CUED - Engineering Tripos Part IIB 2023-2024   Module Coursework

Module	**4M17**	Title of report	**Assignment 2: Optimisation Algorithm Performance Comparison Study**

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4M17 Coursework #2
Optimisation Algorithm Performance Comparison

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December 19, 2023

1 Introduction

This report conducts a comparative analysis of two optimisation algorithms applied to minimise Keane's Bump Function, (KBF). In particular, the study focuses on a Continuous Genetic Algorithm, (CGA), as well as an alternative algorithm not covered in the lectures: Parallel Tempering, (PT). The initial sections involve fine-tuning the algorithms on the two-dimensional KBF to enhance their performance and investigate their respective capabilities. Following this, the algorithms are deployed on the eight-dimensional KBF, and a comprehensive performance evaluation is conducted to discern differences and similarities between them.
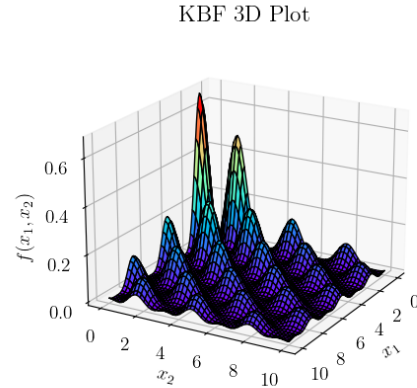
2 Keane's Bump Function

To compare the performances of the two algorithms, the Keane's Bump Function, (KBF), is used as the objective function. In particular, the n-dimensional constrained optimisation problem is defined as the maximisation of:

$$f(\mathbf{x}) = \left| \frac{\sum_{i=1}^{n}(\cos(x_i))^4 - 2\prod_{i=1}^{n}(\cos(x_i))^2}{\sqrt{\sum_{i=1}^{n} i \cdot x_i^2}} \right| \quad (1)$$
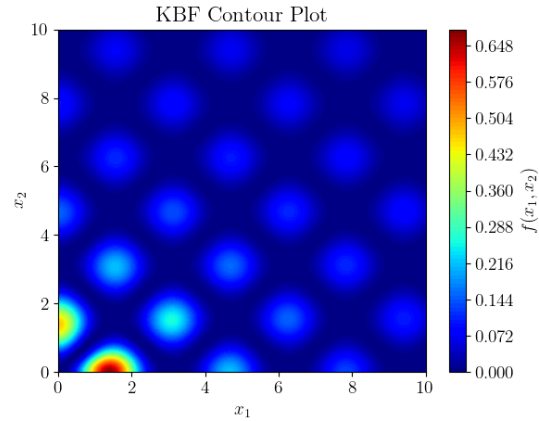
$$\text{subject to} \quad 0 \le x_i \le 10 \quad \forall i \in \{1, \dots, n\}$$

$$\prod_{i=1}^{n} x_i > 0.75$$
$$\sum_{i=1}^{n} x_i < \frac{15n}{2} \quad (2)$$

The two-dimensional form of the function has been plotted in Figure 1. Some notable properties are as follows:

(a) Surface plot.

(b) Contour plot.

Figure 1: Two-dimensional visualisation of the Keane's Bump Function, (KBF).

- The function is undefined at the origin, (0, 0). This is due to the division by zero in the denominator of Equation 1. Otherwise, the function is continuous and differentiable everywhere.

- The function is highly multi-modal. Its global maximum is located on the constaint boundary $x_n = 0$, where x_n denotes the final variable in the n-dimensional space. However, there are many

local maxima located inside the feasible region, all of which have quite similar amplitudes.

- The function is nearly symmetric about the line $x_1 = x_2$. This stems from its construction in 1, using the sums of squared, symmetric terms, x_i^2, $(\cos(x_i))^2$, and $(\cos(x_i))^4$. This results in some invariance regarding the order of the input variables. Overall, the peaks consistently manifest in pairs, yet there is a notable pattern wherein one peak always surpasses its counterpart in magnitude.

Given the above properties, the KBF is a challenging function to optimise. The presence of multiple, similar-amplitude local maxima makes it difficult for an optimisation algorithm to converge to the global maximum. On the other hand, all control variables share the same nature, (continuous variables), and exhibit identical scales. Additionally, all constraints are of the inequality type, and the feasible space is non-disjoint.

The problem becomes more complicated with the inclusion of the constraints outlined in 2. Figure 2 illustrates the resulting feasible region carved out of the original function space. Notably, the contstraint boundaries are non-linear. The problem complexity is additionally excaberated by the presence of multiple optima along the constraint boundaries, including the global maxima that we seek to identify.

These properties make the KBF a suitable candidate for the comparative analysis of the two optimisation algorithms, as discussed in the previous work of [3].
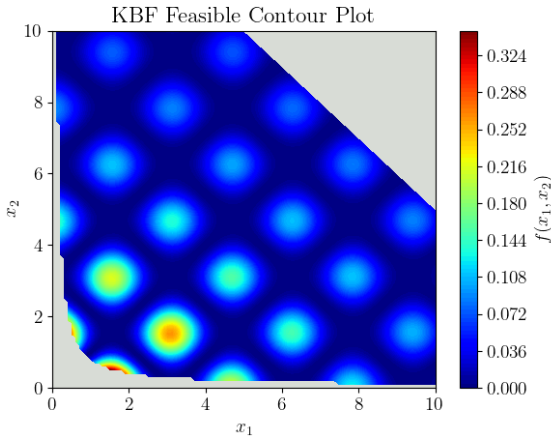

Figure 2: Feasible region carved out from the two-dimensional visualisation of the Keane's Bump Function, (KBF).

3 The Continuous Genetic Algorithm (CGA)

The discrete nature of the GA presented in [9] makes it unsuitable for the optimisation of the KBF. An implementation of a Continuous Genetic Algorithm, (CGA), is used instead, which lends itself better to the problems presented in 1-2.

The CGA, a technique inspired by natural selection and genetics, presents itself as particularly well-suited to tackling challenges associated with multiple local optima. Furthermore, the algorithm lends itself well to parallelisation with low implementation effort, and offers ample opportunities for modifications and adaptations, supported by a rich body of literature on the subject.

The primary difference between the CGA and the GA in [9] is the representation of individuals, (solutions of the state space), within the population. Rather than representing an individual as a vector of binary values or bits, (0s and 1s), the CGA uses a real-valued vector of floating-point numbers to represent each individual, as discussed in [4]. This allows for a direct representation of the problem, and eliminates the need for a decoding function, which reduces overhead in function evaluations.

This adjustment marks a significant departure from conventional GAs, aligning the algorithm more closely with Evolution Strategies (ES), another member of the evolutionary algorithms family presented in [12]. However, the algorithm presented in 3.1 is still classified as a GA in accordance with the differences presented in [5], given that mutation does not serve as the primary search mechanism for exploring the state space. Instead, it functions as a non-adaptive, background operator.

3.1 Implementation

In accordance with the terminology presented in [9], a vector solution of the state space will be referred to as an *individual* or *chromosome*. Correspondingly, a collection of such individuals arranged in a matrix format will be denoted as a *population*. Each individual is delineated as an $n \times 1$ vector of real-valued (floating-point) numbers, where n signifies the number of variables in the state space. The population itself is represented as a $m \times n$ matrix, where m designates the count of individuals in the population. This count is explicitly defined as a hyperparameter within the code, and is referred to as *POPULATION_SIZE*.
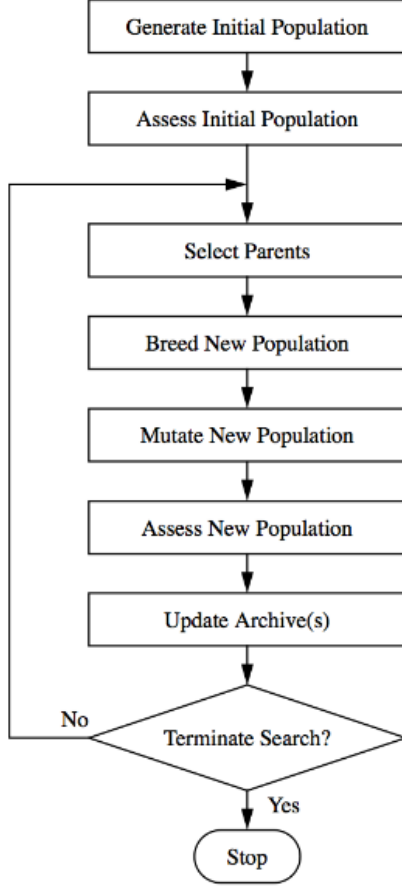
Figure 3: A flowchart depicting the CGA process, taken from [9].

The CGA process is outlined in Figure 3. Notably, three selection strategies and two mutation procedures were deliberately implemented to harness the flexibility inherent in the CGA, tailoring it to the optimisation challenges posed by the KBF. The subsequent section, 3.2, elucidates the selection method and mutation procedure choices that form the basis of the forthcoming comparison.

The CGA can be can be finely tuned for a specific objective function by modifying its fitness function, which assesses the quality of an individual. The management of constraints is woven into the selection process, as outlined later in Section 3.1.2.

3.1.1 Initialisation

The population is initialised with random values uniformly distributed within the range of 0 to 10, which represents the bounds of the state space, encompassing both feasible and infeasible values. This population comprises 250 individuals, as defined by the *POPULATION_SIZE* hyperparameter.

3.1.2 Parent Selection

Three selection methods were implemented: proportional selection, tournament selection, and stochastic remainder selection without replacement (SRS). The hyperparameter governing the quantity of parents chosen, denoted as *NUM_PARENTS*, is established at 25% of the population size, (rounded down to the nearest even number to facilitate the creation of parent pairs).

Another important aspect of the selection process is the handling of constraints. In particular, the selection process is repeated until only feasible individuals are selected. Infeasible individuals are simply not chosen as parents, a strategy advised by [9], which was deemed suitable considering that the feasible space is non-disjoint, and the constraints are of the inequality type.

Proportional Selection

The probability of an individual being selected for mating is proportional to its fitness:

$$P_i = \frac{f_i}{\sum_{i=1}^{n} f_i}$$

Here, f_i denotes the fitness of the ith individual. This is the simplest selection method, and is implemented in accordance with the theory presented in [9].

As noted in [9], this approach is susceptible to high variance in individual selection, primarily because there is no assurance of choosing the optimal individual. Alternatively, the following two procedures show greater potential, incorporating a degree of determinism into the selection process.

However, it would be premature to disregard the proportional selection method. There is a chance that the determinism inherent in the other two methods could negatively impact the KBF optimisation process. A notable degree of stochasticity may improve the algorithm's effectiveness in exploring the search space, which may prove vital given the multi-modal nature of the KBF.

Tournament Selection

As outlined in [9], this strategy involves taking a small subset of the population, and selecting the top two individuals with the highest fitness. This is repeated until the required number of parents is achieved. Selection pressure can then be adjusted by varying the size of the subset, controlled by the *TOURNAMENT_SIZE* hyperparameter.

This is a popular selection method, as it is simple to implement, and is known to perform well in practice. It can be improved by including some of the concepts presented in [7], however, these have been avoided to

reduce the complexity of the algorithm's implementation.

Stochastic Remainder Selection without Replacement (SRS)

This strategy draws inspiration from [9]. Specifically, a group of chosen individuals is curated by generating an expected number of copies for each individual, denoted as:

$$E_i = N * P_i$$

Here, N represents the population size, and P_i is elucidated above in the context of proportional selection. The anticipated number of duplicates is subsequently divided into an integer part, $I_i = \lfloor E_i \rfloor$, and a remainder, $R_i = E_i - I_i$.

The integer part is used for deterministic selection of individuals. The ith indivdual is selected I_i times. Subsequently, the remained, R_i, is then used to stochastically augment the collection of individuals until the required number of parents is achieved. This is done by selecting the ith individual with a probability of R_i.

The discussion in [9] highlights that this approach appears to yield superior performance, ascribed to the inclusion of a degree of determinism in the selection criteria. Nevertheless, it remains worthwhile to evaluate the performance of the other two methods, as they might present distinct advantages within the framework of the KBF.

3.1.3 Mating Procedure

Similarly, two mating procedures have implemented: crossover and heuristic crossover. The entire population is replaced by offspring, bred from two randomly allocated parents from the pool of selected parents.

Crossover

The crossover procedure adheres to the principles detailed in [9]. Initially, a crossover point is randomly chosen. Genes from the first parent are incorporated into the offspring until this point, beyond which genes from the second parent take their place. Specifically, the sequencing of the parents is governed by the probability specified by the hyperparameter *CROSSOVER_PROB*.

Heuristic Crossover

Heuristic crossover is presented in [6]. By this variation, a random number β in the interval $[0, 1]$ is generated. The genes of the offspring are then determined as a blend of the original two parents, p_1 and p_2, as follows:

$$o_i = \beta(p_{1i} - p_{2i}) + p_{2i}$$

With this inspiration in mind, heuristic crossover was implemented in the CGA. Specifically, the sequence of parents in the above formula is determined by the *CROSSOVER_PROB* hyperparameter, aligning with the approach used previously in the original crossover procedure.

A crucial factor to bear in mind is that certain offspring may be produced outside the feasible region. This implementation deviates from the recommendation in [6] by not outright rejecting these offspring during the mating procedure. Rather, they are simply excluded from consideration as parents in the subsequent selection process.

The decision to incorporate this mutation procedure stems from the continuous nature of the state space. While the conventional crossover methods may be well-suited to binary representations, a more intuitive approach emerges when grappling with real-valued variables - using a blend of characteristics from both parents.

Moreover, the use of the heuristic crossover method aims to address previous limitations associated with standard crossover. Unlike conventional crossover, which confines offspring values to those of the parents, blending permits the generation of offspring beyond the parent values, allowing for potentially new information. This feature may prove particularly advantageous in the context of the KBF, enhancing the algorithm's capability to navigate the search space adeptly and thoroughly explore local optima.

An additional noteworthy observation is that the introduction of β serves to bring the CGA into closer alignment with Evolutionary Strategies (ES). This resemblance becomes evident as the formulation above bears some similarity to the intermediate recombination strategy outlined in [12]. Nevertheless, it is essential to emphasise, as mentioned earlier, that mutation does not serve as the primary search mechanism in the CGA. Consequently, the CGA can still be appropriately categorised as a GA, as per the classification seen in [5].

3.1.4 Mutation

The mutation procedure proposed by [4] involves perturbing a gene within a chromosome by a normally distributed random number with a mean of zero and a standard deviation of σ. However, the effectiveness of this procedure is constrained by the selection of σ as an additional hyperparameter, necessitating careful tuning.

Instead, a simpler approach was adopted, where genes within the population have an probability, given by the

mutation rate, of being reset to a random value drawn from a uniform distribution within the confines of the state space, mirroring the initialisation procedure.

3.1.5 Evaluation

The population is then evaluated, and the individuals are ranked in order of fitness. Here, the fitness is defined as the negative of the KBF cost function, outlined in 1. This is done to align the algorithm with the maximisation of the KBF.

3.1.6 Termination

For this section of the report, the algorithm terminates after a maximum number of iterations, (defined as a hyperparameter). A more stringent convergence criterion is adopted for the comparison between the two algorithms in Section 5. The individual with the lowest fitness value is then returned as the optimal solution to the optimisation problem.

3.2 Tuning the CGA

Given the flexibility of the CGA, multiple selection methods and mutation procedures were implemented within the codebase, as discussed previously. These are then selected as hyperparameters within the experiments presented in 10, to take advantage of the flexibility offered by the CGA.

To choose a selection method and mutation procedure going forwards into the main comparison of this report, code 10 was used as a platform for experimentation. Each selection method and mutation procedure was evaluated over 10 and 100 iterations, with a constant mutation rate of 0.05, and a crossover probability of 0.7. The number of parents was established at 25% of the population size, (rounded down to the nearest even number to facilitate the creation of parent pairs). The population size itself was set at 250, and the tournament size was similarly defined as 25% of this.

Supplementary results regarding this initial exploration of hyperparameter tuning are detailed in Section 6.1. Specifically, the final fitness values are outlined in Table 2. At a first glance, it would appear that all selection methods and mutation procedures perform similarly, offering convergences to similar fitness values. Minor variations could be attributed to the stochastic nature of the CGA, and the small number of iterations.

(a) Mutation Procedure: Crossover
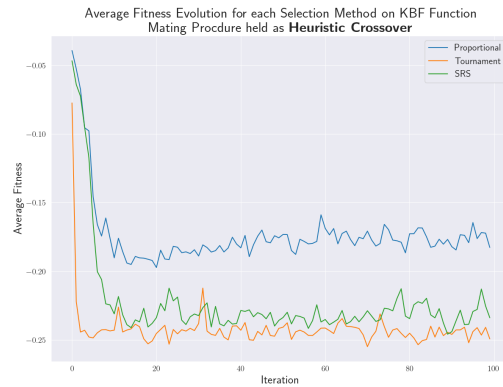
(b) Mutation Procedure: Heuristic Crossover

Figure 4: Evolution of the average fitness values of the CGA population over 100 iterations for each of the selection methods. The results are presented for both mutation procedures: crossover and heuristic crossover. Here, the mutation rate was set to 0.05, and the crossover probability was set to 0.7.

However, more insightful conclusions can be drawn from the figures presented in 4, which illustrate the evolution of the average fitness values of the CGA population over 100 iterations for each of the selection methods. They illustrate that tournament selection seemed to outperform the other two selection methods when maximising the KBF, which is surprising given the favourable description in [9] regarding SRS.

The experiment was repeated several times, yielding results that were admittedly variable, attributed to the inherent stochastic nature of the CGA. At times, the superiority of SRS over tournament selection was evident, yet proportional selection generally did not prove to perform better. Despite this variability, the outcomes exhibited sufficient consistency to justify the designation of tournament selection as the primary method for the upcoming comparison.

The observed differences in performance may be attributed to the distinct characteristics of the KBF. Tournament selection appears to demonstrate greater efficacy in navigating the search space compared to SRS, perhaps due to its less deterministic nature. This becomes particularly significant in light of the multimodal nature of the KBF, where a certain level of stochasticity may prove essential for thorough exploration of the search space.

