Fast Algorithms for the Capacitated Vehicle Routing Problem using Machine Learning Selection of Algorithm's Parameters

Roberto Asín-Achá¹^{Da}, Olivier Goldschmidt²^{bb}, Dorit S. Hochbaum³^{Dc} and Isaías I. Huerta¹^{Dd}

¹Department of Computer Science, Universidad de Concepción, Chile ²Riverside County Office of Education, U.S.A.

³Department of Industrial Engineering and Operations Research, University of California, Berkeley, U.S.A.

Keywords: Vehicle Routing, Machine Learning, Model Selection.

Abstract: We present machine learning algorithms for automatically determining algorithm's parameters for solving the Capacitated Vehicle Routing Problem (CVRP) with unit demands. This is demonstrated here for the "sweep algorithm" which assigns customers to a truck, in a wedge area of a circle of parametrically selected radius around the depot, with demand up to its capacity. We compare the performance of several machine learning algorithms for the purpose of predicting this threshold radius parameter for which the sweep algorithm delivers the best, lowest value, solution. For the selected algorithm, KNN, that is used as an oracle for the automatic selection of the parameter, it is shown that the automatically configured sweep algorithm delivers better solutions than the "best" single parameter value algorithm. Furthermore, for the real worlds instances in the new benchmark introduced here, the sweep algorithm has better running times and better quality of solutions compared to that of current leading algorithms. Another contribution here is the introduction of the new CVRP real world data benchmark based on about a million customers locations in Los Angeles and about a million customers locations in New York city areas. This new benchmark includes a total of 46000 problem instances.

1 INTRODUCTION

The Capacitated Vehicle Routing Problem (CVRP) is a well known NP-hard problem that has been extensively studied due to its importance in applications in logistics and transportation. An instance of this problem consists of a depot, where trucks are located, and a distribution of customers and their demands. The goal is to devise tours for trucks that visit the customers and deliver their demands, subject to the given truck capacity, and so that the sum of distances traversed by the trucks is minimum. A large number of exact and heuristic algorithms have been devised for the CVRP. In addition to algorithms, there are also multiple benchmarks of data sets that are available for the purpose of testing algorithms for CVRP. These include synthetic and real world data and consist mostly of small instances (with fewer than 1000 customers).

One exception is the Gendreau benchmark (Arnold et al., 2019) that includes large instances of size up to 30000.

In general, when there are several algorithms to solve a problem, no single algorithm dominates the others on all problem instances. Algorithm selection attempts to build machine-learning-based oracles capable of determining, in advance, which algorithm can perform best for a given input instance. Similarly, for a single algorithm, several configurations of the algorithm are possible (i.e. different values for the algorithm's parameters). Again, it is often the case that no single configuration performs best on all possible scenarios. Algorithm Configuration is the task of building machine-learning-based oracles that can output the best configuration for a given instance.

In this work we present a case study for automatic algorithm configuration for the "Sweep Algorithm". The sweep algorithm assigns customers to a truck, in a wedge area of a circle of parametrically selected radius around the depot, with demand up to the truck capacity. This radius parameter affects the output of the algorithm, and its best value depends on an instance

^a https://orcid.org/0000-0002-1820-9019

^b https://orcid.org/0000-0002-6727-5565

^c https://orcid.org/0000-0002-2498-0512

^d https://orcid.org/0000-0002-0343-4539

Asín-Achá, R., Goldschmidt, O., Hochbaum, D. and Huerta, I

Fast Algorithms for the Capacitated Vehicle Routing Problem using Machine Learning Selection of Algorithm's Parameters. DOI: 10.5220/0011405400003335

In Proceedings of the 14th International Joint Conference on Knowledge Discovery, Knowledge Engineering and Knowledge Management (IC3K 2022) - Volume 1: KDIR, pages 29-39 ISBN: 978-989-758-614-9; ISSN: 2184-3228

Copyright © 2022 by SCITEPRESS - Science and Technology Publications, Lda. All rights reserved

characteristics. In our study, we propose and compare several Machine Learning (ML) algorithms for identifying the appropriate parameter for each input instance. We compare the algorithms' performance with the Single Best Solver (i.e. the by-default best parameter value across all the instances) and the Virtual Best Solver (i.e. a perfect solver that identifies the best parameter value for each instance without overhead).

Our contributions here include:

- The generation of new benchmark sets based on real world addresses in New York and Los Angeles cities. With our instance generator, one can generate random subset instances of sizes up to one million customers.
- An automatically selected algorithm that generates very fast feasible solutions, which, when compared to the first solutions found by OR tools (Perron and Furnon, 2019) public solver, and by the state-of-the-art FILO solver, publicly available, solver from (Accorsi and Vigo, 2021), deliver better quality solutions in dramatically faster running times.
- Demonstrating the feasibility of building machine-learning-based oracles capable of identifying a "best" parameter value of an algorithm, resulting in considerable speed up and improved solution quality.

