TU Wien – WS 2023/24
Heuristic Optimization Techniques
Programming Assigmnent 2

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Group 30

Genetic Algorithm for WsPEP

Algorithm 1 Genetic Algorithm

$t \leftarrow generation$ 0
initialize $P(t)$
evaluate $P(t)$
while not termination condition **do**
    $parent\_1 \leftarrow selection(P(t))$
    $parent\_2 \leftarrow selection(P(t))$
    $child \leftarrow crossover(parent\_1, parent\_2)$
    $child \leftarrow mutation(child)$
    $P(t+1) \leftarrow replace(P(t), child)$
    $t \leftarrow t+1$
end while
return $P(t)$

Initialization

The algorithm is implemented as a class and the initialization of the population is performed when the class is instantiated. The population is an attribute of the created object and its length is by default 100, although it is possible to set this parameter differently.
To ensure diversity in the initial population, individuals are created using various random greedy construction methods; in particular:

- 75% of individuals are generated by *randomized_Karger_construction*
  (Nodes are clustered first, followed by the addition of edges to form s-plexes)
- 25% of individuals are generated by *reinserting_greedy_construction* in a randomized setting.
  (we reinsert edges in a random way guaranteeing that clusters are always s-plexes)
- 1 individual is result of a deterministic greedy construction

Selection

At each step two parents are selected among the population and recombined to create a new individual. The new solution is added to the population and then the one with the worst fitness is discarded.
The selection can be performed either uniformly at random or through roulette-wheel selection. In our experiments, we opted for a random selection to favor the exploration of the solution space.

Crossover

Given two parents, crossover aims to create a child whose clusters satisfy these two principles:

- Nodes connected in both parents are connected in the child
- Nodes separated in both parents are separated in the child

In our implementation we guarantee only the first claim creating a cluster for each node as intersection of the two parents' clusters which the node belongs to. This operation results in some clusters being very small, and therefore, there is a need to merge some of them according to some rule. One possible way is to exploit a heuristic which estimates the goodness of the final merged clusters and then decide if to perform or not the operation.
We instead opted for another way, two clusters are selected and are merged with a certain probability. The clusters are selected with a probability inversely proportional to their length and merged with a certain probability depending on a parameter alpha. The operation is performed 10 times in a crossover and small clusters are more likely to be selected for the merging. Parameter alpha ideally controls how much randomness is added to the recombination of the clusters: with $\alpha = 0$ a lot of information from parents is kept, whereas $\alpha = 1$ means that only a little information is preserved.

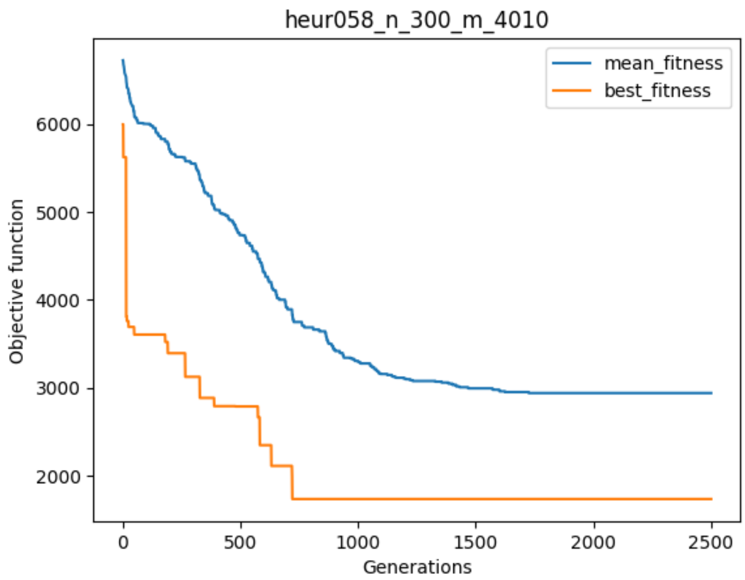
Mutation

The task of crossover is to cluster nodes according to the parents, mutation adds some randomness and tries to improve the quality of the s-plexes.
First swap node exchanges nodes in two clusters, then we use a fixed length local search to improve the quality of the s-plexes with neighbourhood *Flip_Edge*.

