Evolutionary Algorithms: Final report

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1 Metadata

• Group members during group phase: Kostantinos Gkentsidis and Jeffrey Quicken

Time spent on group phase: 15 hours
Time spent on final code: 45 hours
Time spent on final report: 12 hours

2 Modifications since the group phase

2.1 Main improvements

Greedy Heuristic Initialization: Added a heuristic initialization of candidate solutions in order to inject some good initial candidates to the random initial population and speed up the search of the optimum. For more information see Subsection 3.2.

Local Search: Converted the evolutionary algorithm to a memetic algorithm through the inclusion of 2-opt local search after the variation step of each iteration. This addition significantly improved convergence to really good candidate solutions. For more information see Subsection 3.7.

Diversity Promotion: Fitness sharing was added to the $(\lambda + \mu)$ elimination step to improve the diversity of the population across iterations and prevent premature convergence. For more information see Subsections 3.6 and 3.8.

Greedy Mutation: Added a new mutation operator that uses a greedy approach to adapt an individual in the optimal way. For more information see Subsection 3.4

2.2 Issues resolved

Depleting Diversity: In the group phase, we detected a problem with diversity, meaning that our algorithm converged prematurely to locally optimal candidate solutions, thus preventing the discovery of better solutions. This issue was fixed through the addition of diversity promotion, increased mutation strength, and varying mutation operators.

Premature convergence: In the group phase, we used the $(\lambda + \mu) - elimination$ in combination with a convergence criterion of matching mean to best fitness. This resulted in a mostly exploitative behavior resulting in premature convergence. This issue was fixed by implementing methods for diversity promotion.

Loss of Best Candidate: In the individual phase it was discovered that sometimes the best candidate was lost across iterations. This was easily visible as unexplained spikes in the corresponding graph across iterations. This happened due to an unwanted modification of the original population during mutation. Fixing this bug cleared this error.

Inefficient Crossover Operator: The code used for the Order Crossover operator was taken from stackoverflow. In an effort to refine this code and remove needless code repetition, the operator was rewritten from scratch and ended up being more efficient, shorter and more readable.

3 Final design of the evolutionary algorithm

3.1 Representation

In Davis et al [2], five different representations are presented for TSP: Binary, Path, Adjacency, Ordinal, and Matrix representations. Based on a review of the different methods in the same research, it was decided in the group phase to select the **Path / Permutation Representation**, because of its better performance, operator variety, and explainability. The same representation was kept in the individual phase. This Path representation was implemented as a python class called Individual that stores a list of integers representing indices of cities with respect to the given distance matrix. The route of the candidate solution is checked against errors on update and hence the use of python sets was deemed redundant.

3.2 Initialization

In the group phase, a random initialization was used for the population resulting in high diversity with a high probability given a big enough population size λ . In order to achieve good results, it was decided to use a quite large population (1000-2000).

In the individual phase, the initialization step was augmented with a number of greedy heuristic candidate solutions in order to provide some direction to the search and avoid reinventing the wheel. The greedy heuristic search starts from a random city keeps following the shortest path from city to city until all cities are visited exactly once and finally ends up on the first city.

The use of really good candidate solutions entails the danger of taking over the population fairly quickly. However, this issue can be mitigated by limiting the number of heuristic candidate solutions or limiting the steps of the greedy search. Both methods were implemented and based on experiments it was decided to apply greedy search for 10% of the initial population

Furthermore, the addition local search and diversity promotion, allowed the use of a population and offspring size that's two magnitudes smaller ($\lambda = 10, \mu = 5$). Using a lower population and offspring size resulted in better performance with more iterations and no impact on the final results.

3.3 Selection operators

Similarly to the group phase, k-tournament selection was picked for the individual phase as well. This selection method performed really well before and offered a nice balance between exploration and exploitation, hence it was kept in this phase as well. The only tunable parameter of this selection operator is the number k of individuals that take part in a tournament.

