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# Zero Training Overhead Portfolios for Learning to Solve Combinatorial Problems

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## Abstract

There has been an increasing interest in harnessing deep learning to tackle combinatorial optimization (CO) problems in recent years. Typical CO deep learning approaches leverage the problem structure in the model architecture. Nevertheless, the model selection is still mainly based on the conventional machine learning setting. Due to the discrete nature of CO problems, a single model is unlikely to learn the problem entirely. We introduce **ZTop**, which stands for Zero Training Overhead Portfolio, a simple yet effective model selection and ensemble mechanism for learning to solve combinatorial problems. **ZTop** is inspired by algorithm portfolios, a popular CO ensembling strategy, particularly restart portfolios, which periodically restart a randomized CO algorithm, de facto exploring the search space with different heuristics. We have observed that well-trained models acquired in the same training trajectory, with similar top validation performance, perform well on very different validation instances. Following this observation, **ZTop** ensembles a set of well-trained models, each providing a unique heuristic with *zero training overhead*, and applies them, sequentially or in parallel, to solve the test instances. We show how **ZTopping**, i.e., using a ZTop ensemble strategy with a given deep learning approach, can significantly improve the performance of the current state-of-the-art deep learning approaches on three prototypical CO domains, the hardest unique-solution Sudoku instances, challenging routing problems, and the graph maximum cut problem, as well as on multi-label classification, a machine learning task with a large combinatorial label space.

## 1. Introduction

Deep learning has achieved tremendous success in many areas, including visual object recognition, neural machine translation, and autonomous driving. In contrast, combinatorial optimization problems are challenging for deep learning given that, in general, they are unsupervised or weakly supervised and have a large combinatorial solution space (Bengio et al., 2020; Kool et al., 2018). A classical approach to solving CO problems is to design useful heuristics manually to guide the algorithm on exploring the large combinatorial search space. Nevertheless, a heuristic is typically specialized for a specific problem, and it is not trivial to adapt to other CO problems. Deep reinforcement learning (DRL) is becoming a go-to approach for learning heuristics for CO problems (Bello et al., 2016; Mazyavkina et al., 2020). The hope is that DRL generalizes well to tackle several CO problems by learning heuristics from scratch. The architecture design of a deep learning framework leverages the specific problem structure, e.g., it employs the attention mechanism for routing problems (Kool et al., 2018). However, the model selection method still follows the conventional machine learning style, i.e., it selects only the model with the best validation performance from the same training trajectory. Due to the problems' combinatorial nature, we conjecture that a single model typically is not enough to capture the entire problem structure well and learn a useful heuristic for solving the potentially very different problem instances. We propose a new model selection and ensemble method to tackle this challenge.

The runtime and performance of combinatorial optimization algorithms for a given problem can vary significantly from instances to instances, depending on the heuristics used. Even when solving the same instance, a randomized heuristic can also vary dramatically. In fact, the run time distributions of combinatorial optimization algorithms often exhibit heavy tails (Gomes et al., 2000). To remedy and even exploit the heavy-tailed phenomena and large performance variance of CO search methods, *algorithm portfolios*, and in particular *restart portfolios*, are widely used in the CO community (Gomes & Selman, 2001; Xu et al., 2008; Gomes et al., 1998; Biere & Fröhlich, 2018). Essentially, in restart portfolios, the CO algorithms are periodically restarted to

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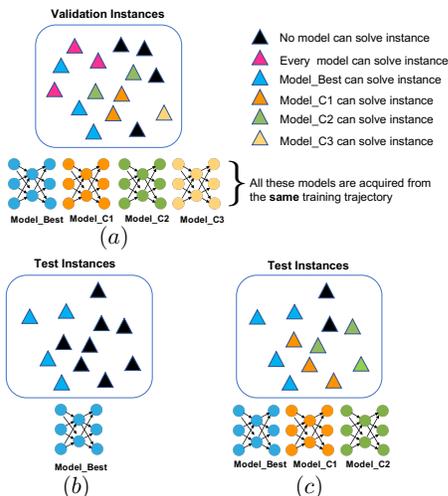