The paper is structured as follows: Section 2 presents the basic concepts and terminology used in the rest of the paper. It also presents relevant related work in the field. In Section 3, we present and elaborate on our automatically configured sweep algorithm. Experimental results are presented in Section 4. Section 5 includes conclusions and pointers to future research.

2 PRELIMINARIES AND RELATED WORK

2.1 The Capacitated Vehicle Routing Problem and Algorithms

In the Capacitated Vehicle Routing Problem (CVRP) there is a set of customers with known demands and an unlimited collection of trucks, of limited capacity, located at the "depot" which are to deliver the goods to the customers so as to satisfy their demands. A solution to the problem is a set of routes for the trucks, such that each route begins and ends at the depot, the total demand is satisfied, and no truck's capacity is exceeded. The goal is to minimize the sum of the lengths of the tours traversed by all the trucks.

CVRP is a well known NP-hard problem, which generalizes the Travelling Salesperson Problem. Due to its difficulty, and its importance in applications, a large number of algorithms were devised for CVRP, most of which are heuristic algorithms that do not guarantee optimality. A recent review of such algorithms is provided in (Elshaer and Awad, 2020). Exact algorithms have also been proposed for the problem, one of which, (Pessoa et al., 2021), is considered particularly influential. Recently, Machine-Learningbased heuristics have been proposed, mostly for small-size problem instances (Bogyrbayeva et al., 2022; Alesiani et al., 2022; Fellers et al., 2021).

Recall that we address here CVRP with unit demands-that is, all customers demands are equal to 1 unit.

2.2 Our Sweep Algorithm implementation

The sweep algorithm (Haimovich and Rinnooy Kan, 1985; Dondo and Cerdá, 2013; Gillett and Miller, 1974) consists of two phases. In the first phase customers are allocated to trucks and in the second phase a short route for each truck is computed, starting from the depot, serving its customers, and returning to the depot. The second phase can use any Travelling Salesperson Problem (TSP) algorithm. In our implementation we solve the TSP using the Lin-Kernigan (Lin and Kernighan, 1973) heuristic, as implemented in the Concorde (Applegate et al., 2009) package, in C language.

The first phase of the sweep algorithm, in which customers are allocated to trucks, consists of two sub-phases:

- 1. Customers are partitioned into two groups. The first group consists of the customers which are within a given distance parameter, **radius**, from the depot. The remaining customers form the second group.
- 2. In each group:
 - (a) With respect to the depot, compute the polar coordinates of each customer and sort the customers by increasing angle to the depot.
 - (b) One by one, assign the sorted customers such that the total demand of customers assigned to a truck doesn't exceed the truck capacity. Note that customers allocated to a truck in the first group are located in a wedge of the circle centered at the depot, see Figure 1.



Figure 1: For the case of truck capacity 4 and unit demands, this figure illustrates an inner wedge and an outer wedge for the sweep algorithm.

In the special case of unit demands, we also implement a variation of the sweep algorithm where the total number of customers in the outer circle is an integer multiple of the truck capacity. In case the selected radius is such that the number of customers on the outer circle is not an integer multiple of the truck capacity, we move the extra customers to the inner circle by effectively increasing the radius. The rationale behind this is to avoid sending a truck serving fewer customers than its capacity far from the depot. This variation is referred as the *second algorithm*.

The Sweep Algorithm's Parameter: We will use the "radius" parameter r, which is computed as the ratio of the radius of the inner circle divided by the distance to the furthest customer from the depot. This parameter r takes values in the range [0, 1]. We use negative values of r to indicate the use of the second algorithm with the parameter |r|.

Figure 2 shows the number of instances that are "best" solved by a given parameter value for the LA and NY benchmark sets (to be discussed in Subsection 3.2.1). This figure implies that, on average, the second variant of the algorithm performs better than the first. Furthermore there is no uniform "best" parameter for all instances. Therefore, the prediction on a "best" parameter value for a given instance is non trivial and we will show that it can successfully be done with machine learning methods.

We further note, from the results in Figure 2, that the dominant best parameter values depend on the benchmark set (NY or LA).

Overall, Table 1 lists the first 10 parameter values that perform best. We observe that parameter value 0 seems to work best, with values close to -0.5 (i.e. -0.49, -0.4, -0.51, -0.42, -0.39, -0.48, -0.41, -0.43) performing next best. We use this list of pa-



Figure 2: Number of instances which are best solved by parameter value.

rameter values when evaluating the effectiveness of the oracle, in Section 4.

Table 1: List of best 10 parameter values ordered according to the percentage of best solved instances.