3.4 Mutation operators

In the group phase, two mutation methods were used, namely inversion mutation and swap mutation. Both mutation operators, were extended in the individual phase with a new parameter called mutation strength σ_{μ} , which determines the number of successive applications of the operator on an individual.

Besides, those two mutation operators, a new greedy mutation operator was implemented in the individual phase. This operator removes four edges from a route randomly, resulting in five unconnected segments, which are greedily reconnected by finding the segment permutation with the best fitness.

Initially each mutation operator was assigned equal probability 33.333% to be chosen. However, in a trial of adaptive parameter control with a reward system, it was discovered that the greedy mutation operator improved solutions more consistently and took over the operator selection, so in the end it was decided to use only the greedy mutation operator.

3.5 Recombination operators

In the individual phase, it was decided to reuse the *Order Crossover* [2] operator, since it performs really well for order-based permutation problems like TSP according to the literature eg. [5] and based on experiments. The only change regarding this operator was the rewritting of its code to make it more efficient and readable.

The operator consists of the following steps:

- 1. Copy a segment between two randomly generated crossover points of the first parent to the first child.
- 2. Starting from the second crossover point on the second parent this time, start copying its genes/alleles that are not already contained on the child, until the child is full.
- 3. Create the second child like the first but with the reverse order of the parents.

One advantage of this operator is that it ensures the generation of only valid offspring and thus doesn't require the need to implement a repair mechanism. Moreover, the fact that the operator preserves the order of the cities from the parents is especially beneficial to Asymetric TSP problems, since it preserves good edges more effectively.

The operator, in general, preserves a segment of the first parent on the child and then tries to fill the rest with the city order of the second parent, thus preserving useful information from both parents. At the same time, because of the combination of two random parents that may or may not have much overlap, the resulting children can be similar to the parents and explore new space, while always producing valid candidate solutions.

Two enhancements ideas were considered regarding recombination operators. First was the possibility to add more recombination operators that vary significantly to Order Crossover and then self-adaptively select the best performing one per individual. This would provide some extra variation in the solutions, while at the same time, one operator might perform better in the beginning and another at the end close to convergence. Secondly, it seemed beneficial to implement the Distance Preserving Crossover (DPX) operator [4] which removes the edges that do not exist in both parents and then greedily reconnects the resulting segments.

3.6 Elimination operators

In the group phase, there was no choice but to use the $(\lambda + \mu) - elimination$ operator, which did not achieve a good balance between exploration and exploitation. This method chooses the top- λ candidates and eliminates worse candidate solutions that could result in better results after a few generations. Instead it even promotes similar candidates that have high fitness, which often causes premature convergence.

In the individual phase, two more elimination operators were implemented, namely, *fitness-sharing-based elimination* and *replace-worst elimination*. Both aimed at preserving diversity.

Fitness-sharing-based elimination is basically implemented as $(\lambda + \mu) - elimination$ with a recalculated fitness of each individual based on the number of its neighbouring individuals. The idea behind fitness sharing, according to [3], is to prevent very similar candidate solutions from overtaking the population by increasing their cost during selection or elimination based on their number of closely resembling neighbours. The distance metric that was used to determine the similarity of two individuals is the number of uncommon edges.

Replace-worst elimination results in a more diverse population than the simple $(\lambda + \mu) - elimination$ by keeping the $\lambda - \mu$ best individuals from the original population and replacing the rest with new offspring. This requires that $\lambda > \mu$.

Out of all three, the fitness-sharing-based elimination achieved the best and most consistent results and was the most successful at preventing premature convergence.

3.7 Local search operators

The absence of a local search operator in the group phase meant that the implemented evolutionary algorithm required a considerable amount of iterations and a really large population in order to find a good solution. As a result, it was deemed imperative to implement a local search operator for the individual phase. After a thorough literature review of the available methods, it was decided to proceed with k-opt local search, proposed by Croes et al [1].

