

Resolución de problemas con metaheurísticas Master Universitario en Investigación en Inteligencia Artificial (UIMP)

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INTRODUCTION

Multidimensional Knapsack Problem: generalization of the basic binary Knapsack Problem to multiple knapsacks or dimensions.

Given a list of n items, the profit p_j for item j, a number m of dimensions ('knapsacks'), the weight (required capacity) w_{ij} of item j for knapsack i, and a total per-dimension capacity W_i :

Maximize

$$\sum_{j=1}^{n} p_j x_j \quad x_j \in \{0, 1\},\$$

subject to

$$\sum_{j=1}^{n} w_{ij} x_j \le W_i \quad \forall i = 1, ..., m$$

DISAMBIGUATION

Multiple knapsacks - not to be confused with physical dimensions

When an item is selected, it consumes a certain capacity from **all** knapsacks/dimensions

Better problem formulation or real use case by [Petersen, 1967]:

- Each item is an R&D project
- A knapsack is a required resource: R&D, marketing, implementation, etc.
- Each R&D project consumes a certain amount of each resource
- Each resource is limited, there's a maximum amount or capacity

PROBLEM FORMULATION (FOR A GENETIC ALGORITHM)

Problem data:

- \circ number of items (n),
- o profit of the items $(p_1, ..., p_n)$,
- \circ number of knapsacks/dimensions (m),
- \circ total capacity of each knapsack (W_1 , ..., W_m),
- o weight or consumed capacity of each item for each dimension (m times n matrix containing w_{ii} weights).
- **Solution representation**: binary vector of length n, position j is 1 if the jth item is selected, otherwise it's 0.
 - Infeasible solutions exist

$$\exists i = 1, ..., m : \sum_{i=1}^{n} w_{ij} x_j > W_i$$

• Size of the state space depends on the problem instance, upper bounded by 2^n .

SSGA IMPLEMENTATION

Base implementation (NEO investigation group, Universidad de Málaga):

- Selection scheme: binary tournament
- Operators:
 - 1. Single-point crossover applied given a probability, only one child is generated.
 - 2. Mutation: per-gene (bit) evaluation given the specified probability.
- Insertion: generated individual replaces the worst individual.

Our modifications/additions:

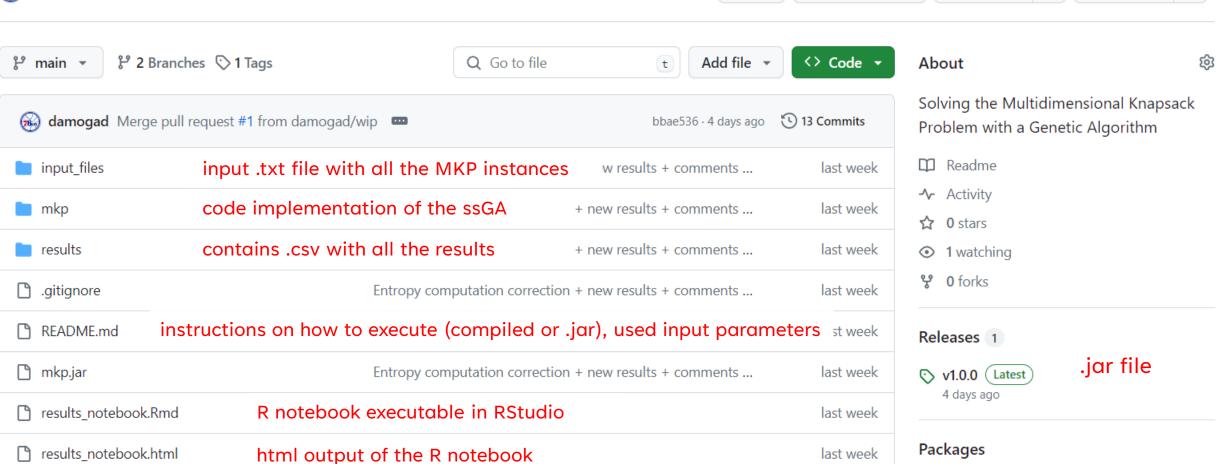
- New class (ProblemMKP.java) with the required attributes to hold the problem instance data and the functionality to compute whether a solution is feasible and depending on that the fitness (infeasible solutions are tolerated, their fitness is -1).
 - [Chu and Beasly, 1998] proposes different alternatives to deal with these solutions.
- Execution functions to carry out the execution/evaluation/gathering of results (Exe.java)