Figure 1. **High-level concept of the ZTop ensemble method.** Assume we use a deep learning model to solve Sudoku. The top rectangle represents Sudoku validation instances. A model (heuristic) can solve the validation instances with the same color. All the well-trained models can solve pink instances. No model can solve black instances. Specific models (other colors) can solve other instances (a) The model selection mechanism of ZTop. We observe that well-trained models (i.e., with similar validation performance) acquired in the same training trajectory can solve significantly diverse instances. (b) Traditional model selection method, i.e., selecting the model with the best validation performance. Due to the combinatorial nature of CO problems, a single model typically cannot learn the problem entirely, so it can only solve few instances. (c) The ZTop method selects several additional models with zero training overhead. These models have similar validation performance but the test instances they can solve are quite different. Thus, applying these models sequentially or in parallel to solve instances and taking the best output can work well for most instances.

explore different search space parts, using randomized or pseudo-randomized heuristics and caching useful run information. De facto *restarts* correspond to using thousands of heuristic variants, with low heuristic switching costs.

We have also observed a large variance in the deep learning models’ performance when considering CO problems. In a deep learning setting, we acquire lots of models during the same training trajectory, and each model can be viewed as a heuristic. However, using thousands of models in the test phase would be computationally intractable. Our goal is to select a few models covering very diverse heuristics.

**Our Contributions:** (1) ZTop, a simple yet *effective mechanism to select a diverse set of models covering different heuristics* with *zero training overhead* (see Fig. 1). The basic idea is to find a few models from the same training trajectory with similar *average* performance (near the best model’s performance) but with a high variance with respect

to the instances they can solve. Near best performance assures these models are well-trained, while the variance indicates they potentially capture uniquely different heuristics. (2) ZTop also provides *an ensemble technique to leverage different models*. Conventional ensemble methods (averaging the decisions of different models) do not work well, as we show in the experimental section, since one heuristic typically works only for a group of instances. Averaging all the heuristics may cancel out each heuristic’s contribution. So we propose a new ensemble method that applies each model sequentially or in parallel to each test instance and takes the best output per instance. ZTop’s training time is identical to the training time of a *single* model, since ZTop selects the models from the same training trajectory. During the test time, we have a similar computing overhead as the traditional ensemble. For each test instance, we compute every models’ output and take the best one instead of averaging their outputs. (3) ZTop *substantially improves the performance of very different learning frameworks on three prototypical CO domains*, the hardest unique solution Sudokus (Chen et al., 2020), the routing problem (Kool et al., 2018), and the graph maximum cut problem (Barrett et al., 2020), as well as *multi-label classification (MLC), a machine learning task with a large combinatorial label space, with zero training overhead*. These frameworks cover *various architecture and learning methods*: for Sudoku, a modified Long Short Term Memory (LSTM) (Hochreiter & Schmidhuber, 1997) with weakly supervised learning, for routing problems, a pointer network with attention encoder with reinforcement learning (RL), for Maximum Cut, structure2vector (s2v) with RL, and for MLC, Label Message Passing (LaMP) (Lanchantin et al., 2019) and Higher Order correlation VAE (HotVAE) (Zhao et al., 2021).