The local search operator was implemented for k=2 and k=3. However, the 3-opt operator proved quite inefficient especially for the larger problems and thus was abandoned in favor of 2-opt, despite it being more suitable for the Asymetric TSP. A basic 2-opt local search algorithm will try all possible swap combinations that will result in an improvement of the fitness of an individual.

Although, 2-opt increases the computational complexity of the algorithm, at the same time, it results in quicker discovery of really good solutions. For really large problems, however, the operator proves extremely slow and thus a two-pronged approach has been implemented to optimize the evolutionary algorithm. Firstly, a new parameter has been introduced that determines the probability threshold p_l for executing local search in a generation. Secondly, a timeout has been added to the operator. As a result, the operator will perform the maximum number of improvements it manages in the one allowed time window.

3.8 Diversity promotion mechanisms

In the individual phase, two diversity promotion mechanisms were implemented. The first one involves a varying mutation rate and strength, but it didn't manage to preserve diversity very well and was thus abandoned. The second one is fitness sharing, it is implemented in the elimination step and it's described in more detail in Subsection ??.

The fitness sharing mechanism has two tunable parameters, the shape α and distance σ that determine its

sensitivity. A larger α value results in a higher penalty for each neighbour and σ represents the distance between two individuals for them to be considered neighbours.

3.9 Stopping criterion

In the individual phase, two convergence criteria were combined. The first one was the same that was used in the group phase. This criterion stops the algorithm when the mean fitness converges to the best fitness of the population. However, because of the diversity promotion mechanisms that was implemented, this criterion never activates. As a result a second criterion was added that simply checks if there was no improvement of the best fitness in the last 100 iterations.

3.10 The main loop

The order of the operators that are applied to the population in each generation can be seen on Fig. 1. It follows the classic order of evolutionary algorithms, starting with selection to produce offspring, then recombination, mutation, and finally elimination. In addition, local search is applied after mutation for each of the generated offspring with a p_l probability in each generation.

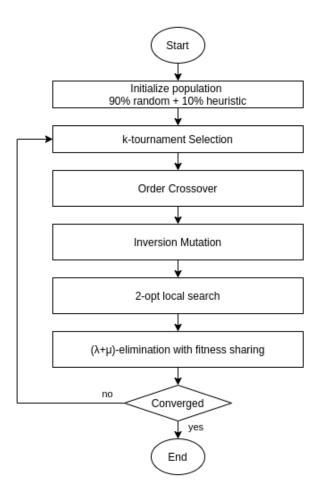


Figure 1: A high level flowchart of the developed evolutionary algorithm.

Selection is done with replacement, so that there is increased probability to pick really good individuals multiple times to recombine with other individuals. We basically desire good genes to be reused in the next generation.

A $(\lambda + \mu) - elimination$ operator selects the new population by combining the old population with the new offspring, sorting the combined population and keeping the $top - \lambda$ individuals. Because of the fitness sharing scheme that is used, the elimination method selects individuals sequentially and not in parallel, with replacement. After each selection the combined population plus offspring are reweighted, so as to avoid several similar solutions from surviving to the next generation.

3.11 Parameter selection

Because of the addition of local search and fitness sharing, the algorithm grew more computationally expensive. As a result the population size and the offspring size were significantly reduced by two orders of magnitude to allow the algorithm to run for more generations before time runs out. In particular, λ was reduced from 2000 to 10 and μ was reduced from around 2000/3 to 5. These parameters were tuned to achieve good performance in all problems, big and small. Fig. 2 presents the performance of the algorithm on tour194 for λ values between 10 and 100 and μ values defined as $\lambda/2$.

Furthermore, the reduction of the population and offspring size, meant that local search could be performed to all offspring with 100% probability even for the large tour929 problem. Although, to increase the number of generations, the local search method had to be constrained with a timeout of 0.2s. Without timeout, a single full run of local search for the tour929 would take 4 to 10 seconds and the algorithm would reach a timeout in just 2-3 generations.