The results additionally indicate that when combined with tournament selection, the heuristic crossover procedure generally outperformed the standard crossover method. This is evident in the typically steeper decline in average fitness values, as illustrated in Fig. 4b. Furthermore, the heuristic crossover exhibited greater result consistency across repeated experiments and generally converged to higher maximas compared to the standard crossover. Although the observed differences were note always significant, the overall trend supports the choice of heuristic crossover as the preferred mating procedure for the forthcoming comparison.

This may be attributed to the heuristic crossover's capacity to generate offspring beyond the existing genotypes present within a generation. This attribute is especially beneficial within the framework of the KBF, enhancing the algorithm's ability to navigate the search space adeptly and systematically explore the numerous local optima.

Having cemented the selection method and mutation procedure choices as tournament selection and heuristic crossover respectively, the CGA was further tuned to optimise its performance.

Specifically, choices for the mutation rate and crossover probability were explored. The results are presented in Figure 5, which showcases two heat maps of the final fitness values after 100 iterations for the CGA using the chosen procedures. The plots are presented for both the average final fitness, as well as the final fitness of the best individual.

Notbaly, as depicted in Fig. 5a, it is evident that an increased stochasticity of the CGA, indicated by higher crossover probabilities, leads to improved average final fitness. This aligns with expectations, as a broader and more randomly distributed population enhances the likelihood of individuals being situated in the proximity of local maxima. Consequently, a greater number of individuals within the population receive lower fitness values, a trend reflected in the observed average final fitness.

Fig. 5b offers deeper insights. It is evident that the crossover probability stands out as the most influential hyperparameter, while the fine-tuning of the mutation rate plays less of a role in shaping the performance of the CGA.
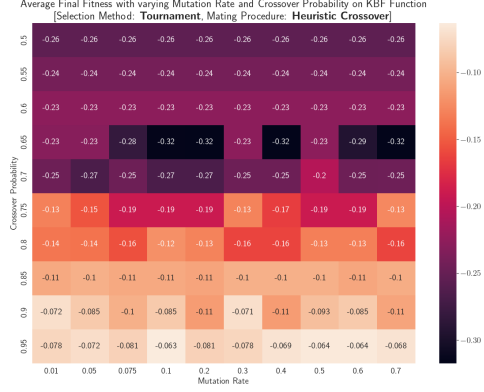
(a) Average final fitness across entire population.
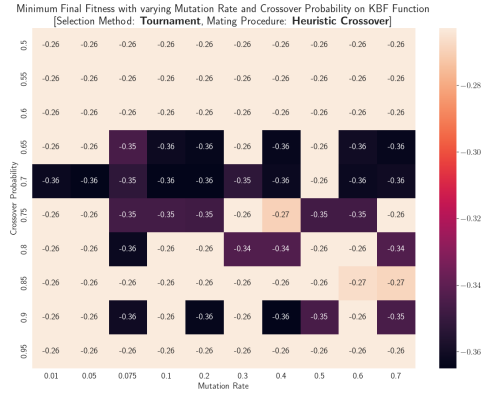
(b) Final (minimum) fitness of best individual.

Figure 5: Heat maps of the final fitness values after 100 iterations for the CGA using tournament selection and heuristic crossover. Here, the mutation rates and crossover probabilities were varied to assess their impact on performance.

Overall, a clear optimal set of hyperparameters emerges. Moving forward, the mutation rate is fixed at 0.1, and the crossover probability is set to 0.65. These values have proven to yield a consistently optimal performance for the algorithm, comfortably lying within the darker regions of the heat maps.

To reiterate and summarise this section of the report, the CGA is now constructed as follows:

- **Selection Method:** Tournament Selection
- **Mutation Procedure:** Heuristic Crossover

- **Mutation Rate:** 0.1

- **Crossover Probability:** 0.65

- **Tournament Size:** 62

- **Number of Parents:** 62

- **Population Size:** 250

Fig. 6 depicts the evolution of the fitness values over 100 iterations using the optimal hyperparameters delineated above. Note that the (minimum) fitness attributed to the best individual remains constant, because an individual within the population is stochastically initialised near the local maxima that the algorithm converges to. This is less likely to occur in the 8-dimensional comparison, where the minimum fitness is expected to evolve more noticeably, given that the search space is significantly larger, and initialisation will be handled with more care.

Fig. 7 depicts the convergence of the population to the second largest maxima over 4 and 80 iterations using the optimally-tuned CGA. Note that the horizontally and vertically distributed outliers are attributed to crossover. Regrettably, global maximum convergence remained elusive even after 100 iterations. However,

there does seem to be a discernible trend of the algorithm converging towards the second-largest maxima in Fig. 7, offering a promising indication of progress.

The primary challenge lies in the fact that both the first and second largest maxima are situated along the non-linear constraint boundary of the optimisation problem, posing a difficult navigational challenge.
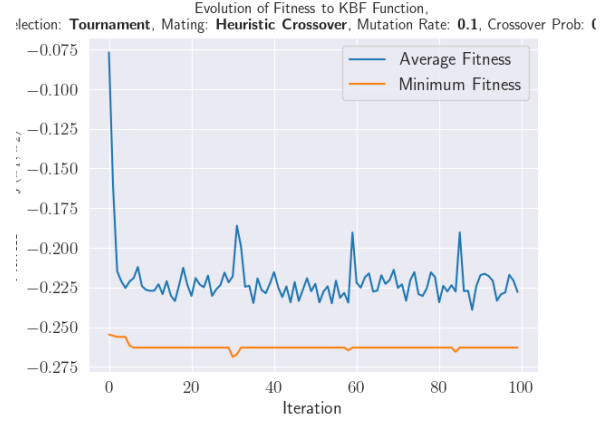
Figure 6: Evolution of the fitness values of the CGA population over 100 iterations for optimally-tuned CGA.
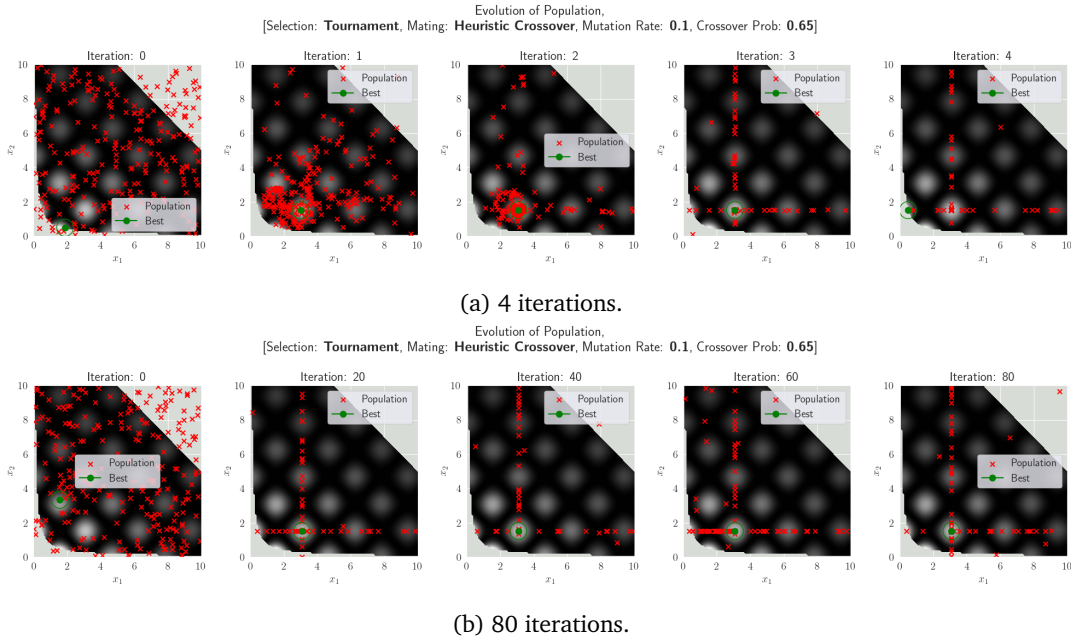

(a) 4 iterations.

(b) 80 iterations.

Figure 7: Evolution of the CGA population over 4 and 80 iterations using the optimal hyperparameters outlined at the end of Section 3.2. The second plot depicts the algorithm converging to a local maxima as a result of an individual being initialised near it.

4 Parallel Tempering (PT)

Having obsererved the CGA's performance and its difficulty in identifying global maxima effectively, an informed decision was made to introduce Parallel Tempering (PT) as the second algorithm for comparison.

This is a Markvo Chain Monte Carlo (MCMC) optimisation approach presented in [2]. Similar to simulated annealing, (SA), it revolves around the idea of smoothening the search space by introducing a temperature parameter, t.

By incorporating a Metropolis-Hasting acceptance probability that is proportional to $\exp(1/t)$, exploration of the solution space is encouraged at high temperatures, while exploitation of the local nature of the function is facilitated at low temperatures. At high temperatures, the acceptance distribution is is smoothened out by this proportionalilty, and the algorithm is then able to explore the search space more thoroughly. As the temperature diminishes, the acceptance distribution becomes more dependent on the fitness of the proposed solution to the KBF, enabling the algorithm to explore the local nature of the function.

However, PT incorporates the novel concept of Replica Exchange Monte Carlo. Unlike SA, which operates along a single tragectory, starting with a high temperature that gradually decreases, PT maintains multiple replicas of the system at different temperatures simultaneously. Each replica explores its own solution space, and exchanges of the solutions can occur between replicas at adjacent temperature levels. This exchange mechanism enhances global exploration by facilitating the movement of solutions between replicas operating at high and low temperature.

This parallel exploration across temperatures improves the algorithm's ability to escape local optima, providing a valuable alternative to traditional single-trajectory methods like SA. Consequently, PT could emerge as a well-suited approach for maximising the highly multi-modal KBF.

Unfortunately, this introduces an elevated computational cost, due to the management of multiple replicas and the periodic exchange of solutions. However, the potential advantages in terms of global exploration of the KBF outweigh the added computational expense. This is especially true, considering the highly parallelisable nature of PT, which may allow for even more efficient utilisation of parallel computing resources than the CGA.

4.1 Implementation

The discourse presented in [2] emphasises a delicate trade-off between optimising MCMC sampling outcomes and minimising computational efforts. Hence, the PT implementation presented here is deliberately crafted for flexibility, offering the ability to fine-tune the algorithm, as shown in Section 4.2.

As per the guidance in [10], constraints are handled by simply rejecting any proposed changes that violate the constraints. This is accomplished within the Metropolis-Hastings criterion regarding the acceptance or rejection of a proposed change. This was determined as a suitable approach, given that the feasible space is non-disjoint, and the constraints are of the inequality type.

The approach can additionally be characterised as population-based, incorporating 10 replicas in accordance with the *NUM_REPLICAS* hyperparameter. Within each replica, there are 25 chains of solutions determined by the *NUM_CHAINS* hyperparameter. Consequently, the total number of solutions being evaluated at any given time is 250, which is equivalent to the population size of the CGA.

4.1.1 Initialisation

The chains are initialised within the range of 0 to 1, as advised by the guidance provided in [11], specifically under the SA-derived solution generation framework presented in Section 4.1.4.

This range persists throughout the algorithm, until function evaluations are necessitated, at which point the *scale_up* lambda function is called to return the solution in the original state space.

Mirroring the CGA implementation, solutions were initialised without consideration for their feasibility. Whilst initialising within the feasible solution space was observed to enhance performance, this approach was deliberately omitted to ensure fair comparisons between the PT and CGA. However, the performance was notably compromised, given that solutions initialised deep within the infeasible zones of the search space faced challenges in escaping under the Metropolis-Hastings acceptance criterion.

4.1.2 Temperature Scheduling

A significant source of flexibility in PT lies in setting and adapting the temperatures of the replicas, as discussed in [2]. Drawing insights from the previous work of [1] on an unrelated, yet similar problem, this was taken advantage of by parameterising the temperature

schedule between 0 and 1, as follows:

$$T_i = \left(\frac{i}{N_{\text{replicas}}}\right)^p \quad \forall i \in \{1, \ldots, N_{\text{replicas}}\} \quad (3)$$

Here, T_i denotes the temperature of the ith replica, and N_{replicas} is the total number of replicas. The exponent p is a hyperparameter referred to as *POWER_TERM* that can be tuned to optimise the performance of the algorithm.

Fig. 8 illustrates the influence of parameter p on the temperature schedule. It intuitively demonstrates how p affects the balance between exploration and exploitation. A higher value of p corresponds to a slower and more gradual increase in temperature, promoting a conducive environment for exploration. A smaller value of p results in a more rapid increase in temperature, encouraging exploitation of the local nature of the function.
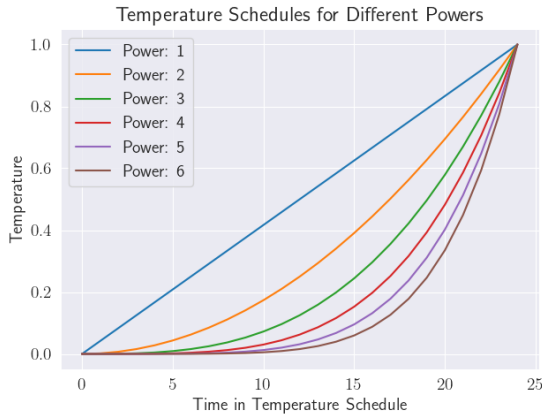

Figure 8: Temperature schedule 3 for the PT algorithm for different values of the *POWER_TERM* hyperparameter.

Tuning this balance is crucial for the algorithm's performance against the KBF, and is conducted in Section 4.2. While alternative approaches, such as geometric progression [2] are recommended in most literature, the above formulation was made to enhance control over the replica temperatures.

4.1.3 Replica Exchange

The most popular approach to replica exchange, as outlined in [2], involves periodic execution. The interchange of solutions between replicas at adjacent temperature levels occurs at regular intervals. In this implementation, periodic exchange is guided by the hyperparameter *EXCHANGE_PARAM*. This hyperparameter assumes values in the range of 0 to 1, representing

the proportion of total iterations that must pass before another swap takes place. A value of 0.05 indicates that a swap occurs every 5 iterations when the maximum number of iterations is set to 100.

However, a second approach has also been implemented, which will be referred to as stochastic exchange. In this configuration, the possibility of replica exchange exists in every iteration, and the hyperparameter *EXCHANGE_PARAM* now functions as the probability governing the occurrence of this swap.

Both have been introduced to enhance the flexibilty of the algorithm, allowing for either a more deterministic or stochastic approach to replica exchange. The optimal choice is determined in Section 4.2.

Upon meeting the conditions for a swap, the replicas are sequentially traversed in ascending order of temperature. Each replica undergoes an attempt to exchange all of its solutions with the subsequent replica in the sequence. The likelihood of accepting such a swap is dictated by the adapted Metropolis-Hastings acceptance criterion, as detailed in Section 4.1.5.

4.1.4 Metropolis Update

The inspiration for proposing a new solution stems from [11], which introduces a routine that leverages accumulated experience from prior iterations to generate SA update steps. Given the similarity between SA and PT, this approach was deemed suitable for the PT implementation.

In particular, a new solution is generated by:

$$\mathbf{x}_{\text{new}} = \mathbf{x}_{\text{old}} + \mathbf{D}\mathbf{u} \quad (4)$$

In this context, $\mathbf{u}$ represents a vector of uniformly distributed random numbers within the range of $[-1, 1]$, while $\mathbf{D}$ is a diagonal matrix specifying the maximum permissible step size in each dimension of the state space. In this PT implementation, $\mathbf{D}$ is uniquely defined for each solution across all replicas. Following the acceptance of a new solution, the matrix $\mathbf{D}$ is updated using the formula:

$$\mathbf{D}_{\text{new}} = (1 - \alpha)\mathbf{D}_{\text{old}} + \alpha\omega\mathbf{R}$$

Here, the constants α and ω are set at 0.1 and 2.1 respectively, in accordance with the guidlines presented in [11]. The matrix $\mathbf{R}$ is a diagonal matrix whose elements represent the magnitudes of the successful changes made to each dimension within a specific solution.

4.1.5 Metropolis-Hastings Acceptance Criterion

The probability of accepting a proposed solution is determined by the Metropolis-Hastings acceptance criterion. This has been specifically formulated to work alongside the "adapting" update step, 4, with additional insights drawn from the works of [11] and [8]. The probability of accepting a new solution generated by Eq. 4 is given by:

$$P_{\text{accept}} = \min \left[1, \exp \left(\frac{f(\mathbf{x}_{\text{new}}) - f(\mathbf{x}_{\text{old}})}{k \cdot T_i \cdot \tilde{d}} \right) \right]$$

In the above formulation, the negation of the objective function: $-f(\mathbf{x})$, represents the fitness of a solution $\mathbf{x}$, k is the Boltzmann constant, T_i is the temperature of the $i$tj replica, and $\tilde{d}$ is euclidean normed distance between the old and new solutions.

However, when judging the swap of two solutions through a replica exchange, the acceptance probability is instead adapted to:

$$P_{\text{accept}} = \min \left[1, \exp \left(\frac{f(\mathbf{x}_{\text{new}}) - f(\mathbf{x}_{\text{old}})}{k\tilde{d}} \left(\frac{1}{T_{\text{old}}} - \frac{1}{T_{\text{new}}} \right) \right) \right]$$

in accordance with [8]. This imposes a harsher standard for the acceptance of a swap between replicas operating at vastly different temperatures, which is a desirable feature, especially when the power term, p, is set to a high value.

4.1.6 Termination

Again, the algorithm terminates after a maximum number of iterations, (defined as a hyperparameter), in this section of the study. A more stringent convergence criterion is adopted for the comparison between the two algorithms in Section 5. The solution with the lowest fitness value across all replicas is then returned as the optimal solution to the optimisation problem.

The total number of iterations is fixed at 100, which generally proved insufficient for the algorithm to achieve complete convergence. Rather than emphasising complete convergence, the assessment centers around tracking the evolution of average fitness values. This approach provides insights into the algorithm's effectiveness and speed, gauging its progress within the limited span of 100 iterations.

4.2 Tuning the PT

As with Section 3.2, the flexibility offered by PT was first explored using the parallelised experiments presented in code 11.

