

Stochastic Offline Programming^{*}

Yuri Malitsky and Meinolf Sellmann
Brown University
Department of Computer Science
P.O. Box 1910, Providence, RI 02912, U.S.A.
ynm,sello@cs.brown.edu

Abstract

We propose a framework which we call stochastic off-line programming (SOP). The idea is to embed the development of combinatorial algorithms in an off-line learning environment which helps the developer choose heuristic advisors that guide the search for satisfying or optimal solutions. In particular, we consider the case where the developer has several heuristic advisors available. Rather than selecting a single heuristics, we propose that one of the heuristics is chosen randomly whenever the heuristic guidance is sought. The task of SOP is to learn favorable instance-specific distributions of the heuristic advisors in order to boost the average-case performance of the resulting combinatorial algorithm.

1. Introduction

Solving hard combinatorial problems efficiently requires search. One of the most difficult tasks when designing combinatorial solvers is to make good heuristic decisions which guide the search. While related communities have only recently started to exploit automatic tuning potential (see, e.g., the performance tuning tool in Cplex 11), the constraints community has a long history of research in this direction and has proposed some pioneering ideas for the automatic configuration of algorithms (see, e.g., [12]). This paper follows in the same tradition by proposing a framework for automatically selecting and combining heuristic advisors. This is achieved by extrapolating experience gathered off-line by experimenting with a given benchmark of representative problem instances.

Several seminal papers have advocated the idea of exploiting statistics and machine learning technology to in-

crease the efficiency of combinatorial algorithms. In [15] it has been suggested to protocol during the solution process of a constraint satisfaction problem which variable assignments cause a lot of filtering and to base future branching decisions on this data. This technique, called *impact-based search*, is one of the most successful in constraint programming and has become part of Ilog CP Solver. For incomplete solvers, [3] proposed to adapt parameters of a tabu search algorithm online and thus created *reactive tabu search*. [5] devised an algorithm that learns online which starting points for simple local search heuristics (such as hill-climbing) lead to good solutions. With respect to off-line learning, [9, 1] developed systems that automatically tune algorithm parameters for a given set of benchmark instances. Moreover, [8, 13] introduced so-called *algorithm portfolios*. The idea is to consider a set of algorithms for a given problem and to base the decision of which algorithm to employ on certain features of the given problem instance, whereby informative features and their correlation with the goodness of the algorithms in the portfolio (such as shortage of running time) are learned offline.

All these approaches have two things in common. First, it is possible to construct *worst-case* scenarios where any statistical inference method fails completely. The second aspect is that they have all led to very impressive improvements in practice – despite the above worst-case argument. That is to say, there is substantial *practical evidence* that exploiting (online or offline) statistical knowledge can boost the *average-case* performance of combinatorial solvers. In some sense one may argue that the very fact that statistical inference does not work in the worst-case is what *makes* it statistical inference. That is because, if we could draw any hard conclusions, we would revert to deterministic inference and filter variable domains or derive new redundant constraints. However, statistical inference only kicks in when our ability to reason about the given problem deterministically is exhausted.

In this paper, based on the above mentioned practical

^{*}This work was supported by the National Science Foundation through the Career: Cornflower Project (award number 0644113).

evidence, we introduce a framework which exploits offline learning as part of the programming process.

2. Algorithm Families and Instance-Specific Tuning

Our approach is motivated and heavily builds upon the previous work on algorithm portfolios by [8, 13] as well as the previous work on automatic parameter tuning and automatic algorithm configuration by [9, 1]. Particularly, we introduce *stochastic offline programming* which intertwines the development of combinatorial algorithms with *automated, instance-specific* selection of an algorithm from an entire family of algorithms.

Our vision is that the algorithm development must not be limited to one fixed algorithm. Instead, the developer ought to have the freedom to propose an entire family of algorithms. Then, provided with a method which associates any given benchmark problem instance with a vector of meaningful feature values, machine learning technology learns which algorithm in the family is best suited for a given instance.

We call this very general framework stochastic offline programming (SOP) since it makes automated offline learning part of the programming process. The adjective 'stochastic' is used because the learning is based on the assumption that the given training instances and their associated feature vectors are indicative of the instances that the resulting algorithm will be used on later.

SOP is similar to and yet differs in some essential ways from existing approaches. Algorithm portfolios like SATzilla for example, suffer from having to evaluate the performance of each algorithm before settling on the best one for a specific instance. This exhaustive evaluation limits the approach to work with only a few algorithms, relying on the *accidental variance* in algorithm performance on different input instances. In contrast, SOP is meant to consider an entire family of algorithms (usually infinitely many) with the developer actively *providing* variance through instance-specific algorithm performance. The idea to consider an entire family of algorithms resembles the situation of tuning algorithm parameters, as done by algorithms like ParamILS. The main difference of our framework is that algorithm parameters are not chosen universally and instead, the choice of parameters depends on the specific features of the instance that needs to be solved.