Termination Condition

The termination conditions are as follows:

- $max\ number\ of\ generations = 3000$
- 600 consecutive generations without any improvement



Genetic Algorithm Tuning

Parameter *alpha* controls the probability of merging two selected clusters in the crossover: $alpha = 0$ corresponds to never merging them, while $\alpha = 1$ corresponds to always merging them.
The table below shows results obtained by tuning instances with different settings of α.
For each instance we report:

- mean and best fitness of final population after in 10 different runs
- average mean and best fitness achieved by the algorithm
- improvement with respect to initial population

Difference between $\alpha = 0.0$ and $\alpha = 0.5$ is statistically significant
- level of significance: 0.05
- $H_0 :=$ "The difference is not significant"
- $H_1 :=$ "The difference is significant"

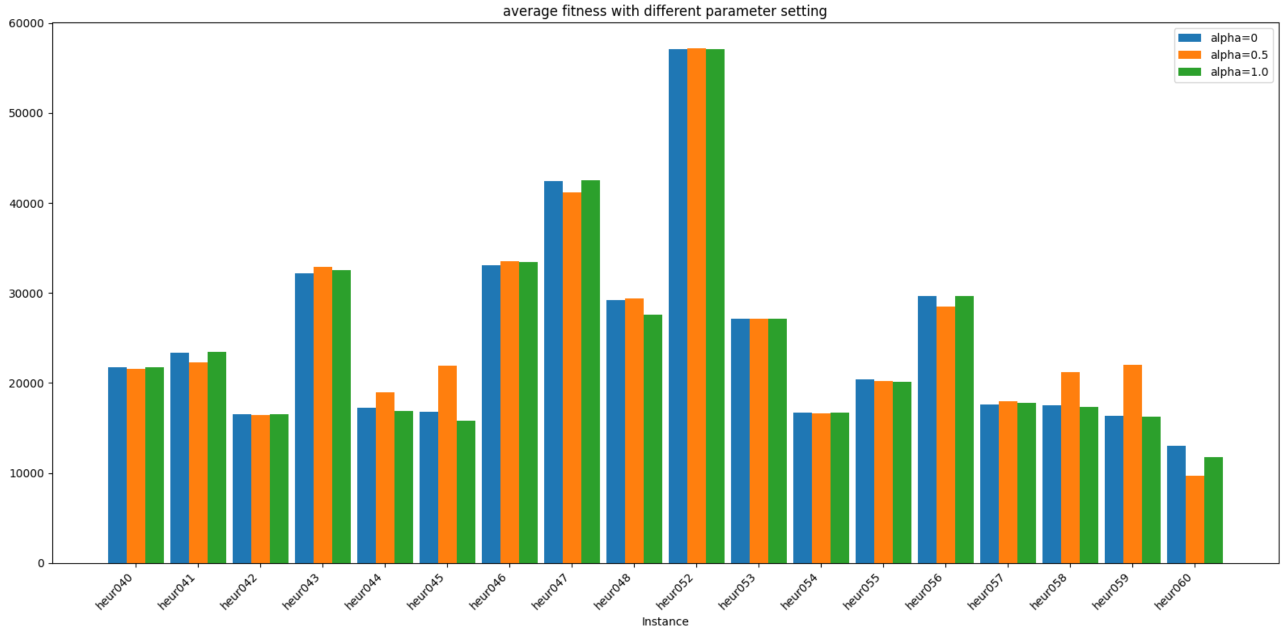
Test Result:
p-value = 0.0178
H_0 can be rejected on a level of significance of 0.05.