For mutation, the idea of mass mutation from Eiben et al [3] was applied. This mass mutation approach refers mostly to memetic algorithms, which find really good locally optimal solutions using local search operators. The goal of mass mutation is to apply mutation with a really high rate so that the algorithm can find solutions that escape from local minima. This approach is implemented with a mutation probability $p_m=0.9$. Fig. 3 presents the best fitness for various mutation rates from 0.1 to 1.0 on tour194.

The number k of participants in the tournament selection was chosen via hyperparameters search. The results are shown in Fig. 4, where a k=4 was chosen due to its nice balance between performance and computational load.

The fitness sharing parameters α and σ were selected as 1 and $num_cities/5$ (38 for tour194) respectively, balancing performance and diversity. The shape parameter α is average with regard to punishment of similar candidates, while the distance σ is selected with respect to the size of the problem. It wouldn't be prudent to select the same distance threshold for all problem sizes, since a threshold of $\sigma=5$ might be suitable for the smallest tour29 problem, but it would result in a very homogeneous population for the largest problem tour929. Fig. 5 presents the best fitness for various σ values in range of one tenth of the number of cities N to N on tour194.

All of the aforementioned parameters were tested with regard to whether they allowed the algorithm to run for enough generations on each problem and whether they produced good enough solutions. The full list of selected hyperparameters can be seen in Subsection 4.1.

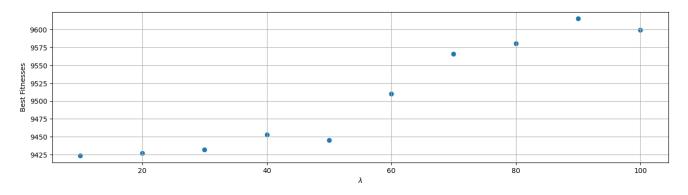


Figure 2: Hyperparameter search of λ

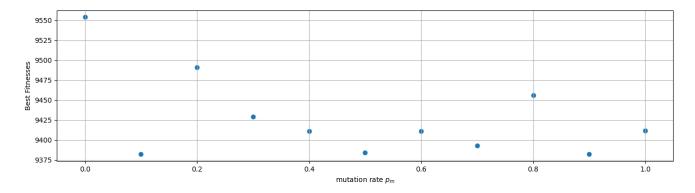


Figure 3: Hyperparameter search of mutation rate p_m

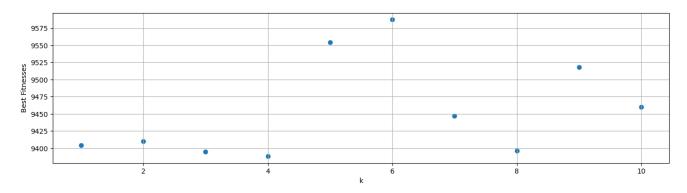


Figure 4: Hyperparameter search of k in k-tournament selection

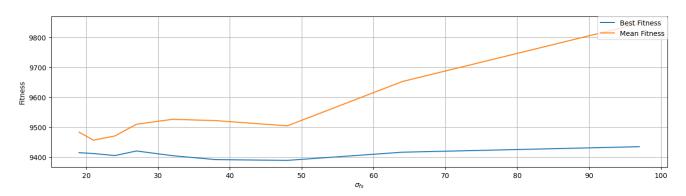


Figure 5: Hyperparameter search of fitness sharing σ for $\sigma = num_cities/d$, where $d\epsilon\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$

4 Numerical experiments

4.1 Metadata

The following list presents the different parameters that were chosen for the experiments presented in the following subsections.

- $\lambda = 10$: size of population
- $\mu = 5$: size of offspring
- $\lambda_h = 0.2 \times \lambda = 2$: number of heuristic solutions calculated during initialization
- k = 4: number of individuals in the k-tournament selection
- $p_c = 0.9$: recombination probability per generation
- $p_m = 0.9$: mutation probability per generation
- $p_l = 1.0$: local search probability per generation
- $\sigma_m = 1$: mutation strength
- $\alpha_{fs} = 1$: Fitness sharing shape
- $\sigma_{fs} = \frac{N}{5}$: Fitness sharing distance threshold, where N is the size of the problem (eg. for tour29 N = 29)

All experiments were run in a laptop with an Intel i7 processor with 4 physical cores, 8 logical cores, 8GB Ram, and a clock speed of 1.3GHz (3.9GHz turbo speed). No parallelization was used, so execution was limited to one core. Finally, all experiments were run with *Python 3.8.5*.