Unlike the CGA table (Table 2), the preliminary exploratory findings presented for PT (Table 3) imply a

subtle correlation between the power term of the temperature schedule and the algorithm's performance. Final fitness values exhibit relative constancy, hinting at no potential connection. However, the variability in algorithm performance appears more pronounced when considering the approach to replica exchange.
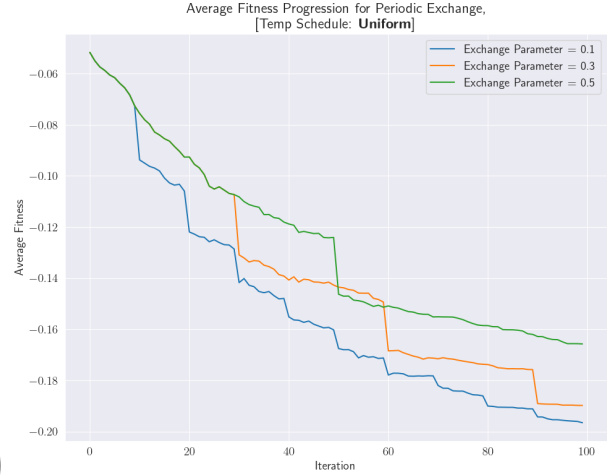
(a) Periodic Exchange
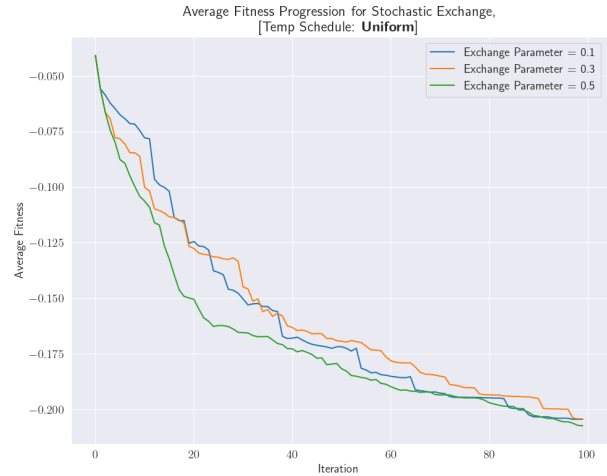
(b) Stochastic Exchange

Figure 9: Evolution of average fitness values of the PT solutions over 100 iterations for the two approaches to replica exchange. Temperature scheduling was kept uniform.

Fig. 9 instead illustrates the evolution of the average fitness values across all 100 iterations for both exchange procedures. The result present a clear distinction between the two approaches that remains consistent with repitition.

The periodic exchange approach seems to exhibit a higher dependency on the value assigned to the ex-

change parameter. In contrast, the stochastic exchange approach appears to follow a consistent descent, irrespective of the exchange parameter value. This observation is unexpected, considering that the exchange parameter is anticipated to exert a similarly significant influence on both approaches. In both cases, the exchange parameter affects the frequency of swaps, which is expected to impact the algorithm's ability to escape local optima.

Additionally, the descent depicted in Fig. 9a seems steeper when the exchange parameter assumes smaller values. This aligns with expectations, as a smaller exchange parameter corresponds to a higher frequency of swaps in the periodic case. Here, the exchange parameter is interpreted as the proportion of total iterations that transpire before another swap takes place. When applied to the KBF, PT demonstrates greater efficacy when the algorithm is permitted to exchange solutions more frequently. This implies that increased exploration of the search space is well-suited to optimising the KBF.

Figures 11 and 12 present a final analysis of these hyperparameters. However, the stochastic heatmap, 12b, did not exhibit any consistency or superiority over the periodic heatmap, 11b, leading to no further consideration of stochastic exchange, given its suboptimal and unpredictable behavior.

In contrast, a consistent pattern unveiled itself in Fig. 11b, which persisted across repetitions. The PT algorithm, when applied to the KBF, consistently demonstrated a inclination towards a lower exchange parameter paired with a low power term. This may be rationalised by the fact that a lower exchange parameter corresponds to a heightened frequency of swaps, facilitating dialogue between the replicas and encouraging more exploration. Conversely, a low power term fosters a delicate equilibrium between exploration and exploitation, as evident in Fig. 8. The preference for uniform temperature scheduling likely stems from its enhanced capability to focus on local changes, after arriving at a particular optimum. Any exploratory capabilities stem from replica exchange, after which the algorithm can then focus on exploiting the local nature of the function.

Overall, these results imply that optimal settings for the PT algorithm on the KBF involve a power term of 1 and an exchange parameter of 0.01. These values are associated with a uniform temperature schedule and replica exchange taking place at every iteration. They position the PT algorithm favorably within the lighter regions of Fig. 11b.

In summary and to reiterate, the PT algorithm is now constructed as follows:

- **Number of Replicas:** 10
- **Number of Chains:** 25
- **Power Term:** 1
- **Exchange Procedure:** Always
- **Exchange Parameter:** N/A

Fig. 10 depicts the evolution of the fitness values over 100 iterations using the optimal hyperparameters delineated above. The fitness of the best solution drops noticeably once better solutions are identified and arrived at through the MCMC updating process.
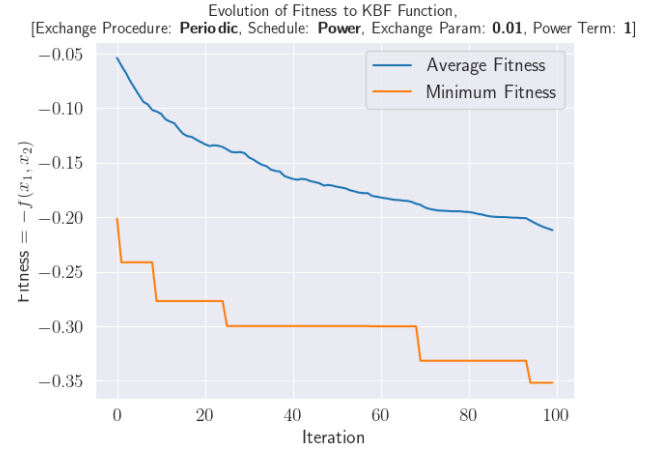
Figure 10: Evolution of the fitness values of the optimally-tuned PT solutions over 100 iterations.

The top row in Fig. 13 depicts the iterative evolution of the solutions. Notably, all solutions consistently converge towards the prominent maxima, and the global maximum is successfully identified in every repetition. The PT algorithm has demonstrated superior capabilities in exploration compared to the CGA.

The optimal solution is denoted by a green circle. For a more insightful comprehension of the Markov Chain Monte Carlo (MCMC) updating process, a particular solution within the final replica is emphasised in yellow. This solution is monitored throughout all iterations and it seems to become ensnared in a local optimum during the earlier iterations. However, it then successfully breaks free through the exchange mechanism and begines to converge towards a larger maximum in subsequent iterations.

The bottom row in Fig. 13 showcases the final solutions of each replica, organised by temperature and superimposed over the temperature-smoothed KBF con-

tours. The arrangement follows an ascending temperature order, with the replica at the lowest temperature positioned on the left. These results shed light on the fundamental dynamics of the algorithm.

At lower temperatures, all solutions exhibit a clear inclination toward the higher, global maxima of the KBF. This preference arises from ample exploration of the search space. In contrast, solutions at higher temperatures display a more dispersed distribution, converging around local optima.

Additionally, although these higher temperatures encourage localised exploration, the replica exchange mechanism facilitates the movement of solutions within the final temperature towards the larger maximas. Subsequent iterations are anticipated to drive convergence of solutions at higher temperatures towards the global maxima as well.
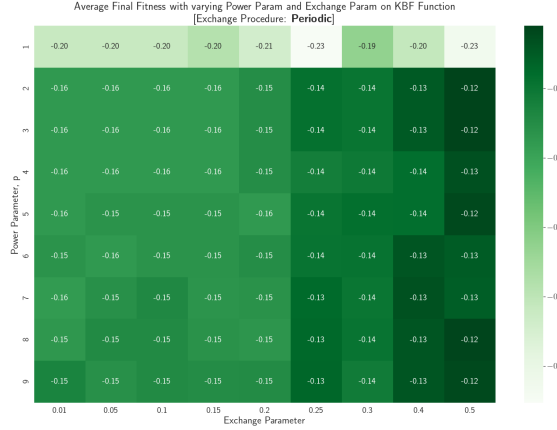
(a) Average Fitness Values
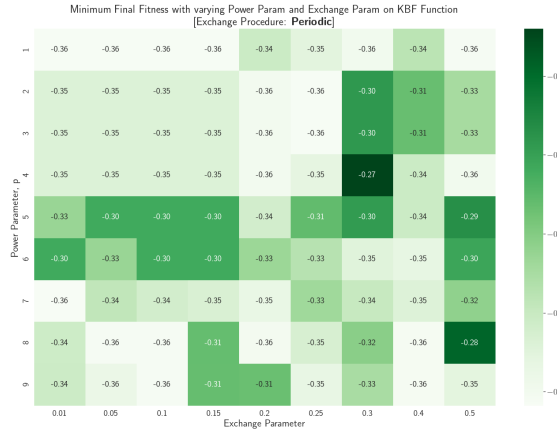
(b) Minimum Fitness Values

Figure 11: Heatmaps of the final fitness values after 100 iterations for the PT algorithm using periodic exchange. Here, the power term and exchange parameter were varied to assess their impact on performance. Despite the somewhat varied outcomes between repitition, a consistent trend emerges - the PT algorithm demonstrates a preference for a lower exchange parameter coupled with a moderate power term.
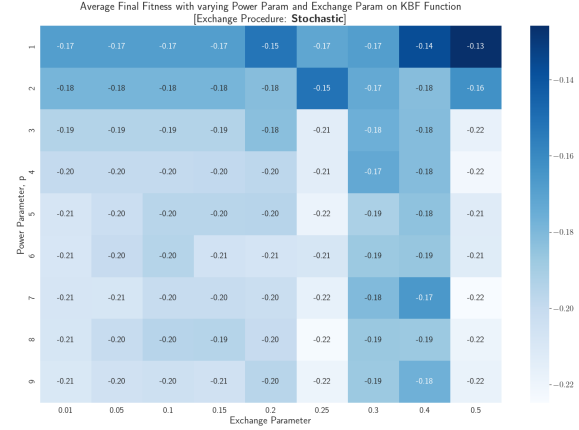
(a) Average Fitness Values
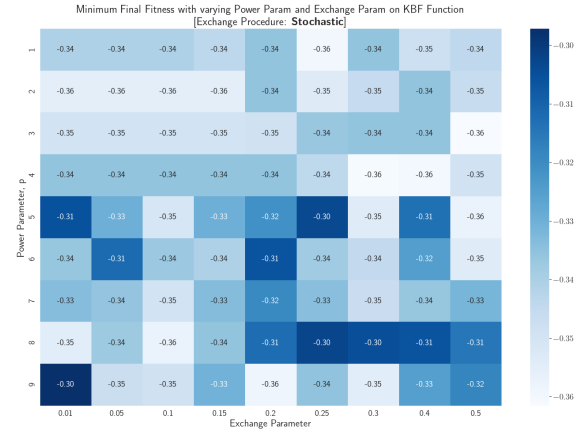
(b) Minimum Fitness Values

Figure 12: Heatmaps of the final fitness values after 100 iterations for the PT algorithm using stochastic exchange. Here, the power term and exchange parameter were varied to assess their impact on performance. The values for the best (minimum) final fitness varied greatly upon repitition. Generally, performance was outmatched by periodic exchange, which was also more consistent and controllable.
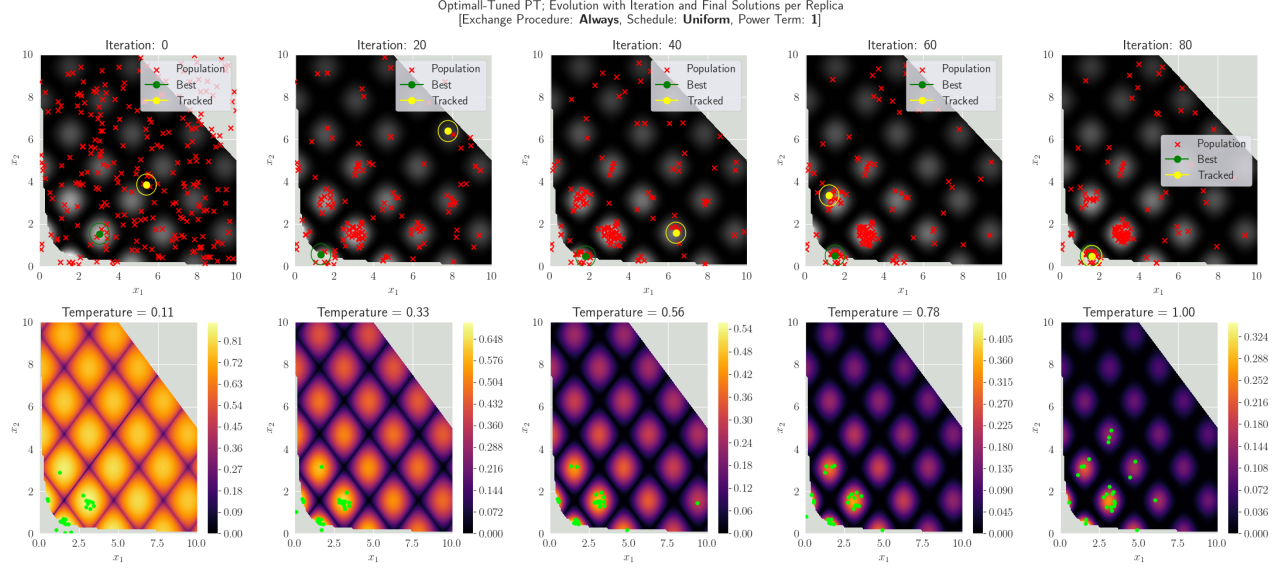
Figure 13: Visualisation of the optimally-tuned PT algorithm. The first row illustrates the evolution of the solution with each iteration. The optimal solution is marked with a green circle. To enhance the understanding of the MCMC updating process, a specific solution within the final replica is highlighted in yellow. The second row displays the final solutions arranged for each replica, overlaid across the smoothened KBF, $f(\mathbf{x})^T$, to help visualise the theory of PT. Lower temperatures facilitate exploration, while higher temperatures encourage exploitation. However, exchange ensures that solutions at higher temperatures are also driven towards the global maxima.

5 Comparison

After fine-tuning both algorithms for the 2-dimensional KBF, a comparative analysis was conducted to assess their performances in optimising the 8-dimensional KBF using the code presented in 12. 50 optimisation loops were conducted for each algorithm, each with a different initialisation. Collected data included expected values and standard deviations of fitness values, as well as the mean CPU time taken to complete all 10,000 iterations and the average iteration count at which convergence occurred.

To uphold fairness and reproducibility, these initialisations were shared between both algorithms. They were generated using random number seeds within the *generate_initial* function, which is part of the *helper_functions.py* file 7. The implementation of this function was crucial for ensuring reproducible outcomes and guaranteeing that solutions were initialised away from the global maxima. This was achieved by imposing a constraint that the maximum function value of these initial collections never exceeded 0.3.

Each run was limited to a maximum of 10,000 function evaluations, and convergence was identified as the point where the l_2-normed difference between the minimum fitness values of consecutive iterations stayed within a tolerance of 0.00025 for 1300 consec-

utive iterations. This was deemed appropriate after the trial run outlined in Section 5.1.

5.1 Trial Run

Prior to the experiment, a trial run of 15,000 funcation evaluations was conducted using one initialisation to assess the suitability of the convergence criterion, and to set expectations.

The outcomes are detailed in Table 1 and illustrated in Fig. 14. These findings underscore a particularly noteworthy result.

The two algorithms yielded fairly divergent solutions, as described in the last row of Table 1. The CGA underwent significant change within the initial 1% of iterations, after which it stabilised near its ultimate solution. In contrast, the PT algorithm consistently evolved over the entire span of 15,000 iterations. Consequently, the CGA demonstrated superior performance in the early iterations, but the PT algorithm ultimately surpassed it by converging to a lower minimum fitness value. This observation is a promising indication of the PT's capacity to escape local optima and explore the search space more efficiently.

However, this advantage comes with a trade-off in terms of increased computational demands. Specifi-

14

cally, the PT algorithm required approximately double the time to finish the 15,000 iterations compared to the CGA. Additionally, the PT algorithm required an extra 2551 iterations to converge to its optimal solution, resulting in a greater time investment of approximately 335.9 seconds, with respect to the CGA.

	CGA	PT
Final Avg. Fitness	-0.4971	-0.4646
Final Min. Fitness	-0.6901	-0.7081
Total Time Taken	299.2	592.7
Iters to Convergence	9349	11990
Optimal Solutions	3.104 3.027 1.624 0.5872 0.5363 0.6130 0.5294 0.4808	3.111 2.948 3.071 1.643 0.3356 0.4636 0.4284 0.2457

Table 1: Trial comparison between CGA and PT, after 15,000 iterations with one shared initialisation, (random seed = 538405).

(a) Average fitnesses.

(b) Minimum fitnesses.

Figure 14: Evolution of fitness values over 15,000 iterations for the CGA and PT algorithms, using a single initialisation as a trial run, (random seed = 538405).

Upon repeated trials, the PT algorithm was unable to consistently overtake the CGA within 10,000 iterations. As a result, it is unlikely that this dynamic will be evident in the final comparison. Nevertheless, the trial run yields valuable insights into the relative performance of the two algorithms and sheds light on potential trade-offs. Additionally, it reinforces the appropriateness of the convergence criterion, which was subsequently employed in the final comparative analysis.

5.2 Final Comparison

Having validated the experiment with a trial run, the final comparison was conducted using 50 different intialisations, generated with the following random seeds:

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6 Appendix

6.1 Supplementary Results regarding CGA Tuning

Selection Method	Mating Procedure	Iterations	Final Avg. Fitness	Final Min. Fitness
Proportional	Crossover	10	-0.19890798	-0.247328018
		100	-0.212384457	-0.24867806
	Heuristic Crossover	10	-0.199296791	-0.258198948
		100	-0.22656183	-0.250977443
Tournament	Crossover	10	-0.309572335	-0.331996331
		100	-0.309235401	-0.342745604
	Heuristic Crossover	10	-0.241261775	-0.262876797
		100	-0.247574635	-0.262876811
SRS	Crossover	10	-0.189986008	-0.208434151
		100	-0.288766718	-0.319667279
	Heuristic Crossover	10	-0.177779432	-0.207148488
		100	-0.182101833	-0.338823558

Table 2: Raw results from an initial exploration of the selection method and mutation procedure hyperparameters within the CGA. Presented as the final fitness values of the CGA population after 10 and 100 iterations. Here, minimum fitness refers to the fitness of the best (feasible) individual within the population. Additionally, the mutation rate was set to 0.05, and the crossover probability was set to 0.7.