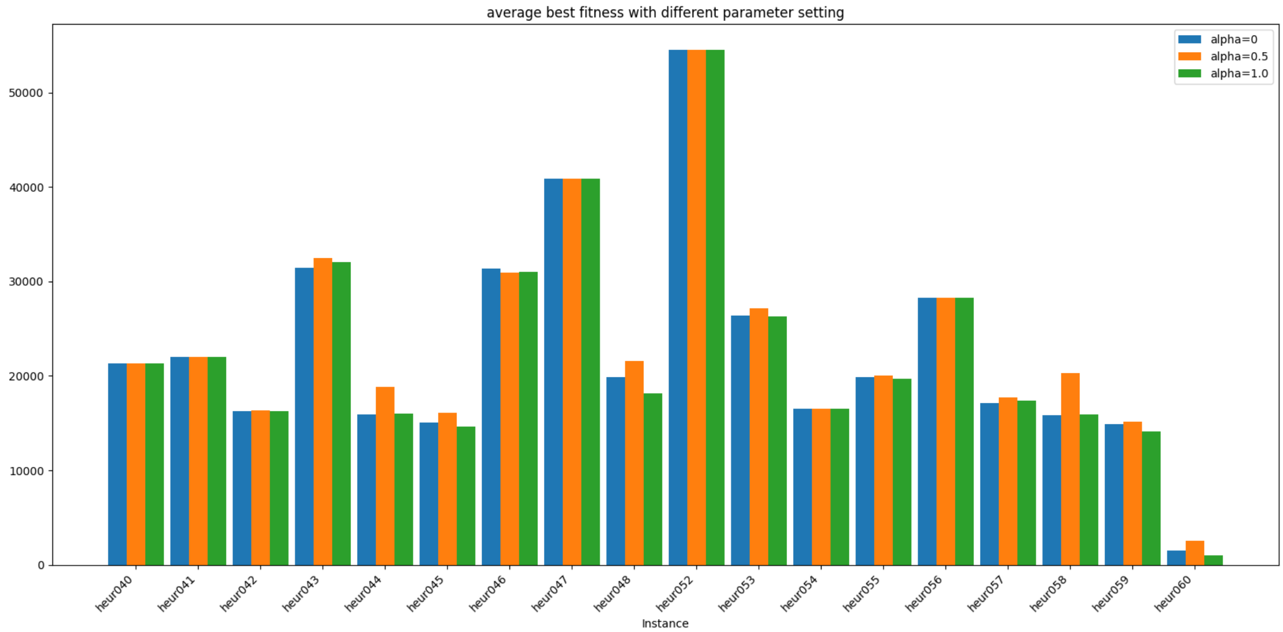
Results with $\alpha = 0.5$ are greater than ones with $\alpha = 0.5$
- level of significance: 0.05
- $H_0 :=$ "Results with $\alpha = 0.5$ are lower or equl to the ones with $\alpha = 0.5$"
- $H_1 :=$ "Results with $\alpha = 0.5$ are greater than ones with $\alpha = 0.0$"

Test Result:
p-value = 0.0089
H_0 can be rejected on a level of significance of 0.05.

Difference between $\alpha = 0.0$ and $\alpha = 1.0$ is statistically significant
- level of significance: 0.05
- H_0 := "The difference is not significant"
- H_1 := "The difference is significant"

Test Result:
p-value = 0.1315
H_0 cannot be rejected on a level of significance of 0.05.





istance		run 1	run 2	run 3	run 4	run 5	average
heur040	mean	6728.56	6694.46	6736.04	6740.42	6735.36	6745.974
	best	6384	6279	6361	6378	6371	6365.4
heur041	mean	8417.01	8206.55	8353.46	8353.75	8445.24	8395.596
	best	7039	7039	7039	7039	7039	7039
heur042	mean	1539.89	1505.31	1517.13	1536.74	1512.99	1518.123
	best	1323	1258	1239	1278	1226	1242.7
heur043	mean	16933.81	17563.57	16992.52	17190.13	17312.08	17150.35
	best	16327	17125	16725	16858	16994	16423.7
heur044	mean	2405.09	2333.69	1870.92	2647.45	2146.68	2280.766
	best	564	627	1264	939	1272	933.2
heur045	mean	2137.4	941.68	2106.51	2282.71	1555.62	1804.784
	best	154	212	442	-34	-369	81.0
heur046	mean	18839.56	17331.27	18957.86	17096.66	18090.42	18063.154
	best	16825	15564	17496	15628	16092	16321.0
heur047	mean	27496.3	27397.13	27573.2	27504.37	27382.75	27470.75
	best	25893	25905	25879	25901	25910	25897.6
heur048	mean	14135.35	14287.07	14280.42	13026.6	15223.64	14190.616
	best	6743	3169	4559	4266	5720	4891.4
heur052	mean	42271.24	41967.6	42052.98	41983.49	42027.17	42060.496
	best	39500	39522	39444	39444	39588	39499.6
heur053	mean	12155.9	12141.08	12129.29	12144.05	12150.61	12144.186
	best	11589	11217	11222	11422	11278	11345.6
heur054	mean	1715.32	1714.04	1720.21	1703.05	1707.6	1712.04
	best	1563	1573	1572	1574	1548	1566.0
heur055	mean	5562.2	4731.02	5559.22	5407.2	5614.7	5374.868
	best	5005	4417	4991	5046	5023	4896.4
heur056	mean	14670.74	14722.92	14623.08	14677.68	14559.82	14650.848
	best	13240	13237	13242	13240	13238	13239.4
heur057	mean	2680.81	2775.21	2375.06	2663.67	2641.77	2627.304
	best	2217	1860	2011	2301	2198	2117.4
heur058	mean	2518.19	2667.96	2028.02	2228.38	3023.32	2493.174
	best	1054	649	772	73	1819	873.4
heur059	mean	1343.89	1627.86	1012.8	927.62	1697.48	1321.93
	best	-56	504	-685	0	-146	-76.6
heur060	mean	-1149.66	-2188.28	-2646.34	-1231.64	-2892.24	-2021.632
	best	-13602	-13714	-12518	-13718	-13833	-13477.0