3. SOP for Homogeneous Benchmarks

We consider the following scenario: Given a combinatorial problem, the developer has devised an algorithm which,

at some point, needs to make heuristic decisions. For example, a branch-and-bound algorithm where a branching assignment needs to be chosen at every choice point in the search tree. Or, the developer may have devised a constructive greedy algorithm which, at every step, uses a heuristic criterion to assign the value of a new variable.

Now, rather than choosing one heuristic out of the several available heuristics, we propose that the developer leaves the choice of the heuristic *at every step* to chance. That is, when a new choice must be made, one of the heuristics is chosen according to a predefined *distribution of heuristics (DoH)*. The objective of stochastic offline programming is then to automatically devise an algorithm which chooses the DoH that is best suited for a given problem instance. To this end, SOP is provided with the combinatorial algorithm, an algorithm which associates an input instance with a vector of instance-characterizing features, as well as a set of training instances.

3.1. Selecting a DoH for Homogeneous Instances

We first consider the case when the benchmark instances are homogeneous in the sense that the feature vectors associated with the instances show no (or only very little) variance. Out of the given algorithm family, we are then to select one algorithm which works well for a set of these homogeneous instances. This setting differs from algorithm portfolios in that we are dealing with an infinite number of potential DoHs, which renders infeasible approaches which try to learn the performance for each algorithm in the portfolio. On the other hand, the homogeneous benchmark setting of SOP also differs from and is strictly simpler than standard parameter tuning (this will change when we consider the heterogeneous case where we tune parameters instance specific): we know what the parameters mean (in our case probabilities associated with each potential heuristic). In particular, we must expect that small changes in the DoH will likely result in small changes in algorithm performance.

We propose Algorithm 1 to compute a good DoH for a set of homogeneous benchmark instances. The procedure presented is provided with an algorithm family 'A' for a combinatorial problem as well as a set 'S' of training instances which are considered to have similar features. The procedure returns a DoH for the given algorithm and benchmark set.

The problem of computing this favorable DoH 'distr' can be stated as a continuous optimization problem: Minimize_{distr} $\sum_{i \in S} \text{Perf}(A, \text{distr}, i)$ such that 'distr' is a probability distribution over the advisors used by 'A.' To solve this problem, we employ a local search procedure. We initialize 'distr' randomly. In each iteration, we randomly pick two heuristic advisors a, b and redistribute their

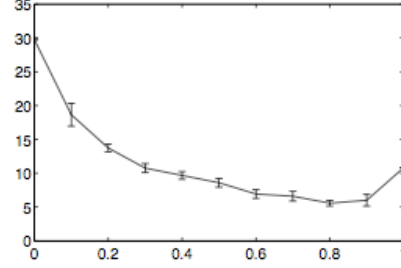
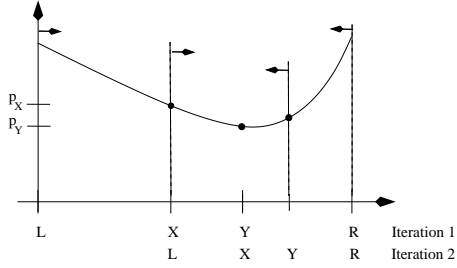


Figure 1. Left: Minimizing a One-Dimensional Convex Function by Golden Section. Right: Optimality Gap when Mixing Advisors “ $\min c$ ” and “ $\min c/k^2$.”

```

1: SOP-Homogeneous (Algorithm A, BenchmarkSet S)
2:  $\text{distr} \leftarrow \text{RandDistr}()$ 
3:  $\lambda_l \leftarrow \frac{\sqrt{5}-1}{\sqrt{5}+1}, \lambda_r \leftarrow \frac{2}{\sqrt{5}+1}$ 
4: while termination criterion not met do
5:    $(a, b) \leftarrow \text{ChooseRandPair}(), m \leftarrow \text{distr}_a + \text{distr}_b$ 
6:    $X \leftarrow \lambda_l, Y \leftarrow \lambda_r$ 
7:    $L \leftarrow 0, R \leftarrow 1, \text{length} \leftarrow 1$ 
8:    $p_X \leftarrow \sum_{i \in S} \text{Perf}(A, \text{distr}[a=m X, b=m(1-X)], i)$ 
9:    $p_Y \leftarrow \sum_{i \in S} \text{Perf}(A, \text{distr}[a=m Y, b=m(1-Y)], i)$ 
10:  while  $\text{length} > \epsilon$  do
11:    if  $p_X < p_Y$  then
12:       $p_Y \leftarrow p_X$ 
13:       $R \leftarrow Y, \text{length} \leftarrow R - L$ 
14:       $Y \leftarrow X, X \leftarrow L + \lambda_l \text{length}$ 
15:       $p_X \leftarrow \sum_{i \in S} \text{Perf}(A, \text{distr}[a=m X, b=m(1-X)], i)$ 
16:    else
17:       $p_X \leftarrow p_Y$ 
18:       $L \leftarrow X, \text{length} \leftarrow R - L$ 
19:       $X \leftarrow Y, Y \leftarrow L + \lambda_r \text{length}$ 
20:       $p_Y \leftarrow \sum_{i \in S} \text{Perf}(A, \text{distr}[a=m Y, b=m(1-Y)], i)$ 
21:    end if
22:  end while
23:   $\text{distr} \leftarrow \text{distr}[a=m X, b=m(1-X)]$ 
24: end while
25: return  $\text{distr}$ 