(a) Mutation Procedure: Crossover

(b) Mutation Procedure: Heuristic Crossover
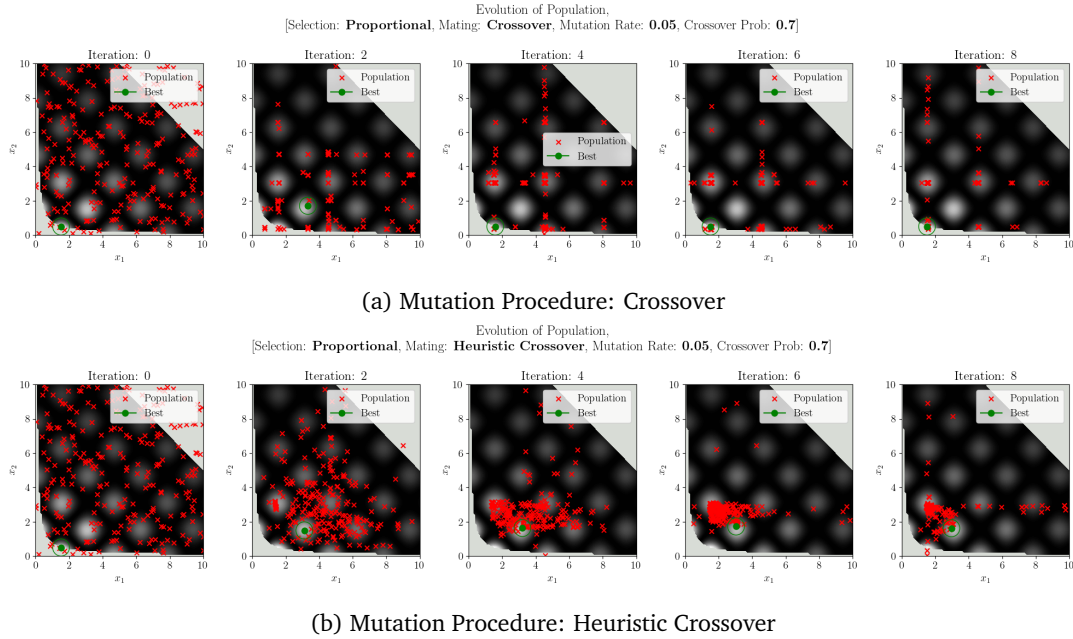
Figure 15: Evolution of the CGA population over 8 iterations using proportional selection. Proportional selection proved to be a somewhat effective selection method. However, it was not chosen over tournament selection as the primary selection method for the reasons outlined in Section 3.2.
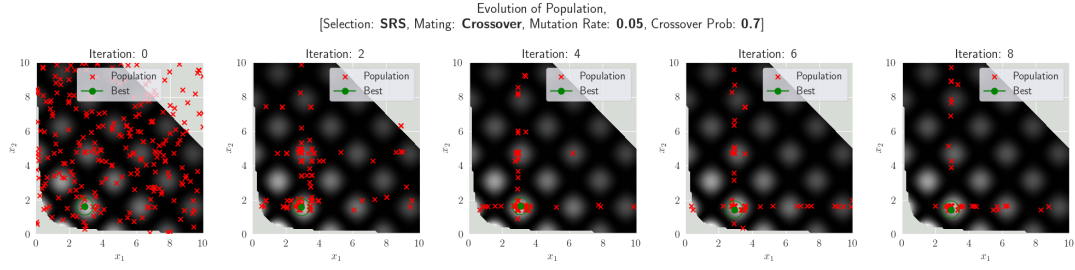
(a) Mutation Procedure: Crossover
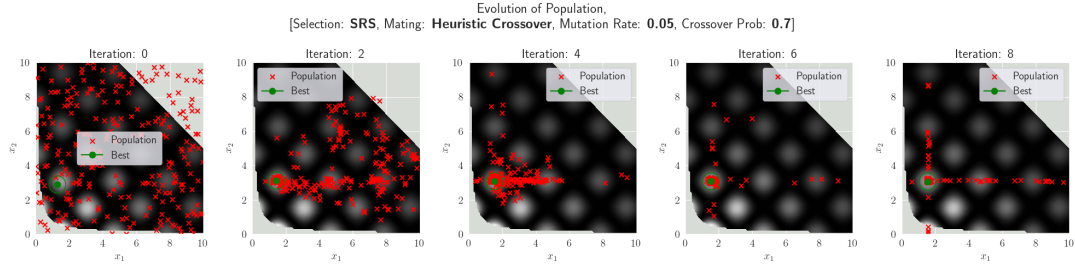
(b) Mutation Procedure: Heuristic Crossover

Figure 16: Evolution of the CGA population over 8 iterations using stochastic remainder selection without replacement (SRS). SRS proved to be the second most effective selection method, when compared to Proportional Selection and Tournament Selection, as discussed in 3.2.

6.2 Supplementary Results regarding PT Tuning

Exchange Procedure	Exchange Parameter	Power Term	Final Avg. Fitness	Final Min. Fitness
Periodic	0.1	1	-0.186415811	-0.34081297
		3	-0.186415811	-0.34081297
		5	-0.192142049	-0.34081297
	0.3	1	-0.183591253	-0.335207939
		3	-0.183591253	-0.335207939
		5	-0.178574074	-0.310814711
	0.5	1	-0.166370319	-0.355617525
		3	-0.166370319	-0.355617525
		5	-0.162769374	-0.31189813
Stochastic	0.1	1	-0.182496471	-0.327434397
		3	-0.182496471	-0.327434397
		5	-0.197887075	-0.328011329
	0.3	1	-0.191162383	-0.310872726
		3	-0.191162383	-0.310872726
		5	-0.196042151	-0.314329893
	0.5	1	-0.206621007	-0.347483314
		3	-0.206621007	-0.347483314
		5	-0.211224821	-0.349273739

Table 3: Raw results from an initial exploration of the exchange procedure, exchange parameter, and power term hyperparameters within PT. Presented as the final fitness values of the PT solutions after 100 iterations. Here, minimum fitness refers to the fitness of the best (feasible) solution across all chains.
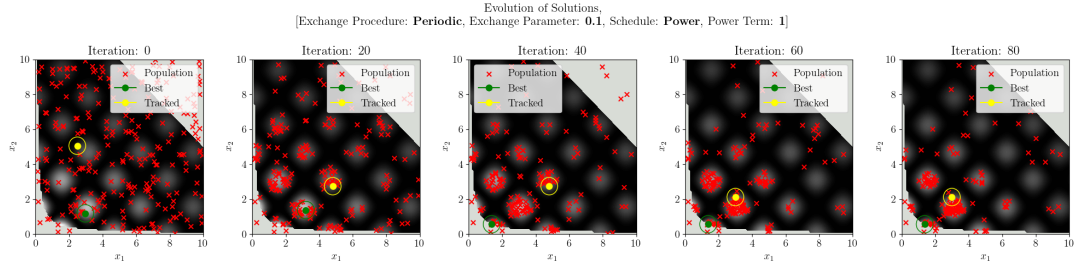
Figure 17: Evolution of the chain across all replicas over 100 iterations using periodic replica exchange and a uniform temperature scheduling, (power term of 1). Here, replica exchange occurs every 10% of the time, (exchange parameter set to 0.1). The 'tracked' solution is distinct from the 'best' solution. It is a random solution within the final replica that is observed to verify the MCMC evolution.
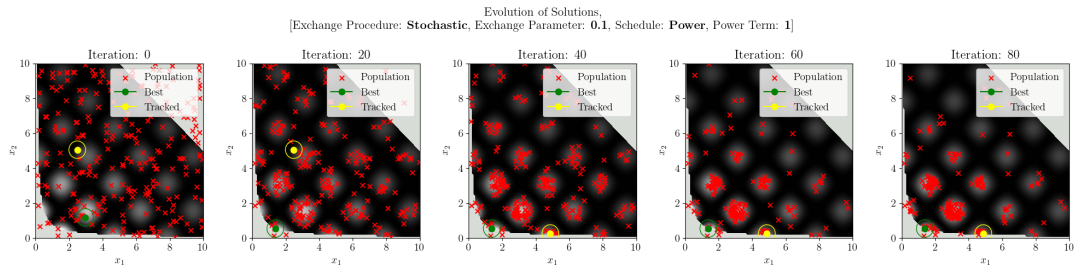
Figure 18: Evolution of the chain across all replicas over 100 iterations using stochastic replica exchange and a uniform temperature scheduling, (power term of 1). Here, replica exchange occurs with a probability of 10%. The 'tracked' solution is distinct from the 'best' solution. It is a random solution within the final replica that is observed to verify the MCMC evolution.

7   Code

To ease development, the codebase has been modularised in the manner presented below:

   src/

      algorithms/

         CGA/

            CGA.py

            mating_functions.py

            selection_functions.py

         PT/

            PT.py

            replica_exchange_functions.py

            temp_prog_functions.py

      utils/

         helper_functions.py

         plotting_functions.py

      functions.py

   FinalComparison.py

   CGA_TuningExperiments.py

   PT_TuningExperiments.py

7.1 algorithms

7.1.1 CGA

```python
"""
Candidate No : 5730E, Module: 4M17

Description :
    This file contains the class for the continous genetic algorithm.
"""

import numpy as np
import sys; sys.path.append('..')

from src.algorithms.CGA.selection_functions import proportional_selection,
    tournament_selection, SRS_selection
from src.algorithms.CGA.mating_functions import crossover, heuristic_crossover
from src.utils.helper_functions import satisfy_constraints

class ContinousGeneticAlgorithm():
    """
    Class for continous genetic algorithm.
    """
    def __init__(self, population_size, chromosome_length, num_parents, objective_function,
    tournament_size, range=(0,10), mutation_rate=0.1, crossover_prob=0.8, selection_method='
    Tournament', mating_procedure='Heuristic Crossover', constraints=True):
        """
        Constructor for continous genetic algorithm.

        Parameters:
        - population_size (int): Number of individuals in population
        - chromosome_length (int): Size of vector individual, (number of genes), i.e.
    dimension of solution space
        - num_parents (int): Number of parents to select for mating
        - objective_function (function): Objective function to optimise
        - tournament_size (int): Size of subset of population for tournament selection
        - range (tuple): Range of values for genes, determined by constraints of problem
        - mutation_rate (float): Mutation rate
        - crossover_prob (float): Crossover rate
        - selection_method (str): Selection method used for parent selection
        - mating_procedure (str): Mating procedure used for reproduction
        - constraints (bool): Whether to satisfy constraints with parent selection or not
        """
        self.population_size = population_size
        self.chromosome_length = chromosome_length # n in R^n, dimension of the search space
        self.num_parents = num_parents
        self.func = objective_function
        self.tournament_size = tournament_size
        self.lb = range[0]
        self.ub = range[1]
        self.mutation_rate = mutation_rate
        self.crossover_prob = crossover_prob
        self.constraints = constraints

        # Dictionaries to map string to function call. Function imported from directory files
        selection_mapping = {'Proportional': proportional_selection,
                            'Tournament': tournament_selection,
                            'SRS': SRS_selection # SRS = Stochastic Remainder Selection
    without Replacement
                            }

        mating_mapping = {'Crossover': crossover,
                        'Heuristic Crossover': heuristic_crossover
                        }

        # Check if selection method and mating procedure are valid
        if selection_method not in ['Proportional', 'Tournament', 'SRS']:
            raise ValueError(f"Invalid selection method: {selection_method}")
        else:
            self.selection_process = selection_mapping[selection_method]
```

```python
62
63          if mating_procedure not in ['Crossover', 'Heuristic Crossover']:
64              raise ValueError(f"Invalid mating procedure: {mating_procedure}")
65          else:
66              self.mating_process = mating_mapping[mating_procedure]
67
68          # Initialise population
69          self.initialise_population()
70
71      def initialise_population(self):
72          """
73          Initialise population with random values between lb and ub.
74          """
75          self.population = np.random.uniform(low=self.lb,
76                                              high=self.ub,
77                                              size=(self.population_size, self.chromosome_length
     )
78                                              )
79
80          self.fitness = np.zeros(self.population_size) # Initialise fitness of population
81          self.evaluate_fitness() # Update fitness of population with starting individual
82
83      def evaluate_fitness(self):
84          """
85          Evaluate fitness of population.
86
87          Parameters:
88          - fitness_function (function): Fitness function to evaluate fitness of population
89          """
90          for i in range(self.population_size):
91              self.fitness[i] = - self.func(self.population[i])
92
93          # Evaluate rankings of individuals in population by fitness
94          self.parent_rankings = np.argsort(self.fitness) # Indices of individuals in order of
     fitness
95
96          # Update best individual and best fitness
97          self.best_individual = self.population[self.parent_rankings[0]]
98          self.min_fitness = self.fitness[self.parent_rankings[0]]
99
100         # Best individual must satisfy constraints, if not, find next best individual that
     does
101         i = 1
102         while not satisfy_constraints(self.best_individual):
103             self.best_individual = self.population[self.parent_rankings[i]]
104             self.min_fitness = self.fitness[self.parent_rankings[i]]
105             i += 1
106
107     def select_parents(self):
108         """
109         Select parents for mating.
110
111         Returns:
112         - parents (np.array): Indices of parents selected for mating
113         """
114         return self.selection_process(self)
115
116     def mate(self):
117         """
118         Mate parents to produce offspring.
119
120         Returns:
121         - offspring (np.array): Offspring of parents
122         """
123         return self.mating_process(self)
124
125     def mutate(self):
126         """
127         Mutate offspring. Every gene has a mutation rate chance of being mutated.
```

```
128            """
129            for i in range(self.population_size):
130                for j in range(self.chromosome_length):
131                    if np.random.rand() < self.mutation_rate:
132                        self.population[i][j] = np.random.uniform(low=self.lb, high=self.ub)
133
134    def evolve(self):
135            """
136            Evolve population for one generation.
137            """
138            offspring = self.mate()
139            self.population = offspring
140            self.mutate()
141            self.evaluate_fitness()
```

Listing 1: CGA.py

```
1      """
2      Candidate No : 5730E, Module: 4M17
3
4      This file contains the mating functions for the CGA algorithm.
5      """
6
7      import numpy as np
8
9      def crossover(CGA):
10            """
11            Crossover mating procedure.
12            """
13            # Select parents
14            selected_parents = CGA.select_parents()
15
16            # Reshape them into a set of potential parent pairs
17            parent_pairs = np.array(selected_parents).reshape(-1, 2)
18
19            # Initialise new offspring to replace population
20            offspring = np.zeros((CGA.population_size, CGA.chromosome_length))
21
22            # Iterate through population
23            for i in range(CGA.population_size):
24
25                # Assign random pair of parents from parent_pairs
26                parent1, parent2 = parent_pairs[np.random.randint(len(parent_pairs))]
27
28                # Assign random crossover point
29                p = np.random.randint(1, CGA.chromosome_length)
30
31                # Swap genes from parents to create offspring
32                if np.random.rand() < CGA.crossover_prob:
33                    offspring[i][:p] = CGA.population[parent1][:p]
34                    offspring[i][p:] = CGA.population[parent2][p:]
35                else:
36                    offspring[i][:p] = CGA.population[parent2][:p]
37                    offspring[i][p:] = CGA.population[parent1][p:]
38
39            return offspring
40
41    def heuristic_crossover(CGA):
42            """
43            Heuristic crossover mating procedure. Inspired by the relevant section in https://doi.
       org/10.1002/0471671746.ch3
44            """
45
46            # Select parents
47            selected_parents = CGA.select_parents()
48
49            # Reschape them into a set of potential parent pairs
50            parent_pairs = np.array(selected_parents).reshape(-1, 2)
51
52            # Initialise new offspring to replace population
```

```
53          offspring = np.zeros((CGA.population_size, CGA.chromosome_length))
54
55          # Iterate through population
56          for i in range(CGA.population_size):
57
58              # Assign random pair of parents from parent_pairs
59              parent1, parent2 = parent_pairs[np.random.randint(len(parent_pairs))]
60
61              # Iterate through all the genes of an individual/chromosome
62              for j in range(CGA.chromosome_length):
63
64                  # Heuristic crossover with probability, CGA.crossover_prob
65                  b = np.random.rand() # b is a random number between 0 and 1
66
67                  if np.random.rand() < CGA.crossover_prob:
68                      # p_new = b * (p1 - p2) + p2
69                      offspring[i][j] = b * (CGA.population[parent1][j] - CGA.population[parent2
    ][j]) + CGA.population[parent2][j]
70                  else:
71                      # p_new = b * (p2 - p1) + p1
72                      offspring[i][j] = b * (CGA.population[parent2][j] - CGA.population[parent1
    ][j]) + CGA.population[parent1][j]
73
74          return offspring
```

