating restriction upon the population, and where all recombinations are possible.
5.6 Detailed analysis of the Parallel Genetic Algorithm: Master-Slave approach

A sound solution design and implementation of the CUDA kernels is of paramount importance to the successful implementation of an efficient cluster analysis algorithm. Apart from CUDA’s Mersenne Twister implementation, the source code for the whole cluster analysis algorithm is self-developed. Best Practices were applied consistently in the writing of the kernels, as stipulated by Czapinski, Robilliard, Langdon, Chen, Stratton and the CUDA Programming and Best Practises Guide compiled by NVIDIA [52–60]. For random number generation, I made use of CUDA’s Curand API [61] and the CUDA Mersenne Twister implementation, opting for the latter in terms of reliability when executing the CUDA PGA clustering application. I also made use of the CUDA THRUST Standard Template Library (STL) [62] in order to sort, merge data and perform summation operations in the cluster analysis algorithm. CUDA THRUST Standard Template Library (STL) is a C++ template library for CUDA based on the Standard Template Library (STL) standard. Thrust allows me to develop high performance parallel applications with minimal programming effort through a high-level interface that wraps the CUDA C framework.

5.6.1 Data Parallelism

Data parallelism aims at distributing the data across the fine-grained units of execution in the most efficient manner. In the PGA implementation, the main objective was to have a very fine-grained distribution of the population of individuals, so that I can optimally map data elements, or the individual’s genes, to parallel processing threads [7]. As described in Section 5.2, the individuals in the population typify a cluster configuration.
and its representation is as following:

\[
Individual = \{c_1, c_2, \ldots, c_{i-1}, c_i\}, c = 1, \ldots, K, i = 1, \ldots, N. \tag{5.5}
\]

The variable \(c_i\) is the \(i-th\) gene which denotes the cluster that \(i-th\) object or asset belongs to. The numbers of objects or assets is \(N\). For example, if I had to create a population of \(N = 400\) individuals and was analysing the data for 16 objects or assets the population could have the following constitution:

\[
\begin{align*}
Individual_1 &= (1, 2, 4, 5, 7, 8, 2, 8, 9, 1, 2, 3, 4, 5, 6) \\
Individual_2 &= (9, 2, 1, 1, 1, 3, 2, 8, 8, 5, 6, 4, 3, 1, 2) \\
Individual_3 &= (3, 1, 3, 4, 6, 8, 2, 1, 1, 9, 2, 2, 2, 2, 2) \\
Individual_4 &= (2, 1, 3, 3, 7, 9, 9, 1, 1, 9, 2, 2, 2, 1, 1) \\
\vdots \\
Individual_{400} &= (8, 1, 9, 8, 7, 6, 5, 10, 5, 3, 6, 5, 4, 4, 3, 3)
\end{align*}
\]

One can envisage the population, the individuals and the genes as data on a two-dimensional data grid. The data grid cells are mapped to threads, where each thread executes a kernel processing the data cell at that \(x,y\)-coordinate. Thus one can envisage the mapping as depicted in Figure 5.2.
5.6.2 Initialisation

The initialisation basically encompasses the memory allocation of the algorithm’s various variables and data containers. The initialisation code takes a two-pronged approach:

1. Allocate host memory to variables and data containers.

2. Allocate device memory to variables.

The data containers include containers for results from the computations, statistics and time measurement data. The C STRUCT complex data type is utilised to store the GA data, configuration-specific information, statistics and GA state data. The reasoning stems from the approach to have a data structure that aggregates cohesive attributes or fields, which allows for flexibility and ease of maintainability as I am able to maintain and extend the functionality of the code base without having to make many code changes to the interfaces or methods utilised and have all the information encapsulated in one data structure.
5.6.3 Grid, block and thread heuristics

In line with the 'best practises' listed in section 4.3.6 in Chapter 4, I need to compute the dimension and size of the blocks per grid and the dimension and size of threads per block, whilst being cognisant of the constraints imposed to achieve optimal efficiency. The algorithm code computes the appropriate size metrics for each of the kernels. If I look at the GA execution model in Figure 5.2, I would require a thread block dimension of 16x16 (256 threads) and a grid dimension of 1x25 blocks. It is quite evident that the GPU is nowhere near full utilisation, but this is the limitation imposed by the nature of the data in the research undertaken.

The sizing for the training set with 40 simulated stocks is not as trivial as the number of assets is not a multiple of the recommended warp size. If I take the population size to be 400, the thread dimensions will still be 16x16 (256 threads), but the grid dimensions will be 25x3. This will activate 48 threads to compute 40 objects. The code implementation features checks in place that will interrogate the thread ID and index, and will prohibit it from processing, if there is no logical mapping between the gene and the thread.

5.6.4 Master-slave GA computation parallelisation

The Master-slave implementation features 44 kernels, each addressing a different aspect of the PGA and depicted in the following listing:

```c
#if defined(MERSENNE_TWISTER)
    createPopulation<<<dimGrid, dimBlock>>>(...);
#elif defined(CURAND)
    createPopulation<<<dimGrid, dimBlock>>>(...);
#endif
```

//Start evolution
for (int currGen = 1; currGen <= gaConfig.generations; ++currGen) {

    // Evaluate fitness of population
    evaluateFitnessOfPopulation<<<dimGrid, dimBlock>>>(..);

    consolidateFitnessValues<<<dimGridFitness, dimBlock>>>(..);

    // Sorting of population according to fitness score
    thrust::sort_by_key(thrust::device_ptr<float>(..),
                        thrust::device_ptr<float>(..),
                        thrust::device_ptr<int>(..),
                        thrust::greater<float>()) ;

    // Compute sum of all fitness values
    sumFitnessValues = thrust::reduce(..);

    // Evaluate the current state of the GA and compute GA statistics
    evaluateGAState<<<dimGridSingleExecution, dimBlockSingleExecution>>>(..);

    // Isolate the fittest individuals
    evaluateFittestIndividual<<<dimGridEvalFittest, dimBlockEvalFittest>>>(..);

    if (terminateEvolutionHost == true) {
        break;
    }

    // Apply elitism
    if (gaConfig.applyElitism) {
        applyGeneticOperator_Elitsim<<<dimGridElitism, dimBlock>>>(..);
    }

    // Apply scaling
    applyScaling<<<dimGridScaling, dimBlock>>>(scaledScores, metrics.columns);
```cpp
int sumScaledScores = thrust::reduce(...);

// Apply
performGeneticOperatorPreSelector<<<dimGridSingleExecution, dimBlockSingleExecution>>>(...);

// Apply Crossover
performGeneticOperatorCrossover(...);

// Apply Mutation
#if defined(MARSENNE_TWISTER)
applyGeneticOperator_Mutation<<<dimGridGeneticOperator, dimBlockGeneticOperator>>>(...);
#elif defined(CURAND)
applyGeneticOperator_Mutation<<<dimGridGeneticOperator, dimBlockGeneticOperator>>>(...);
applyGeneticOperator_Replacement<<<dimGrid, dimBlock>>>(...);
#endif
```