```

Algorithm 1: SOP for Homogeneous Benchmarks

joint probability mass ‘ m ’ among themselves while keeping the probabilities of all other advisors the same.

We heuristically expect that the one-dimensional problem which optimizes which percentage of ‘ m ’ is assigned to advisor a (the remaining percentage is then already determined to go to advisor b) is convex. We search for the best percentage using a method for minimizing one-dimensional convex functions over closed intervals which is based on the golden section (see left side of Figure 1): We consider two points $X < Y$ within the interval $[0, 1]$ and measure their performance ‘ p_X ’ and ‘ p_Y .’ The performance at X is assessed by running the algorithm ‘ A ’ on the given benchmark with distribution ‘ $\text{distr}[a=m X, b=m(1-X)]$ ’, which denotes the distribution resulting from ‘ distr ’ when assigning probability mass ‘ Xm ’ to advisor ‘ a ’ and probability

mass ‘ $(1-X)m$ ’ to advisor ‘ b ’. Now, if the function is indeed convex, if $p_X < p_Y$ ($p_X \geq p_Y$), then we know that the minimum of this one-dimensional function lies in the interval $[0, Y]$ ($[X, 1]$). We continue splitting the remaining interval (which shrinks geometrically fast) until the interval size ‘ length ’ falls below a given threshold ‘ ϵ .’ By choosing points X and Y based on the golden section, in each iteration we only need to evaluate one new point rather than two.

3.2. A Greedy Heuristic for Set Covering

To make the discussion less abstract let us consider a specific example of an optimization problem and algorithm whose average-case performance we hope to boost by computing a favorable distribution of heuristic advisors. Given items $1 \dots n$ and a set of sets of these items, which we call *bags*, and a cost associated with each bag, the *set covering problem (SCP)* consists in finding a set of bags such that the union of all bags contains all items and the cost of the selection is minimized.

Note: As with any other tuning algorithm, our benchmark is **not** the set covering problem but the specific complete or incomplete algorithms for its optimization. Just like in [9] where the benchmarks were solvers for SAT, and not SAT itself, here we show how the performance of two concrete algorithms for set cover can be boosted.

Greedy Algorithm: A simple greedy algorithm for the SCP is to select bags one by one until we cover all items. Several heuristics have been proposed in the literature on how the next bag ought to be selected. For instance, we can select the bag

- that costs the least ($\min c$),
- that covers the most new items ($\max k$),
- that minimizes the ratio of costs over the number of newly covered items ($\min c/k$),
- that minimizes the ratio of costs over newly covered items times the logarithm of newly covered items ($\min \frac{c}{k \log k}$),

```

1: SCP-Greedy ( $S_1, \dots, S_m, c_1, \dots, c_m$ )
2: bestValue  $\leftarrow \infty$ 
3: for  $i = 1 \dots 200$  do
4:   solution  $\leftarrow \emptyset$ , cost  $\leftarrow 0$ 
5:   while  $\bigcup_{i \in \text{solution}} S_i \neq \{1, \dots, n\}$  do
6:      $r \leftarrow \text{PickAdvisor}()$ 
7:      $j \leftarrow \text{SelectBag}_r(\text{solution}, S_1, \dots, S_m, c_1, \dots, c_m)$ 
8:     solution  $\leftarrow \text{solution} \cup \{j\}$ 
9:     cost  $\leftarrow \text{cost} + c_j$ 
10:  end while
11:  if bestValue > cost then
12:    bestValue  $\leftarrow$  cost
13:    bestSolution  $\leftarrow$  solution
14:  end if
15: end for
16: return bestSolution

```

Algorithm 2: Randomized Greedy Set Covering Algorithm

- that minimizes the ratio of costs over the square of newly covered items ($\min \frac{c}{k^2}$),
- and the bag that minimizes the ratio of square root of costs over the square of newly covered items ($\min \frac{\sqrt{c}}{k^2}$).