## 2. Related Work

**Deep Learning for Combinatorial Optimization (CO):** Several CO deep learning model architectures leverage the problem structures for learning better heuristics. Structure2Vector (s2v) (Dai et al., 2016; Khalil et al., 2017b) was proposed for graph instances. For each node of the graph, a feature vector can be learned, capturing the properties of itself and its neighbors. A Pointer Network (PN) (Vinyals et al., 2015) computes the permutation of variable length sequence data. This subtle model can naturally capture many CO constraints. Graph Neural Networks are also employed for SAT instances (Selsam et al., 2018; Kurin et al., 2019). A modified LSTM, i.e., each LSTM step’s input is multiplied with a constraint graph capturing the Sudoku constraints, performs very well on weakly-supervised learning to solve challenging Sudoku problems (Chen et al., 2020). Creating a large labeled dataset is computationally intractable for CO problems. So, deep reinforcement learning or weakly

supervised learning is used to learn CO problems, ranging from routing problems (Bello et al., 2016; Kool et al., 2018), the maximum cut problem (Khalil et al., 2017a; Barrett et al., 2020) to the minimum vertex cover problem (Khalil et al., 2017a; Song et al., 2020). Several approaches combine deep models with search algorithms (Kool et al., 2018; Deudon et al., 2018; Abe et al., 2019) to further improve the performance. *ZTop can further significantly improve the performance on top of these learning approaches.*

**Ensemble Methods in Deep Learning:** Neural network ensembles (Zhou et al., 2002; Polikar, 2006; Rodriguez et al., 2006) have been widely used to boost the model’s performance in the machine learning community. However, they mainly focus on (weighted) averaging the output of the models and training a set of heterogeneous models requiring substantial computational resources. Due to the considerable overhead of traditional ensemble methods, the deep learning community proposes several methods to remedy this issue. “Implicit” ensembles (Srivastava et al., 2014; Wan et al., 2013; Huang et al., 2016; Singh et al., 2016; Krueger et al., 2016; Han et al., 2017) are proposed as an alternative to traditional ensemble methods given their minor overhead in both the training and test phase. One example of “implicit” ensembles is Dropout (Srivastava et al., 2014), which randomly zeros some hidden neurons during each training step. At the test time, every neuron is kept and scaled by the keeping probability of the training phase. An explanation of dropout is that there are a considerable number of models created by dropping neurons, and these models are implicitly ensembled at the test phase. Similar to the dropout mechanism, stochastic depth (Huang et al., 2016) proposes to randomly drop some layers during the training time to create different models with various depths. These implicit ensemble methods create many shared-weights models and ensemble them in the test phase implicitly. Several works focus on efficiently acquiring many good models (Huang et al., 2017; Zhang et al., 2020) to decrease the training cost. Snapshot ensemble (Huang et al., 2017) leverages the cyclic learning rates (Loshchilov & Hutter, 2016) to force the model to jump from one local minimum to another local minimum, and ensemble these models of different local minimum to reduce the training phase overhead. However, cyclic learning rates can potentially damage the model’s performance, and it is designed for only convolution neural networks. Another line of research focuses on reducing the test time overhead (Buciluă et al., 2006; Hinton et al., 2015; Shen et al., 2019; Ian et al., 2018). Distill (Hinton et al., 2015) proposes to employ the ensemble of many models as the training label of a single model (similar or smaller size). Learning to improve (L2I) (Lu et al., 2019) proposes a new way to leverage models. L2I employs the model to guide their local search, and they find that taking the best results of many models with

small rollout steps is better than one model with much larger rollout steps. However, L2I requires to train these models separately, and the training method is designed specifically for their learning framework.

Ensemble methods for MLC fall into three groups: the first group is to ensemble binary relevance classifiers (Read et al., 2011; Wang et al., 2016); the second group is to ensemble label powerset classifiers (Read et al., 2008; Tsoumakas et al., 2010); and, the third group uses random forest of predictive clustering trees (Kocev et al., 2007). All the ensemble methods above except for L2I rely on (weighted) averaging the outputs of many models.