LISTING 5.1: Master-slave PGA algorithm (Focus has been placed on the core functionality and thus certain code details omitted)

### 5.6.5 Initial Population generation

The PGA initialises the population of the GA at the beginning, having two random number generators at our disposal: namely CURAND, a library that offers efficient generation of high-quality pseudo-random and quasi-random numbers and the CUDA Marsenne Twister implementation, NVIDIA’s implementation of a generator for uniform pseudo-random numbers. The initial population was created by multiplying a random number in the range of [0,1] with the number of objects or assets in the data-set. The population and data pertinent to the evolution process resides in global GPU memory throughout the execution of the PGA.
5.6.6 Evaluation of the fitness function

Analogous to the computation for population generation, the following computations execute on a very fine-grained level, where each thread allotted to the computation computes values for each gene in the individual or in the case of the evaluation of the fitness value, the number of clusters $K$ is equal to the number of objects $N$ or the length of chromosome. I proceed to evaluate the fitness $L_c$ of the individuals in the population. It is a two pass approach:

- **Pass 1**: Calculate the values for $ns$ and $cs$ for each of the clusters in each individual by calling kernel `evaluateFitnessOfPopulation()`.

- **Pass 2**: Collate the results and compute the fitness value $L_c$ for each individual by calling `consolidateFitnessValues()`.

In **Pass 1** the algorithm interrogates the individual and determines the number of objects $ns$ in each of the clusters. The kernel initialises storage in the device’s shared memory and sums up the number of objects for each of the cluster indexes from 1, $\ldots$, $N$, $N$ being the number of objects or the chromosome length. The cluster indices for which there are no objects are given the value 0 and are eliminated from further computations. Subsequently, the internal correlation $cs$ of the cluster indices with $ns > 0$ is computed.

In **Pass 2** the kernel reads the computed values for variables $cs$ and $ns$. It filters out the cluster indexes. Analogous, all the cluster indexes with $ns = 0$ are not considered, i.e. those are indexes for clusters that are not represented in the individual depicting a possible residual cluster configuration. This means, for example, that Individual 2 in Section 5.6.1 would have not have any asset or object belonging to a cluster of index 7. Analogous to the fitness function implementation by Gebbie[12, 14] in his serial GA
algorithm, I put another constraint on the permissible values for the computation. The constraint is that if $n_s = 1$, the value for the internal correlation must be $c_s < 1$. If the value is $c_s \leq 1$, the the fitness value is set to 0. The algorithm then computes the value for the $L_c$ for all individuals in the population.

Computation of the statistics and current state of the algorithm ensues by calling the kernel `evaluateGAState()`. Determination of the fittest individuals follows by computing the index of the fittest individuals within the population. In case of elitism being applied, the fittest individuals, in number determined by configuration, are promoted directly to the next generation. Scaling, denoted by the kernel call `applyScaling()` is applied to the fitness values of the remainder of the population upon which selection of the parents for the mating process takes place.

### 5.6.7 Genetic Operators and Genetic Algorithm configuration

After determining the parents’ artefacts, crossover and mutation operations ensue and children are created that constitute the individuals of the next generation. The evolution process stops upon meeting the termination criteria for the GA. Once the optimal individual has been determined, the data, including statistics for each of the generations, is copied back to the host.

Genetic operators and certain Genetic Algorithm configurations are the key factors which will determine the performance of the GA. Finding a balance between explorative and exploitative features of GA is paramount to the success of the GA and henceforth parameter tuning of the operators and the GA configuration is unavoidable[26]. Adewumi and Ali[26] state that this includes the tuning of parameters such as mutation probability, the crossover operator and the population size. They also state that the parameters
should be dependent on the internal dynamics of the algorithm. Although the paper by Adewumi and Ali [26] focuses on a multi-stage space allocation problem in the realm of domain specific combinatorial optimisation problems, the methodology of tuning the parameters is generic in nature and can be applied to any type of GA problem and served as the basis for the PGA algorithm tuning.

5.6.7.1 Scaling

A call is issued to the kernel `applyScaling()` to initiate scaling on the GPU. As discussed in Section 3.1.1.1, prior to selecting the operator that will be applied to the population, I need to adjust and scale the fitness value. The decision was taken to opt for rank fitness scaling, analogous to the approach used by MATLAB’s GA library. Rank fitness scaling initially adjusts the fitness value of the individuals in such a manner that the fittest individual is assigned the value of rank 1 and the least fit the value of P, where P is the population size. This represents the first transform. In the second transform, the following formula is applied:

\[
\text{score}_{\text{Individual}_n} = \frac{1}{\text{Rank}_{\text{Individual}_n}}, \quad N \leq P
\]

This allows for full exploitation of the search space, giving all the weakest individuals the opportunity to partake in the mating process.

5.6.7.2 Selection

A call is issued to the kernel `performGeneticOperatorPreSelector()` to initiate selection on the GPU. In terms of the selection approach, I applied the stochastic uniform selection method (see Section 3.1.1.1 for description). This method provides a more
favourable selection pressure as it exhibits zero bias to the selection approach and improves the chances of selection of weaker individuals, which increases diversity\[6\]. The method creates contiguous segments of a line, where each parent’s segment is proportional in length to its scaled value. The algorithm moves along the sequence in steps of equal size. At each step, the algorithm allocates a parent from the section it lands on. After applying selection, the individuals are committed to the GPU’s global memory

![Selection Line](image)

**Figure 5.3:** Stochastic uniform selection approach

and I proceed with the application of the crossover and mutation genetic operators.