Greedy algorithms like this are frequently used to find high quality solutions within complete solution approaches. The traditional way of designing algorithms is to try all greedy variants on some training problems and to select the one which yields the best results on average. An innovative idea was presented in [2]. Rather than choosing just one greedy variant or to choose a random variant each time the greedy algorithm is employed, it has been suggested to choose a random heuristic for selecting the next bag *within* the greedy algorithm. It was reported that significantly improved solutions are found when this randomized greedy algorithm is run 30 times every time the complete algorithm calls the primal heuristic. This approach is outlined in Algorithm 2. Note that, if we are to run the greedy construction 30 times anyway, we could also run each of the pure heuristics of which there are only 6. The significance of the finding in [2] is that hybridizing the heuristics by choosing one of them uniformly at random at each step of the greedy construction and repeating this randomized construction 30 times yields results which are *better* than running the best pure heuristic. We test Algorithm 1 on this randomized greedy algorithm. Rather than choosing a selection heuristic uniformly at random in Lines 6-7, we intend to learn which distributions of selection heuristics are most promising.

Benchmark Sets: To experiment with our SOP framework, we require training and test sets for the SCP. We consider three different randomly generated benchmark sets whereby each set has instances with 100 items and 10,000 bags each.

- **Set 1:** Each bag contains exactly 4% of the items which are chosen uniformly without replacement. The

cost of each bag is chosen uniformly at random between 1 and 1,000.

- **Sets 2:** For each item, for each bag we flip a coin and with a probability of 8% we insert the item into that bag. The cost of each bag is chosen uniformly at random between 1 and 1,000.
- **Sets 3:** For each bag, we repeatedly sample an item from the set of items for insertion into the bag. We assume the items are numbered and that the sample is taken from a Gaussian distribution which has its mean at a random (yet fixed) item. The standard deviation of this distribution is 50. The process of sampling and inserting items is repeated until the bag contains exactly 4% of the items. Again, the cost of each bag is chosen uniformly at random between 1 and 1,000.

For each of the five classes above, there are really two benchmark sets, one for training and one for test purposes, and each containing 100 SCP instances.

Experimental Results: In each iteration of Algorithm 1 we assume that the one-dimensional subproblem that is solved by the golden section is convex. In the right side of Figure 1 we plot the average solution quality (over 5 runs of Algorithm 1 for each DoH) that is achieved when mixing heuristics advisors “min c ” and “min c/k^2 ” on an instance in Set 2. The error bars give the standard deviation over 5 runs at each DoH. We observe convex curves like the one shown here for all instances and for all combinations of heuristic advisors that we looked at. Note that Algorithm 1 would also work when the convexity assumption was in fact false, but then it may only provide a locally optimal solution. However, for our application we may expect that Algorithm 1 provides near-optimal DoHs.

In Table 1 we compare the solution quality achieved by different DoHs in terms of percent of optimality gap closed. To this end, we pre-computed optimal SCP solutions for all training and test instances in Set 1, Set 2, and Set 3. The initial gap is defined by the solution quality that is achieved when using the single advisor which gives, on average, the

Benchmark	Gap	All	Uniform	SOP	Oracle	
Set 1	Train	7.0%	22.8 (2.7)	20.4 (2.3)	41.0 (2.5)	41.1 (1.7)
	Test	7.7%	26.3 (2.6)	24.4 (2.0)	40.5 (1.9)	40.8 (2.3)
Set 2	Train	8.9%	32.6 (3.5)	44.3 (3.2)	57.4 (2.7)	58.8 (2.3)
	Test	8.5%	29.4 (3.5)	46.9 (3.0)	56.0 (2.7)	58.0 (2.9)
Set 3	Train	7.1%	20.8 (3.2)	23.0 (2.4)	39.1 (2.2)	40.0 (2.1)
	Test	8.3%	26.8 (3.2)	25.3 (2.4)	38.5 (2.1)	42.3 (2.0)

Table 1. Percent of Optimality Gap Closed over the Best Single-Advisor Heuristic. The standard deviations are provided inside the parentheses.

best solutions for the training instances. In column “Gap” we observe that the best pure greedy approach leaves an optimality gap between 7% and 9%.

We compare the following choices for the advisor selection in Line 6 of Algorithm 2. “All” performs a round-robin through all advisors. That is, in the i th construction of a greedy solution it always returns the same advisor, and moves on to the next advisor in iteration $i + 1$. Note that, for this way of choosing advisors, it is of course not necessary to perform 200 iterations, since there are only 6 different advisors. Clearly, we expect a much better performance from mixing advisors and running the randomized algorithm 200 times to make up for the additional time spent. “Uniform” denotes the algorithm proposed in [2] where, in each iteration of the greedy construction, we choose a different advisor by picking one uniformly at random. “SOP” denotes the greedy algorithm which uses the DoH which SOP found for the given training set. Finally, “Oracle” denotes the performance when we use the best DoH for each individual instance which we pre-computed and use as an upper bound on the solution quality that can be achieved by the simple greedy heuristic that we are trying to tune.