Listing 2: mating_functions.py

```
1       """
2       Candidate No : 5730E, Module: 4M17
3
4       This file contains the selection functions for the CGA algorithm.
5       """
6
7       import numpy as np
8       import sys; sys.path.append('..')
9       from src.utils.helper_functions import satisfy_constraints
10
11      def proportional_selection(GCA):
12          """
13          Proportional selection of parents.
14
15          Args:
16          - GCA (CGA): Continuous Genetic Algorithm object passed into this function using self.
    select_parents(self)
17
18          Returns:
19          - selected_individuals (list): List of indices of selected individuals for mating,
    length = GCA.num_parents
20          """
21          # Calculate probabilities
22          probabilities = GCA.fitness / np.sum(GCA.fitness)
23
24          # Select individuals based on probabilities
25          selected_individuals = list(np.random.choice(GCA.population_size, size=GCA.num_parents
    , p=probabilities))
26
27          # Retry - reject parents that do not satisfy constraints
28          if GCA.constraints == True:
29              for i in range(GCA.num_parents):
30                  while not satisfy_constraints(GCA.population[selected_individuals[i]]):
31                      selected_individuals[i] = np.random.choice(GCA.population_size, p=
    probabilities)
32
33          return selected_individuals
34
35      def tournament_selection(GCA):
36          """
37          Tournament selection of parents.
38
39          Args:
```

```python
        - GCA (CGA): Continuous Genetic Algorithm object passed into this function using self.
    select_parents(self)

        Returns:
        - selected_individuals (list): List of indices of selected individuals for mating,
    length = GCA.num_parents
        """

        # Initialise list of selected individuals
        selected_individuals = []

        # Select top two parents for each tournament, so need 'GCA.num_parents // 2'
    tournaments
        for i in range(GCA.num_parents//2):

            # Take subset of population
            subset = np.random.choice(GCA.population_size, size=GCA.tournament_size, replace=
    False)

            # Take top two parents
            parent1 = subset[np.argmin(GCA.fitness[subset])]
            subset = np.delete(subset, np.argmin(GCA.fitness[subset]))
            parent2 = subset[np.argmin(GCA.fitness[subset])]

            # Retry, reject parents that do not satisfy constraints
            if GCA.constraints == True:
                while not satisfy_constraints(GCA.population[parent1]):
                    subset = np.delete(subset, np.argmin(GCA.fitness[subset]))
                    parent1 = subset[np.argmin(GCA.fitness[subset])]
                while not satisfy_constraints(GCA.population[parent2]):
                    subset = np.delete(subset, np.argmin(GCA.fitness[subset]))
                    parent2 = subset[np.argmin(GCA.fitness[subset])]

            # Add parents to list of selected individuals
            selected_individuals += [parent1, parent2]

        return selected_individuals

    def SRS_selection(GCA):
        """
        Stochastic Remainder Selection without Replacement (SRS) of parents.

        Args:
        - GCA (CGA): Continuous Genetic Algorithm object passed into this function using self.
    select_parents(self)

        Returns:
        - selected_individuals (list): List of indices of selected individuals for mating,
    length = GCA.num_parents
        """

        # Calculate probabilities
        probabilities = GCA.fitness / np.sum(GCA.fitness)

        # Calculate expected number of copies of each individual
        expected_num_copies = probabilities * GCA.num_parents

        # Calculate integer number of copies of each individual
        num_copies = np.floor(expected_num_copies)

        # Calculate remainder, which later serves as the probability of further selection
        remainder = expected_num_copies - num_copies

        # Initialise list of selected individuals
        selected_individuals = []

        # Duplicate individuals "num_copies" times
        for i in range(GCA.population_size):
```

```python
103            # Add only feasible individuals
104            if satisfy_constraints(GCA.population[i]):
105                selected_individuals += [i] * int(num_copies[i]) # Add i to list num_copies[i]
     times
106
107        # Remainer must satisfy sum(remainder) = 1, since it serves as the probabilities for
     further selection
108        remainder = remainder / np.sum(remainder)
109
110        # Calculate remaining number of individuals that need to be selected
111        remaining_number = GCA.num_parents - len(selected_individuals)
112
113        # Cannot be negative
114        remaining_number = remaining_number if remaining_number > 0 else 0
115
116        # Select individuals using remainder probabilities
117        selected_individuals += list(np.random.choice(GCA.population_size, size=
     remaining_number, p=remainder))
118
119        # Reject parents that do not satisfy constraints
120        if GCA.constraints == True:
121            for i in range(len(selected_individuals)):
122                while not satisfy_constraints(GCA.population[selected_individuals[i]]):
123                    selected_individuals[i] = np.random.choice(GCA.population_size, p=
     remainder)
124
125        return selected_individuals
```

Listing 3: selection_functions.py

7.1.2 PT

```python
1     """
2     Candidate No : 5730E, Module: 4M17
3
4     Description :
5         This file contains the class for the parallel tempering algorithm.
6     """
7     import numpy as np
8
9     import sys; sys.path.append('..')
10    from src.algorithms.PT.temp_prog_functions import power_progression, geometric_progression
11    from src.algorithms.PT.replica_exchange_functions import period_exchange,
     stochastic_exchange, always_exchange
12    from src.utils.helper_functions import satisfy_constraints
13
14    class ParallelTempering():
15        """
16        Class for parallel tempering algorithm.
17        """
18        def __init__(self, objective_function, x_dim, range=(0,10), alpha=0.1, omega=2.1,
     num_replicas=10, num_chains=25, exchange_procedure='Periodic', exchange_param=0.2,
     schedule_type='Power', power_term=1, total_iterations=100, constraints=True):
19            """
20            Constructor for parallel tempering algorithm.
21
22            Parameters:
23            - objective_function (function): Objective function to optimise
24            - x_dim (int): Dimension of solution space
25            - range (tuple): Range of values for x, determined by constraints of problem
26            - alpha (float): Dampening constant for max. allowable step size update
27            - omega (float): Weighting for max. allowable step size update
28            - num_replicas (int): Number of replicas
29            - num_chains (int): Number of solutions per replica
30            - exchange_procedure (str): Procedure for exchanging solutions between replicas
31            - exchange_param (float between 0 and 1):
32                if exchange_procedure = 'Periodic', this is the percentage of iterations after
     which to exchange solutions
33                if exchange_procedure = 'Stochastic', this is the probability of exchanging
     solutions between replicas during each iteration
```

```python
34              - progression_type (str): Type of progression for temperature scheduling
35              - power_term (float > 1): Temperature progression power term, if using power
        progression. Schedule is (i/N)^power_term
36              - total_iterations (int): Total number of iterations the algorithm will run for
37              - constraints (bool): Whether to satisfy constraints with Metropolis criterion or
        not
38              """
39              self.func = objective_function
40              self.x_dim = x_dim
41              self.lb = range[0]
42              self.ub = range[1]
43              self.alpha = alpha
44              self.omega = omega
45              self.num_replicas = num_replicas
46              self.num_chains = num_chains
47              self.exchange_param = exchange_param
48              self.total_iterations = total_iterations
49              self.constraints = constraints
50
51              # The update step suggested by Parks et al. (1990) requires control variables to
        be scaled to [0, 1]
52              # Therefore, we need to scale up solutions to original range when evaluating the
        objective function
53              self.scale_up = lambda x: x * (self.ub - self.lb) + self.lb
54
55              # Energy difference = (f(x_new) - f(x)) / (k * d * T), the term in the exponent of
         the Metropolis criterion
56              k = 1.38064852e-23 # Boltzmann constant
57              self.deltaE = lambda x, x_new, d, T: (self.func(self.scale_up(x_new)) - self.func(
        self.scale_up(x))) / (k * d * T)
58
59              # Check if temperature schedule type is valid
60              if schedule_type not in ['Geometric', 'Power']:
61                  raise ValueError("Invalid progression type")
62
63              # Dictionaries to map string to function call. Function imported from directory
        files
64              schedule_mapping = {'Geometric': geometric_progression,
65                                  'Power': power_progression
66                                  }
67
68              # Check if power term is valid, if it's needed
69              if schedule_type == 'Power':
70                  if power_term is None or power_term < 1:
71                      raise ValueError(f"Power term not specified correctly: {power_term}. Must
        be greater than 1.")
72
73              # Generate temperature schedule
74              self.temperature_schedule = schedule_mapping[schedule_type](num_replicas,
        power_term)
75
76              # Check if exchange procedure is valid
77              if exchange_procedure not in ['Periodic', 'Stochastic', 'Always']:
78                  raise ValueError(f"Invalid exchange procedure: {exchange_procedure}.")
79
80              # Check if exchange parameter is valid, should be either a probability or a
        percentage
81              if exchange_param < 0 or exchange_param > 1:
82                  raise ValueError(f"Exchange parameter must be between 0 and 1: {exchange_param
        }.")
83
84              # Dictionaries to map string to function call. Function imported from directory
        files
85              exchange_mapping = {'Periodic': period_exchange,
86                                  'Stochastic': stochastic_exchange,
87                                  'Always': always_exchange
88                                  }
89
90              # Set exchange procedure
```

```python
 91            self.exchange_procedure = exchange_mapping[exchange_procedure]

 92
 93            # Initialise solutions
 94            self.initialise_solutions()

 95
 96        def initialise_solutions(self):
 97            """
 98            Initialise solutions for each replica.
 99            """
100            # Array of solutions for each replica, between 0 and 1 recommended by Parks et al.
        (1990)
101            self.current_solutions = np.random.uniform(0, 1, (self.num_replicas, self.
     num_chains, self.x_dim))

102
103            # Diagonal matrix of max. allowable step sizes for each solution
104            # Each item in the matrix pertains to the max step size for each dimension of the
        solution
105            D = np.eye(self.x_dim)

106
107            # Copy matrix for each solution in each replica
108            # Each one will be updated individually, as the algorithm progresses
109            self.max_change = np.tile(D, (self.num_replicas, self.num_chains, 1, 1))

110
111        def get_best_solution(self, all_solutions=None):
112            """
113            Return best solution out of all replicas and solutions.

114
115            Parameter, all_solutions, is optional. All solutions are already at hand in the
     fitness function,
116            so we can directly pass it into this to reduce overhead. If not passed in,
     get_all_solutions() is called.
117            """
118            if all_solutions is None:
119                # Get a list of all solutions
120                all_solutions = self.get_all_solutions()

121
122            # Evaluate function at each solution
123            all_solutions_eval = np.array([self.func(x) for x in all_solutions])

124
125            # Find index of best solution
126            best_idx = np.argmax(all_solutions_eval)

127
128            # Only consider candidates from feasible region
129            if self.constraints:
130                while not satisfy_constraints(all_solutions[best_idx]):
131                    all_solutions_eval[best_idx] = -np.inf
132                    best_idx = np.argmax(all_solutions_eval)

133
134            # Return best solution
135            return all_solutions[best_idx]

136
137        def metropolis_criterion(self, x, x_new, T, T_new=None):
138            """
139            Metropolis-Hastings criterion for accepting new solution.
140            Acceptance probability as advised by Simulated Annealing lecture notes (Parks et
        al.)

141
142            Despite efforts to avoid overflow, the small Boltzmann constant still causes
     problems.
143            However, the algorithm needs to be sensitive, and only seems to work with the
     inclusion of k.
144            It works completely fine, but it is not ideal from a performance perspective.

145
146            Parameters:
147            - x (np.array): Current solution
148            - x_new (np.array): New solution
149            - T (float): Temperature
150            - T_new (float): New temperature, if a replica exchange has occurred
151
```

```python
152             Returns:
153             - bool: Whether to accept new solution or not
154             """
155             # If constraints are to be satisfied, check if new solution satisfies constraints
156             if self.constraints:
157                 if not satisfy_constraints(self.scale_up(x_new)):
158                     return False # Reject solution if it doesn't satisfy constraints
159
160             # Calculate the L2 norm of the step size
161             d = np.linalg.norm(x_new - x)
162
163             # Avoid division by 0, if denominator is too small, probability of acceptance is 1
164             if T * d < 1e-6:
165                 return True
166
167             # If a replica exchange has occurred
168             elif T_new is not None:
169
170                 # Avoid division by zero
171                 if T < 1e-6:
172                     return True
173                 elif T_new < 1e-6:
174                     return False
175                 else:
176                     # More likely to accept replica exchanges that see a small change in
    temperature
177                     # Small change in temp = larger acceptance probability, p = exp(-deltaE /
    delta_T)
178                     delta_T = ((1 / T) - (1 / T_new))**(-1)
179
180                 # Avoid division by 0
181                 if delta_T * d < 1e-6:
182                     return True
183
184                 # Acceptance probability, change in temp is sent into denominator of
    acceptance probability
185                 return np.random.uniform() < min(1, np.exp(self.deltaE(x, x_new, d, delta_T)))
186
187             else:
188
189                 # Acceptance probability with no replica exchange
190                 return np.random.uniform() < min(1, np.exp(self.deltaE(x, x_new, d, T)))
191
192     def update_max_change(self, x, x_new, i, j):
193         """
194         Function to update max. allowable step size whenever a solution is accepted.
195         See Parks et al. (1990) for more details.
196         """
197         # Absolute difference between new and current solution
198         R = np.diag(np.abs(x_new - x))
199
200         # Update max. allowable step size
201         self.max_change[i][j] = (1-self.alpha) * self.max_change[i][j] + self.alpha * self
    .omega * R
202
203     def update_chains(self):
204         """
205         One step of the algorithm. Update solutions for each replica. Easily
    parallelisable.
206         """
207         # Loop through each replica, i.e. each temperature
208         for i in range(self.num_replicas):
209
210             # Loop through each solution in replica
211             for j in range(self.num_chains):
212
213                 # Generate new solution, [ x_new = x + D * U(-1, 1) ], where D is max.
    allowable step size
214                 x_new = self.current_solutions[i, j] + self.max_change[i][j] @ np.random.
```

```
          uniform (-1, 1, self.x_dim)

215
216                      # Metropolis - Hastings criterion
217                      if self.metropolis_criterion(self.current_solutions[i, j], x_new, self.
          temperature_schedule[i]):

218
219                          # Update current solution if new solution is accepted
220                          self.current_solutions[i, j] = x_new

221
222                          # Update max. allowable step size if new solution is accepted
223                          self.update_max_change(self.current_solutions[i, j], x_new, i, j)

224
225
226      def replica_exchange(self, iter):
227          """
228          Function to exchange solutions between replicas.
229          """
230          # Call exchange procedure
231          self.exchange_procedure(self, iter)

232
233      def get_fitness(self):
234          """
235          Function to calculate average and min fitness of population. Fitness is negative
          of objective function.
236          """
237          all_solutions = self.get_all_solutions()

238
239          avg = np.mean([-self.func(x) for x in all_solutions])
240          best_solution = self.get_best_solution(all_solutions)
241          min = -self.func(best_solution)

242
243          return avg, min

244
245      def get_all_solutions(self):
246          """
247          Return all solutions reshaped into a n-dim array, scaled up to original range of
          problem.
248          """
249          return self.scale_up(self.current_solutions.flatten().reshape(-1, self.x_dim))
```

Listing 4: PT.py

```
1      """
2      Candidate No : 5730E, Module: 4M17
3
4      Description :
5          This file contains the functions for exchanging solutions between replicas.
6      """
7
8      import numpy as np
9
10     def swap(PT):
11         """
12         Swap solutions between adjacent replicas, (subject to Metropolis criterion).
13         """
14         # Loop through each replica
15         for i in range(PT.num_replicas - 1):
16
17             # Temperatures of adjacent replicas to swap
18             T_1 = PT.temperature_schedule[i]
19             T_2 = PT.temperature_schedule[i + 1]
20
21             # Loop through each solution in replica
22             for j in range(PT.num_chains):
23
24                 # If solutions are the same, no need to swap
25                 if np.array_equal(PT.current_solutions[i, j], PT.current_solutions[i + 1, j]):
26                     continue
27
28                 # Check Metropolis criterion for both directions.
```

```python
29              # Acceptance is now dependent on temp difference, so now both temps are sent
   in as args
30              check_criterion = [
31                  PT.metropolis_criterion(PT.current_solutions[i, j], PT.current_solutions[i
   + 1, j], T_1, T_2),
32                  PT.metropolis_criterion(PT.current_solutions[i+1, j], PT.current_solutions
   [i , j], T_2, T_1)
33                  ]
34
35              # Only swap solutions if both directions satisfy Metropolis criterion
36              if all(check_criterion):
37
38                  # Swap solutions
39                  PT.current_solutions[i, j], PT.current_solutions[i + 1, j] = PT.
   current_solutions[i + 1, j], PT.current_solutions[i, j]
40
41                  # Update max. allowable step size
42                  PT.update_max_change(PT.current_solutions[i, j], PT.current_solutions[i +
   1, j], i, j)
43
44
45  def period_exchange(PT, iter):
46      """
47      Periodic exchange of solutions between replicas, swaps solutions every PT.
   exchange_param*NUM_ITERS.
48      """
49      # Check if it is time to swap solutions between replicas
50      if iter % (PT.exchange_param * PT.total_iterations) == 0:
51          swap(PT)
52
53  def stochastic_exchange(PT, iter):
54      """
55      Random exchange of solutions between replicas, with probability PT.exchange_param.
56      """
57      # Chance to swap solutions between replicas
58      if np.random.uniform() < PT.exchange_param:
59          swap(PT)
60
61  def always_exchange(PT, iter):
62      """
63      Always exchange solutions between replicas.
64      """
65      swap(PT)
```

Listing 5: replica_exchange_functions.py

```python
1      """
2      Candidate No : 5730E, Module: 4M17
3
4      Description : This file contains temperature scheduling functions for parallel tempering.
5                    Each temerature scheduling function returns a list of temperatures ranging
    from 0 to 1.
6      """
7      import numpy as np
8
9      def power_progression(num_replicas, p=1):
10         """
11         Uniform progression for temperature scheduling.
12         Returns (i / num_replicas)^p for i in [0, num_replicas].
13
14         Parameters:
15         - num_replicas (int): Number of replicas
16
17         Returns:
18         - schedule (list): List of temperatures
19         """
20         return np.linspace(0, 1, num_replicas)**p
21
22     def geometric_progression(num_replicas, p=1):
23         """
```

```
24          Geometric progression for temperature scheduling.
25          Returns 2^i / 2^num_replicas for i in [0, num_replicas].
26          (Was not used, because power progression allows for more flexibility).
27
28          Parameters:
29          - num_replicas (int): Number of replicas
30
31          Returns:
32          - schedule (list): List of temperatures
33          """
34          return np.logspace(-2, 0, num_replicas)
```