*Algorithm Portfolios*, used by the CO community (Gomes & Selman, 2001; Leyton-Brown et al., 2003; Xu et al., 2008), ensemble different algorithms and solvers to solve a CO problem. In particular, *restart portfolios (restarts)* are widely used in the SAT community (Gomes et al., 1998; Biere & Fröhlich, 2018), since they are an effective way of combating long and heavy tailed runtime distributions (Gomes et al., 2000). They are also used in stochastic optimization to solve non-convex problems (Dick et al., 2014; Gagliolo & Schmidhuber, 2007). *Restarts* periodically restart an algorithm, de facto trying different (pseudo) randomized heuristics, with low heuristic-switching cost.

**Restarts in Deep Learning (DL):** As an example of *restarts* in DL, the learning rate is reset based on some manually designed metrics to speed up the training or improve the performance (Gotmare et al., 2018; Loshchilov & Hutter, 2016). DRNets (Chen et al., 2020) also employ restarts in the optimization phase to improve performance, with different random seeds. Nevertheless restarts are not often employed in the deep learning community.

*A key feature that differentiates ZTop is that it leverages different models from the same training trajectory in the test phase to improve performance, with zero training overhead.*

### 3. ZTop, a Novel Ensemble Method

**ZTop** is a novel ensemble method that selects a set of diverse models for learning to solve CO problems incurring zero training overhead, inspired by the *restart portfolios*. The selected models are applied sequentially or in parallel to solve the test instances, taking the best output per instance. **ZTop** can be used on top of any weakly supervised or reinforcement CO learning framework, or even in some cases on top of a supervised framework, to significantly improve the performance, with zero training overhead and the same test overhead as traditional ensemble methods.

Due to the discrete nature of many CO problems, an oracle heuristic, i.e., a heuristic that works for almost every instance, is unlikely to exist. In the CO community, *restarts*

**Algorithm 1** ZTop method workflow

**Input:** Split Dataset  $D_{train}, D_{val}, D_{test}$ , performance metric  $\phi$ , number of ensemble models  $n$   
**for** epoch= 1 **to**  $max\_epoch$  **do**  
    Update model’s parameters using  $D_{train}$   
    Test model on  $D_{val}$ , **save the test result along with model’s parameters in  $val\_res$  object**  
**end for**  
Compute the performance metric  $\phi$  based on  $val\_res$ .  
Select the top  $n$  models, denoted as  $M_1, \dots, M_n$ , w.r.t  $\phi$ .  
**for**  $i = 1$  **to**  $n$  **do**  
    Test model  $M_i$  on  $D_{test}$ , and save the result as  $res_i$   
**end for**  
**for all**  $x \in D_{test}$  **do**  
    Take the best output of  $x$  in  $res_{i,i=1\dots n}$   
**end for**

are widely employed to remedy this issue by periodically switching to a new heuristic. We postulate that it is also difficult for a single deep learning model to perfectly solve all kinds of instances. Surprisingly, we have observed that several models acquired through the **same** training trajectory contain quite diverse heuristics. These models have similar validation performance, but the subsets of the validation set they perform well vary significantly. It is then promising to select several models from the same training trajectory instead of a single one.

**Selecting diverse models from the same training trajectory.** The goal is to select several models with similar validation performance, but they should perform well on different subsets of the validation set. Often, in CO problems, we naturally have a metric  $\phi$  to validate the model’s performance, e.g., the average length of the route in the TSP problems. Surprisingly, selecting top-k models with respect to the metric  $\phi$  on the validation set can achieve the goal. The resulting set of models have very comparable performance as the optimal set of models found by enumerating all the possible combinations, as we show in the experimental section. In terms of the training time overhead, we mark the additional training operation of **ZTop** in blue in the Alg. 1. We only need to store each model’s validation performance along with its parameters. This additional operation incurs zero training cost since traditional model selection also needs to validate these models.

How to leverage these models is another issue. Each model can be viewed as a heuristic, and different heuristics typically work for different instance groups. So averaging these models’ output may cancel out each heuristic’s contribution.