https://github.com/damogad/MKP







● Unwatch 1 ▼

☆ Star 0

왕 Fork 0

METHODOLOGY

- Employed instances:
 - 3 different different instances, each of a different relative size (small, medium, large), extracted from [Petersen, 1967]. 3rd, 5th and 7th problems in http://people.brunel.ac.uk/~mastjjb/jeb/orlib/files/mknap1.txt
 - o Fixed population size: 100, 100 and 200, respectively.
- Types of studies:
 - 1. Fixed number of evaluations: evaluate obtained fitness
 - 2. Reach the optimal fitness: evaluate the needed number of evaluations
- 25 candidates/combinations of these hyperparameters:
 - Crossover probability: {0.6, 0.7, 0.8, 0.9, 1.0}
 - O Mutation probability: x / n, where x is $\{1, 2, 3, 4, 5\}$ and n is the number of items (number of genes). Meaning: average expected number of mutated genes per individual.

METHODOLOGY

Metrics:

- Required number of evaluations (2nd study). 1st study: 1000, 10000 and 1000000, respectively
- o Fitness of the best individual in the last population. Relevant for both studies, as we may obtain an 'unfinished' execution in the 2nd study (50000000 max. evaluations).
- Average fitness in the complete last population
- Measure of the variety in the last population genotype: Shannon Entropy

$$\frac{1}{n} \sum_{i=1}^{n} H(x_i)$$

where

$$H(x_i) = \begin{cases} 0 & \text{if } p_i^1 = 0 \lor p_i^1 = 1\\ -p_i^1 \log_2(p_i^1) - p_i^0 \log_2(p_i^0) & \text{otherwise} \end{cases}$$

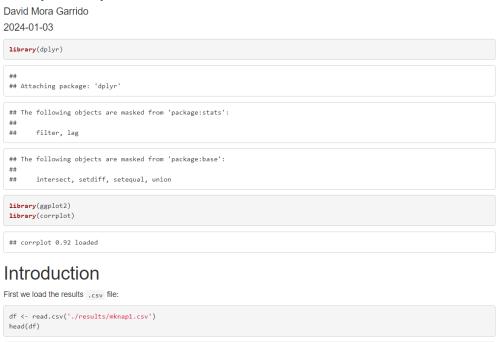
METHODOLOGY

- The ssGA is executed 30 times for each combination of hyperparameters (crossover+mutation)
- Statistical hypothesis testing:
 - o Parametric methods:
 - Shapiro-Wilk normality test
 - ANOVA
 - Non-parametric methods:
 - Kruskal-Wallis test
 - Wilcoxon rank-sum test (Mann-Whitney U test) with [Benjamini and Hochberg, 1995] correction to avoid inflating the Type I error
- Tested variables:
 - 1st study: relative deviation from the target fitness -> (target obtained)/target
 - o 2nd study: number of evaluations
- **0.02** level of significance (α)

RESULTS

Processing/evaluation of the results in R: https://github.com/damogad/MKP/blob/main/results_notebook.Rmd Already generated output (html): https://github.com/damogad/MKP/blob/main/results_notebook.html