Listing 6: temp_prog_functions.py

7.2 utils

```
1      """
2      Candidate No : 5730E, Module: 4M17
3
4      Description :
5          This file contains some helper functions for the project.
6      """
7
8      import numpy as np
9      import os
10     from src.functions import KBF_function
11
12     def satisfy_constraints(x):
13          """
14          Function to check if a given vector x satisfies the constraints of the problem.
15
16          Args:
17          - x (np.ndarray): Vector to check.
18
19          Returns:
20          - bool: True if x satisfies constraints, False otherwise.
21          """
22
23          # List of boolean values for each constraint satisfied
24          constraints = [
25              np.all(x >= 0) and np.all(x <= 10),
26              np.prod(x) > 0.75,
27              np.sum(x) < 15 * x.shape[0] / 2,
28          ]
29
30          # Return True if all constraints are satisfied, False otherwise
31          return all(constraints)
32
33     def evaluate_2D(func, x_range=(0,10), constraints=False):
34          """
35          Function for generating a meshgrid and evaluating a function in R^2.
36          """
37
38          # Create a meshgrid
39          x1 = np.linspace(x_range[0], x_range[1], 100)
40          x2 = np.linspace(x_range[0], x_range[1], 100)
41          X1, X2 = np.meshgrid(x1, x2)
42
43          # Compute the function values
44          f = np.zeros_like(X1)
45          for i in range(X1.shape[0]):
46              for j in range(X1.shape[1]):
47                  f[i, j] = func(np.array([X1[i, j], X2[i, j]]))
48
49                  # If constraints are enabled, set f to nan if constraints are not satisfied
50                  if constraints == True:
51                      if not satisfy_constraints(np.array([X1[i, j], X2[i, j]])):
52                          f[i, j] = np.nan
53
54          return X1, X2, f
```

```python
def create_figure_directories_CGA(name, selection_methods, mating_procedures, iters_list):
    """
    Function for creating directories for figures generated in my simulations.
    """
    # Create parent directory
    if not os.path.exists('figures'):
        os.makedirs('figures')

    # Create directory for specific function
    function_dir = os.path.join('figures', name)
    if not os.path.exists(function_dir):
        os.makedirs(function_dir)

    # Create directory for each number of iterations
    for iters in iters_list:
        iters_dir = os.path.join(function_dir, f'{iters}_iters')
        if not os.path.exists(iters_dir):
            os.makedirs(iters_dir)

    # Create directories for each selection method and mating procedure
    for selection_method in selection_methods:
        for mating_procedure in mating_procedures:
            for iters in iters_list:
                selection_dir = os.path.join(function_dir, f'{str(iters)}_iters',
    selection_method)
                if not os.path.exists(selection_dir):
                    os.makedirs(selection_dir)

                mating_dir = os.path.join(selection_dir, mating_procedure)
                if not os.path.exists(mating_dir):
                    os.makedirs(mating_dir)

def create_figure_directories_PT(name, exchange_procedures, schedule_types, iters_list):
    """
    Function for creating directories for figures generated in my simulations.
    """
    # Create parent directory
    if not os.path.exists('figures'):
        os.makedirs('figures')

    # Create directory for specific function
    function_dir = os.path.join('figures', name)
    if not os.path.exists(function_dir):
        os.makedirs(function_dir)

    # Create directory for each number of iterations
    for iters in iters_list:
        iters_dir = os.path.join(function_dir, f'{iters}_iters')
        if not os.path.exists(iters_dir):
            os.makedirs(iters_dir)

    # Create directories for each exchange procedure and schedule type
    for exchange_procedure in exchange_procedures:
        for schedule_type in schedule_types:
            for iters in iters_list:
                exchange_dir = os.path.join(function_dir, f'{str(iters)}_iters',
    exchange_procedure)
                if not os.path.exists(exchange_dir):
                    os.makedirs(exchange_dir)

                schedule_dir = os.path.join(exchange_dir, schedule_type)
                if not os.path.exists(schedule_dir):
                    os.makedirs(schedule_dir)

def generate_initial(x_dim=8, pop_size=250):
    """
    Function for generating a collection of populations for comparison section.
    Each population is generated using a different random seed.
```

```
122          Only initialisations which do not contain a solution close to the optimum are kept.
123
124          Args:
125          - x_dim (int): Dimension of the vectors.
126          - pop_size (int): Size of each collection of initial solutions.
127
128          Returns:
129          - initialisations (list): List of initial populations.
130          - seeds (list): List of seeds used for each initialisation.
131          """
132
133          # Initialise variables
134          seeds = []
135          initialisations = []
136
137          # Generate 50 initialisations
138          i = 0
139          while i < 50:
140              # Generate a random number seed
141              seed = np.random.randint(0, 1000000)
142
143              # Set the seed
144              np.random.seed(seed)
145
146              # Generate a random initialisation
147              initialisation = np.random.uniform(0, 10, (pop_size, x_dim))
148
149              # Make sure no solution is close to the optimum
150              f_x = np.array([KBF_function(x) for x in initialisation])
151
152              if np.max(f_x) < 0.3:
153                  initialisations.append(initialisation)
154                  seeds.append(seed)
155                  i += 1
156
157          return initialisations, seeds
```

Listing 7: helper_functions.py

```
1      """
2      Candidate No : 5730E, Module: 4M17
3
4      Description :
5          This file contains various functions used for plotting figures.
6      """
7
8      import matplotlib.pyplot as plt
9      from mpl_toolkits.mplot3d import Axes3D
10     from matplotlib import rc
11     import seaborn as sns
12     from src.utils.helper_functions import evaluate_2D
13     from src.algorithms.PT.temp_prog_functions import power_progression
14
15     # Set LaTeX font
16     rc('font', **{'family': 'serif', 'serif': ['Computer Modern']}, size=14)
17     rc('text', usetex=True)
18
19     def plot_2D(X1, X2, f, name, constraints=False):
20         """
21         Function for visualising a function in R^2.
22         Creates both a contour plot and a 3D surface plot.
23
24         Args:
25         - X1 (np.ndarray): Meshgrid of x1 values.
26         - X2 (np.ndarray): Meshgrid of x2 values.
27         - f (np.ndarray): Function values.
28         - name (str): Name of function.
29         - constraints (bool): Whether to plot with carved out feasible region or not.
30         """
31
```

```python
        # Change visualisation depending on whether we're plotting the carved out feasible
region or not
        if constraints == True:
            name_png = f'{name} Feasible'
            angle = -10
            elevation = 30

        else:
            name_png = name
            angle = 30
            elevation = 20

        # Plot contour
        plt.figure()
        plt.gca().set_facecolor('xkcd:light grey')
        plt.contourf(X1, X2, f, 100, cmap='jet')
        plt.xlabel(r'$x_1$')
        plt.ylabel(r'$x_2$')
        plt.title(f'{name_png} Contour Plot')
        cbar = plt.colorbar()
        cbar.set_label(r'$f(x_1, x_2)$')
        plt.savefig(f'figures/{name}/{name_png}_contour.png')

        # Plot 3D surface
        fig = plt.figure()
        ax = fig.add_subplot(111, projection='3d')
        ax.plot_surface(X1, X2, f, cmap='rainbow', edgecolor='k')
        ax.set_xlabel(r'$x_1$')
        ax.set_ylabel(r'$x_2$')
        ax.zaxis.set_rotate_label(False)
        ax.set_zlabel(r'$f(x_1, x_2)$', rotation=90)
        ax.set_title(f'{name_png} 3D Plot')
        ax.view_init(elev=elevation, azim=angle)  # Set the view angle
        plt.savefig(f'figures/{name}/{name_png}_surf.png')

    def plot_population(population, plot, best=None, last=None):
        """
        Function for overlaying a particular generation from the CGA's optimisation on a
contour plot in R^2.

        Args:
        - population (np.ndarray): Population of individuals.
        - plot (matplotlib.pyplot): Plot to overlay on.
        - best (np.ndarray): Best individual.
        - last (np.ndarray): Last individual in collection, (for highlighting to visualise
MCMC moves).
        """

        # Plot population
        plot.scatter(population[:,0], population[:,1], marker='x', label='Population', color='
red')

        # Plot circle around best individual
        if best is not None:
            plot.plot(best[0], best[1], marker='o', markersize=8, label='Best', color='green')
            plot.add_patch(plt.Circle((best[0], best[1]), 0.5, color='green', fill=False))

        # Plot circle around last individual
        if last is not None:
            plot.plot(last[0], last[1], marker='o', markersize=8, label='Tracked', color='
yellow')
            plot.add_patch(plt.Circle((last[0], last[1]), 0.5, color='yellow', fill=False))

        plot.legend()

    def plot_sub_contour(X1, X2, f, plot, x_range=(0,10), colour='gray'):
        """
        Function for plotting the grey contour plot which will be overlayed with the
population during optimisation.
```

```
95
96            Args:
97            - X1 (np.ndarray): Meshgrid of x1 values.
98            - X2 (np.ndarray): Meshgrid of x2 values.
99            - f (np.ndarray): Function values.
100           - plot (matplotlib.pyplot): A subplot within the grid of contours to plot the contour
      on.
101           - x_range (tuple): Range of x values.
102           """
103           plot.contourf(X1, X2, f, 100, cmap=colour)
104           plot.set_facecolor('xkcd:light grey')
105           plot.set_xlabel(r'$x_1$')
106           plot.set_ylabel(r'$x_2$')
107           plot.set_xlim(x_range)
108           plot.set_ylim(x_range)
109
110       def plot_fitness(avg_fitness, min_fitness, type, PT=False):
111           """
112           Function for plotting the evolution of the average and minimum fitness of a population
      .
113
114           Args:
115           - avg_fitness (np.ndarray): Array of average fitness values.
116           - min_fitness (np.ndarray): Array of minimum fitness values.
117           - name (str): Name of function.
118           - type (list): List of parameters used for the optimisation.
119           - PT (bool): Whether the optimisation was performed using parallel tempering or not.
120           """
121           plt.figure()
122           sns.set_style('darkgrid')
123           plt.plot(avg_fitness, label='Average Fitness')
124           plt.plot(min_fitness, label='Minimum Fitness')
125           plt.xlabel('Iteration')
126           plt.ylabel(r'Fitness = $-f(x_1, x_2)$')
127
128           # Set naming based on algorithm used
129           if PT:
130               hyperparams = ['Exchange Procedure', 'Schedule', 'Exchange Param', 'Power Term']
131
132           else:
133               hyperparams = ['Selection', 'Mating', 'Mutation Rate', 'Crossover Prob']
134
135           plt.title("Evolution of Fitness to " + type[0] + " Function, \n"
136                     + f"[{hyperparams[0]}: " + r"\textbf{" + type[2]
137                     + r"}, " + hyperparams[1] + r": \textbf{" + type[3]
138                     + r"}, " + hyperparams[2] + r": \textbf{" + str(type[4])
139                     + r"}, " + hyperparams[3] + r": \textbf{" + str(type[5])
140                       + r"}]", fontsize=12)
141
142           plt.legend()
143           plt.savefig(f'figures/{type[0]}/{str(type[1])}_iters/{type[2]}/{type[3]}/{type[4]}_{
      type[5]}_Fitness.png')
```

Listing 8: plotting_functions.py

7.3   functions

```
1     """
2     Candidate No : 5730E, Module: 4M17
3
4     Description :
5         This file contains the implementation of the Keane's Bump Function and the Rosenbrock
      function.
6     """
7
8
9     import numpy as np
10
11    def KBF_function(x, eps=1e-8):
12        """
```

```
13        Function implements Keane's Bump Function for a given input vector x of shape n x 1.
14
15        Args:
16            x (np.ndarray): Input vector of shape n x 1.
17            eps (float): Small value to avoid division by zero.
18
19        Returns:
20            f (float): Function value at x.
21        """
22
23        # Get the number of dimensions
24        n = x.shape[0]
25
26        # Compute the numerator
27        num = np.sum(np.cos(x)**4) - 2*np.prod(np.cos(x)**2)
28
29        # Compute the denominator
30        den = np.sqrt(np.sum(np.arange(1, n+1)*x**2))
31
32        # Avoid division by zero
33        if den == 0:
34            den = eps
35
36        # Compute the function value
37        f = np.abs(num/den)
38
39        return f
40
41    def Rosenbrock_function(x):
42        """
43        Function implements the Rosenbrock function for a given input vector x of shape n x 1.
44        Used for testing optimisation algorithms.
45
46        Args:
47            x (np.ndarray): Input vector of shape n x 1.
48
49        Returns:
50            f (float): Function value at x.
51        """
52
53        # Get the number of dimensions
54        n = x.shape[0]
55
56        # Compute the function value
57        f = 0
58        for i in range(n-1):
59            f += 100*(x[i+1] - x[i]**2)**2 + (1 - x[i])**2
60
61        return f
```