**Ensembling models at test time.** **ZTop** applies its models sequentially or in parallel to solve each test instance and selects the best output per instance (see Alg. 1). For weakly-

supervised or reinforcement learning (RL) settings, it is natural to have a metric, e.g., the reward used in RL, to select the best output. Consider using a deep model to solve Sudoku. We employ ZTop’s models to solve test Sudoku instances sequentially. If any model solves a test instance, no need to try other models. Note that each test instance is only fed once into each model, so our test time overhead is identical to that of traditional ensemble methods.

**4. Experiments**

We show the performance of the **ZTop** approach on various CO problems learning frameworks and two MLC learning frameworks.

**4.1. General Experiment Settings**

**Baselines.** **ZTop** has zero training overhead, thus we compare it with methods that share similar training overhead with us. The first baseline is the conventional machine learning model selection scheme (denoted as **Single**), i.e., it selects a single model with the best validation performance. Note here, the learning framework’s training strategy consists of proper implicit ensemble methods. So we are also comparing **ZTop** with these implicit ensemble methods. In terms of leveraging the models, we also compare **ZTop** with the conventional ensemble method, i.e., averaging the output of all models. We denote this baseline as **Average**: picking top models w.r.t metric  $\phi$  and averaging the outputs of them. The last method is our method **ZTop**: selecting top models w.r.t metric  $\phi$  and taking the best output per instance.

**Settings for the learning framework.** **ZTopping** a given learning approach involves adapting released codes and following the original paper’s settings (for training/test instances, train models, and test models’ performance).

**4.2. Hardest unique solution Sudoku**

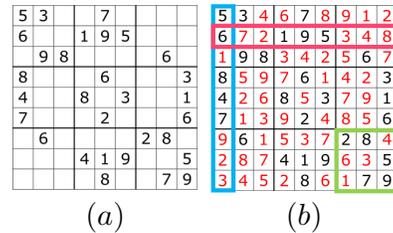


Figure 2. **Sudoku:** (a) a  $9 \times 9$  Sudoku with 30 hints. (b) The solution to (a); the three rectangles represent the three types of constraints (no repetition of digits per row, column, or block).

Sudoku is an NP-hard combinatorial number-placement puzzle on an  $n \times n$  board. We focus on the Sudoku problems on  $9 \times 9$  boards, as they are most widely studied. The object is to complete a  $9 \times 9$  board, pre-filled with several hints

Single (0)	Single (10)	# Ensemble Models	Average (0)	ZTop (0)	Average (10)	ZTop (10)
0.289	0.387	3	0.364	<b>0.549</b>	0.569	<b>0.588</b>
		5	0.443	<b>0.652</b>	0.651	<b>0.707</b>
		10	0.469	<b>0.753</b>	0.670	<b>0.815</b>
		20	0.475	<b>0.813</b>	0.452	<b>0.867</b>

Table 1. **ZTopping DRNets, on 1,000 17 hint Sudokus.** DRNets is the state of the art for unsupervised Sudoku (Chen et al., 2020). Sudoku accuracy of 17 hint Sudokus for single and ensemble models, under two test modes: 0 and 10 optimization steps. The number in parentheses next to the modality is the optimization step used in the test mode. We mark ZTop’s results in blue and bold the best results. ZTop significantly improves the DRNets’ performance and outperforms the traditional averaging ensemble method on the two test modes.

(numbers pre-assigned to cells), with numbers 1 to 9. In a Sudoku, each row, column, and pre-defined  $3 \times 3$  box cannot have a repeated digit (see Fig. 2). It has been showed that 17 is the minimum number of hints for which a Sudoku has a unique solution (McGuire et al., 2012). So we focus on solving  $9 \times 9$  Sudokus with 17 hints.

We select DRNets (Chen et al., 2020) as the learning framework since it is the state-of-the-art weakly-supervised learning Sudoku framework, supervised **only** by the Sudoku rules. It employs continuous relaxation to convert the discrete constraints to differentiable loss functions. The training and test of DRNets only require Sudokus without labels.