Practical study of a basic genetic algorithm on the Knapsack problem



crossover probability

0.6

0.6

0.6

0.6

mutation probability search optimal

0.06666667 false

0.06666667 false

0.06666667 false

0.06666667 false

<dbl> <chr>

problem index

<int>

2

2

population_size

<int>

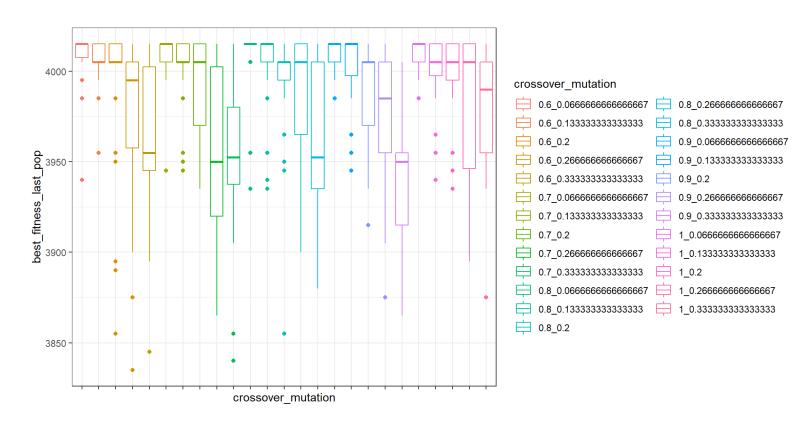
100

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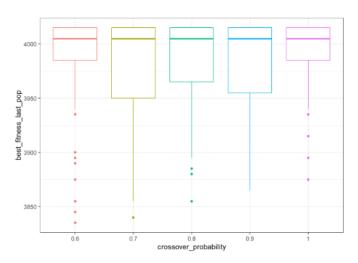
100

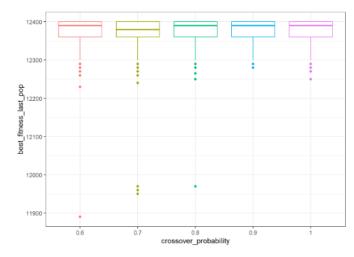
Graphical depiction of the results for each combination of crossover and mutation probabilities (small instance):



See the similarities/pattern?

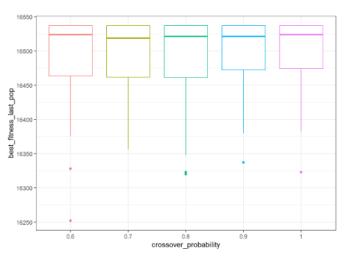
Crossover probability does not seem to have a big effect...





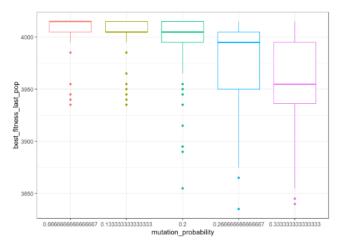
(a) Small instance

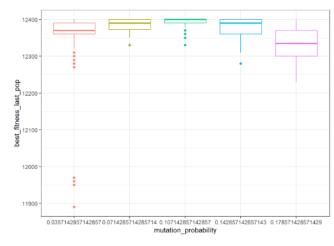
(b) Medium instance



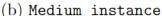
(c) Large instance

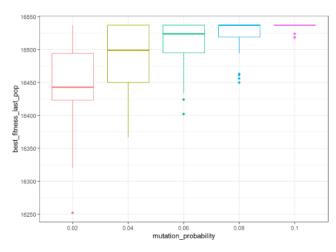
However, the mutation probability **does** seem to influence the best obtained fitness





(a) Small instance





(c) Large instance

Verification of assumptions: hypothesis tests

Shapiro-Wilk normality test: null hypothesis rejected for most combinations, for the 3 instances

```
## [1] "0.6,0.066666666666667"
   Shapiro-Wilk normality test
## data: df_study1_small[df_study1_small$crossover_mutation == combination, "optimal_deviation_best_last_pop"]
## W = 0.50817, p-value = 6.545e-09
## [1] "0.6,0.133333333333333333333333
## Shapiro-Wilk normality test
## data: df_study1_small[df_study1_small$crossover_mutation == combination, "optimal_deviation_best_last_pop"]
## W = 0.69397, p-value = 1.276e-06
## [1] "0.6,0.2"
## Shapiro-Wilk normality test
## data: df_study1_small[df_study1_small$crossover_mutation == combination, "optimal_deviation_best_last_pop"]
## W = 0.61915, p-value = 1.26e-07
## [1] "0.6,0.26666666666667"
   Shapiro-Wilk normality test
## data: df study1 small[df study1 small$crossover mutation == combination, "optimal deviation best last pop"]
## W = 0.78276, p-value = 3.23e-05
```