Listing 9: functions.py

7.4 Experiments

7.4.1 CGA_TuningExperiments

```
1     """
2     Candidate No : 5730E, Module: 4M17
3
4     Description :
5         This file serves as a platform to run multiple simulations of the CGA algorithm.
6         Used to generate the results for the table and figures in Section 3.2 of the report.
7     """
8
9     import sys; sys.path.append('..')
10    from src.utils.helper_functions import evaluate_2D, create_figure_directories_CGA
11    from src.utils.plotting_functions import plot_2D, plot_sub_contour, plot_population,
      plot_fitness
12    from src.functions import KBF_function, Rosenbrock_function
```

```python
from src.algorithms.CGA.CGA import ContinousGeneticAlgorithm

import numpy as np
import matplotlib.pyplot as plt
from multiprocessing import Pool
import pandas as pd
import seaborn as sns

# Hyperparameters
X_RANGE=(0,10)
FUNCTION = KBF_function
POPULATION_SIZE = 250
CHROMOSOME_LENGTH = 2
NUM_PARENTS =  POPULATION_SIZE // 4 # 25% of population size
MUTATION_RATE_LIST = [0.05, 0.1]
CROSSOVER_PROB_LIST = [0.7, 0.65]
SELECTION_METHOD_LIST = ['Proportional', 'Tournament', 'SRS']
MATING_PROCEDURE_LIST = ['Crossover', 'Heuristic Crossover']
ITERS_LIST = [5, 10, 100]
TOUNAMENT_SIZE = POPULATION_SIZE // 4 # 25% of population size

NAME = 'Rosenbrock' if FUNCTION == Rosenbrock_function else 'KBF'

# Make sure NUM_PARENTS is a multiple of 2
if NUM_PARENTS % 2 != 0:
    NUM_PARENTS += 1

# Create directories for figures
create_figure_directories_CGA(NAME, SELECTION_METHOD_LIST, MATING_PROCEDURE_LIST,
ITERS_LIST)

# 2D Visualisation of function
X1, X2, f = evaluate_2D(FUNCTION, x_range=X_RANGE)
plot_2D(X1, X2, f, name=NAME)

# Visualise with carved out feasible region
X1, X2, f_feasible = evaluate_2D(FUNCTION, x_range=X_RANGE, constraints=True)
plot_2D(X1, X2, f_feasible, name=NAME, constraints=True)

### Function used to generate results for table and figures in Section 3.2/Appendix of the
 report ###
def selection_mating_tuning(params):
    """
    Parallelisable function to run multiple simulations of the CGA algorithm and
    assess the impact of different hyperparameters on the algorithm's performance.
    The results are saved to a csv file and figures are generated to visualise the results
.
    """

    # Parse parameters
    SELECTION_METHOD, MATING_PROCEDURE, MUTATION_RATE, CROSSOVER_PROB, NUM_ITERS = params

    # Instantiate CGA
    CGA = ContinousGeneticAlgorithm(
        population_size=POPULATION_SIZE,
        chromosome_length=CHROMOSOME_LENGTH,
        num_parents=NUM_PARENTS,
        objective_function=FUNCTION,
        tournament_size=TOUNAMENT_SIZE,
        range=X_RANGE,
        mutation_rate=MUTATION_RATE,
        crossover_prob=CROSSOVER_PROB,
        selection_method=SELECTION_METHOD,
        mating_procedure=MATING_PROCEDURE,
    )

    # Evaluate initial population
    CGA.evaluate_fitness()
```

```python
 79        # Make a grid of 2D plots to show evolution of population
 80        PLOT_EVERY = NUM_ITERS // 5
 81        num_plots = (NUM_ITERS // PLOT_EVERY)
 82        fig, axs = plt.subplots(1, num_plots, figsize=(20, 5))
 83        fig.suptitle("Evolution of Population, \n"
 84                     + r"[Selection: \textbf{" + SELECTION_METHOD
 85                     + r"}, Mating: \textbf{" + MATING_PROCEDURE
 86                     + r"}, Mutation Rate: \textbf{" + str(MUTATION_RATE)
 87                     + r"}, Crossover Prob: \textbf{" + str(CROSSOVER_PROB)
 88                     + r"}]", fontsize=18)
 89
 90        # Plot grey contour plots of function on each subplot in grid
 91        # This will be overlayed with populations at different iterations
 92        for idx in range(num_plots):
 93            plot_sub_contour(X1, X2, f_feasible, plot=axs[idx], x_range=X_RANGE)
 94
 95        # Initialise arrays to store fitness values
 96        avg_fitness = np.zeros(NUM_ITERS)
 97        min_fitness = np.zeros(NUM_ITERS)
 98
 99        for iter in range(NUM_ITERS):
100
101            # Overlay population on grey contour every "PLOT_EVERY" iterations. (Periodic
    break to allow for visualisation).
102            if iter % PLOT_EVERY == 0:
103                plot_num = (iter // PLOT_EVERY)
104                idx = plot_num % num_plots
105                axs[idx].set_title(f'Iteration: {iter}')
106                plot_population(CGA.population, plot=axs[idx], best=CGA.best_individual)
107
108            # Evolve population
109            CGA.evolve()
110
111            # Update fitness arrays
112            avg_fitness[iter] = np.mean(CGA.fitness)
113            min_fitness[iter] = CGA.min_fitness
114
115        plt.tight_layout()
116        plt.savefig(f'figures/{NAME}/{str(NUM_ITERS)}_iters/{SELECTION_METHOD}/{
    MATING_PROCEDURE}/{MUTATION_RATE}_{CROSSOVER_PROB}_Population.png')
117
118        # Plot fitness evolution with iteration
119        plot_fitness(avg_fitness, min_fitness, type=(NAME, NUM_ITERS, SELECTION_METHOD,
    MATING_PROCEDURE, MUTATION_RATE, CROSSOVER_PROB))
120
121        # Return results to dataframe
122        return {
123            'Selection Method': SELECTION_METHOD,
124            'Mating Procedure': MATING_PROCEDURE,
125            'Mutation Rate': MUTATION_RATE,
126            'Crossover Rate': CROSSOVER_PROB,
127            'Iterations': NUM_ITERS,
128            'Final Avg Fitness': avg_fitness[-1],
129            'Final Min Fitness': min_fitness[-1]
130        }
131
132    ### Function used to generate fitness evolutions in Section 3.2 of the report ###
133    def plot_fitnesses():
134        """
135        Function to plot fitness evolution for each selection method.
136        """
137        for MATING in MATING_PROCEDURE_LIST:
138
139            # Make a plot for each mating procedure to show fitness evolution for the three
    selection method
140            plt.figure(figsize=(14, 10))
141            sns.set_style('darkgrid')
142            plt.title(f'Average Fitness Evolution for each Selection Method on {NAME} Function
    \n'
```

```
143                             + r"Mating Procdure held as \textbf{" + MATING + r"}", fontsize=24)
144                 plt.xlabel('Iteration', fontsize=20)
145                 plt.ylabel('Average Fitness', fontsize=20)
146
147                 for SELECTION_METHOD in SELECTION_METHOD_LIST:
148                     # Instantiate CGA
149                     CGA = ContinousGeneticAlgorithm(
150                         population_size=POPULATION_SIZE,
151                         chromosome_length=CHROMOSOME_LENGTH,
152                         num_parents=NUM_PARENTS,
153                         objective_function=FUNCTION,
154                         tournament_size=TOUNAMENT_SIZE,
155                         range=X_RANGE,
156                         mutation_rate=0.05,
157                         crossover_prob=0.7,
158                         selection_method=SELECTION_METHOD,
159                         mating_procedure=MATING,
160                         )
161
162                     # Evaluate initial population
163                     CGA.evaluate_fitness()
164
165                     # Initialise arrays to store fitness values
166                     avg_fitness = np.zeros(100)
167                     min_fitness = np.zeros(100)
168
169                     for iter in range(100):
170                         # Evolve population
171                         CGA.evolve()
172
173                         # Update fitness arrays
174                         avg_fitness[iter] = np.mean(CGA.fitness)
175                         min_fitness[iter] = CGA.min_fitness
176
177                     # Plot fitness evolution with iteration
178                     sns.lineplot(x=range(100), y=avg_fitness, label=SELECTION_METHOD)
179
180                 plt.legend(fontsize=16)
181                 plt.savefig(f'figures/{NAME}/Fitness_Evolution_{MATING}.png')
182
183     ### Function used to generate heat maps in Section 3.2 of the report ###
184     def rate_prob_mesh(params):
185         """
186         Parallelisable function to create mesh grids for heat map plots to assess
187         the impact of mutation rate and crossover probability on the
188         algorithm's performance.
189         """
190
191         # Parse parameters
192         i, j, MUTATION_RATE, CROSSOVER_PROB = params
193
194         # Instantiate CGA
195         CGA = ContinousGeneticAlgorithm(
196             population_size=POPULATION_SIZE,
197             chromosome_length=CHROMOSOME_LENGTH,
198             num_parents=NUM_PARENTS,
199             objective_function=FUNCTION,
200             tournament_size=TOUNAMENT_SIZE,
201             range=X_RANGE,
202             mutation_rate=MUTATION_RATE,
203             crossover_prob=CROSSOVER_PROB,
204             selection_method=SELECTION_METHOD,
205             mating_procedure=MATING_PROCEDURE,
206         )
207
208         # Evaluate initial population
209         CGA.evaluate_fitness()
210
211         # Evolve population
```

```python
212            for iter in range(100):
213                CGA.evolve()
214
215            # Return the results
216            return i, j, np.mean(CGA.fitness), CGA.min_fitness
217
218        ### Now run the above three functions ###
219
220        # Create a list of parameter combinations
221        params_list = [(SELECTION_METHOD, MATING_PROCEDURE, MUTATION_RATE, CROSSOVER_PROB,
        NUM_ITERS)
222                        for SELECTION_METHOD in SELECTION_METHOD_LIST
223                        for MATING_PROCEDURE in MATING_PROCEDURE_LIST
224                        for MUTATION_RATE in MUTATION_RATE_LIST
225                        for CROSSOVER_PROB in CROSSOVER_PROB_LIST
226                        for NUM_ITERS in ITERS_LIST]
227
228        print('Starting simulations for table and figure generation...')
229
230        # Create a pool of worker processes
231        pool = Pool()
232
233        # Create a dataframe to store results for CSV table
234        results = pd.DataFrame(columns=['Selection Method',
235                                        'Mating Procedure',
236                                        'Mutation Rate',
237                                        'Crossover Rate',
238                                        'Iterations',
239                                        'Final Avg Fitness',
240                                        'Final Min Fitness'])
241
242        # Run the simulations in parallel
243        for result in pool.map(selection_mating_tuning, params_list):
244            results.loc[len(results)] = result # Append result to dataframe
245
246        # Close the pool
247        pool.close()
248        pool.join()
249
250        # Save results to csv file
251        results.to_csv(f'figures/{NAME}/CGAresults.csv')
252
253        print('Done!')
254
255        print('Starting simulations for fitness plots generation')
256
257        # Plot fitness evolution for each selection method
258        plot_fitnesses()
259
260        print('Done!')
261
262        print('Starting simulations for contour plot generation')
263
264        # Optimal selection and mating chosen as Tournament and Heuristic Crossover respectively
265        # as discussed in Section 3.2 of the report
266        SELECTION_METHOD = 'Tournament'
267        MATING_PROCEDURE = 'Heuristic Crossover'
268
269        # Particular mutation rates and crossover probabilities I want to test
270        MUTATION_RATE_LIST = [0.01, 0.05, 0.075, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7]
271        CROSSOVER_PROB_LIST = [0.5, 0.55, 0.6, 0.65, 0.7, 0.75, 0.8, 0.85, 0.9, 0.95]
272
273        # Initialise meshgrids of variables, X = mutation rate, Y = crossover probability
274        X, Y = np.meshgrid(MUTATION_RATE_LIST, CROSSOVER_PROB_LIST)
275
276        # Initialise array to store final avg and min fitnesses, used as Z in heat maps
277        AVG = np.zeros((len(MUTATION_RATE_LIST), len(CROSSOVER_PROB_LIST)))
278        MIN = np.zeros((len(MUTATION_RATE_LIST), len(CROSSOVER_PROB_LIST)))
279
```

```
280    # Create a pool of workers
281    pool = Pool()
282
283    # Create a list of parameters for parallel execution
284    params_list = [(i, j, MUTATION_RATE, CROSSOVER_PROB)
285                    for i, MUTATION_RATE in enumerate(MUTATION_RATE_LIST)
286                    for j, CROSSOVER_PROB in enumerate(CROSSOVER_PROB_LIST)]
287
288    # Run the simulations in parallel
289    results = pool.map(rate_prob_mesh, params_list)
290
291    # Update fitness arrays
292    for i, j, fitness, min_fitness in results:
293        AVG[i, j] = fitness
294        MIN[i, j] = min_fitness
295
296    # Close the pool
297    pool.close()
298    pool.join()
299
300    # Plot average fitness heat map
301    plt.figure(figsize=(14, 10))
302    plt.title(f'Average Final Fitness with varying Mutation Rate and Crossover Probability on
       {NAME} Function \n'
303            + r"[Selection Method: \textbf{" + SELECTION_METHOD + r"}, "
304            + r"Mating Procedure: \textbf{" + MATING_PROCEDURE + r"}]", fontsize=18)
305    sns.heatmap(AVG, annot=True, xticklabels=MUTATION_RATE_LIST, yticklabels=
       CROSSOVER_PROB_LIST)
306    plt.xlabel('Mutation Rate', fontsize=14)
307    plt.ylabel('Crossover Probability', fontsize=14)
308    plt.savefig(f'figures/{NAME}/AVGContour_{SELECTION_METHOD}_{MATING_PROCEDURE}.png')
309
310    # Plot minimum fitness heat map
311    plt.figure(figsize=(14, 10))
312    plt.title(f'Minimum Final Fitness with varying Mutation Rate and Crossover Probability on
       {NAME} Function \n'
313            + r"[Selection Method: \textbf{" + SELECTION_METHOD + r"}, "
314            + r"Mating Procedure: \textbf{" + MATING_PROCEDURE + r"}]", fontsize=18)
315    sns.heatmap(MIN, annot=True, xticklabels=MUTATION_RATE_LIST, yticklabels=
       CROSSOVER_PROB_LIST)
316    plt.xlabel('Mutation Rate', fontsize=14)
317    plt.ylabel('Crossover Probability', fontsize=14)
318    plt.savefig(f'figures/{NAME}/MINContour_{SELECTION_METHOD}_{MATING_PROCEDURE}.png')
319
320    print('Done!')
```

Listing 10: CGA_TuningExperiments.py

7.4.2 PT_TuningExperiments

```
1     """
2     Candidate No : 5730E, Module: 4M17
3
4     Description :
5         This file serves as a platform to run multiple simulations of the PT algorithm.
6         Used to generate the results for the table and figures in Section 4.2 of the report.
7     """
8
9     import matplotlib.pyplot as plt
10    import numpy as np
11    from multiprocessing import Pool
12    import pandas as pd
13    import seaborn as sns
14
15    from src.algorithms.PT.PT import ParallelTempering
16    from src.functions import KBF_function, Rosenbrock_function
17    from src.utils.helper_functions import evaluate_2D, create_figure_directories_PT
18    from src.utils.plotting_functions import plot_sub_contour, plot_population, plot_fitness,
       plot_temp_progressions
19
```

```python
      # Hyperparameters
20    X_RANGE=(0,10)
21    FUNCTION = KBF_function
22    X_DIM = 2
23    NUM_REPLICAS = 10
24    NUM_SOL_PER_REPLICA = 250 // NUM_REPLICAS # 250 solutions overall, same as CGA population
25    EXCHANGE_PROCEDURE_LIST = ['Periodic', 'Stochastic']
26    EXCHANGE_PARAM_LIST = [0.1, 0.3, 0.5, 0.01]
27    TEMP_TYPE = 'Power'
28    PROGRESSION_POWER_LIST = [1, 3, 5] # 1 is uniform
29    NUM_ITERS_LIST = [100]
30
31
32    FUNC_NAME = 'Rosenbrock' if FUNCTION == Rosenbrock_function else 'KBF'
33
34    # Create figure directories
35    create_figure_directories_PT(FUNC_NAME, EXCHANGE_PROCEDURE_LIST, [TEMP_TYPE],
      NUM_ITERS_LIST)
36
37    ### Function used to generate results for table and figures in Section 4.2/Appendix of the
       report ###
38    def PT_initial_tuning(params):
39        """
40        Parallelisable function to run multiple simulations of the PT algorithm and
41        assess the impact of different hyperparameters on the algorithm's performance.
42        The results are saved to a csv file and figures are generated to visualise the results
      .
43        """
44
45        # Parse parameters
46        EXCHANGE_PROCEDURE, EXCHANGE_PARAM, PROGRESSION_POWER, NUM_ITERS = params
47
48        # Set schedule name for files and plots
49        SCHEDULE_NAME = TEMP_TYPE + " " + str(PROGRESSION_POWER) if TEMP_TYPE == 'Power' else
      TEMP_TYPE
50
51        # Instantiate PT object
52        PT = ParallelTempering(
53            objective_function=FUNCTION,
54            x_dim=X_DIM,
55            range=X_RANGE,
56            num_replicas=NUM_REPLICAS,
57            num_chains=NUM_SOL_PER_REPLICA,
58            exchange_procedure=EXCHANGE_PROCEDURE,
59            exchange_param=EXCHANGE_PARAM,
60            schedule_type=TEMP_TYPE,
61            power_term=PROGRESSION_POWER
62        )
63
64        # Make a grid of 5 2D plots to show evolution of population
65        PLOT_EVERY = NUM_ITERS // 5
66        num_plots = (NUM_ITERS // PLOT_EVERY)
67        fig, axs = plt.subplots(1, num_plots, figsize=(20, 5))
68        plt.suptitle(f"Evolution of Solutions, \n"
69                    + r"[Exchange Procedure: \textbf{" + EXCHANGE_PROCEDURE
70                    + r"}, Exchange Parameter: \textbf{" + str(EXCHANGE_PARAM)
71                    + r"}, Schedule: \textbf{" + TEMP_TYPE
72                    + r"}, Power Term: \textbf{" + str(PROGRESSION_POWER)
73                    + r"}]", fontsize=16)
74
75        # Plot grey contour plots of function on each subplot in grid
76        # This will be overlayed with populations at different iterations
77        X1, X2, f_feasible = evaluate_2D(FUNCTION, x_range=X_RANGE, constraints=True)
78        for idx in range(num_plots):
79            plot_sub_contour(X1, X2, f_feasible, plot=axs[idx], x_range=X_RANGE)
80
81        # Initialise arrays to store fitness values
82        avg_fitness = np.zeros(NUM_ITERS)
83        min_fitness = np.zeros(NUM_ITERS)
84
```

```python
85          # Initial avg. and min. fitness
86          avg_fitness[0], min_fitness[0] = PT.get_fitness()
87
88          for iter in range(NUM_ITERS):
89              # Overlay population on grey contour every "PLOT_EVERY" iterations. (Periodic
    break to allow for visualisation).
90              if iter % PLOT_EVERY == 0:
91                  plot_num = (iter // PLOT_EVERY)
92                  idx = plot_num % num_plots
93                  axs[idx].set_title(f'Iteration: {iter}')
94                  final_replica = PT.get_all_solutions()
95                  plot_population(final_replica, axs[idx], best=PT.get_best_solution(), last=
    final_replica[-1])
96
97              # Algorithm update
98              PT.update_chains()
99              PT.replica_exchange(iter)
100
101              # Update fitness arrays
102              avg_fitness[iter], min_fitness[iter] = PT.get_fitness()
103
104          plt.tight_layout()
105          plt.savefig(f'figures/{FUNC_NAME}/{str(NUM_ITERS)}_iters/{EXCHANGE_PROCEDURE}/{
    TEMP_TYPE}/{EXCHANGE_PARAM}_{PROGRESSION_POWER}_Solutions.png')
106
107          plot_fitness(avg_fitness, min_fitness, [FUNC_NAME,
108                                                   NUM_ITERS,
109                                                   EXCHANGE_PROCEDURE,
110                                                   TEMP_TYPE,
111                                                   EXCHANGE_PARAM,
112                                                   PROGRESSION_POWER], PT=True)
113
114          # Return results to dataframe
115          return {
116              'Exchange Procedure': EXCHANGE_PROCEDURE,
117              'Exchange Parameter': EXCHANGE_PARAM,
118              'Schedule': TEMP_TYPE,
119              'Power Term': PROGRESSION_POWER,
120              'Iterations': NUM_ITERS,
121              'Final Avg. Fitness': avg_fitness[-1],
122              'Final Min. Fitness': min_fitness[-1],
123              'Avg. Fitness Progression': avg_fitness
124          }
125
126      ### Function used to generate heatmaps in Section 4.2/Appendix of the report ###
127      def power_exchange_mesh(params):
128          """
129          Parallelisable function to create mesh grids for heat map plots to assess
130          the impact of exchange rate and temperature scheduling on the
131          algorithm's performance.
132          """
133
134          # Parse parameters
135          i, j, EXCHANGE_PROCEDURE, EXCHANGE_PARAM, PROGRESSION_POWER = params
136
137          # Instantiate PT object
138          PT = ParallelTempering(
139              objective_function=FUNCTION,
140              x_dim=X_DIM,
141              range=X_RANGE,
142              num_replicas=NUM_REPLICAS,
143              num_chains=NUM_SOL_PER_REPLICA,
144              exchange_procedure=EXCHANGE_PROCEDURE,
145              exchange_param=EXCHANGE_PARAM,
146              schedule_type='Power',
147              power_term=PROGRESSION_POWER
148          )
149
150          # Run algorithm for 100 iterations
```

```python
151        for iter in range(100):
152            PT.update_chains()
153            PT.replica_exchange(i)
154
155        # Get final fitness
156        final_avg_fitness, final_min_fitness = PT.get_fitness()
157
158        return i, j, final_avg_fitness, final_min_fitness
159
160    # Create a list of all combinations of parameters
161    params_list = [(EXCHANGE_PROCEDURE, EXCHANGE_PARAM, PROGRESSION_POWER, NUM_ITERS)
162                   for EXCHANGE_PROCEDURE in EXCHANGE_PROCEDURE_LIST
163                   for EXCHANGE_PARAM in EXCHANGE_PARAM_LIST
164                   for PROGRESSION_POWER in PROGRESSION_POWER_LIST
165                   for NUM_ITERS in NUM_ITERS_LIST]
166
167    print('Starting simulations for table and figure generation...')
168
169    # Create a pool of worker processes
170    pool = Pool()
171
172    results = pd.DataFrame(columns=['Exchange Procedure',
173                                    'Exchange Parameter',
174                                    'Schedule',
175                                    'Power Term',
176                                    'Iterations',
177                                    'Final Avg. Fitness',
178                                    'Final Min. Fitness',
179                                    'Avg. Fitness Progression'])
180
181    # Run the simulations in parallel
182    for result in pool.map(PT_initial_tuning, params_list):
183        results.loc[len(results)] = result # Append result to dataframe
184
185    # Save results to csv
186    results.to_csv(f'figures/{FUNC_NAME}/PT_initial_tuning.csv', index=False)
187
188    # Close the pool of workers
189    pool.close()
190    pool.join()
191    print('Done!')
192
193    print('Generating fitness figures...')
194
195    ### Used to gerenate fitness figures in Section 4.2 of the report ###
196    # Plot fitness progression for each exchange procedure with varying power term
197    for EXCHANGE_PROCEDURE in EXCHANGE_PROCEDURE_LIST:
198        plt.figure(figsize=(10, 8))
199        sns.set_style('darkgrid')
200
201        # Get results pertaining to that exchange procedure
202        periodic_results = results[results['Exchange Procedure'] == EXCHANGE_PROCEDURE]
203
204        # Get results corresponding to uniform schedule
205        periodic_results_1 = periodic_results[periodic_results['Power Term'] == 1]
206
207        # Get results correctponding to 'Exchange Parameter' = 0.1, 0.3, 0.5
208        periodic_results_1_01 = periodic_results_1[periodic_results_1['Exchange Parameter'] ==
    0.1]
209        periodic_results_1_03 = periodic_results_1[periodic_results_1['Exchange Parameter'] ==
    0.3]
210        periodic_results_1_05 = periodic_results_1[periodic_results_1['Exchange Parameter'] ==
    0.5]
211
212        # Plot fitness progression for each 'Exchange Parameter'
213        plt.plot(periodic_results_1_01['Avg. Fitness Progression'].values[0], label='Exchange
    Parameter = 0.1')
214        plt.plot(periodic_results_1_03['Avg. Fitness Progression'].values[0], label='Exchange
    Parameter = 0.3')
```

```
215         plt.plot(periodic_results_1_05['Avg. Fitness Progression'].values[0], label='Exchange
       Parameter = 0.5')
216
217         plt.title(f'Average Fitness Progression for {EXCHANGE_PROCEDURE} Exchange, \n'
218                   + r"[Temp Schedule: \textbf{Uniform}]")
219         plt.xlabel('Iteration')
220         plt.ylabel('Average Fitness')
221         plt.legend()
222         plt.tight_layout()
223
224         plt.savefig(f'figures/{FUNC_NAME}/100_iters/{EXCHANGE_PROCEDURE}/
       PT_Avg_Fitness_Evolution.png')
225
226     print('Done!')
227
228     print('Starting heatmap generation...')
229
230     EXCHANGE_PROCEDURE = 'Stochastic'
231     EXCHANGE_PARAM_LIST = [0.01, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5]
232     PROGRESSION_POWER_LIST = range(1, 10)
233
234     # Create mesh grid for exchange parameters and power terms
235     X, Y = np.meshgrid(EXCHANGE_PARAM_LIST, PROGRESSION_POWER_LIST)
236
237     # Initialise arrays to store fitness values
238     AVG = np.zeros((len(EXCHANGE_PARAM_LIST), len(PROGRESSION_POWER_LIST)))
239     MIN = np.zeros((len(EXCHANGE_PARAM_LIST), len(PROGRESSION_POWER_LIST)))
240
241     params_list = [(i, j, EXCHANGE_PROCEDURE, EXCHANGE_PARAM, PROGRESSION_POWER)
242                    for i, EXCHANGE_PARAM in enumerate(EXCHANGE_PARAM_LIST)
243                    for j, PROGRESSION_POWER in enumerate(PROGRESSION_POWER_LIST)]
244
245     # Create a pool of worker processes
246     pool = Pool()
247
248     results = pool.map(power_exchange_mesh, params_list)
249
250     for i, j, final_avg_fitness, final_min_fitness in results:
251         AVG[i, j] = final_avg_fitness
252         MIN[i, j] = final_min_fitness
253
254     # Close the pool
255     pool.close()
256     pool.join()
257
258     # Plot average fitness heat map
259     plt.figure(figsize=(14, 10))
260     plt.title(f'Average Final Fitness with varying Power Param and Exchange Param on {
       FUNC_NAME} Function \n'
261               + r"[Exchange Procedure: \textbf{" + EXCHANGE_PROCEDURE + r"}]", fontsize=18)
262     sns.heatmap(AVG, annot=True, fmt='.2f', xticklabels=EXCHANGE_PARAM_LIST, yticklabels=
       PROGRESSION_POWER_LIST, cmap='Blues')
263     plt.xlabel('Exchange Parameter', fontsize=16)
264     plt.ylabel('Power Parameter, p', fontsize=16)
265     plt.tight_layout()
266     plt.savefig(f'figures/{FUNC_NAME}/PT_Avg_Fitness_Heatmap_{EXCHANGE_PROCEDURE}.png')
267
268     # Plot minimum fitness heat map
269     plt.figure(figsize=(14, 10))
270     plt.title(f'Minimum Final Fitness with varying Power Param and Exchange Param on {
       FUNC_NAME} Function \n'
271               + r"[Exchange Procedure: \textbf{" + EXCHANGE_PROCEDURE + r"}]", fontsize=18)
272     sns.heatmap(MIN, annot=True, fmt='.2f', xticklabels=EXCHANGE_PARAM_LIST, yticklabels=
       PROGRESSION_POWER_LIST, cmap='Blues')
273     plt.xlabel('Exchange Parameter', fontsize=16)
274     plt.ylabel('Power Parameter, p', fontsize=16)
275     plt.tight_layout()
276     plt.savefig(f'figures/{FUNC_NAME}/PT_Min_Fitness_Heatmap_{EXCHANGE_PROCEDURE}.png')
277
```

```python
278     print('Done!')
279
280     print('Generating optimal PT evolution and temperature schedule plot...')
281
282     ### The rest of the code is used to plot the final plot in 4.2, showing the evolution of
        the solutions for the optimal PT ###
283     # Optimally-tuned PT
284     PT = ParallelTempering(
285             objective_function=FUNCTION,
286             x_dim=X_DIM,
287             range=X_RANGE,
288             num_replicas=NUM_REPLICAS,
289             num_chains=NUM_SOL_PER_REPLICA,
290             exchange_procedure='Always',
291             exchange_param=0.5,
292             schedule_type='Power',
293             power_term=1
294         )
295
296     # Make a grid of 10 2D plots to show evolution of population
297     PLOT_EVERY = 100 // 5
298     num_plots = 100 // PLOT_EVERY
299
300     # Two rows, one for evolution with iterations, one for solutions for each replica/
        temperature
301     fig, axs = plt.subplots(2, num_plots, figsize=(22, 10))
302     plt.suptitle(f"Optimall-Tuned PT; Evolution with Iteration and Final Solutions per Replica
        \n"
303             + r"[Exchange Procedure: \textbf{Always}, Schedule: \textbf{Uniform}"
304             + r", Power Term: \textbf{" + str(1)
305             + r"}]", fontsize=16)
306
307     # On first row, plot grey contour plots of function on each subplot in grid
308     X1, X2, f_feasible = evaluate_2D(FUNCTION, x_range=X_RANGE, constraints=True)
309     for idx in range(num_plots):
310         plot_sub_contour(X1, X2, f_feasible, plot=axs[0][idx], x_range=X_RANGE)
311
312     # Make a new array of every t_index'th temperature, (excluding idx 0)
313     t_index = len(PT.temperature_schedule) // num_plots
314     temps = PT.temperature_schedule[1::t_index]
315
316     for idx in range(num_plots):
317         # Raise function to power of temperature!!! Good for visualising how the temperature
        affects the function
318         f_temp = f_feasible ** temps[idx]
319
320         plot_sub_contour(X1, X2, f_temp, axs[1][idx], x_range=X_RANGE, colour='Greys')
321         axs[1][idx].set_title(f'Temperature = {temps[idx]:.2f}')
322         plt.colorbar(axs[1][idx].contourf(X1, X2, f_temp, 100, cmap='inferno'), ax=axs[1][idx
        ])
323
324     # Plot evolution for 100 iterations
325     for iter in range(100):
326         if iter % PLOT_EVERY == 0:
327             plot_num = (iter // PLOT_EVERY)
328             idx = plot_num % num_plots
329             axs[0][idx].set_title(f'Iteration: {iter}')
330             final_replica = PT.get_all_solutions()
331             plot_population(final_replica, axs[0][idx], best=PT.get_best_solution(), last=
        final_replica[-1])
332
333         PT.update_chains()
334         PT.replica_exchange(iter)
335
336     replica_solutions = PT.current_solutions[1::t_index]
337
338     # Overlay replica solutions on second row
339     for idx in range(num_plots):
340         solutions = PT.scale_up(replica_solutions[idx])
```

```
341        axs[1][idx].scatter(solutions[:, 0], solutions[:, 1], c='lime', s=15, label='Replica
       Solutions')
342
343    plt.tight_layout()
344    plt.savefig(f'figures/{FUNC_NAME}/PT_Optimal_Tuning.png')
```