Table 1: $\alpha = 0.0$

Note: the reported fitness may appears negative in the table because is not scaled.
To encourage insertion of already present edges their weights are set negative, however we forgot to scale the results in the fitness function and there was no time to run all instances again. The minimum can therefore be negative but this should not be an issue when we compare results obtained with different parameter settings cause we focus on the difference of the two performances.

istance		run 1	run 2	run 3	run 4	run 5	average
heur040	mean	6614.04	6611.25	6607.81	6610.21	6609.48	6610.558
	best	6358	6369	6358	6364	6395	6368.8
heur041	mean	7264.96	7326.48	7279.5	7274.61	7265.68	7282.256
	best	7039	7039	7039	7039	7039	7039.0
heur042	mean	1474.97	1449.84	1465.32	1468.31	1462.38	1464.164
	best	1379	1386	1362	1388	1384	1379.8
heur043	mean	17871.42	17898.28	17916.37	17846.77	18054.6	17917.488
	best	17453	17437	17417	17421	17463	17438.2
heur044	mean	4004.41	3992.71	4006.42	3984.87	4009.16	3999.514
	best	3882	3876	3879	3879	3868	3876.8
heur045	mean	7606.31	4522.44	7195.58	7576.24	7951.74	6970.462
	best	1699	1205	1314	555	522	1059.0
heur046	mean	18750.47	18240.46	17754.42	18990.14	18712.85	18489.668
	best	16675	14494	16204	16832	15248	15890.6
heur047	mean	26267.45	26206.66	26123.7	26182.95	26163.69	26188.89
	best	25901	25901	25893	25901	25899	25899.0
heur048	mean	14442.85	14111.43	14965.64	14487.3	13931.26	14387.696
	best	6727	7270	8251	4979	5532	6551.8
heur052	mean	42146.91	42231.79	42146.04	42150.05	42246.59	42184.276
	best	39407	39585	39496	39444	39586	39503.6
heur053	mean	12165.97	12170.19	12163.47	12169.53	12184.22	12170.676
	best	12162	12162	12162	12162	12162	12162.0
heur054	mean	1642.64	1647.19	1648.56	1652.11	1649.25	1647.95
	best	1559	1556	1555	1555	1576	1560.2
heur055	mean	5196.07	5218.11	5220.33	5201.86	5189.1	5205.094
	best	5038	5049	5006	4999	5001	5018.6
heur056	mean	13509.7	13498.08	13515.82	13450.31	13425.06	13479.794
	best	13238	13240	13240	13238	13240	13239.2
heur057	mean	2931.65	2925.49	2874.4	2963.3	2948.4	2928.648
	best	2702	2665	2650	2794	2820	2726.2
heur058	mean	6189.15	6163.29	6175.37	6171.86	6189.94	6177.922
	best	5988	4680	5542	4478	5987	5335.0
heur059	mean	9121.68	9576.07	9323.38	2621.43	4623.5	7053.211
	best	-458	297	-717	759	929	162.0
heur060	mean	-4166.99	-5791.13	-7729.5	-2950.81	-5766.2	-5280.926
	best	-12103	-12734	-12462	-12139	-12637	-12415.0