For Set 1 we observe that running the greedy heuristic 6 times rather than just once while using a different advisor each time and returning the best cover in the end closes around 22% of the optimality gap that the best pure greedy construction left open. Surprisingly, for this benchmark set we do not find it worthwhile to invest the time to construct 200 covers while mixing advisors uniformly at random in the construction of each cover. In fact, the solution quality even slightly declines compared to “All.” The situation is similar for benchmark Set 3. Only for Set 2 we find that mixing advisors and spending 194 extra iterations results in significantly better covers.

Looking at column “Oracle,” we find that by spending an extra 199 iterations we can expect at most to close around 40% of the optimality gap for Sets 1 and 3, and around 60% for Set 2. Comparing with SOP, we see that the latter comes surprisingly close to realizing this potential! Moreover, when comparing the training and test performances that SOP achieves, we see that extrapolating the off-line experience gained on the training set is feasible and results in only slightly decreased performances on the test sets.

4. SOP for Heterogeneous Benchmarks

We now consider the general case where we are given a set of benchmark instances which show significant diversity with respect to their associated feature vectors. In this scenario we intend to learn a function which associates any given feature vector not represented in the training set with

a DoH which we can expect to work well for instances with respective features.

4.1. Selecting a DoH for Heterogenous Instances

For this task we tried two different algorithms. The first followed the standard machine learning approach of multinomial logistic regression [10]. The idea aimed to learn a weight for each feature/advisor pair. Then, with the help of those weights, compute a distribution of heuristics (DoH) by taking, for each advisor, the weighted sum of the features of the instance times the respective feature/advisor weights and using this as the argument to the exponential function. This way, each advisor is associated with a weight, and the distribution is then computed through normalizing the weights.

While there are good statistical arguments for choosing a logarithmic regression function (see [10]), the high dimensionality of the search space and the high cost of evaluating the objective function make the continuous optimization problem difficult to solve efficiently. Therefore, we propose a second algorithm for the heterogenous case.

Our second algorithm is based on the idea of grouping the benchmark instances in clusters and pre-computing a promising DoH for each cluster. Treating each such cluster as a set of homogeneous instances we can then employ Algorithm 1 which works on a much lower-dimensional space. In order to cluster the instances, we require a distance metric in the feature space, though. Naturally, the distance between two feature vectors ought to reflect how well a DoH works on instances with respective features. In particular, we want to separate (and thus introduce a large distance between) feature vectors v_1, v_2 where a promising DoH for instances with features v_1 works badly for instances with features v_2 , and vice versa.

The idea is realized in Algorithm 3. First we initialize the metric in the feature space arbitrarily (for example using the Euclidean norm). Then, in each iteration we cluster the benchmark set in k groups of instances, whereby we assume that k is a parameter of the algorithm. To cluster the instances we use Lloyd’s k-means clustering algorithm [11]. For each cluster, we compute the optimal DoH using Algorithm 1 as well as the center of gravity. We now assess what the distance between individual instances and the centers of gravity of the different clusters ought to be. To this end, for each pair of clusters $i \neq j$, we compute the difference between the performance on all instances in cluster i which is achieved by the best DoH for that cluster and the DoH of the other cluster.

The distance between an instance a in cluster C_i and the centers of gravity of cluster C_j is then the maximum of this regret and 0. Using these desired distances, we adjust the

```

1: SOP-Heterogeneous-Cluster(Algorithm A, BenchmarkSet S, Int
k)
2: Init(featureMetric)
3: repeat
4:    $[C_1, \dots, C_k] \leftarrow \text{Cluster}(S, k, \text{featureMetric})$ 
5:   for  $i=1$  to  $k$  do
6:      $f_i \leftarrow \text{SOP-Homogeneous}(A, C_i)$ 
7:      $c_i \leftarrow \text{Center}(C_i)$ 
8:   end for
9:   for all  $1 \leq i \neq j \leq k$  do
10:    for all instances  $a \in C_i$  do
11:       $d_{a, c_j} \leftarrow \max\{\text{Perf}(A, f_j, a) - \text{Perf}(A, f_i, a), 0\}$ 
12:    end for
13:  end for
14: until Adjust(featureMetric, d) = false
15: return  $([f_1, \dots, f_k], [c_1, \dots, c_k], \text{featureMetric})$ 

```

Algorithm 3: Cluster-Based SOP for Heterogeneous Benchmarks

feature metric and iterate until the feature metric does not change anymore. Then, we return the best DoHs as well as the centers of gravity for each cluster, and the final feature metric. Equipped with this tuple, any formerly unseen instance with associated feature vector can easily be assigned to one of the clusters and the appropriate DoH can then be used for its optimization.