Listing 11: PT_TuningExperiments.py

7.4.3 FinalComparison

```
1    """
2    Candidate No : 5730E, Module: 4M17
3
4    Description :
5        This file serves to compare the optimally-tuned CGA and PT algorithms in section 5 of
       the report.
6    """
7
8    import sys; sys.path.append('..')
9    from src.utils.helper_functions import generate_initial
10   from src.algorithms.CGA.CGA import ContinousGeneticAlgorithm
11   from src.algorithms.PT.PT import ParallelTempering
12   from src.functions import KBF_function
13
14   import numpy as np
15   import matplotlib.pyplot as plt
16   import seaborn as sns
17   from time import time
18   import pandas as pd
19
20   # Generate initial solutions for both functions.
21   # No solution has a function value > 0.3, (away from global optimum)
22   initial_pop_list, seeds = generate_initial(x_dim=8, pop_size=250)
23
24   # Max number of iterations, as required by assignment handout
25   MAX_NUM_ITERS = 10000
26
27   # Convergence criteria
28   eps = 0.00025
29   conv_iters = 1300
30
31   ### CGA Gather Results ###
32   CGA_AvgFit_ALL = np.zeros((50, MAX_NUM_ITERS))
33   CGA_MinFit_ALL = np.zeros((50, MAX_NUM_ITERS))
34   CGA_times_ALL = np.zeros(50)
35   CGA_best_Xs = np.zeros((50, 8))
36   CGA_converg_iters = np.zeros(50)
37
38   # Run CGA 50 times with different initialisations
39   for run_iter, initialisation in enumerate(initial_pop_list):
40
41       # Instantiate optimally-tuned CGA
42       CGA = ContinousGeneticAlgorithm(population_size = 250,
43                                       chromosome_length = 8,
44                                       num_parents = 62,
45                                       objective_function = KBF_function,
46                                       tournament_size = 62,
47                                       range=(0,10),
48                                       mutation_rate=0.1,
49                                       crossover_prob=0.65,
50                                       selection_method='Tournament',
51                                       mating_procedure='Heuristic Crossover',
52                                       constraints=True)
53
54       # Now forcibly reset population to the initialisation
55       CGA.population = initialisation
56
57       # Initialise arrays for storing fitness
58       avg_fitness = np.zeros(MAX_NUM_ITERS)
59       min_fitness = np.zeros(MAX_NUM_ITERS)
```

47

```python
60
61          # Max number of iterations = MAX_NUM_ITERS
62          conv_count = 0
63          CGA_tic = time()
64          for i in range(MAX_NUM_ITERS):
65
66              # Evolve population
67              CGA.evolve()
68
69              # Update fitness arrays
70              avg_fitness[i] = np.mean(CGA.fitness)
71              min_fitness[i] = CGA.min_fitness
72
73              # Check if the algorithm has converged, |f(x) - f(x_prev)| < eps for 'conv_iters'
    iterations
74              if i != 0 and np.linalg.norm(min_fitness[i] - min_fitness[i-1]) < eps:
75                  conv_count += 1
76              else:
77                  conv_count = 0
78
79              # If the algorithm has converged, store the iteration at which it converged
80              if conv_count == conv_iters:
81                  CGA_converg_iters[run_iter] = i - conv_iters
82
83          # Time taken to run algorithm
84          CGA_toc = time()
85          CGA_times_ALL[run_iter] = CGA_toc - CGA_tic
86
87          # Update arrays
88          CGA_AvgFit_ALL[run_iter, :] = avg_fitness
89          CGA_MinFit_ALL[run_iter, :] = min_fitness
90          CGA_best_Xs[run_iter, :] = CGA.best_individual
91
92      ### PT Gather Results ###
93      PT_AvgFit_ALL = np.zeros((50, MAX_NUM_ITERS))
94      PT_MinFit_ALL = np.zeros((50, MAX_NUM_ITERS))
95      PT_times_ALL = np.zeros(50)
96      PT_best_Xs = np.zeros((50, 8))
97      PT_converg_iters = np.zeros(50)
98
99      # Run PT 50 times with different initialisations
100     for run_iter, initialisation in enumerate(initial_pop_list):
101
102         # Instantiate optimally-tuned PT
103         PT = ParallelTempering(objective_function=KBF_function,
104                                x_dim=8,
105                                range=(0,10),
106                                alpha=0.1,
107                                omega=2.1,
108                                num_replicas=10,
109                                num_chains=25,
110                                exchange_procedure='Always',
111                                power_term=1,
112                                constraints=True)
113
114         # Forcibly reset the PT solutions
115         initialisation = initialisation / 10 # Scale down to the range of the PT algorithm
    (0-1)
116         initialisation = initialisation.reshape(10, 25, 8) # Share solutions between replicas,
     i.e. from shape: (250, 8) to (10, 25, 8)
117         PT.current_solutions = initialisation
118
119         # Initialise arrays for storing fitness
120         avg_fitness = np.zeros(MAX_NUM_ITERS)
121         min_fitness = np.zeros(MAX_NUM_ITERS)
122
123         # Max number of iterations = MAX_NUM_ITERS
124         conv_count = 0
125         PT_tic = time()
```

```
126         for i in range(MAX_NUM_ITERS):
127
128             # Algorithm update
129             PT.update_chains()
130             PT.replica_exchange(iter)
131
132             # Update fitness arrays
133             avg_fitness[i], min_fitness[i] = PT.get_fitness()
134
135             # Check if the algorithm has converged, |f(x) - f(x_prev)| < eps for 'conv_iters'
        iterations
136             if i != 0 and np.linalg.norm(min_fitness[i] - min_fitness[i-1]) < eps:
137                 conv_count += 1
138             else:
139                 conv_count = 0
140
141             # If the algorithm has converged, store the iteration at which it converged
142             if conv_count == conv_iters:
143                 PT_converg_iters[run_iter] = i - conv_iters
144
145         # Time taken to run algorithm
146         PT_toc = time()
147         PT_times_ALL[run_iter] = PT_toc - PT_tic
148
149         # Update arrays
150         PT_AvgFit_ALL[run_iter, :] = avg_fitness
151         PT_MinFit_ALL[run_iter, :] = min_fitness
152         PT_best_Xs[run_iter, :] = PT.get_best_solution()
153
154     # Find the expectation of the average and min fitness across all 50 initialisations
155     CGA_AvgFit_mean = np.mean(CGA_AvgFit_ALL, axis=0)
156     PT_AvgFit_mean = np.mean(PT_AvgFit_ALL, axis=0)
157     CGA_MinFit_mean = np.mean(CGA_MinFit_ALL, axis=0)
158     PT_MinFit_mean = np.mean(PT_MinFit_ALL, axis=0)
159
160     # Find the expected iteration at which CGA and PT converge
161     CGA_Avg_i = np.mean(CGA_converg_iters)
162     PT_Avg_i = np.mean(PT_converg_iters)
163
164     # Plot expected average fitness values for CGA and PT
165     plt.figure()
166     sns.set_style('darkgrid')
167     plt.plot(CGA_AvgFit_mean, label='CGA', color='green')
168     plt.plot(PT_AvgFit_mean, label='PT', color='red')
169     plt.axvline(CGA_Avg_i, color='green', linestyle='--', label=f'CGA Best Converges at {int(
        CGA_Avg_i)} Iterations')
170     plt.axvline(PT_Avg_i, color='red', linestyle='--', label=f'PT Best Convergence at {int(
        PT_Avg_i)} Iterations')
171     plt.xlabel('Iterations')
172     plt.ylabel('Average Fitness')
173     plt.title('Expected Average Fitness across 50 Different Initialisations')
174     plt.legend()
175     plt.savefig('figures/Final Comparison/CGA vs PT Average Fitness.png', dpi=300)
176
177     # Plot expercted min fitness values for CGA and PT
178     plt.figure()
179     sns.set_style('darkgrid')
180     plt.plot(CGA_MinFit_mean, label='CGA', color='green')
181     plt.plot(PT_MinFit_mean, label='PT', color='red')
182     plt.axvline(CGA_Avg_i, color='green', linestyle='--', label=f'CGA Best Converges at {int(
        CGA_Avg_i)} Iterations on Avg.')
183     plt.axvline(PT_Avg_i, color='red', linestyle='--', label=f'PT Best Convergence at {int(
        PT_Avg_i)} Iterations on Avg.')
184     plt.xlabel('Iterations')
185     plt.ylabel('Minimum Fitness')
186     plt.title('Expected Minimum Fitness across 50 Different Initialisations')
187     plt.legend()
188     plt.savefig('figures/Final Comparison/CGA vs PT Minimum Fitness.png', dpi=300)
189
```

```python
190    # Save final results to csv
191    CGA_final_avg = CGA_AvgFit_mean[-1]
192    CGA_final_std = np.std(CGA_AvgFit_ALL[:, -1])
193    CGA_final_min = CGA_MinFit_mean[-1]
194    CGA_final_min_std = np.std(CGA_MinFit_ALL[:, -1])
195    CGA_final_time = np.mean(CGA_times_ALL)
196    CGA_final_time_std = np.std(CGA_times_ALL)
197    CGA_AVG_best_X = np.mean(CGA_best_Xs, axis=0)
198
199    PT_final_avg = PT_AvgFit_mean[-1]
200    PT_final_std = np.std(PT_AvgFit_ALL[:, -1])
201    PT_final_min = PT_MinFit_mean[-1]
202    PT_final_min_std = np.std(PT_MinFit_ALL[:, -1])
203    PT_final_time = np.mean(PT_times_ALL)
204    PT_final_time_std = np.std(PT_times_ALL)
205    PT_AVG_best_X = np.mean(PT_best_Xs, axis=0)
206
207    data = {'CGA': [CGA_final_avg, CGA_final_std, CGA_final_min, CGA_final_min_std,
       CGA_final_time, CGA_final_time_std, CGA_Avg_i, CGA_AVG_best_X],
208            'PT': [PT_final_avg, PT_final_std, PT_final_min, PT_final_min_std, PT_final_time,
       PT_final_time_std, PT_Avg_i, PT_AVG_best_X]}
209    df = pd.DataFrame(data, index=['Final Avg. Fitness', 'Final Avg. Fitness Std', 'Final Min.
        Fitness', 'Final Min. Fitness Std', 'Total Time Taken', 'Time Taken Std', 'Mean Iters to
       Convergence', 'Mean Best Solution'])
210    df.to_csv('figures/Final Comparison/CGA vs PT Final Results.csv')
211
212    print(seeds) # These are the random seeds used to generate the initial populations
```

Listing 12: FinalComparison.py