### 5.6.7.3 Crossover Operator

The *Master-Slave* algorithm feature 3 types of crossover algorithms, namely *Single-Point Crossover* 3.1.1.2, *Two-Point Crossover* 3.1.1.2 and a *Knowledge-based Crossover* 3.1.3 techniques. The *Knowledge-based Crossover* genetic operator was developed specifically for the problem of increasing the efficiency of the *Master-Slave* and is Parallelisation Scheme agnostic and can be applied to any type of Genetic Algorithm. It needs to be underlined that it is not featured anywhere in literature and is a novel approach. Section 3.1.3 motivates why I chose to utilise that operator. The genetic operator is a hybrid between *Single-Point Crossover* and the use of a guiding function namely the Giada and Marsili log-likelihood function 2.14, which uses the function, to determine which segment from the respective two individuals to copy over to the child. The explanation to use
the likelihood function as described in Section 2.4.1, in order to determine the 'fitter' segment, is motivated by the fact that the application of the measure of likelihood for cluster structure should not be restricted only to the whole data-set, but can also be applied to subsets of data. Initially, a separate algorithm randomly determines crossover sites for all selected parents in the population. Each parent is assigned a different locus. Due to the nature of a Single-Point Crossover, there will be two segments per parent, a segment left of the randomly selected crossover site and the segment right, or segment with a starting index bigger or equal than the computed crossover site. The guiding function is used to ascertain which of the two segments at the pre-determined loci will be copied. A random number is generated and compared to $P_{cf}$. Should the random number be bigger than the crossover probability, then the algorithm will copy over the segment with the highest segment fitness value as determined by Equation 5.6, in the event that the random value is smaller, the 'less' fit segment is copied over, i.e. the segment from the other individual. Two parents are selected which yield one child, that will be injected in to the population undergoing evolution.

$$f = \arg \max \| \prod_{s \geq 1} \left[ \frac{1}{2} \sum_{s: n_s > 1} \left[ \log \frac{n_s}{c_s} + (n_s - 1) \log \frac{n_s^2 - n_s}{n_s^2 - c_s} \right] \right]$$ \hspace{1cm} (5.6)$$

Algorithm 7 depicts the novel Knowledge-based Crossover: The crossover operation is initiated by the call to method `performGeneticOperatorCrossover()`. This in turn calls one kernel to compute the segment scores and the other to apply the crossover operator.

5.6.7.4 Mutation Operator

Creep mutation The mutation operation is initiated by the call to method `applyGeneticOperatorMutation()`. Two distinct mutation operators were implemented. The first operator employs an
**Algorithm 7** Custom Knowledge-based Crossover operator

Randomly determine crossover sites for parents selected for mating

Generate random number $R_c$

Determine fitness of segments $F_{\text{SegmentLeft}}^{P_1}, F_{\text{SegmentLeft}}^{P_2}, F_{\text{SegmentRight}}^{P_1}$

for $\text{locus} \leq \text{genomeLength}$ do in parallel

  if $\text{locus} < \text{crossover site}$ then
  
  if $F_{\text{SegmentLeft}}^{P_1} \geq F_{\text{SegmentLeft}}^{P_1}$ then \(\triangleright\) Isolate first segment to be copied over to the offspring.

  if $R_c > P_{cf}$ then \(\triangleright\) Isolate second segment to be copied over to the offspring.

  $\text{OffSpringSegmentLeft} \leftarrow \text{Parent}^{1}_{\text{SegmentLeft}}$ \(\triangleright\) Copy Over segment from individual 1

  else
  
  $\text{OffSpringSegmentLeft} \leftarrow \text{Parent}^{2}_{\text{SegmentLeft}}$ \(\triangleright\) Copy Over segment from individual 2

  end if

  else
  
  if $R_c > P_{cf}$ then
  
  $\text{OffSpringSegmentLeft} \leftarrow \text{Parent}^{2}_{\text{SegmentLeft}}$ \(\triangleright\) Copy Over segment from individual 2

  else
  
  $\text{OffSpringSegmentLeft} \leftarrow \text{Parent}^{1}_{\text{SegmentLeft}}$ \(\triangleright\) Copy Over segment from individual 1

  end if

  end if

else

  if $F_{\text{SegmentRight}}^{P_1} \geq F_{\text{SegmentRight}}^{P_1}$ then \(\triangleright\) Isolate right segment to be copied over to the offspring.

  if $R_c > P_{cf}$ then \(\triangleright\) Isolate second segment to be copied over to the offspring.

  $\text{OffSpringSegmentRight} \leftarrow \text{Parent}^{1}_{\text{SegmentRight}}$ \(\triangleright\) Copy Over segment from individual 1

  else
  
  $\text{OffSpringSegmentRight} \leftarrow \text{Parent}^{2}_{\text{SegmentRight}}$ \(\triangleright\) Copy Over segment from individual 2

  end if

else

  if $R_c > P_{cf}$ then
  
  $\text{OffSpringSegmentRight} \leftarrow \text{Parent}^{2}_{\text{SegmentRight}}$ \(\triangleright\) Copy Over segment from individual 2

  else
  
  $\text{OffSpringSegmentRight} \leftarrow \text{Parent}^{1}_{\text{SegmentRight}}$ \(\triangleright\) Copy Over segment from individual 1

  end if

end parallel for
approach as utilised by [24] in a genetic algorithm-based clustering technique, called GA-clustering, which searches for appropriate cluster centres. A number is generated in the range between [0,1] with uniform distribution. In order to facilitate this, the **Mersenne-Twister random number generator** is invoked. If the value of a gene at a pre-defined locus is \( v \), then the mutation approach, as depicted in 5.7 is applied to the integer-based chromosome as following:

\[
v^{t+1} = \begin{cases} 
  v^t \pm 2 \times \delta \times v^t & \text{if } v^t \neq 0 \\
  v^t \pm 2 \times \delta & \text{if } v^t = 0
\end{cases}
\]  

(5.7)

5.6.7.5 Random replacement

The replacement operation is trigger by the call to method `applyGeneticOperator_Replacement()`. The second mutation operator utilises the **Mersenne-Twister random number generator** to generate a number in the range [0, 1] and multiply that number with the upper bound value pertaining to a cluster affiliation. In the case of the training set of 40 simulated stocks, we have 40 objects, which can either belong to either a singleton or represent 40 disjoint data points. Therefore, I would have to ensure that the generated mutation value is within the bounds of [0,40), otherwise I would have an invalid cluster configuration.

5.6.7.6 Replacement Operator

There are a few replacement operators, as discussed in 3.1.1.5. I chose using a weak parent replacement scheme 3.1.1.5, where the stronger parent and the offspring are promoted to the next phase of evolution. This introduces bias towards fitter individuals,
thus increasing the overall fitness of the population, but reduces the diversity of the mating pool.

### 5.6.8 Termination Criteria

There are two significant termination criteria, namely

- Once a pre-defined number of maximum evolutions has been executed, the algorithm terminates.

- If there is no notable improvement in the fitness value of the fittest individual, representing the most optimal cluster configuration resident in the data-set being analysed, the algorithm will continue to iterate through a pre-defined number of evolutions, denoted stall generations $G_{stall}$. The fittest individual from the previous evolution is compared to the fittest individual of the current evolution and if the difference between the two values is smaller than a pre-defined error tolerance, one would classify this as a stall generation.