4.2 tour29.csv

Fig. 6a presents a typical convergence graph of the algorithm run on *tour29*. As we can see, the algorithm finds the optimal solution very quickly before the 10th generation, although it takes a while for the algorithm to converge due to the hard limit of 100 generations without improvement. In the graph we can see with the dotted lines, where are the greedy heuristic and optimal solutions to this problem. The best solution of the algorithm starts very close to the greedy heuristic and reaches the optimal in less than 10 iterations. Furthermore, the mean fitness never converges fully to the best fitness because of the fitness sharing scheme that is used, which indicates good preservation of diversity across generations.

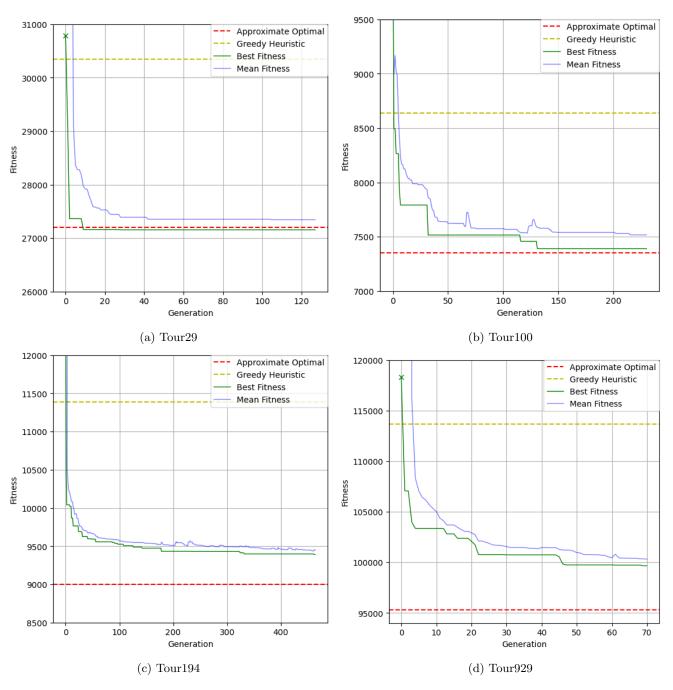


Figure 6: Typical convergence graphs on the various datasets.

The best tour that was found has a fitness - tour length of approximately **27154m**. The corresponding tour sequence is the following:

[2, 6, 8, 12, 13, 15, 23, 24, 26, 19, 25, 27, 28, 22, 21, 20, 16, 17, 18, 14, 11, 10, 9, 5, 0, 1, 4, 7, 3]

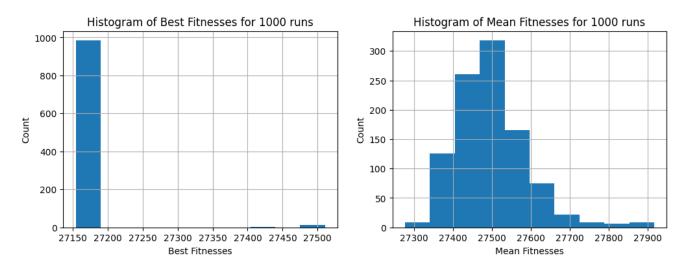


Figure 7: Tour29 1000 run histograms of best and mean fitness

Based on Fig. 7, the algorithm seems to perform really well on *tour29*, consistently finding the optimal or a near optimal solution for a 1000 runs. At the same time, the histogram of the mean fitness illustrates the fact that even at convergence the algorithm manages to preserve some diversity in the population, since mean fitness is always greater than the best fitness. The mean and std of the 1000 runs for the best and the mean fitness are shown in Table 1.