The procedure is straight-forward. The only issue is the parameter k which determines the number of clusters and thus the final number of different algorithms which will be used to optimize different instances. We need to strike a good balance here between our wish to provide many different algorithms so that we can provide a tailor-made algorithm for new instances and the need to devise robust algorithms which work well on a variety of instances with the same or similar features. In the end, the choice of k must be determined heuristically by the user, as the variance in performance depends on the algorithm A as well as the optimization problem and the features used.

4.2. Tuning a Greedy Heuristic for Heterogeneous Set Covering Benchmarks

We consider again the greedy heuristic for the SCP and the different advisors from Section 3.2. To make the choice of DoH instance-specific, we require features which characterize an instance.

Features: We gather the following data for SCP instances:

- the normalized cost vector $c' \in [1, 100]^m$,
- the vector of bag densities $(|S_i|/n)_{i=1\dots m}$,
- the vector of item costs $(\sum_{i, j \in S_i} c'_i)_{j=1\dots n}$,
- the vector of item coverings $(|\{i \mid j \in S_i\}|/m)_{j=1\dots n}$,
- the vector of costs over density $(c'_i/|S_i|)_{i=1\dots m}$,
- the vector of costs over square density $(c'_i/|S_i|^2)_{i=1\dots m}$,

- the vector of costs over $k \log k$ -density $(c'_i/(|S_i| \log |S_i|))_{i=1\dots m}$, and
- the vector of root-costs over square density $(\sqrt{c'_i}/|S_i|^2)_{i=1\dots m}$.

As features we compute the maxima, minima, averages, variances, standard deviations, and the logarithms of all these statistics for all vectors. To assess the performance achieved by a particular DoH (see the calls to function 'Perf' in Algorithm 3), we run the modified Algorithm 2 again five times and take the average of the solutions returned.

Benchmark Sets: To experiment with our SOP framework, we also require heterogenous training and test sets for the SCP. We consider two more benchmark sets, whereby again each set consists in a training set and a test set of SCP instances.

- **Set 4:** The training set consists in 90 instances, 30 from each of the sets Set 1, Set 2, and Set 3. The test set is the union of all test sets of Set 1-3.
- **Set 5:** For each instances, we first choose at random whether the constraint matrix is filled by row or by column and whether the respective row or column density is constant or variable. Then, we randomly select the density or desired mean density at 4% or 8%, and flip a coin to decide whether row or column densities that are set to one are chosen uniformly at random or with a Gaussian-bias. Costs are uniformly chosen from $[1, 1000]$. A training set with 200 instances and a test set with 100 instances are generated this way. Additional test sets are benchmark classes SCP 4, SCP 5, and SCP 6 from the OR library [14].

Experimental Results: As in Section 3.2, we run various algorithms on our benchmarks, whereby the offline learning algorithms are run on the training set and evaluated on the training as well as the test sets. We compute again the optimality gap of the pure greedy heuristic that works best for the training set. The percentage of this gap that is closed by the contenders is given in Table 2. Again, we observe that using a uniform distribution is often not much better and sometimes even worse than using all of the advisors in a pure round-robin fashion. Our homogenous SOP approach already provides significantly improved DoHs, even though the effect on these heterogenous sets of SCP instances is not as dramatic as seen before on the homogenous benchmarks Set 1-3. In particular, the comparison with the 'Oracle' data where we computed the best DoH for each individual instance shows that there is still room for improvement.

On Set 4 we observe that the heterogenous SOP-clustering approach comes close to realizing the total potential that running the simple greedy algorithm 200 times

Benchmark	Gap	All	Uniform	SOP-homo	SOP-hetero		Oracle	
					Regress	Cluster		
Set 4	Train	7.3%	26.0 (3.0)	30.6 (2.7)	39.6 (2.2)	40.5 (2.4)	46.0 (2.4)	49.2 (2.1)
	Test	8.2%	27.6 (3.1)	30.6 (2.8)	40.5 (2.5)	40.3 (2.5)	45.4 (2.5)	46.0 (2.5)
Set 5	Train	7.2%	22.3 (4.8)	31.9 (3.9)	39.0 (3.3)	32.8 (3.6)	47.7 (2.4)	64.1 (2.5)
	Test	7.6%	30.9 (4.2)	35.0 (4.1)	43.4 (3.6)	38.1 (3.7)	50.3 (3.7)	63.9 (2.9)
	SCP 4	12.4%	25.6 (2.9)	25.0 (2.8)	29.5 (3.3)	41.8 (2.3)	41.1 (2.3)	49.9 (2.2)
	SCP 5	11.8%	34.2 (3.0)	22.5 (1.8)	33.7 (2.5)	35.5 (1.4)	44.9 (2.3)	47.1 (2.4)
	SCP 6	12.4%	20.0 (6.0)	29.6 (3.9)	38.3 (5.9)	34.1 (4.3)	42.7 (3.7)	48.5 (3.5)