Table 2: $\alpha = 0.5$

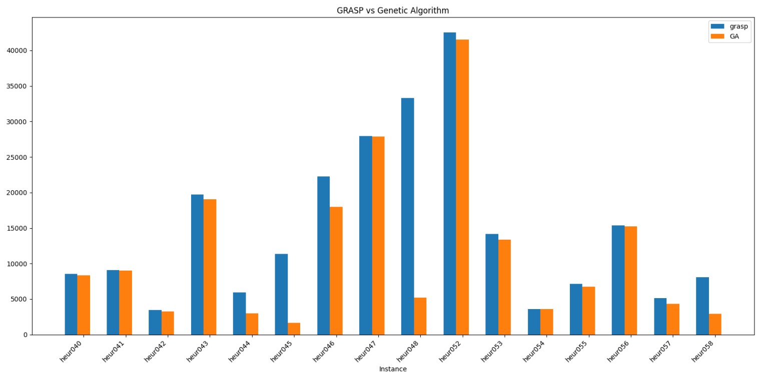
istance		run 1	run 2	run 3	run 4	run 5	average
heur040	mean	6785.91	6754.69	6730.94	6712.12	6751.33	6746.998
	best	6405	6398	6206	6390	6361	6352.0
heur041	mean	8489.1	8415.52	8415.39	8352.28	8474.46	8429.35
	best	7039	7039	7039	7039	7039	7039.0
heur042	mean	1528.2	1494.83	1523.06	1523.52	1520.44	1518.01
	best	1256	1218	1255	1280	1214	1244.6
heur043	mean	17346.17	16651.81	17329.49	17417.41	18895.17	17528.01
	best	17315	15807	17262	17312	17431	17025.4
heur044	mean	3249.38	1714.0	1084.64	1456.41	2012.1	1903.306
	best	2513	663	167	541	1081	993.0
heur045	mean	494.19	750.5	1256.66	595.88	827.19	784.884
	best	-893	-630	97	-361	53	-346.8
heur046	mean	18884.72	19866.44	17852.56	19354.47	16460.46	18483.73
	best	16995	19057	15668	15621	12564	15981.0
heur047	mean	27564.9	27515.34	27613.38	27403.61	27462.98	27512.042
	best	25894	25901	25920	25896	25898	25901.8
heur048	mean	13020.54	12043.05	11952.52	13137.55	12989.61	12628.654
	best	4701	890	3010	3472	3859	3186.4
heur052	mean	41985.35	42158.81	42126.85	42039.56	42053.09	42072.732
	best	39444	39433	39586	39500	39544	39501.4
heur053	mean	12172.78	12153.45	12127.43	12147.7	12157.99	12151.87
	best	11407	11435	11213	11181	11457	11338.6
heur054	mean	1708.1	1706.04	1717.25	1699.46	1706.11	1707.392
	best	1557	1566	1568	1573	1551	1563.0
heur055	mean	5282.43	4399.5	4625.06	5564.78	5575.94	5089.542
	best	5030	4110	4389	5017	5004	4710.0
heur056	mean	14624.64	14629.14	14715.61	14652.55	14630.14	14650.416
	best	13239	13240	13239	13240	13240	13239.6
heur057	mean	2932.89	2696.88	2950.29	2569.97	2910.66	2812.138
	best	2720	229	2656	1792	2341	2360.4
heur058	mean	1735.36	2159.35	2709.28	2658.95	2572.55	2367.098
	best	635	632	1107	103	1357	953.2
heur059	mean	945.34	1285.29	1301.28	766.46	1980.49	1255.772
	best	-1229	-1491	-640	-559	-446	-873.0
heur060	mean	-3068.41	-4115.9	-4067.09	-2306.19	-2859.7	-3283.47
	best	-14381	-13703	-14145	-14234	-13414	-13975.4

Table 3: $\alpha = 1.0$

Genetic Algorithm vs GRASP

Statistical test - level of significance: 0.05
- H_0 := "Results with the Genetic Algorithm are not worse than with GRASP"
- H_1 := "Results with the Genetic Algorithm are better than with GRASP"