DRNets assign each digit a learnable embedding and a tensor represents a Sudoku instance. A modified LSTM computes the missing digits given the Sudoku tensor as input. We create 100,000 Sudoku with 18 to 25 hints for training and validating the models and 1000 Sudoku with 17 hints for testing the model. The other training/validating/testing settings also strictly follow the original paper.

To ensure the model candidates are well-trained, we save the top 100 models from the training phase in terms of the validation performance. Then we select models based on the performance metric  $\phi$ , which in this case is the Sudoku accuracy, i.e., the number of Sudoku this model correctly solved. We do not assign partial credits. We evaluate the ensemble performance of 3, 5, 10, and 20 models.

**Sudoku Accuracy.** The results are summarized in Table 1. We consider two test modes of the DRNets framework: 0-step optimization mode and 10-step optimization mode. Since the loss function of DRNets is derived only from the Sudoku rules, it can still be optimized for the test instances. Here 0-step mode fixes the models’ parameters while 10-step mode optimizes the loss function 10 steps in the test phase. In all the cases, **ZTop** substantially outperforms the single model and standard averaging ensemble methods. We only require 10 models to achieve 75.5% Sudoku accuracy, considerably higher than the single model’s 28.9% Sudoku accuracy, reaching 86.7% with 20 models and 10 optimization steps. These results show that a set of diverse models are more effective than a single model to capture the varied

structure of 17 hint Sudoku instances.

### 4.3. A Series of Routing Problems

Routing problems are intensively studied in the CO community and have many real-world applications (Ross et al., 2019). We consider four routing problems and their variants. **Traveling Salesperson Problems (TSP):** Given a set of cities and the distance between any two cities, the goal is to find the shortest route that can traverse every city and return to the start city. **Vehicle Routing Problems (VRP):** This problem (Toth & Vigo, 2014) is a generalized TSP problem. Given a set of cities and a depot, each city has a demand, i.e., how many people intend to visit the city, the goal is to find an optimal set of routes to meet all the demands. We focus on two variants of this problem. **Capacitated VRP (CVRP):** The total cities’ demands in one route cannot exceed a pre-set threshold. **Split Delivery VRP (SDVRP):** This variant has the same constraint as CVRP, but here the demand of a city can be split through multiple routes. **Orienteering Problem (OP) (Golden et al., 1987):** We have a set of cities and know the distance between any two cities. Each city contains a prize. The object is to find a route whose length cannot surpass a threshold and we want to maximize the summation of the cities’ prizes in this route. **Prize Collecting TSP (PCTSP) (Balas, 1989):** This is a more challenging variant of the TSP problem. Each city is assigned a prize and a penalty. We need to find a route collecting at least a minimum total prize to minimize the route length plus the sum of missed cities’ penalty. **Stochastic PCTSP (SPCTSP):** This problem is quite similar to the PCTSP problem. The only difference is that the prize of each city is sampled from a fixed distribution. The salesperson only knows the *expected* prize of each city, and the true prize is revealed when visiting a city.

We select Kool et al.’s (Kool et al., 2018) learning framework (denoted as AM) for these routing problems since it is one of the state-of-the-art methods. This framework employs reinforcement learning (REINFORCE algorithm (Williams, 1992) with baselines) to learn efficient heuristics unsupervisedly. Thus, the training, validation, and test of this framework only require problem instances. The model