Parameter Value r	% Wins
0	14.58
-0.5	4.09
-0.49	4.04
-0.4	3.72
-0.51	3.4
-0.42	3.36
-0.39	3.33
-0.48	3.32
-0.41	3.22
-0.43	2.92
	•
	:

Figures 3 and 4 show how the normalized cost (i.e. the length of the tour normalized by dividing it by the best (minimal) known value of each instance) varies for different values of the parameter. Figure 3 shows one line for the median value of all instances grouped by different truck capacity. Besides observing that the value can vary significantly for close parameter values, particularly for the first algorithm), we also notice that the trend is different depending on the capacity of the trucks. For instance, we can see that the best value for instances for large capacities are among the worst values for instances with small capacities. We observe that the difference between "best" and "worst" parameter values correspond to a magnitude that is around 14% of the value of the "best solution". The behavior for the parameters corresponding to the second algorithm is different than the one for the first algorithm due to the effect of the "padding" of the outer circle customers to multiples of the truck capacity, since many close values deliver exactly the same solution.

Analogously, Figure 4 shows one line for the median values of all instances grouped by number of customers. Again, we notice that close parameter values in the first algorithm can generate solutions of very different quality. Here, we see that the normalized difference between best and worse solutions can scale



Figure 3: Normalized mean cost variation across possible parameter's values by truck capacity of all 46000 instances.

up to 15%. As in the previous case, the trend of the normalized cost across the different parameter values varies depending on the number of clients. For example, we can see that good parameter values for big instances are among the worse parameter values of the smaller ones.



Figure 4: Normalized mean cost variation across possible parameter's values by number of customers of al 46000 instances.

2.3 Machine Learning

Machine Learning (ML) is an Artificial Intelligence field that has seen huge development during the last decade (Alpaydin, 2021). It is considered one of the most powerful tools for processing and analyzing big data volumes. Algorithms proposed for the different ML models seek to identify hidden patterns in the data, from which they can learn. In general, ML models seek to learn, from given data, called training set, a function f that maps an input instance to a corresponding scalar (vector) output, referred to as label(s). ML models can be classified based on how f is learned. When the learning process is based on the use of ground truth, consisting of a set of input instances and the associated correct output labels (discrete or continuous), then the model is known as supervised, e.g. (Burkart and Huber, 2021). When labels are not available, the model finds patterns by analyzing the nature of the input data, then the model is said to be unsupervised, e.g. (Alloghani et al., 2020). If the learning process of the model is based on both ground-truth data and pattern analysis of the input data, then it is known as semi-supervised, e.g. (Zhu

and Goldberg, 2009).

We also classify ML models depending on the nature of the output of the mapping f. If the output assumes discrete values, known as "classes", that are used to separated the possible inputs on different categories, the model is said to be a **classification** model. If the output is given as real (floating-point) values, then the model is called a **regression** model.

The ML algorithms used here are:

- **Random Forests (RF)** (Breiman, 2001): is an ensemble method (Breiman, 1996) that constructs a parameterized (*n_estimators*) number of decision trees (Quinlan, 1986), that are trained, each one, with a different subset of instances belonging to the training set. To compute the output label, each of the trees "proposes" a result. The final result is determined by a consensus scheme that varies depending if the model is a regression or a classification one. In the regression case, the consensus corresponds to the average of all the decision trees' outputs, while for the classification version, the final output corresponds to the label that repeats (is voted) the most, among the trees' outputs.
- *k*-Nearest Neighbors (KNN) (Fix and Hodges, 1989): is a ML algorithm that bases the output label on the labels of the *k* closest training examples to the input point we want to label. Although several distance metrics can be used, the euclidean distance between feature vectors is the most common one. For classification tasks, KNN assigns the output label as the most repeated label among the *k* neighbors. In case of a regression task, the label corresponds to the average of the labels of the *k* neighbors.
- Ada Boost (AB) (Schapire, 2013): belongs to a class of ensemble methods known as boosting (Schapire, 1997). This technique consists on, iteratively, refining the "weakest model" in the ensemble (e.g. a decision tree). First, this model is trained with the complete training set, then a higher weight is assigned to the data points which accumulate bigger deviations on the metric being optimized (e.g. the error). The weights are computed from a parameter called *learning_rate*. A new iteration with another "weak" model is performed using the new weights from the previous step, in order to correct the highest deviations of the previous model. This is repeated for a number of iterations which is given as a parameter (*n_estimators*).
- **Gradient Boosting (GB)** (Friedman, 2001): is also a boosting model that generalizes the ideas be-

hind Ada Boost. For it, different parameterized loss functions can be defined. For the learning, the model, consecutively, learns a parameterized number ($n_estimators$) of new "weak" models that are given as input to the next iteration. For each new model, in a similar way of gradient descent, a negative gradient is computed based on the past model which is weighted according to a parameterized scheme (*learning_rate*), and a move in the opposite direction for reducing the loss is performed.