Table 2. Percent of Optimality Gap Closed over the Best Single-Advisor Heuristic

with a mix of our six different advisors holds in store for us. On the test set that was generated by the same generator as the training set, the results are outstanding. On Set 5, which is much more diverse, we observe that instance-specific parameter tuning significantly outperforms all other algorithms, although it clearly does not achieve the performance of a perfect oracle. What is remarkable is that the quality of the clustering approach does not decline much for the test sets SCP 4-6 which are drawn from the OR library! Moreover, note that both heterogenous SOP approaches keep their performance much more stable and closer to the training set over all four test sets in this benchmark than homogenous SOP.

5. SOP for Tree Search

Now we consider a complete tree search approach. For optimization problems like set covering, systematic approaches are commonly based on branch-and-bound. The latter draws its strength from the upper and lower bounds which are used for pruning purposes. For the lower bound, we use a linear relaxation which is computed by SoPlex 1.4 [16]. There exist techniques to strengthen the lower bound, especially by adding valid inequalities. These techniques are outside the scope of this paper. Here, we focus on strengthening the upper bound which is commonly computed by a primal heuristic like the one presented in Algorithm 2. With the help of SOP, we intend to improve the upper bound so that our branch-and-bound approach provides high quality solutions very quickly.

In principle, the situation is similar to that in the previous sections. There are some fundamental differences, though. First, we have seen before that the simple greedy heuris-

tic, even when run multiple times and with high-quality DoHs, leaves an optimality gap of 3%-4%, depending on the benchmark set that is tackled. Embedded in a branch-and-bound approach, we expect the upper bound to converge to (near) optimality with as little search as possible. The second difference is that the primal heuristic is now called for every choice point. The distribution of problem instances encountered at the various choice points is likely to differ a lot from that represented by the input benchmark set.

Consequently, we set up the following algorithm that will be optimized by SOP. At every choice point, we compute an upper bound with the help of Algorithm 2, whereby we use an iteration limit of 30 instead of 200 in Line 3 since the primal heuristic is being called at every choice point for only slightly varying problems anyway. Also at every choice point, we compute an LP-based lower bound and backtrack if the optimal relaxation is integer or when the global upper bound is already lower or equal to the local lower bound. If that is not the case, we branch and continue search in depth-first manner. For SOP training purposes, we stop this tree-search after 50 nodes and note the final solution quality.

In Table 3 we show the optimality gap left open when using the best single advisor for the training set. We observe that this gap is now much smaller due to the search that is performed by our target algorithm. We also note that the best pure advisor for the training sets of Sets 2 and 3 work comparably well on the corresponding test sets. For Set 1, however, we find that the best pure advisor overtunes: It leaves a rather small optimality gap on the training set but loses a lot of quality (more than 60%) when used on the generalized test set. Note that this effect influences all

Benchmark	Gap	All (stdev)	Uniform (stdev)	SOP (stdev)	Offline (stdev)	
Set 1	Train	1.05%	-7.39 (1.5)	-0.91 (1.6)	7.02 (1.4)	4.9 (1.4)
	Test	1.61%	16.9 (1.7)	14.4 (1.7)	24.53 (1.5)	20.1 (1.6)
Set 2	Train	1.95%	10.44 (2.2)	15.7 (2.2)	33.14 (1.8)	26.2 (1.9)
	Test	2.07%	17.05 (2.1)	32.3 (1.8)	37.23 (1.8)	36.3 (1.8)
Set 3	Train	1.12%	2.8 (1.5)	10.5 (1.3)	13.2 (1.3)	14.4 (1.4)
	Test	1.17%	1.8 (1.7)	12.1 (1.6)	14.0 (1.5)	10.4 (1.6)

Table 3. Percent of Optimality Gap Closed by the Tree-Search Algorithm over the Best Single-Advisor Heuristic.