Test Result: p-value = 0.0190 H0 can be rejected on a level of significance of 0.05.



	heur040	heur041	heur042	heur043	heur044	heur045	heur046	heur047	heur048
run 1	6588	7044	1497	17496	3939	9508	20184	25909	31551
run 2	6589	7066	1441	17523	3925	9537	20138	25890	30999
run 3	6448	7109	1424	17796	4001	9171	20197	25917	31820
run 4	6588	7065	1448	17497	3866	9164	20216	25889	31486
run 5	6612	7039	1407	17632	3909	9169	20401	25904	31422
run 6	6585	7200	1453	17554	3915	9430	20340	25982	31057
run 7	6592	7104	1443	17503	3953	9208	20173	25916	31209
run 8	6588	7066	1429	19617	3957	9424	20340	25900	30858
run 9	6359	7040	1488	17469	3896	9420	20592	25956	31320
run 10	6626	7056	1492	17460	3948	9317	20178	25922	31280
best	6359	7039	1407	17460	3866	9164	20138	25889	30858
mean	6557.5	7078.9	1452.2	17727.9	3930.9	9334.8	20275.9	25915.2	31300.25

	heur052	heur053	heur054	heur055	'heur056	heur057	heur058	heur059	heur060
run 1	42268	12159	1560	5110	13308	3104	6040	13008	20399
run 2	40339	12159	1621	5070	13297	3373	6036	13395	21925
run 3	40230	12159	1578	5115	13307	3095	6016	12965	20452
run 4	41670	12159	1597	5231	13327	3076	6001	12826	20836
run 5	40218	12159	1542	5250	13440	3091	6088	13064	20878
run 6	39825	12159	1561	5095	13443	3123	6048	13024	20427
run 7	40201	12159	1576	5088	13295	3070	6024	12781	20549
run 8	40076	12159	1549	5226	13443	3179	5976	12856	22577
run 9	40156	12159	1560	5056	13272	3081	6233	13023	20345
run 10	40275	12159	1589	5085	13420	3041	6029	13011	22045
best	39825	12159	1542	5056	13272	3041	5976	12781	20345
mean	40525.8	12159.0	1573.3	5132.6	13355.2	3123.3	6049.1	12995.3	21043.3

Adaptive Large Neighbour Search

Algorithm 2 ALNS

given a problem instance I and the hyperparameters γ : momentum for ρ, T : initial temperature, α : cooling factor.

$x_0 \leftarrow$ greedy construction
$\rho_d \leftarrow [1, ..., 1]^T$
$\rho_r \leftarrow [1, ..., 1]^T$
while $T \geq$ stop_temp **do**
  repeat #epochs **times**
    $D(\cdot) \leftarrow$pick *destroy* function at random proportional to ρ_d
    $R(\cdot) \leftarrow$pick *repair* function at random proportional to ρ_r
    $x_1 \leftarrow R(D(x_0))$
    metropolis acceptance of x_1 against x_0
    record best solution so far
  end
  update ρ_d, ρ_r, T
end while
return best recorded solution

The ALNS we implemented is a class that takes in input a number of hyperparameters and two lists:

- **destroy functions**: functions that take in input a solution x_0 and return an altered solution with something changed, note that this solution may not respect the constraints of the problem.
- **repair functions**: functions that repair a solution which doesn't respect the problem constraint.

Then we initialize two lists with ones, representing the initial probabilities of picking one or another destroy/repair functions.

At each loop we're going to extract at random (proportional to ρ) a destroy and a repair function, apply them to x_0. Then, using the metropolis acceptance, we accept the result with a certain probability, depending on the difference of the objective function values of x_0 and x_1 and the current temperature T.

We're going to run this in a nested loop. The outer loop is going to run until the value of the temperature reaches a value which is small enough: 50 during hyperparameter tuning, 1 when performing the final evaluation.