### 5.7 Parallel Genetic Algorithm tuning

In order to ensure an efficient implementation of the Master-slave algorithm, I need to find a balance between exploration of the search space and exploitation of the discoveries in the search space. The more exploitation of the discoveries that is made, the faster the PGA will converge towards a solution, but will fail at finding the true global optimum. The more exploration will lead to finding the true optimum, but will slow down convergence. I opted for tuning the mutation probability, the crossover operator parameter and the population size, analogous to the approach taken and motivated by Adewumi and
Ali[26]. I additionally looked at finding an efficient mutation operator, finding an ideal setting for the novel and self-developed knowledge-based crossover operator (see Section 5.6.7.3) and at tuning the number of elite individuals that get promoted to the next generation. The following algorithm parameter tuning experiments were compiled in order to arrive at the optimal algorithm configuration settings, as the PGA parameters affect the algorithms search quality and efficiency[30]:

- Investigation into the effect of population size on the efficiency of the PGA
- Investigation into the effect of crossover probability $P_c$ on the efficiency of the PGA
- Investigation into the effect of crossover probability $P_c$ on the efficiency of the PGA
- Investigation into the effect of mutation probability $P_m$ on the efficiency of the PGA
- Investigation into the effect of knowledge-based crossover fragment operator probability $P_{cf}$ on the efficiency of the PGA
- Investigation into the effect of crossover genetic operator on the efficiency of the PGA
- Investigation into the effect of mutation genetic operator on the efficiency of the PGA
- Investigation into the effect of the number of elite individuals promoted to the next generation on the efficiency of the PGA.
5.8 Measurement metrics

The tuning exercise was performed on the training set of 4 disjoint clusters and in such it represents the optimal GA parameters for the training set data set.

5.8.1 Performance metric

In order to analyse the efficiency of an algorithm, I would usually apply time complexity analysis to get an estimate of the running time as a function of the size of the input data. This result is normally expressed using Big O notation. This is useful for comparing algorithms in cases where a large amount of data is to processed, which is not the case in this research. This research focuses on a small set of data-and the goal of returning a result in the shortest possible time. This will in turn lead to faster computation of high-frequency, low-latency data feeds, where a high throughput of data needs to be processed efficiently. Secondly, algorithms which include parallel processing may be more difficult to analyse using the Big O notation. Thus, in order to be able to measure the efficiency of the algorithm, measurements of the time taken to execute a clustering analysis on a data set were conducted. Two common time measures are: CPU time and Elapsed time. CPU time is the actual time it takes the Central Processing Unit (CPU) to process the instructions of a computer program or the Operating System (OS). This does not include the waiting for Input/Output resources (I/O) to complete their operations or the context switching operations in the OS. The Elapsed time measures the total time pertaining to the execution of a computer program, which means the duration from when the process was started until the time it terminated. Execution time trails of each of the implementations were executed. The decision was taken to use the elapsed time as a benchmarking metric. It is quite an involved process to be able to
compare computational times for an algorithm that can both run on a CPU and a GPU and in such somehow try to quantify its efficiency. The CUDA framework provides a profiling workbench, which reports benchmarking metrics to a fine level of granularity. It will report on CPU and GPU time spent on executing a piece of CUDA code and for example, on the time taken to for transfer of data between the host and device; such a level of detail is beyond the scope of this research. I rather opted for introducing time measuring barriers, localised in such places in the code base so that they give a good enough indication as to the execution times of the different manifestations of a PGAs run on various platforms under different configurations and run on multiple environments as listed in Section 6.1.

5.8.2 Average calculations

Algorithm tuning experiments described in Section 6.2.2 employed the calculation of the arithmetic average value for the fitness of all individuals in the population for that generation, which was calculated in the following manner: $F_{\text{ave}} = \frac{1}{n} \sum_{i=1}^{N} F_{\text{individual}},$ where $n$ denotes the number of the individuals, $F_{\text{ave}}$ the average fitness and $F_{\text{individual}}$ the respective fitness value of the individual. This metric will indicate the quality of the successive population of individuals generated by the PGA.
Chapter 6

Experiments and Measurements

This chapter reports on the algorithm tuning and execution time trials of the CUDA PGA implementation being executed on two OS platforms, and against the serial GA implementation[14]. The following algorithm parameter tuning experiments were compiled in order to arrive at the optimal algorithm configuration settings as described and motivated in Section 5.7:

- Investigation into the effect of population size on the efficiency of the PGA.
- Investigation into the effect of crossover probability $P_c$ on the efficiency of the PGA.
- Investigation into the effect of crossover probability $P_c$ on the efficiency of the PGA.
- Investigation into the effect of mutation probability $P_m$ on the efficiency of the PGA.
- Investigation into the effect of knowledge-based crossover fragment operator probability $P_{cf}$ on the efficiency of the PGA.
• Investigation into the effect of crossover genetic operator on the efficiency of the PGA.

• Investigation into the effect of mutation genetic operator on the efficiency of the PGA.

• Investigation into the effect of the number of elite individuals promoted to the next generation on the efficiency of the PGA.

It also presents clustering analysis results, depicted in the form of Minimum Spanning Trees, as described in Section 5.1, of 1780 time units of real-word stock prices taken from the Johannesburg Stock Exchange (JSE) spanning over the time period from 28th September 2012 until 10th of October 2012.

6.1 Environment

The CUDA algorithm and the respective test harness were primarily developed on the Linux platform. It was successively ported to the Windows environment. Multiple environments were configured as per the configuration depicted in Table 6.1 in order to provide a high-level overview of the versatility of the CUDA cluster analysis algorithm and highlight that its efficiency is not confined to one platform and thus is platform-independent. All the CUDA code was compiled with the the CUDA C compiler `nvcc`, version 5.0. The code was compiled against two configuration sets, namely the DEBUG configuration for debugging and testing, and a RELEASE configuration, optimised to perform code execution time measurements. The code was compiled with CUDA compute capabilities of 2.0 and 3.0. The CUDA compute capability designates a ‘feature set’, being both software and hardware features, that a device supports. In the RELEASE
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<table>
<thead>
<tr>
<th>Environment</th>
<th>Configuration</th>
<th>Algorithm execution environment or framework</th>
</tr>
</thead>
<tbody>
<tr>
<td>LINUX</td>
<td>Linux Mint 13 Maya (3.2.0-23-generic(x86_64)), Intel Core i7-2600 CPU @ 3.4 GHz, 8 GB of RAM, Geforce 560 Ti and Geforce 660 Ti with 2 GB of RAM</td>
<td>CUDA 5.0</td>
</tr>
<tr>
<td>WINDOWS</td>
<td>Windows 7 Home Premium 64-bit, Intel Core i7-3630QM CPU @ 2.4 GHz, 8 GB of RAM, Geforce GTX 660M with 2 GB of RAM</td>
<td>CUDA 5.0</td>
</tr>
<tr>
<td>WINDOWS</td>
<td>Windows 7 Home Premium 64-bit, Intel Core i7-3630QM CPU @ 2.4 GHz, 8 GB of RAM, Geforce GTX 660M with 2 GB of RAM</td>
<td>MATLAB 2011b</td>
</tr>
</tbody>
</table>

Table 6.1: Development and Testing environment

configuration, the compiler switch \texttt{-use\_fast\_math} and the the flag \texttt{-03} were set. The CUDA compiler switch \texttt{-use\_fast\_math} was utilised to increase the performance of the code, by coercing every \texttt{functionName()} call to the equivalent \texttt{\_functionName()} call.