Convolutional Neural Networks(CNN)

(Fukushima and Miyake, 1982): are a special type of Neural Networks (McCulloch and Pitts, 1943) that specialize in processing topological data in form of matrices (i.e. an image). Its structure is typically composed by three types of layers: convolutional layer, pooling layers and fully connected layers. The main operation of this kind of networks is that of convolution consisting of computing the dot product between two matrices: a submatrix of the input matrix and another matrix called kernel (also called filter). The kernel contains parameters that are learnt during the training phase. The result of performing several convolutions of the image is a new set of features that is fed to the next layer, which in turn corresponds to high level characteristics of the input data (e.g. borders, corners, colors, etc). The pooling layers are used in order to reduce the dimensionality of each feature map resulting of the convolution phase. This is done by performing single operations over the matrices like obtaining the maximum or the average of its values. This way, each matrix is "compressed" into one single value that is later fed to the fully connected layers, which usually correspond to the last layers of the network. These layers map this "compressed data" into the corresponding output of the model (i.e. the labels).

2.4 Per Instance Automatic Algorithm Configuration

According to (Kerschke et al., 2019), *automatic algorithm configuration* consists of determining the parameter values of a given algorithm (its configuration) in order to optimize its average performance across the instances of a given benchmark set. *Perinstance algorithm configuration* is a generalization of this problem, where the configuration is optimized for a specific input instance. For the latter, we can identify two phases: a *training phase*, where the per-

instance configurator learns from the characteristics and performance metrics of known training instances, for which training set labels exist, and a production phase where it is used to select the best configuration for a given, new, instance. In contrast, (per-set) automatic algorithm configuration (see (López-Ibáñez et al., 2016)) sets "good average" values that are used for all the test instances, once it is trained. One approach for Per-instance algorithm configuration is to consider it as an special case of automatic algorithm selection (Lindauer et al., 2015), where a finite number of different configurations correspond to a finite number of algorithms, and the task consists on finding which, among such configurations, would perform best in a given input instance (Rice, 1976). Formally, as defined in (Lindauer et al., 2019), the goal is to select, for a given instance and a given metric *m*, an algorithm A, whose performance metric value is best.

Previous work on algorithm selection/configuration for CVRP, include (Fellers et al., 2021), where the authors present a CNN-based meta-solver that is capable of identifying, from a set of 4 heuristic algorithms, for up to 79% of instances, the one that performs best, in a set of diverse instances automatically generated by the authors. The instances considered in such study vary the number of customer in the range [100 - 1000]. Also, a recent survey on learning-based algorithms for the CVRP can be found in (Bogyrbayeva et al., 2022).

2.5 Performance Metrics

To evaluate algorithm selection methods, two baselines are frequently used:

- **Single Best Solver (SBS):** relates to the performance of the solver with best average behavior across all the instances used for the first phase (i.e. the best solver on average for the training set).
- **Virtual Best Solver (VBS):** relates to a virtual solver that delivers perfect selection of the best performing algorithm for each individual instance.

An algorithm selector is reasonable if it performs at least as well as the SBS. Hence, it is common to normalize the performance metric m with respect to this baselines. For this problem, we take m as the length of all trucks' tours. This normalized metric is known as \hat{m} and is defined as follows:

$$\hat{m} = \frac{m - m_{VBS}}{m_{SBS} - m_{VBS}} \tag{1}$$

Values of $\hat{m} = 0$ mean that the selector performs as well as the VBS and $\hat{m} = 1$ means that it performs as well as the SBS. Greater than 1 values of \hat{m} mean that the use of the selector is worse than using a single algorithm/configuration for all the instances in the test.

For evaluating the performance of different ML models on the quality of the predicted parameter r, we use the Mean Squared Error (Carbone and Armstrong, 1982) (MSE). This measures the average of the squares of the differences between the predicted values of r and the best possible values of r. This best value is determined for each instance by running all possible values of r and picking the one which gives the lowest value of the length of the tours. This best value is referred to as the *ground-truth* label of the instance.

3 META-SWEEP-ALGORITHM: AUTOMATIC CONFIGURATION OF THE SWEEP ALGORITHM

3.1 Algorithm Configuration as Algorithm Selection

As proposed in (Lindauer et al., 2015), algorithm configuration tasks can be handled the same way as algorithm selection tasks. For this, typically, a continuous domain has to be discretized and bounded. For the Sweep Algorithm, this is straightforward, since its parameter is bounded by the range [0, 1] and such a range can be discretized at a desired level of granularity. The algorithm selector setup for the Sweep algorithm is given in Figure 5.

The process is composed of the following tasks:

- **Training and Testing Data Preparation:** For this task, benchmark sets have to be collected, and all possible configurations of the algorithm have to be tested against those benchmark sets. For each experiment, the cost obtained by the algorithm and the time of the execution is stored.
- **Instance Characterization:** The instances are characterized by devising and selecting a set of features that are ideally informative. It is also important that computation of the features of an instance is done efficiently, since the focus of algorithm selection is low running time overall.
- **Instance Labeling:** Since our approach here is supervised, we need to label our training set. These labels are computed by comparing the quality of the costs of the solutions associated to the corresponding parameter values.



Figure 5: Training process for our supervised algorithm configuration framework.