The inner loop will repeat #epochs=100 times by default, at the end of which we're going to update ρ with the number of successes of each destroy/repair function, and we're going to update also $T \leftarrow \alpha T$.

$$\rho_d[i] \leftarrow (1-\gamma)\rho_d[i] + \gamma \frac{\#successes(i)}{\#attempts(i)}$$

Destroy Functions

All our destroy functions modify the partition of the clusters, without considering the damages to the intra-cluster edges:

- **Merge**: Given 2 random clusters merge them together. This function can be skewed to choose proportionally to the inter-cluster distance;
- **Divide**: given a random cluster divide it in 2 subclusters. This function can be skewed to choose proportionally to intra-cluster distance.
- **SwapNode**: given 2 clusters swap randomly two nodes.

Repair Functions

2 out of 3 of our destroy functions destroy the intracluster edges and the s-plex condition (each node must have at least $|V| - s$ edges with nodes within its plex). To account for this we have two repair functions that rebuild the edges inside a cluster:

- **Insertion heuristic**: consider a plex with no edges; for each node insert edges (starting from the smallest weight) until it has $|V| - s$ edges.
- **Deletion heuristic** consider a fully connected plex; for each node remove s edges (if possible), starting from those with the highest weight.

Hyperparameter tuning

In this process we have a bunch of hyperparameters:

- *stop_temperature*: temperature at which we stop the execution, it's 50 when doing the hyperparameter search (to speed up the process) and 1 otherwise;
- *epochs*: number of repetitions to run in the inner loop, before updating T and ρ, by default it's 100;
- *initial temperature*: it's the starting temperature T;
- *alpha*: it's the cooling factor for the temperature;
- *gamma*: it's the momentum weight for updating ρ.

On the last three parameters we run a grid search on the tuning set to find the best parameters.

temperature	100	1000	10000
gamma	0.7	0.9	
cooling	0.92	0.95	

Table 4: Test hyperparameters

We run each of the possible 12 configurations[4] 10 times on each of the 18 tuning instances, for a total of 2160 runs. Then we compute the gain for each of the different parameter's configurations as the scaled difference to the mean performance.

$$gain = \frac{f(x_0) - avg(f)}{avg(f)}$$

Now our goal is to find the set of parameters that give us the lowest possible gain (as this is a minimization problem).

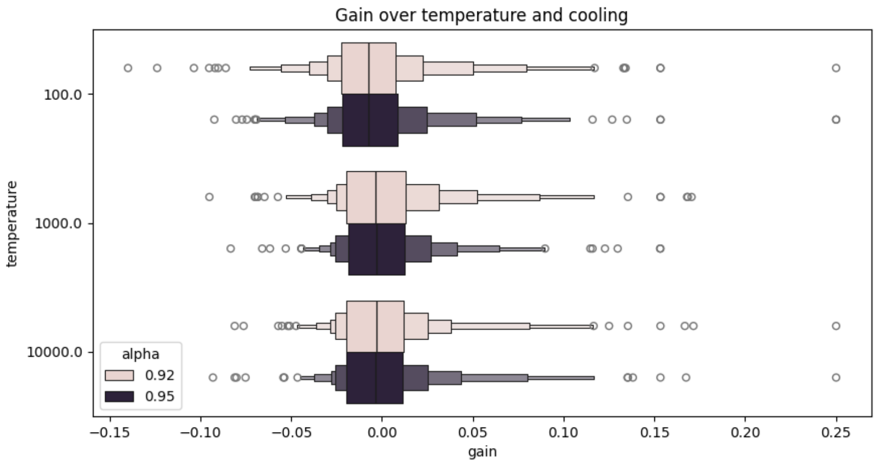


Figure 1: Gain computed for different values of the temperature and cooling factor