### ZTop: Zero Training Overhead Portfolios

Method		n = 20		n = 50		n = 100	
		Obj.	Time	Obj.	Time	Obj.	Time
TSP ↓	Single AM	3.85	1s	5.81	2s	8.11	6s
	Average AM (m=3/5/10)	3.85/3.85/3.85	3s/5s/10s	5.81/5.81/5.81	6s/10s/20s	8.09/8.09/8.09	18s/30s/60s
	ZTopping AM (m=3/5/10)	<b>3.84/3.84/3.84</b>	3s/5s/10s	<b>5.77/5.75/5.74</b>	6s/10s/20s	<b>8.03/8.00/7.97</b>	18s/30s/60s
CVRP ↓	Single AM	6.42	1s	11.02	3s	16.68	8s
	Average AM (m=3/5/10)	6.41/6.41/6.41	3s/5s/10s	11.01/11.01/11.01	9s/15s/30s	16.66/16.66/16.66	24s/40s/80s
	ZTopping AM (m=3/5/10)	<b>6.33/6.30/6.27</b>	3s/5s/10s	<b>10.86/10.80/10.74</b>	9s/15s/30s	<b>16.46/16.40/16.31</b>	24s/40s/80s
SDVRP ↓	Single AM	6.41	1s	10.96	4s	16.70	11s
	Average AM (m=3/5/10)	6.40/6.40/6.40	3s/5s/10s	10.95/10.95/10.95	12s/20s/40s	16.68/16.68/16.68	33s/55s/110s
	ZTopping AM (m=3/5/10)	<b>6.31/6.29/6.27</b>	3s/5s/10s	<b>10.80/10.76/10.70</b>	12s/20s/40s	<b>16.51/16.44/16.37</b>	33s/55s/110s
OP ↑	Single AM	5.18	1s	15.42	1s	31.21	5s
	Average AM (m=3/5/10)	5.19/5.19/5.19	3s/5s/10s	15.46/15.46/15.46	3s/5s/10s	31.21/31.20/31.20	15s/25s/50s
	ZTopping AM (m=3/5/10)	<b>5.27/5.30/5.32</b>	3s/5s/10s	<b>15.76/15.85/15.94</b>	3s/5s/10s	<b>31.77/31.94/32.14</b>	15s/25s/50s
PCTSP ↓	Single AM	3.19	1s	4.60	2s	6.24	5s
	Average AM (m=3/5/10)	3.19/3.19/3.19	3s/5s/10s	4.60/4.60/4.60	6s/10s/20s	6.24/6.24/6.24	15s/25s/50s
	ZTopping AM (m=3/5/10)	<b>3.16/3.15/3.15</b>	3s/5s/10s	<b>4.55/4.54/4.52</b>	6s/10s/20s	<b>6.16/6.14/6.11</b>	15s/25s/50s
SPCTSP ↓	Single AM	3.27	1s	4.66	2s	6.30	5s
	Average AM (m=3/5/10)	3.26/3.26/3.26	3s/5s/10s	4.66/4.66/4.66	6s/10s/20s	6.30/6.30/6.30	15s/25s/50s
	ZTopping AM (m=3/5/10)	<b>3.22/3.20/3.19</b>	3s/5s/10s	<b>4.59/4.57/4.55</b>	6s/10s/20s	<b>6.20/6.18/6.15</b>	15s/25s/50s

Method		n = 20		n = 50		n = 100	
		Obj.	Time	Obj.	Time	Obj.	Time
TSP ↓	ZTopping AM (m=100)	<b>3.84</b>	1.7min	<b>5.72</b>	3.4min	<b>7.93</b>	10min
	AM (sampling)	<b>3.84</b>	5min	5.73	24min	7.94	1h
CVRP ↓	ZTopping AM (m=100)	<b>6.21</b>	1.7min	<b>10.64</b>	5min	<b>16.19</b>	13.4min
	AM (sampling)	6.25	6min	<b>10.62</b>	28min	16.23	2h
SDVRP ↓	ZTopping AM (m=100)	<b>6.22</b>	1.7min	<b>10.61</b>	6.7min	<b>16.25</b>	18.4min
	AM (sampling)	6.25	9min	<b>10.59</b>	42min	16.27	3h
OP ↑ (distance)	ZTopping AM (m=100)	<b>5.36</b>	1.7min	<b>16.08</b>	1.7min	<b>32.41</b>	8.4min
	AM (sampling)	5.30	4min	16.07	16min	<b>32.68</b>	58min
PCTSP ↓	ZTopping AM (m=100)	<b>3.14</b>	1.7min	<b>4.50</b>	3.4min	<b>6.08</b>	8.4min
	AM (sampling)	3.15	5min	4.52	19min	<b>6.08</b>	1h
SPCTSP ↓	ZTopping AM (m=100)	<b>3.14</b>	1.7min	<b>4.52</b>	3.4min	<b>6.11</b>	8.4min
	REOPT (half)	3.31	25min	4.64	3h	6.16	16h