Benchmark	Gap	All (stdev)	Uniform (stdev)	SOP (stdev)	
Set 4	Train	1.3%	3.7 (1.6)	3.1 (1.7)	21.4 (1.5)
	Test	1.5%	13.7 (1.7)	20.0 (1.7)	25.1 (1.7)
Set 5	Train	2.7%	8.5 (3.0)	19.1 (2.8)	25.3 (1.5)
	Test	3.8%	9.7 (3.9)	18.2 (3.6)	24.8 (3.4)

Table 4. Percent of Optimality Gap Closed over the Best Single-Advisor Heuristic

other approaches for which we measure performance percent of optimality gap closed over the best pure advisor: The training performance of the other approaches appears worse, and their test performance appears better. Overall, we find that SOP outperforms all other approaches, leaving an average optimality gap of 1% to 1.3% after only 50 nodes of search. In column 'Offline' we show the performance when using the DoHs which were found in the experiment corresponding to Table 1. While these DoHs still perform on par or better than a uniform selection of advisors, learning DoHs which perform well within the tree-search framework is clearly better.

We repeat the same experiment for the heterogeneous benchmarks Set 4 and Set 5. In Table 4 we see once more that offline learning based on training instances that are stochastically related to the test cases offers the possibility of significantly boosting the performance of combinatorial algorithms.

6. Conclusions and Future Work

We have introduced the idea of stochastic offline programming, a programming framework for automatically choosing and combining different heuristic advisors. The instance-specific randomized combination of advisors is based on offline experience gathered on a training set which is sampled from the same distribution as the test sets that the algorithm is expected to perform well on.

Extensive tests on a greedy incomplete algorithm and a systematic tree search algorithm for the set covering problem provide a proof of concept: It is indeed possible to combine heuristic advisors in a randomized fashion, and favorable instance-specific distributions can be learned which clearly outperform the best pure advisor as well as a uniform combination of advisors. Moreover, on heterogeneous benchmarks we found that there is no one best distribution of heuristics (DoH) that works well on all instances. For this case, we showed that we can learn how to select a DoH based on the features of a given problem instance.

Our future work regards the test of SOP on algorithms for other problems. The SOP framework is general enough to cope with any combination of advisors and any objective. For example, we intend to use it to combine branching heuristics to minimize the expected runtime of a con-

straint solver. As this will require a lot more CPU time that we could afford in the development and calibration of the homogeneous and heterogeneous SOP algorithms, we are working towards an efficient parallel implementation of SOP. Moreover, we intend to generalize the framework so that it can learn more than one DoH simultaneously when heuristic guidance is needed for more than one task within a combinatorial algorithm.

References

- [1] B. Adenso-Diaz and M. Laguna. Fine-tuning of Algorithms using Fractional Experimental Design and Local Search. *Operations Research*, 54(1):99–114, 2006.
- [2] E. Balas and M. Carrera. A dynamic subgradient-based branch-and-bound procedure for set covering. *Operations Research*, 44:875–890, 1996.
- [3] R. Battiti and G. Tecchioli. The reactive tabu search. *ORSA Journal on Computing*, 6(2):126–140, 1994.
- [4] M. Birattari, T. Stuetzle, L. Paquete, K. Varrentrapp. A Racing Algorithm for Configuring Metaheuristics. *GECCO*, 11-18, 2002.
- [5] J.A. Boyan and A.W. Moore. Learning Evaluation Functions to Improve Optimization by Local Search. *Journal of Machine Learning Research*, 1:77–112, 2000.
- [6] S.P. Coy, B.L. Golden, G.C. Runger, E.A. Wasil. Using Experimental Design to Find Effective Parameter Settings for Heuristics. *Journal of Heuristics*, 7(1):77–97, 2001.
- [7] A. Fukunaga. Automated discovery of local search heuristics for satisfiability testing. *Evolutionary Computation*, 16(1):31–61, 2008.
- [8] C. Gomes and B. Selman. Algorithm Portfolios. *Artificial Intelligence*, 126(1–2):43–62, 2001.
- [9] F. Hutter, H. Hoos, T. Stuetzle. Automatic Algorithm Configuration based on Local Search. *AAAI*, 1152–1157, 2007.
- [10] M. Jordan. Why the logistic function? A tutorial discussion on probabilities and neural networks. *MIT Computational Cognitive Science Report*, 9503:1995.
- [11] S.P. Lloyd. Least squares quantization in PCM. *IEEE Transactions on Information Theory* 28(2):129–137, 1982.
- [12] S. Minton. Automatically Configuring Constraint Satisfaction Programs. *Constraints*, 1(1):1–40, 1996.
- [13] E. Nudelman, K. Leyton-Brown, H.H. Hoos, A. Devkar, Y. Shoham. Understanding Random SAT: Beyond the Clauses-to-Variables Ratio. *CP*, 438–452, 2004.
- [14] J.E. Beasley. OR-Library. *Journal of the Operational Research Society*, 41(11):1069–1072, 1990.
- [15] Ph. Refalo. Impact-Based Search Strategies for Constraint Programming. *CP*, pp. 557–571, 2004.
- [16] R. Wunderling. Paralleler und objektorientierter Simplex-Algorithmus *Technische Universität Berlin*, 1996.