Machine Learning Models: A machine learning model is defined by its input, output and the function that maps the input into the output. The input consists of the (possibly normalized) features determined in the characterization step above and the output corresponds to the (possibly normalized) labels also described above. The learning of the mapping is then computed by ML algorithms that adjust the parameters of the underlying structure of the model (neural network, decision trees, etc). After this, the model is validated by comparing the model's output with the labels in the testing data.

Next, we elaborate on the details of each of the tasks.

3.2 The Generated Training and Testing Data

3.2.1 Los Angeles and New York Datasets

The customers of each instance are randomly selected either from a set of over one million addresses in Los Angeles, (https://data.lacity.org), or from a set of close to one million addresses in New York City (https://data.cityofnewyork.us). Each customer is defined by its latitude and longitude coordinates. The distance between two customers is calculated as the Euclidean distance. For each instance, we locate the depot at the mid-point between the most south-west and the most north-east customers.

In this study, we set all demands to unit. The number of customers per instance varies from 500 to 6000, randomly selected, and the truck capacity varies from 25 to 200 customers. For every combination of number of customers and truck capacity, we have generated 500 instances from each of the Los Angeles and the New-York City collections of addresses. In total, we generated 46000 instances.

3.3 Instance Characterization and Features

Our models use different features of the CVRP instances as input for suggesting the best configuration of the algorithm. Such features have to be informative and, hopefully, fast to compute. They are normally computed by preprocessing the input instance and by extracting descriptive statistics from it. For CVRP, fast to extract descriptive statistics are: number of customers, average and standard deviation of the demands, statistics on the spatial distribution of the customers, etc.

We choose the following **features** to feed to our models:

- Number of Customers. The total number of customers in the CVRP problem.
- **Capacity:** The capacity of the trucks. For this work, we consider uniform capacity across all the trucks, but this can easily be converted to a vector of capacities if this is not the case.
- Width. The biggest difference across x-coordinates of all customers.
- **Height.** The biggest difference across y-coordinates of all customers.
- **k-circular Convolution.** We take k-concentric circles, centered at the depot, in such a way that the last circle has radius equivalent to the distance of the depot to its furthest customer. The radius for the other k 1 circles are uniformly distributed between the depot and the external circle. For each circle i > 0 of radius r_i , we compute the percentage of customers that lie in the flat donuts formed by the circles of radius r_i and r_{i-1} . For this work, we take k = 100.
- **Customers Matrix.** This matrix is equivalent to the one used in (Huerta et al., 2022): It is a 128×128 matrix that is computed as follows. We uniformly divide the euclidean space in which the customers are disposed in a 128×128 layout and, for each of the 16384 cells, we compute the number of customers that are contained in the cell. For normalization purposes, a top threshold value can be set for really crowded cells.

The first four features are used in all the models, whereas k-circular convolution is used for RF, KNN, AB and GB, and the customers matrix is used only for CNN.

3.4 Instance Labeling

The instance labeling entails the computation of the ground-truth label of each instance. As explained earlier, this is the value of r that gives the best performance of the Sweep algorithm for this instance. This is given to the ML algorithms as the labels for the training set.

3.5 Machine Learning Models Used

For training our regression model, we used several ML algorithms. The parameters for the models were adjusted using *k*-fold cross validation (Stone, 1974), with k = 5. The results of this hyper-parameter tuning and further details on each of the algorithms are as follows:

Random Forests: $n_estimators = 510$

k-Nearest Neighbors: k = 210

Gradient Boost: loss = MSE, $learning_rate = 0.1$, $n_estimators = 100$.

Ada Boost: $learning_rate = 0.1$, $n_estimators = 50$.

- **Convolutional Neural Networks:** The CNN is formed by the following layers:
 - 3 convolutional layers with 16,32 and 48, 3 × 3sized filters,
 - 2 pooling layers of sizes 2×2 ,
 - a dense layer of 32 nodes
 - a layer that concatenates the previous layer with the 4 features corresponding the number of customers, capacity, width, height,
 - 4 fully connected layers of sizes 512, 128, 32 and 10, the last one corresponding to the output of the network.

All layers use the ReLu, a piece-wise linear activation function (Agarap, 2018), with the exception of the last one, which uses a linear activation function.

3.6 Meta-Sweep-Algorithm

The Meta-Sweep-Algorithm (MSA) is a per-instance automatically configured algorithm. This metaalgorithm first computes the features, defined in Subsection 3.3, associated with an input instance, which are then fed to the selected machine-learning-based oracle to predict the best parameter value. Then, the meta-algorithm runs the sweep algorithm with this predicted radius parameter.

4 EXPERIMENTAL RESULTS

4.1 Comparing the Parameter Prediction Quality of Different Machine Learning Algorithms

The training and testing of the five ML algorithms were performed on a machine with a 3.3Ghz AMD Ryzen 9 5900HS processor with 16GB of RAM. A Nvidia RTX 3060 GPU was also used for the training of CNN. We used the Machine Learning Algorithms implemented in the Scikit-learn and Keras (tensorflow) modules of Python.



Figure 6: Quality (in terms of MSE) and running time comparison of ML algorithms.