Fitness	1000-Run Average	1000-Run Sandard Deviation
Best	27160.06137471839	43.44519234412967
Mean	27497.005460551067	92.03286853386737

Table 1: Statistics of 1000 runs on tour 29.

4.3 tour100.csv

Fig. 6b presents the fitness and mean fitness of a run of the algorithm on *tour100*. The best solution that was found comes very close to the optimal solution (red dotted line). The algorithm finds the best solution at about the 130th iteration, but it doesn't converge until the timeout at around the 240th generation, since there haven't been over 100 iterations without improvement. Furthermore, the diversity promotion scheme performed really well as can be seen from the distance between the mean and best fitness across generations.

The best tour that was found has a fitness - tour length of approximately **7390m**. The corresponding tour sequence is the following:

[81, 92, 52, 60, 63, 24, 97, 98, 48, 40, 44, 78, 33, 90, 85, 70, 27, 22, 77, 96, 69, 29, 1, 17, 34, 95, 76, 23, 68, 71, 25, 16, 55, 80, 20, 47, 35, 18, 59, 49, 5, 56, 57, 19, 73, 39, 32, 74, 38, 13, 8, 86, 4, 51, 54, 41, 12, 89, 61, 43, 58, 67, 42, 83, 66, 0, 50, 65, 15, 79, 64, 93, 14, 6, 88, 72, 94, 84, 36, 46, 91, 28, 10, 37, 45, 7, 62, 53, 11, 87, 30, 9, 3, 31, 82, 21, 75, 99, 26, 2]

4.4 tour194.csv

Fig. 6c presents the fitness and mean fitness of a run of the algorithm on *tour194*. The best solution that was found lies between the greedy heuristic (yellow dotted line) and the optimal one (red dotted line). It is closer to the optimal one and a clear improvement rate can be observed across iterations. The algorithm finds the best solution at about the 320th iteration, but it doesn't converge until the timeout at around the 570th generation, since there haven't been over 100 iterations without improvement. Furthermore, the diversity promotion scheme managed to keep enough diversity which can be observed by the nonzero distance between the best and mean fitnesses.

The best tour that was found has a fitness - tour length of approximately **9390m**. The corresponding tour sequence is the following:

[55, 57, 42, 39, 33, 38, 46, 50, 60, 65, 66, 72, 67, 63, 69, 76, 83, 80, 78, 82, 87, 91, 96, 94, 95, 92, 90, 101, 102, 105, 104, 106, 107, 99, 109, 111, 114, 115, 116, 120, 119, 122, 123, 127, 132, 128, 134, 142, 147, 159, 165, 170, 169, 166, 161, 157, 158, 164, 167, 177, 179, 184, 192, 187, 190, 191, 188, 183, 180, 176, 174, 172, 173, 171, 178, 185, 182, 186, 189, 193, 181, 175, 168, 163, 162, 160, 155, 144, 148, 145, 141, 136, 139, 133, 131, 129, 126, 125, 124, 137, 138, 143, 149, 153, 156, 152, 151, 140, 146, 150, 154, 135, 130, 117, 121, 118, 108, 112, 113, 110, 103, 100, 98, 93, 88, 89, 97, 84, 85, 64, 19, 62, 35, 58, 61, 81, 70, 79, 86, 75, 74, 77, 71, 73, 68, 59, 56, 44, 36, 26, 21, 28, 27, 32, 17, 20, 23, 25, 16, 6, 10, 13, 24, 22, 12, 15, 7, 5, 0, 3, 1, 2, 4, 8, 9, 11, 14, 18, 29, 31, 30, 34, 37, 40, 47, 45, 43, 41, 49, 48, 54, 53, 51, 52]

4.5 tour929.csv

Fig. 6d presents the fitness and mean fitness of a run of the algorithm on *tour929*. The best solution that was found lies between the greedy heuristic (yellow dotted line) and the optimal one (red dotted line). It is closer to the optimal one and a clear improvement rate can be observed across iterations. The algorithm finds the best solution at about the 56th iteration, but it doesn't converge until the timeout at the 70th generation since there haven't been over 100 iterations without improvement. Furthermore, the diversity promotion scheme managed to keep enough diversity which can be observed by the nonzero distance between the best and mean fitnesses.