The C++ compiler flag \texttt{-03} ensures that the code is fully optimised. Those flags were omitted in the DEBUG configuration compilation. Please refer to [7, 41] for definitions and further descriptions of technical terms.

6.2 Data: Training Set

The following results are based on a test set of 40 simulated stocks, which features 4 distinct disjoint clusters. This will provide a clear delineation, that the algorithm is processing the data as expected, resulting in a optimal cluster configuration of 4 distinct clusters. The training set was hard-coded and also persisted to a flat file, to be passed into the respective algorithm implementation, so that it can be processed. It was utilised to tune the various genetic operators.
6.2.1 Cluster Analysis in Matlab using a serial Genetic Algorithm

The algorithm runs on a CPU only. Attempts were made to port parts of the code to run on the GPU, but proved to be unsuccessful, due to the fact that MATLAB’s Parallisation Toolbox’s interface for GPU computing has not matured yet. The results obtained are depicted in Figures 6.1, with the first graph depicting the correlation matrix for the training set. The graph clearly depicts 4 coloured regions, depicting highly-correlated data, which represents 4 distinct disjoint clusters.

![Figure 6.1](image)

**Figure 6.1:** Fitness vs. generation with the following GA configuration: 40x40 correlation matrix, 400 generations, a genome length of 40 and population size of 400, 100 stall generations and tolerance value of 0.001.
6.2.2 Experiments for tuning of parameters in Master-Slave PGA Algorithm on the GPU

Optimal cluster configuration for the chosen training set will yield ideally the same value for adjacent genes of the fittest individual, with four distinct segments of values within the instance of the chromosome each denoting a cluster, offset by a stepped transition in value at a specific locus as depicted in figure 6.2 and explained in Section 6.2. The algorithm parameter tuning experiments, as explained in Section 5.7, yielded the following optimal configuration for the Master-Slave PGA: Figure 6.2 depicts the optimal cluster configuration, which was computed by running the cluster analysis on the training set.

6.2.2.1 Variation in Population Size

The size of the population was varied between 0 and 1000 in steps of 200. The following static parameters were used:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population Size</td>
<td>1000/600</td>
</tr>
<tr>
<td>Number of Generations</td>
<td>400</td>
</tr>
<tr>
<td>Crossover Probability ($P_c$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Mutation Probability ($P_m$)</td>
<td>0.1</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations ($G_{stall}$)</td>
<td>50</td>
</tr>
<tr>
<td>Elite size</td>
<td>10</td>
</tr>
<tr>
<td>Crossover Operator</td>
<td>Knowledge-based Operator . See 5.6.7.3</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement . See 5.6.7.5</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ($P_{cf}$)</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Table 6.2: GA parameter configurations
Figure 6.2: Optimal cluster configuration of training set data obtained by Master-Slave PGA

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Generations</td>
<td>400</td>
</tr>
<tr>
<td>Mutation Probability ($P_m$)</td>
<td>0.09</td>
</tr>
<tr>
<td>Crossover Probability ($P_c$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations ($G_{stall}$)</td>
<td>50</td>
</tr>
<tr>
<td>Elite size</td>
<td>4</td>
</tr>
<tr>
<td>Crossover Operator</td>
<td>Knowledge-based Operator .See 5.6.7.3</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement .See 5.6.7.5</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ($P_{cf}$)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 6.3: GA parameter configurations: Variation in Population Size

The results for the variation of the population as illustrated in Figure 6.3 underlines the fact that the population size will depend on the complexity of the problem, the various parameter settings and choice of genetic operators applied. In order to be able to find the most optimal solution to the problem, the population should firstly have a large enough gene pool and exhibit a high degree of diversity in order to be able to traverse and explore the whole search space and not hone in on a local minimum, which will lead to a sub-optimal solution to the exercise. The graph illustrates the fact that the bigger the population, the bigger the resultant fitness value as can be observed by
Effect of Population Size on Convergence Rate and Effectiveness of PGA

Choosing a population size of 1000 or 600 and the lowest at population size of 400. No deduction can be made as to the pattern with the rate of convergence as it is highest at the highest population size, but inconsistent for the stepped decrease in the population thereafter. I can only attribute this to the level of diversity present in the population at the beginning. Summa Summarum, for a GA efficiency to reach a global optimum instead of a local one it is largely dependant on the size of the population [6]. It entails a higher computational cost and utilisation of memory resources, which further cements the case for running the described algorithms on a parallel computing architecture such as CUDA.
6.2.2.2 Variation in Crossover probability $P_c$

Coley[4] recommends to use values between 0.4 and 0.9. In order to gain more insight into how this parameter affects the efficiency of the algorithm, the range was widened and the probability of crossover varied between 0 and 0.9. The following static parameters were used:

<table>
<thead>
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<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Population Size</td>
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<tr>
<td>Number of Generations</td>
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<tr>
<td>Mutation Probability ($P_m$)</td>
<td>0.09</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations ($G_{stall}$)</td>
<td>50</td>
</tr>
<tr>
<td>Elite size</td>
<td>4</td>
</tr>
<tr>
<td>Crossover Operator</td>
<td>Knowledge-based Operator. See 5.6.7.3</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement. See 5.6.7.5</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ($P_{cf}$)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 6.4: GA parameter configurations: Variation in Crossover probability $P_c$

![Effect of crossover probability on average fitness](image-url)
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The increased crossover probability increases the chromosome gene recombination probability, which is favourable, but on the other hand this increase of probability can lead to the loss of favourable genetic make-up, which would in theory yield a lower fitness value. As depicted in Figure 6.4, the average fitness increases with an increase in crossover probability up until a value of 0.6, which would mean that 60% of the population will be formed by selection and crossover and 40% by selection only used in tandem with an additional stochastic operator to either allow or ignore the crossover operation to take place at the respective crossover probability of $P_c$.