Figure 6 shows the performance of the parameter prediction of the five ML-algorithms. The performance is measured in terms of MSE across the training set and the running time (shown as mean and standard deviation). As can be seen, GB and CNN are the algorithms with largest MSE value. Moreover, for AB, the running time is the largest. KNN delivers, on average, predictions of best quality and at the fastest running time. RF and GB perform slightly worse in quality, and take longer times (up to $3 \times$ the time needed by KNN). Hence, for the rest of this section, we report on results obtained by KNN.

In Figure 7 we contrast the ground-truth labels with the predicted labels as computed by the KNN algorithm. The ideal form of such graphic would be a perfect diagonal, but we can observe chunks of values for which the mislabeling is more common. For instance, we notice that the algorithm predicts very different values when the ground-truth values are close to 0. We also notice that the algorithm tends to predict a negative value (i.e. the second algorithm) more often than when the real "best" parameter indeed corre-



Figure 7: Ground truth labels vs predicted labels by KNN.

sponds to the second algorithm. This may not have an impact on the quality of the recommendation, since there may be parameter values for the first and second algorithms that generate very close solutions in the quality of the tour length. How this mislabelling affects the performance in the length of the resulting tour length is explored in the next subsections.

4.2 Comparison with Other CVRP Solvers

We compare the results of our Meta-Sweep-Algorithm (MSA) with other state-of-the-art solvers. Specifically, we compare with OR-tools CVRP solver (Perron and Furnon, 2019) with its default parameters' values, and with the publicly available FILO solver, described in (Accorsi and Vigo, 2021), also with its default parameters' values. The CVRP OR-tools solver is a constraint Programming solver that supports multiple CVRP formulations. The FILO solver is based on Iterated Local Search, which implements several already proposed and new neighborhoods, which acceptance criterion is based on that of Simulated Annealing, in order to continually diversifying and exploiting different regions of the search space. More importantly for this work, FILO's local search initialize with the solution obtained by a C++ implementation of the classic Savings heuristic for the VRP (Clarke and Wright, 1964), which we label CW.

For each of the 15333 instances in the testing set (a third of the benchmark set), we run the three algorithms: MSA, CW and OR-Tools. Figure 8 illustrates the difference in the performances of the algorithms. In this figure, each instance is presented as a point for each of the three algorithms in blue (MSA), orange (OR-Tools) and green (CW). The horizontal x-axis is the computation time (in log-scale) taken by the algorithms to produce a first solution. The vertical y-axis is the solution quality measured as the ratio of the solution value divided by the best value delivered by one of the three algorithms.



Figure 8: Time and quality comparison of MSA, OR-tools and CW algorithms.

As can be seen, compared to OR-Tools, MSA and CW produce better solutions and in dramatically faster time. Compared to CW, MSA is noticeably faster (on average 2x faster) and delivers most of the best solutions computed. The gap between the solutions both algorithms produce oscillates between very small values and up to 18%. The most extreme variations seem to happen for the fastest-to-compute instances, which are the smallest ones.

Table 2: Percentage of best solved instances per algorithm and average runtime, grouped by number of customers. # cust = number of customers. % MSA, % CW, % OT = percentage of instances in the group best solved by meta-sweep-algorithm, CW and OR-tools respectively, and t_MSA, t_CW, t_OT = average time needed to produce the first solution by meta-solver, CW and OR-tools respectively, in seconds.

# cust.	% MSA	t_MSA	% CW	t_CW	% OT	t_OT
500	82.89	0.03	17.11	0.02	0.0	1.77
1000	76.49	0.07	23.51	0.07	0.0	7.01
1500	75.68	0.11	24.32	0.13	0.0	15.61
2000	77.88	0.16	22.12	0.23	0.0	27.53
3000	73.76	0.23	26.24	0.5	0.0	61.43
4000	57.11	0.35	42.89	0.89	0.0	108.89
5000	56.93	0.44	43.07	1.4	0.0	169.41
6000	57.82	0.54	42.18	2.03	0.0	245.26

Table 2 reports the percentage of instances, out of the 15333 instances, that are best solved by each of the algorithms. It also shows the average time needed by each algorithm to compute the solutions. This is reported for each group of instances that share the same number of customers. The results in this table indicate that MSA finds solutions much faster than the other algorithms–up to two orders of magnitude faster than OR-Tools, and about a factor of 2 faster than CW. Also, MSA finds better quality solutions for most instances.

4.3 The Effectiveness of the KNN Oracle

One way of evaluating the effectiveness of the oracle, as proposed in (Dunning et al., 2018), is to make it predict the best p values of r for each instance, and compare them to a "single" best vector of values of r for the entire dataset. This is a generalization of the SBS as discussed in Section 2.5, which we call p-SBS. For this, the model is trained to output not only one, but the p best values of r. Here we set p = 10. For SBS, it is run for the first p parameter values in the ranked list from Table 1, (0, -0.5, -0.49, -0.4, -0.51, -0.42, -0.39, -0.48, -0.41, -0.43).