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Verification of assumptions: hypothesis tests

• Kruskal-Wallis test on the equality of the deviation from the optimal among all the combinations of crossover + mutation probabilities: null hypothesis rejected for the 3 instances → the distribution of at least one combination is not the same as the rest

```
##
## Kruskal-Wallis rank sum test
##
## data: optimal_deviation_best_last_pop by crossover_mutation
## Kruskal-Wallis chi-squared = 350.83, df = 24, p-value < 2.2e-16</pre>
```

• Next step: Wilcoxon rank-sum test between every pair (300 total tests) with BH correction → significant number of pairs that are not equal between them (154, 160 and 186, respectively)

```
## Pairwise comparisons using Wilcoxon rank sum test with continuity correction
0.6,0.02 0.6,0.04 0.6,0.06 0.6,0.08 0.6,0.1 0.7,0.02 0.7,0.04 0.7,0.06
## 0.6.0.04 0.00020 -
## 0.6.0.06 7.0e-07 0.05867 -
## 0.6,0.08 8.4e-09 0.00037 0.02361 -
## 0.6.0.1 2.1e-09 2.7e-05 0.00247 0.34628 -
## 0.7,0.02 0.76371 0.00033 4.8e-07 2.9e-09 1.1e-09 -
## 0.7,0.04 0.00105 0.58696 0.01109 5.2e-05 2.9e-06 0.00319
## 0.7,0.06 1.0e-05 0.41108 0.36796 0.00250 0.00018 1.1e-05 0.14141 -
## 0.7.0.08 3.9e-09 0.00013 0.01239 0.70392 0.57575 2.2e-09 1.4e-05 0.00099
## 0.8.0.02 0.82923 0.00055 4.2e-07 5.7e-09 1.5e-09 0.86481 0.00419 1.8e-05
## 0.8,0.04 0.00631 0.31714 0.00377 1.2e-05 1.0e-06 0.01176 0.66471 0.04676
## 0.8,0.06 1.3e-05 0.15922 0.81985 0.06778 0.00669 1.8e-05 0.05278 0.50741
## 0.8.0.08 1.1e-08 0.00080 0.05056 0.89273 0.28266 5.8e-09 8.8e-05 0.00499
## 0.8.0.1 1.5e-09 9.8e-06 0.00055 0.17742 0.70365 9.5e-10 1.2e-06 5.0e-05
## 0.9.0.02 0.40027 0.00319 6.8e-06 2.5e-08 2.7e-09 0.53254 0.01827 0.00015
## 0.9.0.04 0.00011 0.95870 0.05835 0.00015 9.3e-06 0.00029 0.58917 0.37796
## 0 9 0 06 3 3e-06 0 19380 0 67285 0 00664 0 00059 1 6e-06 0 04812 0 65952
## 0.9,0.08 5.4e-08 0.00520 0.26624 0.51832 0.10920 6.4e-08 0.00081 0.03636
```

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Verification of assumptions: hypothesis tests

But we saw that the crossover probability did not seem to affect the best obtained fitness significantly...

- Grouped by crossover probability (only):
 - Kruskal-Wallis test: null hypothesis not rejected for the 3 instances → obtained fitness can be considered equal regardless of the crossover probability (on the tested set of values)

```
##
## Kruskal-Wallis rank sum test
##
## data: optimal_deviation_best_last_pop by crossover_probability
## Kruskal-Wallis chi-squared = 1.6399, df = 4, p-value = 0.8016
```

- Grouped by mutation probability (only):
 - Kruskal-Wallis test: null hypothesis rejected for the 3 instances → at least one mutation probability yields a different fitness
 - \circ Wilcoxon rank-sum tests (5 mutation probabilities = 10 pairs to be tested) \rightarrow 10, 9 and 10 tests are rejected, respectively, so there's a significant influence of the mutation probability on the fitness