### 6.2.2.3 Variation in Mutation probability $P_m$

The probability of mutation was varied between 0.1 and 0.01. Coley[4], Sivanandam and Deepa [6] recommend that the probability should be

$$P_m = \frac{1}{\sqrt{L}}$$

, where $L =$ genomelength, which is within the range of this investigation. Configurations of have

$$P_m = \frac{1}{N\sqrt{L}}$$

, where $L =$ genomelength, $N =$ PopulationSize

also been implemented, but were not found to be viable. The following static parameters were used:
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population Size</td>
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<td>Number of Generations</td>
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<td>Crossover Probability ($P_c$)</td>
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<tr>
<td>Elite size</td>
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<tr>
<td>Crossover Operator</td>
<td>Knowledge-based Operator. See 5.6.7.3</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement .See 5.6.7.5</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ($P_{cf}$)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 6.5: GA parameter configurations: Variation in Mutation probability $P_m$

![Effect of mutation probability on average fitness](image)

Figure 6.5: Variation in Mutation probability $P_m$

The optimal value for the mutation probability $P_m$ is problem specific. A too high mutation rate increases the probability of searching more regions of the search space, but prevents the algorithm from converging towards an optimum solution. On the other hand, too small a mutation rate may result in premature convergence by honing in on a local optima instead of global optimum. Figure 6.5 depicts the graph for the average fitness of the population with the variation of mutation probability $P_m$ with an apogee
at around the 0.1 mark. The minima for the average fitness value for the mutation probability \( P_m \) for the ranges between 0.03 and 0.06, is reached at \( P_m = 0.05 \) and for \( P_m \) ranges 0.06 and 0.09, at \( P_m = 0.07 \). Figure 6.2 depicts the optimal cluster configuration with 4 clusters of 10 objects each. The troughs in the development of the average fitness value at those specific \( P_m \) values can be attributed to the fact that the rate of mutation applied introduces too much disorder to the residual cluster configuration, in other words introduces too much noise to the hill-climbing algorithm and bumps the GA algorithm into another region of the search space, which leads to non-optimal object constellations. In layman’s term, the optimal \( P_m \) setting is problem specific; devising a heuristic for determining the optimal \( P_m \) for all data sets is quite a complex exercise: the only viable approach known at present would be to apply an adaptive, self-tuning GA with a feedback mechanism that would report on the efficiency of an applied parameter and in such would allow a controller to adjust the \( P_m \) for successive generations.

### 6.2.2.4 Variation in Knowledge-based crossover fragment operator probability \( P_{cf} \)

The probability was varied 0 and 1. The range of values was determined empirically.

The following static parameters were used:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population Size</td>
<td>600</td>
</tr>
<tr>
<td>Number of Generations</td>
<td>400</td>
</tr>
<tr>
<td>Crossover Probability (( P_c ))</td>
<td>0.9</td>
</tr>
<tr>
<td>Mutation Probability (( P_m ))</td>
<td>0.09</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations (( G_{stall} ))</td>
<td>50</td>
</tr>
<tr>
<td>Elite size</td>
<td>4</td>
</tr>
<tr>
<td>Crossover Operator</td>
<td>Knowledge-based Operator .See 5.6.7.3</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement .See 5.6.7.5</td>
</tr>
</tbody>
</table>

Table 6.6: GA parameter configurations: Variation in Knowledge-based crossover fragment operator probability \( P_{cf} \)
Figure 6.6: Variation in Knowledge-based crossover fragment operator probability $P_{cf}$

Figure 6.6 depicts 'seesaw-like' behaviour, analogous to the behaviour observed in 6.2.2.3 with the distinction that a high value for the crossover fragment operator probability $P_{cf}$ is attained at 0.1 with a tapering of the average fitness value, reaching a minimum at 0.7 and then rising sharply, reaching an apogee at 0.9 and then dropping again. Again this can be attributed to the specific dimensions of the training set and that certain $P_{cf}$ yield unfavourable results for the problem I am trying to solve.

6.2.2.5 Variation in Crossover genetic operator

Three different types of crossover operators were implemented and investigated, as per the discussion in 5.6.7.3. The approaches are the following: Single-point crossover, Two-point crossover and the novel and newly-devised Knowledge-based crossover operator.

The following static parameters were used:
Table 6.7: GA parameter configurations: Variation in Crossover genetic operator

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population Size</td>
<td>600</td>
</tr>
<tr>
<td>Number of Generations</td>
<td>400</td>
</tr>
<tr>
<td>Crossover Probability ($P_c$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Mutation Probability ($P_m$)</td>
<td>0.09</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations ($G_{stall}$)</td>
<td>50</td>
</tr>
<tr>
<td>Elite size</td>
<td>4</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ($P_{cf}$)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Figure 6.7: Variation in Crossover genetic operator

Figure 6.2.2.2 motivates the approach taken, as introduced in 3.1.3. I observed that, using a knowledge-based crossover operator guides the algorithm in such a way that it converges towards an optimal fitness value at a faster rate compared to the alternate crossover operators, namely Single-point crossover and Two-point crossover. Single-point crossover is more efficient in guiding the GA towards the maximum fitness, thus allowing me to isolate the optimal residual cluster configuration. The knowledge-based
crossover operator and the single-point crossover share a common trait: they both use only a single locus for the crossover operation. Analogous to the reasoning provided in Section 6.2.2.3, I can deduce that this behaviour is specific to the nature of problem. In reference to Section 6.2.2, I could make the assumption that two-point crossover would add too much diversity and in such create too much noise and divert the GA off the path of finding the optimal solution for this problem.

6.2.2.6 Variation in Mutation genetic operator

Two different mutation operators were implemented and investigated, as per the discussion in Section 5.6.7.4. The approaches are the following: Modified Creep Mutation (see 5.6.7.4) and Random replacement (see 5.6.7.5) The following static parameters were used:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population Size</td>
<td>600</td>
</tr>
<tr>
<td>Number of Generations</td>
<td>400</td>
</tr>
<tr>
<td>Crossover Probability ((P_c))</td>
<td>0.9</td>
</tr>
<tr>
<td>Mutation Probability ((P_m))</td>
<td>0.09</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations ((G_{stall}))</td>
<td>50</td>
</tr>
<tr>
<td>Elite size</td>
<td>4</td>
</tr>
<tr>
<td>Crossover Operator Knowledge-based Operator</td>
<td>Knowledge-based Operator. See 5.6.7.3</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ((P_{cf}))</td>
<td>0.5</td>
</tr>
</tbody>
</table>

**Table 6.8:** GA parameter configurations: Variation in Mutation genetic operator
Chapter 6. Results and Discussion

Figure 6.8: Variation in Mutation genetic operator

Figure 6.8 depicts the typical difference between exploration of the search space and exploitation of discoveries [4]. Random value mutation has a more pronounced effect on the performance of the algorithm: whilst it converges at a slower rate, it enables the GA to hone in on the global optimum. Arithmetic mutation or Modified Creep mutation allows the change of the cluster value in small steps in contrast to random value mutation, which exploits the whole spectrum of permissible random values for the cluster value and henceforth would lend itself to exploitative approach, as can be deduced from the formula applied and illustrated in 5.6.7.4. This is the reason why it converges towards a maximum at a higher rate but does not locate the true global optimum as it hone in on the local minimum of around 1.5 - 1.6.
6.2.2.7 Variation in number of elite individuals promoted to the next generation