Figure 9: Percentage of instances that are best solved using *p* parameter values, for MSA and *p*-SBS.

Figure 9 shows that the use of the oracle in MSA provides significant improvement over *p*-SBS, both of which use the same number of "best" parameter values. Whereas *p*-SBS selects parameter values from a fixed list, the oracle provides MSA parameter values that depend on the instance. As we can see, in the base case in which a single parameter value is used, MSA is able to dynamically pick a best possible parameter value for up to 29% of the instances. This contrasts with SBS, which is only able to do so for 14.58% of the instances using the fix parameter value of 0. We can see that the gap between MSA and *p*-SBS on the percentage of instances for which a best parameter can be found, among the *p* alternatives, increases.

Figure 10 illustrates how the quality of the solution of MSA and *p*-SBS improves as a function of increased number *p* of top-ranked parameter values to be tested in the algorithm. As can be seen, in the base case where a single parameter value is tested, MSA delivers solutions with close to 0.6% gap, on average, compared to the best possible delivered by VBS. In contrast, SBS delivers solutions that have a gap close to 5%. This difference between MSA and SBS diminishes dramatically when picking a second parameter



Figure 10: Gap percentage within the cost using *p* parameter values and the best known cost, for MSA and *p*-SBS.



Figure 11: \hat{m} values for each p in the range $[1, \ldots, 10]$.

to test. For 4 or more parameter values, the difference becomes minimal.

Another evaluation metric that is usually taken into account for automatic algorithm selection tasks is the \hat{m} metric, presented in Subsection 2.5. Figure 11 shows how the \hat{m} value behaves as p increases. We recall that values closer to 0 mean that the meta-solver behaves close to the Virtual Best Solver and that values close to 1 mean that the solver behaves more like the p-SBS. Note that while increasing p, the \hat{m} value tends to get worse because the larger p is, the more likely the performance of p-SBS is to improve.

5 CONCLUSIONS AND FUTURE WORK

We demonstrate here that using ML for automatic selection of an algorithm's parameters improves significantly the quality of the solution provided. This proof of concept is given here for the case of CVRP and the sweep algorithm with the radius parameter. We present a comparison of several ML algorithms for selecting automatically the radius parameter. In our experiments, KNN is the best performing. Using KNN for automatically selecting the radius parameter, we compare the performance of our meta-solver (MSA) with two publicly available state-of-the-art CVRP solvers: OR-tools (Perron and Furnon, 2019) and FILO (Accorsi and Vigo, 2021) showing that automatic selection of the radius parameter provides fast and high quality solutions. Specifically, MSA always dramatically improves on the quality and running time of OR-tools. For comparison with FILO (which entails comparison with Clark-Wright), the improvement is particularly notable for large-scale instances with relatively small number of trucks (i.e. ratio of total number of customers divided by the truck capacity).

We further introduce here two new CVRP benchmark sets based on real addresses in Los Angeles and New York City. These include about one million customers each and a collection of 46000 instances that are random subsets of these benchmarks.

Future research plans are to build a CVRP metasolver that considers a portfolio of additional algorithms based on local search and exact methods. We also plan to expand the functionality of the metasolver by adding capabilities of having user-specified limits on the running time and other computational resources.

ACKNOWLEDGEMENTS

This research was supported in part by AI Institute NSF Award 2112533.

REFERENCES

- Accorsi, L. and Vigo, D. (2021). A fast and scalable heuristic for the solution of large-scale capacitated vehicle routing problems. *Transportation Science*, 55(4):832– 856.
- Agarap, A. F. (2018). Deep learning using rectified linear units (relu). arXiv preprint arXiv:1803.08375.
- Alesiani, F., Ermis, G., and Gkiotsalitis, K. (2022). Constrained clustering for the capacitated vehicle routing problem (cc-cvrp). *Applied Artificial Intelligence*, pages 1–25.
- Alloghani, M., Al-Jumeily, D., Mustafina, J., Hussain, A., and Aljaaf, A. J. (2020). A systematic review on supervised and unsupervised machine learning algorithms for data science. *Supervised and unsupervised learning for data science*, pages 3–21.
- Alpaydin, E. (2021). Machine learning. MIT Press.
- Applegate, D. L., Bixby, R. E., Chvátal, V., Cook, W., Espinoza, D. G., Goycoolea, M., and Helsgaun, K. (2009). Certification of an optimal tsp tour through 85,900 cities. *Operations Research Letters*, 37(1):11– 15.