Numerical results (mean/median/std best fitness, mean/median deviation from optimal) for each mutation probability:

Mutation	Avg. fitness	Median fitness	Std fitness	Avg. deviation	Median deviation
0.06666667	4009.167	4015	13.13861	0.001452885	0.00000000
0.13333333	4002.267	4005	19.57250	0.003171440	0.00249066
0.20000000	3992.900	4005	30.94306	0.005504359	0.00249066
0.26666667	3975.800	3995	39.90374	0.009763387	0.00498132
0.33333333	3958.467	3955	41.71631	0.014080531	0.01494396

Mutation Avg. fitness		Median fitness	Std fitness	Avg. deviation	Median deviation	
	0.03571429	12353.93	12370	82.36355	0.0037150538	0.0024193548
	0.07142857	12386.27	12390	16.28384	0.0011075269	0.0008064516
	0.10714286	12393.67	12400	12.81865	0.0005107527	0.0000000000
	0.14285714	12379.00	12390	24.15693	0.0016935484	0.0008064516
	0.17857143	12333.83	12335	42.50707	0.0053360215	0.0052419355

	Mutation	Avg. fitness	Median fitness	Std fitness	Avg. deviation	Median deviation
_	0.02	16447.07	16443	53.684399	0.0054379069	0.005684223
	0.04	16491.17	16499	43.521408	0.0027715628	0.002297877
	0.06	16511.47	16524	33.840069	0.0015436093	0.000786116
	0.08	16527.70	16537	18.816225	0.0005623753	0.000000000
	0.10	16534.15	16537	6.587956	0.0001725424	0.000000000

Smaller instance, smaller number of expected mutated genes by chance per individual

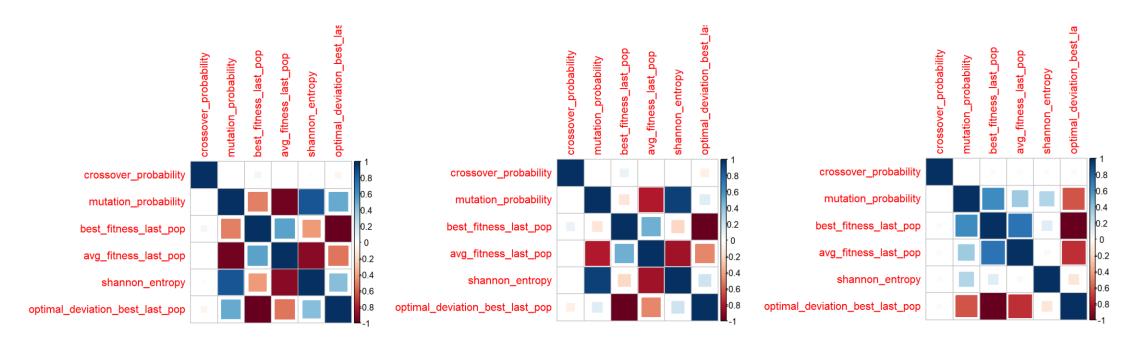
Medium instance, medium number of expected mutated genes by chance per individual

Larger instance, larger number of expected mutated genes by chance per individual

Small and medium instances: negative correlation between the average fitness of last population and the entropy