The best tour that was found has a fitness - tour length of approximately **99669m**. The corresponding tour sequence is the following:

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[703, 712, 727, 731, 750, 749, 739, 735, 733, 746, 751, 755, 741, 736, 763, 761, 772, 781, 778, 764, 769, 780, 773, 789,
  800, 799, 801, 798, 791, 775, 784, 785, 782, 771, 760, 767, 762, 756, 752, 748, 737, 734, 728, 715, 713, 697, 702, 742,
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                                     724, 718, 701, 689, 688, 696, 698, 709, 720, 710]
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5 Critical reflection

Working on this project allowed me the opportunity me to study evolutionary algorithms and understand them in more depth, while also looking at state-of-the-art research to find clues as to how to refine my algorithm for

solving the *Travelling Salesman Problem (TSP)*. Evolutionary algorithms in general are really good at solving nonconvex optimization problems whose solution space contains many local minima, where a popular optimization algorithm like Steepest Descent would get stuck quite easily in a suboptimal solution. TSP is such a non-convex problem and hence evolutionary algorithms are a good approach to solve it. Of course in most cases it's not guaranteed that an evolutionary algorithm will find the global optimum in finite time, but it certainly has the capability to escape local minima and find really good solutions. This is mainly thanks to the random nature of the mutation and recombination steps. On one hand we have the random combination of the useful information that already exists in the population and on the other hand we have the randomness that's inserted into new individuals, which may produce even better solutions than the previous generations.

A good evolutionary algorithm, in general, needs really careful design and needs to be specialized to a problem and use problem specific information to guide the search towards optimal solutions. For example, it's easy to design an evolutionary algorithm for solving the TSP with a lot of randomness, but to make it really efficient, it is very advantageous to seed the initial population or even other steps of the algorithm with heuristic information. This step proved to improve the efficiency of the developed algorithm and speed up the search of good candidate solutions quite considerably. Moreover, an evolutionary algorithm can become even more efficient if it's combined with local search methods like steepest descent or k-opt. Instead of waiting to find local minima after many generations of mutation and recombination it's a lot more efficient to run local search on a lot of individuals from the population and thus find many local minima, thus increasing the probability to find the global minima or at least a really good solution. The introduction of 2-opt proved instrumental in finding really good solutions without letting the algorithm run for thousands of generations.

Of course, evolutionary algorithms are not the perfect tool for solving any problem in many cases there are way better alternatives. One main disadvantage of evolutionary algorithms is that they are very computationally expensive. The developed evolutionary algorithm, in particular, is quite inefficient because of the really expensive local search operator (2-opt) that prevents the larger problems from running for a high number generations given the 5-minute time limit. This could have potentially been alleviated by parallelizing the local search on multiple offspring at the same time. Another issue with the local search operator and the greedy heuristic initialization was that the algorithm was directed towards strong local minima and couldn't escape easily. However, the benefit of those two methods far outweighed the costs.

What surprised me the most in this project was mainly how modular and customizable an evolutionary algorithm can be. There are so many different methods to choose from, yet not all of them are compatible with all problems or with each other and it's a quite complex and time-consuming task to find the right ones to combine. Furthermore, a few methods that I experimented with, such as self-adaptive mutation rate and/or strength failed to provide any measurable improvement to the algorithm, despite them being quite popular in the literature. Another thing that was quite difficult to work out was how to interpret the results. Due to the random nature of evolutionary algorithms, it was difficult for example to evaluate if a modification to the algorithm or the tuning of a parameter made any difference, which resulted in a lot of trial and error to find a good combination of parameters.

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