This section investigates the effect of the number of elite individuals, which are promoted to the next generation, on the overall average fitness value of the population. The elite size was varied between 0 and 10. The following static parameters were used:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Population Size</td>
<td>600</td>
</tr>
<tr>
<td>Number of Generations</td>
<td>400</td>
</tr>
<tr>
<td>Crossover Probability ($P_c$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Mutation Probability ($P_m$)</td>
<td>0.09</td>
</tr>
<tr>
<td>Error tolerance</td>
<td>0.00001</td>
</tr>
<tr>
<td>Stall generations ($G_{stall}$)</td>
<td>50</td>
</tr>
<tr>
<td>Crossover Operator</td>
<td>Knowledge-based Operator .See 5.6.7.3</td>
</tr>
<tr>
<td>Mutation Operator</td>
<td>Random replacement .See 5.6.7.5</td>
</tr>
<tr>
<td>Knowledge-based crossover operator probability ($P_{cf}$)</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 6.9: GA parameter configurations: Variation in number of elite individuals promoted to the next generation

![Graph showing the effect of number of elite individuals on average fitness value](image)

Figure 6.9: Variation in Number of elite individuals promoted to the next generation
Figure 6.9 depicts, with the exception a couple of anomalies, the expected behaviour that, if I allow for the increase of the number of the fittest individuals that are promoted to the next generation, the average fitness will increase due to the increase in probability that the fittest individuals will exchange genetic information. Also, the higher the number of elite individuals, the more pronounced the effect of the fitter individual’s fitness on the average fitness of the population.
6.3 Data: Intra-day stock prices for 18 stocks from the Johannesburg Stock Exchange (JSE)

The following investigation focused on 1780 time units of real-word stock prices taken from the Johannesburg Stock Exchange (JSE), spanning the time period from 28th September 2012 until 10th of October 2012. The computed cluster configurations were used to build a correlation-based Minimal Spanning Tree (MST) for stock prices, taken at a specific point in time during trading hours. The time interval for the ticker data was 3 seconds. The stocks under investigation are listed in table 6.10. The time interval of the ticker data is too narrow to report on any pronounced trends emerging, but I made note of some key observations and developments restricting myself to the time period under investigation. In no way is the interpretation meant to infer some intrinsic behaviour in the South African Market today or at any point in time.

<table>
<thead>
<tr>
<th>Stock JSE identifier</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AGL</td>
<td>Anglo American Plc</td>
</tr>
<tr>
<td>AMS</td>
<td>Anglo American Plat Limited</td>
</tr>
<tr>
<td>ANG</td>
<td>Anglogold Ashanti Limited</td>
</tr>
<tr>
<td>ASA</td>
<td>ABSA Group</td>
</tr>
<tr>
<td>BIL</td>
<td>BHP Billiton Plc</td>
</tr>
<tr>
<td>CFR</td>
<td>Compagnie Fin Richemont</td>
</tr>
<tr>
<td>FSR</td>
<td>Firstrand Limited</td>
</tr>
<tr>
<td>GFI</td>
<td>Gold Fields Limited</td>
</tr>
<tr>
<td>IMP</td>
<td>Impala Platinum Holdings Limited</td>
</tr>
<tr>
<td>KIO</td>
<td>Kumba Iron Ore</td>
</tr>
<tr>
<td>MTN</td>
<td>MTN Group</td>
</tr>
<tr>
<td>NPN</td>
<td>Naspers</td>
</tr>
<tr>
<td>OML</td>
<td>Old Mutual Plc</td>
</tr>
<tr>
<td>SAB</td>
<td>Sabmiller Plc</td>
</tr>
<tr>
<td>SBK</td>
<td>Standard Bank Group</td>
</tr>
<tr>
<td>SHF</td>
<td>Steinhoff International Holdings</td>
</tr>
<tr>
<td>SLM</td>
<td>Sanlam</td>
</tr>
<tr>
<td>SOL</td>
<td>Sasol Limited</td>
</tr>
</tbody>
</table>

Table 6.10: Stocks traded on the Johannesburg Stock Exchange (JSE)

configuration for the GA algo was per the optimal settings, specified in table 6.2. By
close inspection of the Minimum Spanning Trees (MSTs) for the 18 stocks in the time period between 28th September 2012 until 10th of October 2012, I observe that in the early hours of trading there is some notable activity, with the emergence of 1 significant cluster with lower weighted edges and two or three smaller clusters with higher weighted edges as illustrated by Figures 6.10, 6.11 and 6.12. As illustrated in Figure 6.10, I observe low correlations between Old Mutual Plc, Gold Fields Limited, Sanlam, Standard Bank Group, Anglo American Plat Limited, Kumba Iron Ore and Firstrand Limited. I notice three 2-element clusters in Figure 6.10 with high weight edges and thus high correlations between Sasol Limited and Steinhoff International Holdings, between Compagnie Fin Richemont and MTN Group, and between Naspers and Sabmiller Plc. As illustrated
in Figure 6.11, I see low correlations between Old Mutual Plc, Gold Fields Limited, Sanlam, Standard Bank Group, Anglo American Plat Limited, Kumba Iron Ore, Steinhoff International Holdings and ABSA Group. I notice a 2-element cluster with high weight edges and thus high correlations between Anglogold Ashanti Limited and Compagnie Fin Richemont. As illustrated in Figure 6.12, I observe low correlations between Old Mutual Plc, Gold Fields Limited, Sanlam, Standard Bank Group, Anglo American Plat Limited, Kumba Iron Ore, Steinhoff International Holdings and ABSA Group. I notice two smaller clusters with high weight edges and thus high correlations between MTN Group and Compagnie Fin Richemont, and between between Anglo American Plc, Sasol Limited and BHP Billiton Plc.

The early morning trading pattern snapshots depict the trend that the primary stocks...
more or less exhibit the slightly similar trending characteristics, following the same pattern on a daily basis with no notable disturbances with one or two outliers behaving differently, showing high correlations. The low correlations between the majority of the stocks signifies that there is no definitive underlying cause, be it a macroeconomic or microeconomic factor that might drive the trend of the stocks under observation. The following stocks show a similar morning trending pattern in trading: Old Mutual Plc, Gold Fields Limited, Sanlam, Standard Bank Group, Anglo American Plat Limited, Kumba Iron Ore, Steinhoff International Holdings and ABSA Group.

Looking at the outliers, the same applies. All the stocks belong to different industry segments, so there is no evidence that the early morning trending pattern might be intrinsic to either the mining, banking, petroleum, telecommunication, beverage or any
other type of industry sector.