Large instange: (almost) no correlation between the aforementioned variables

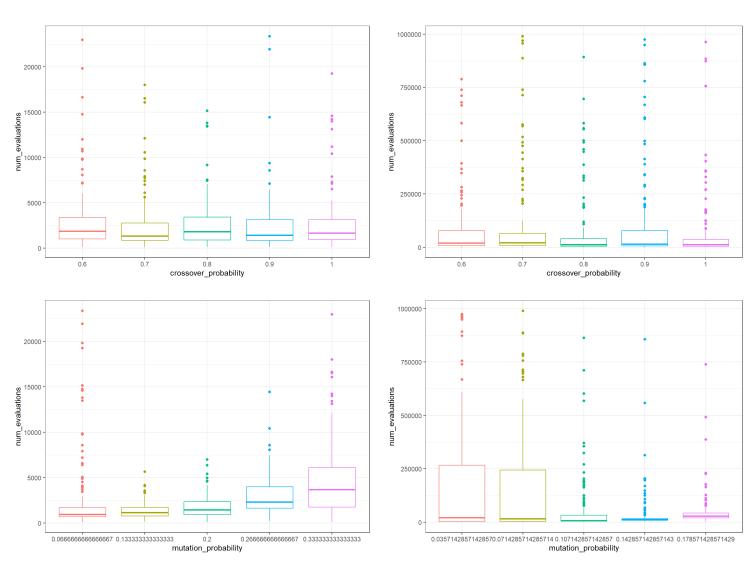
→ Greater num_items/knapsacks may increase the diversity in the genotype?



Small and medium problem instances: same results than 1st study

- Different crossover probabilities yield similar number of evaluations
- Different mutation probabilities yield statistically significant differences in the number of evaluations
 - For a smaller instance, a smaller number of expected mutated genes on avg. yields less evaluations
 - Analogously for the mediumsized instance (medium number in the tested set of values)

(tested again with Kruskal-Wallis + Wilcoxon rank-sum tests)



Large instance: several peculiarities

- Optimal fitness was not always reached ('unfinished' execution)
- Modification: max limit of 50000000 evaluations when targeting a fitness value
 - o If not reached, metrics on current state written as result and execution is reset
 - o Reset until obtaining a 'finished' execution
- We cannot use the unfinished executions for the study (435)
- 'Stripped' results for tests, but number of such executions checked:
 - o Crossover probability: evenly distributed, except for one value
 - Smaller mutation probability, greater number of unfinished executions

optimal_not_reached <int></int>	crossover_probability <db ></db >
87	0.6
70	0.7
70	0.8
88	0.9
120	1.0

mutation_probability <dbl></dbl>	optimal_not_reached <int></int>
0.02	291
0.04	53
0.06	38
0.08	30
0.10	23

Large instance: several peculiarities

- 'Stripped' results:
 - Different crossover probabilities yield a different number of evaluations

```
## ## Kruskal-Wallis rank sum test

## data: num_evaluations by crossover_probability

## Kruskal-Wallis chi-squared = 24.147, df = 4, p-value = 7.462e-05

## Pairwise comparisons using Wilcoxon rank sum test with continuity correction

## data: df_study2_large_optimal$num_evaluations and df_study2_large_optimal$crossover_probability

## 0.6 0.7 0.8 0.9

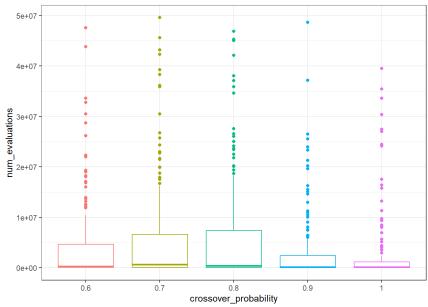
## 0.7 0.5832 - - - -

## 0.8 0.6801 0.7338 - -

## 0.9 0.0308 0.0050 0.0142 -

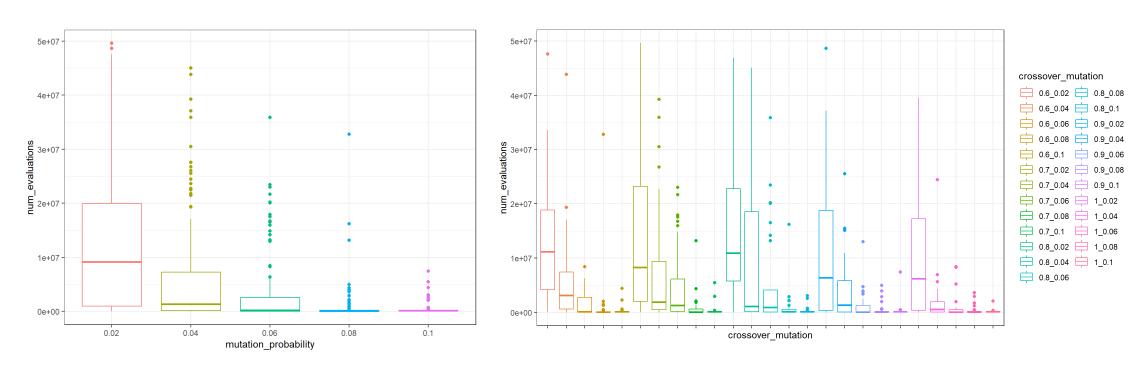
## 1 0.0045 0.0013 0.0036 0.5832

## ## P value adjustment method: BH
```