- Arnold, F., Gendreau, M., and Sörensen, K. (2019). Efficiently solving very large-scale routing problems. *Computers & operations research*, 107:32–42.
- Bogyrbayeva, A., Meraliyev, M., Mustakhov, T., and Dauletbayev, B. (2022). Learning to solve vehicle routing problems: A survey. arXiv preprint arXiv:2205.02453.
- Breiman, L. (1996). Bagging predictors. *Machine learning*, 24(2):123–140.
- Breiman, L. (2001). Random forests. *Machine learning*, 45(1):5–32.
- Burkart, N. and Huber, M. F. (2021). A survey on the explainability of supervised machine learning. *Journal of Artificial Intelligence Research*, 70:245–317.
- Carbone, R. and Armstrong, J. S. (1982). Note. evaluation of extrapolative forecasting methods: results of a survey of academicians and practitioners. *Journal of Forecasting*, 1(2):215–217.
- Clarke, G. and Wright, J. W. (1964). Scheduling of vehicles from a central depot to a number of delivery points. *Operations research*, 12(4):568–581.
- Dondo, R. and Cerdá, J. (2013). A sweep-heuristic based formulation for the vehicle routing problem with cross-docking. *Computers & Chemical Engineering*, 48:293–311.
- Dunning, I., Gupta, S., and Silberholz, J. (2018). What works best when? a systematic evaluation of heuristics for max-cut and qubo. *INFORMS Journal on Computing*, 30(3):608–624.
- Elshaer, R. and Awad, H. (2020). A taxonomic review of metaheuristic algorithms for solving the vehicle routing problem and its variants. *Computers & Industrial Engineering*, 140:106242.
- Fellers, J., Quevedo, J., Abdelatti, M., Steinhaus, M., and Sodhi, M. (2021). Selecting between evolutionary and classical algorithms for the cvrp using machine learning: optimization of vehicle routing problems. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, pages 127–128.
- Fix, E. and Hodges, J. L. (1989). Discriminatory analysis. nonparametric discrimination: Consistency properties. *International Statistical Review/Revue Internationale de Statistique*, 57(3):238–247.
- Friedman, J. H. (2001). Greedy function approximation: a gradient boosting machine. *Annals of statistics*, pages 1189–1232.
- Fukushima, K. and Miyake, S. (1982). Neocognitron: A self-organizing neural network model for a mechanism of visual pattern recognition. In *Competition and cooperation in neural nets*, pages 267–285. Springer.
- Gillett, B. E. and Miller, L. R. (1974). A heuristic algorithm for the vehicle-dispatch problem. *Operations research*, 22(2):340–349.
- Haimovich, M. and Rinnooy Kan, A. H. (1985). Bounds and heuristics for capacitated routing problems. *Mathematics of operations Research*, 10(4):527–542.
- Huerta, I. I., Neira, D. A., Ortega, D. A., Varas, V., Godoy, J., and Asín-Achá, R. (2022). Improving the state-ofthe-art in the traveling salesman problem: An anytime

automatic algorithm selection. *Expert Systems with Applications*, 187:115948.

- Kerschke, P., Hoos, H. H., Neumann, F., and Trautmann, H. (2019). Automated algorithm selection: Survey and perspectives. *Evolutionary computation*, 27(1):3–45.
- Lin, S. and Kernighan, B. W. (1973). An effective heuristic algorithm for the traveling-salesman problem. *Operations research*, 21(2):498–516.
- Lindauer, M., Hoos, H. H., Hutter, F., and Schaub, T. (2015). Autofolio: An automatically configured algorithm selector. *Journal of Artificial Intelligence Research*, 53:745–778.
- Lindauer, M., van Rijn, J. N., and Kotthoff, L. (2019). The algorithm selection competitions 2015 and 2017. *Artificial Intelligence*, 272:86–100.
- López-Ibáñez, M., Dubois-Lacoste, J., Cáceres, L. P., Birattari, M., and Stützle, T. (2016). The irace package: Iterated racing for automatic algorithm configuration. *Operations Research Perspectives*, 3:43–58.
- McCulloch, W. S. and Pitts, W. (1943). A logical calculus of the ideas immanent in nervous activity. *The bulletin of mathematical biophysics*, 5(4):115–133.
- Perron, L. and Furnon, V. (2019). Or-tools.
- Pessoa, A. A., Poss, M., Sadykov, R., and Vanderbeck, F. (2021). Branch-cut-and-price for the robust capacitated vehicle routing problem with knapsack uncertainty. *Operations Research*, 69(3):739–754.
- Quinlan, J. R. (1986). Induction of decision trees. *Machine learning*, 1(1):81–106.
- Rice, J. R. (1976). The algorithm selection problem. In Advances in computers, volume 15, pages 65–118. Elsevier.
- Schapire, R. E. (1997). Using output codes to boost multiclass learning problems. In *ICML*, volume 97, pages 313–321. Citeseer.
- Schapire, R. E. (2013). Explaining adaboost. In *Empirical inference*, pages 37–52. Springer.
- Stone, M. (1974). Cross-validatory choice and assessment of statistical predictions. *Journal of the royal statistical society: Series B (Methodological)*, 36(2):111– 133.
- Zhu, X. and Goldberg, A. B. (2009). Introduction to semisupervised learning. *Synthesis lectures on artificial intelligence and machine learning*, 3(1):1–130.