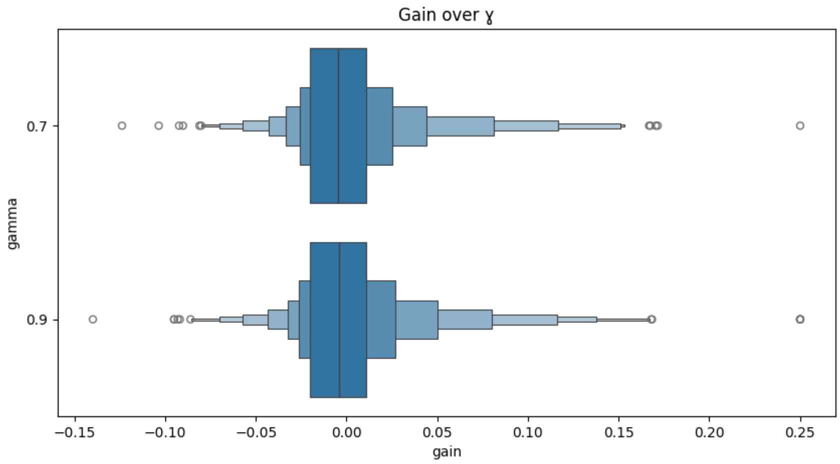


Figure 2: Gain computed over different values of gamma

Only by this plots it doesn't seem that the difference is very significant.
We then plot the mean performance of each triplet of parameters:

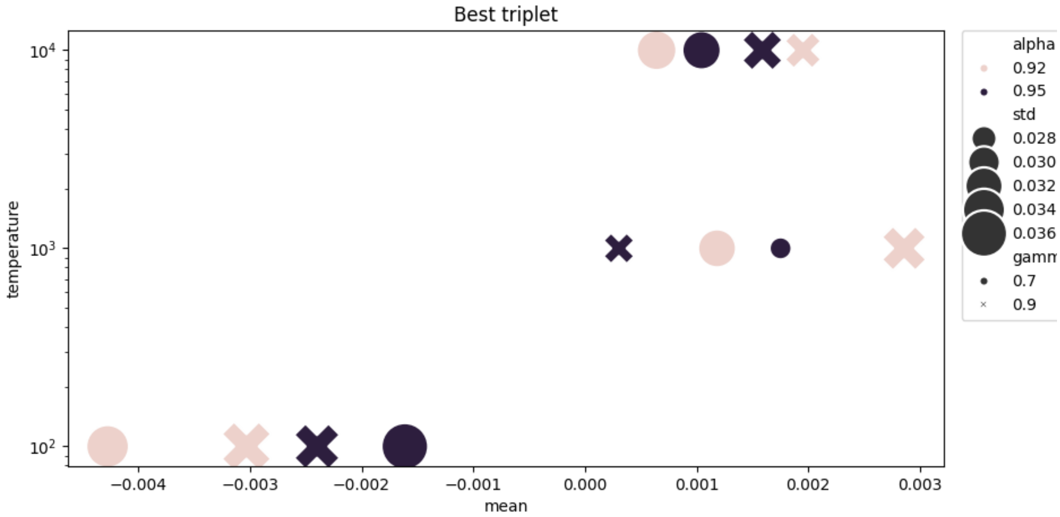


Figure 3: Mean objective value for configuration of parameters

We can see that the distances are very small and the standard deviation is very high, but among these the best triplet is:

temperature	alpha	gamma
100	0.92	0.7

Statistical Testing

Frequentist *t*-Test

We can try to test whether the difference that we see in the plot is significant. The maximum probability that we're willing to consider given the risk of a type I error is 0.05.

- **H0**: the best performing parameters are performing better by chance, their objective values have the same mean as the rest;
- **H1**: the best performing parameters perform better as their mean objective value is lower than objective value than the rest.

We perform a one-sided t-test the result of which is:

$$\textbf{p-value} = 0.024674$$

As such we can reject the null hypothesis with a level of significance of 0.05, and assume that the distribution of the gain for the best triplet found is statistically better than the other parameters. As such this configuration will be the one that we'll use for the final submission.

Bayesian hypothesis testing

Since the size of our population is quite small we can try to perform bayesian hypothesis testing, which should be more robust. We test two hypothesis:

- **H0**: the gamma parameter has no influence on the performance;
- **H1**: the gamma parameter is significant.

We set as a non-informative prior where $p(H_0) = p(H_1) = 0.5$ as we don't have any information about the distribution of performance of parameters. When computing the log-likelihood of the two cases we arrive find out:

$$\textbf{Bayes Factor} = \frac{p(X|H_1)}{p(X|H_0)} = 1.73$$

Which following the Kass and Raftery table[1] should be interpreted as "barely any evidence of statistical significance".

As such we can conclude that the gamma parameter isn't very important when it comes to changes in the performance (although admittedly we had the time and resources to test it only on two values).

[1] Bayes Factor on Wikipedia