Large instance: several peculiarities

- 'Stripped' results:
 - Different mutation probabilities yield a different number of evaluations (already expected)
 - Thus, as Kruskal-Wallis test for the equality of the number of evaluations of all the crossover+mutation combinations is rejected, given the Wilcoxon test results and the balance between median, mean and variance, best combination is (c=1.0, m=0.08).



Large instance: fairer study

- Relaxation of the problem: trying to get as less unfinished executions as possible
 - o 99.5% of the optimal: still many unfinished (77)

crossover_probability <dbl></dbl>	optimal_not_reached <int></int>
0.6	17
0.7	14
0.8	17
0.9	15
1.0	15

optimal_not_reached	mutation_probability <dbl></dbl>
58	0.02
15	0.04
4	0.06
1	0.08
0	0.10

o 99% of the optimal: only 3 unfinished

Large instance: fairer study (99%)

- 'Back to normal':
 - No significant differences among the tested crossover probabilities
 - Kruskal-Wallis rejected for the results grouped by mutation probabilities, with Wilcoxon test and numerically aggregated results, best result is obtained with 0.06 (3 expected mutated genes per individual on average)
- Mutation probability: 0.06 or 3/50 (now) vs 0.1 or 5/50 (then)
 - May be caused by the problem being a 'relaxed' version
 - The original problem may be tailored to be hard to get close to the optimal (100%)
 - Thus, it may be easier to escape a local optimum with a smaller probability than before

Crossover probability	Avg. evaluations	Median evaluations	Std. evaluations	Mutation probability	Avg. evaluations	Median evaluations	Std. evaluations
0.6	680515.9	11079	4653050	0.02	2033935.33	6102.0	8116662.536
0.7	486655.8	9272	4327903	0.04	80863.77	6397.5	891338.375
0.8	333479.7	9462	2977488	0.06	9025.78	8383.5	3034.596
0.9	516886.7	9792	4518431	0.08	12522.85	11697.5	4776.126
1.0	167130.7	8862	1031928	0.10	18869.42	18235.5	6585.632

CONCLUSIONS

- Most results are very similar when comparing the two studies → fixed number of evaluations is better, time is guaranteed to be bounded
- Overall not significant effect of the (tested) crossover probabilities → nature of the problem and number of existing constraints, easier to solve an unfeasible solution by mutating than by applying the crossover operator

Improvements/future work

Applying a 'repair' operator or a heuristic in order not to add unfeasible solutions to the population.

- [Chu and Beasley, 1998] approach: greedy algorithm based on a DROP phase and an ADD phase
- [Shah, 2020]: Lagrangian multipliers + 'greedy crossover'

REFERENCES

[Benjamini and Hochberg, 1995] Benjamini, Y. and Hochberg, Y. (1995). Controlling the false discovery rate: A practical and powerful approach to multiple testing. Journal of the Royal Statistical Society. Series B (Methodological), 57(1):289–300.

[Chu and Beasley, 1998] Chu, P. and Beasley, J. (1998). A genetic algorithm for the multidimensional knapsack problem. Journal of Heuristics, 4(1):63–86.

[Petersen, 1967] Petersen, C. C. (1967). Computational experience with variants of the balas algorithm applied to the selection of rd projects. Management Science, 13(9):736–750.

[Shah, 2020] Shah, S. (2020). Genetic algorithm for the 0/1 multidimensional knapsack problem.