The midday does not deviate from the morning trending pattern, but shows higher weighted edges between the respective stocks in the MST, thus more pronounced correlation between the nodes of the MST, taken from a random midday snapshot in the time period under investigation shown in 6.14. The midday trading periods yields MST star topologies, as illustrated by the following snapshots, namely 6.13 and 6.15.

**Figure 6.13:** Midday trading pattern snapshot on the 1st October 2012
The afternoon and late afternoon trending patterns expose a more pronounced occurrence of Minimum Spanning Tree (MST) star topologies as depicted in Figures 6.16, 6.17 and 6.18. As illustrated in Figure 6.16, one sees Anglo American Plc driving the trending pattern for stocks such as Naspers, Sasol Limited, SAB Miller Plc, etc. As illustrated in Figure 6.17, I notice Sanlam, American Plat Limited and Gold Fields Limited, in other words stocks in the mining sector driving the trending pattern on the securities exchange. As illustrated in Figure 6.18, it is quite evident again that Anglo American Plc (JSE:AGL) drives the trending pattern for all other assets on the exchange for that time snapshot, depicted by higher weighted edges, thus higher correlations with the other stocks. In conjunction with 6.18, I could say that late stock trading is largely dictated by the mining sector, which in turn could be attributed to some underlying
factor. The determination of such would necessitate further and more detailed analysis and investigation.
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Figure 6.16: Afternoon trading pattern snapshot on the 1st October 2012

Figure 6.17: Afternoon trading pattern snapshot on the 1st October 2012
6.4 PGA algo execution time trials of the CUDA cluster analysis algorithm

6.4.1 PGA algo execution time trials results

Execution time trail tests, as illustrated in Figures 6.19, 6.20, 6.21 and 6.22, were run on the environments listed in Section 6.1. The PGA algo execution time trail runs include algorithm tuning tests as described in Section 6.2.2, a single cluster analysis execution of the training set, and the process of cluster analysis of 1000 correlation matrices of real world data as depicted in Section 6.3. Time measurements were conducted using the StopWatch utility by Tommaso Urli[63]. Measurements were taken as per the methodology described in Section 5.8.1.
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Figure 6.19: GA execution time runs in various execution environments

Figure 6.20: PGA execution time runs in various execution environments (Average execution time recorded)
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Variation in Population Size
Variation in Mutation probability
Variation in Crossover probability
Variation in Knowledge-based crossover fragment operator probability
Variation in Mutation genetic operator

Figure 6.21: PGA execution time runs in various execution environments (Maximum execution time recorded)
Chapter 6. Results and Discussion

Variation in Population Size
Variation in Mutation probability
Variation in Crossover probability
Variation in Knowledge-based crossover fragment operator probability
Variation in Mutation genetic operator

Figure 6.22: PGA execution time runs in various execution environments (Minimum execution time recorded)
6.4.2 Analysis of GA algo execution time trials

The results show a clear picture of the efficiency of the CUDA PGA implementation. The performance improvement in the case of the training set cluster analysis run is in the region of 13 000% on the Linux, 6500% on the Windows. This can be attributed to the utilisation of a parallel computation platform, a novel genetic operator and the extensive and comprehensive algorithm tuning techniques employed. Similar performance gains are also observed in the real world data code execution time runs, namely that the CUDA PGA executes at around 100 times faster than the serial MATLAB GA algorithm. Shifting the focus to the various algorithm tuning runs, I noticed that, on average, there is a very notable performance improvement between the LINUX and the WINDOWS platform. The same compilation options were utilised on both platforms, but the code optimised for the Linux platform. This might explain the discrepancy in execution times between LINUX and the WINDOWS environment. In order to make a more substantial assessment, I would have to profile the algorithm on both platforms and investigate the causes for the discrepancies; but this is beyond the scope of this research.
Chapter 7

Conclusions and future prospects

7.1 Conclusions

The range of investigations that were undertaken show that the Giada and Marsili likelihood function[11], inspired by the Noh model, is a viable approach for isolating residual clusters in data-sets. Its key advantages, in comparison to conventional clustering methods, are that it is unsupervised and that the interpretation of results is transparent in terms of the model.

Two evolutionary search heuristics were reviewed, namely the Master-slave Parallel Genetic Algorithm and the Multi-pe-deme Parallel Genetic Algorithm. The implementation of the Master-slave PGA showed that the efficiency depends on various parameter settings and that fine-tuning such an algorithm is not easy. The research shows that the PGA efficiency is largely dependant on the size of the population, a statement which is also supported by literature[6], but entails a higher computational cost and utilisation of memory resources. The increased crossover probability increases the chromosome gene recombination probability and thus, on average, enables the PGA to generate fitter
individuals. The same applies to the mutation probability. A novel knowledge based crossover operator was introduced. The results show that it outperforms traditional crossover operators, such as Single-point crossover and Two-point crossover genetic operators as the PGA achieves higher convergence rates and creates successive populations with higher average fitness values. The type of mutation operator utilised has a pronounced effect on the algorithm’s efficiency to isolate the optimal solution in the search space, whereas other parameter settings primarily impact the convergence rate. The Arithmetic mutation operator allows the PGA to create offspring with optimal fitness values. The final test run investigated the effect of the number of elite individuals, that are promoted to the next generation on the average fitness of the successive generation. I can conclude, that, the higher the number of elite individuals that are promoted, the higher the average fitness value of the successive generation and thus the higher the quality of offspring created. According to the time trial results, the CUDA PGA implementation runs 100-130 times faster than the serial GA implementation in MATLAB, which is the true litmus test of the success of the research undertaken. It illustrates that the application of the Master-slave Parallel Genetic Algorithm (PGA) framework for unsupervised cluster analysis on the CUDA platform, using the Giada and Marsili log-likelihood function as the fitness function, is a novel and promising new cluster analysis approach.

7.2 Future prospects

The current configuration of the Master-slave algorithm only allows for a minimal utilisation of the computational platform, using a fraction of the memory and processing capability due to the small size of the data-sets utilised. In theory, I could improve
on the Master-slave algorithm by fully exploiting the extent of resources that the GPU provides and as such, fully utilise the whole grid of thread blocks and run multiple clustering analysis processes in tandem. This would boost the efficiency of the Master-slave PGA and result in a novel hybrid Master-slave PGA for cluster analysis, where huge low-latency data feeds could be harvested for cluster characteristics in a fraction of the time it would take other algorithms to derive similar results.

Future prospects would include the proper implementation, testing and research of a Multiple-deme PGA on the GPGPU platform. Research, presented in Section 3.2.3, shows that the Multiple-deme approach scheme shows the most promise in terms of computational performance, and that it warrants further investigation.