Figure 3. Performance of ZTop and state-of-the-art AM baselines on 10,000 instances. Ztop’s results are in blue and the best result for each problem is in bold. The variable  $n$  represents the number of cities/nodes of the problem. The variable  $m$  refers to the number of models used for ensemble. The up arrow next to the problem means the larger the better the results are while the down arrow means the smaller the better the results are. The top table compares all *direct* methods, i.e., no search included. While the bottom table compares Ztop using all the models and the sampling method. Due to the stochastic nature of SPCTSP, AM (sampling) does not work. We compare our method with REOPT (half), a C++ ILS-based algorithm proposed in the original paper. From the top table, we observe that ZTopping AM substantially outperforms AM and the conventional ensemble method using only 3 models for the ensemble. ZTopping AM using 100 the models can surprisingly excel the AM (sampling) method with a considerably shorter time in most cases.

architecture of AM is the pointer network (Vinyals et al., 2015) with an attention encoder. The graph of the problem is fed into the attention encoder to compute the graph embedding and node embeddings. Then the decoder of the pointer network generates the policy of the next action.

The solution generation process of AM is *incremental*, i.e., the model selects one node (city) per step conditioned on all the previous actions. The data generation and training processes are strictly following the original paper’s settings (Kool et al., 2018). We select the best 100 models from the training phase. We evaluate the ensemble performance of 3, 5, 10, and all the 100 models. The metric we used for each problem is illustrated below.

**Results.** We introduce one more baseline for the AM

method since it proposes a sampling method based on the model’s output. This method (denoted as **AM (sampling)**) can generate better solutions with considerable time. AM (sampling) samples 1280 solutions and report the best result for each problem. We now introduce the metrics (Obj. column of the table) used to evaluate the performance of each problem. All the metrics we report are averaged across all the test instances. **TSP**: length of the route, **CVRP**, **SDVRP**: length of the route that meets the capacity constraint, **OP**: the summation of prize collected in the route that meets the length constraint and **PCTSP**, **SPCTSP**: length of the route plus the penalty of missing cities. The results are summarized in Fig 3. The top table compares all the *direct* methods, i.e., they do not use any search to generate solutions. We can observe that ZTop significantly outperforms

## ZTop: Zero Training Overhead Portfolios

Method		n=20	n=40	n=60	n=100	n=200
		Max-Cut Approximation Ratio				
ER ( $n=20$ )	Single ECO-DQN	0.973	0.982	0.969	0.954	0.930
	Average ECO-DQN ( $m=3/5/10$ )	0.974/0.973/0.972	0.988/0.988/0.988	0.985/0.984/0.984	0.980/0.980/0.980	0.975
	ZTopping ECO-DQN ( $m=3/5/10$ )	<b>0.979/0.980/0.981</b>	<b>0.997/0.998/0.999</b>	<b>0.995/0.997/0.999</b>	<b>0.991/0.994/0.997</b>	<b>0.986/0.989/0.993</b>
BA ( $n=200$ )	Single ECO-DQN	0.958	0.941	0.935	0.929	0.909
	Average ECO-DQN ( $m=3/5/10$ )	0.943/0.931/0.927	0.904/0.957/0.880	0.892/0.880/0.867	0.883/0.8670.848	0.872/0.831/0.808
	ZTopping ECO-DQN ( $m=3/5/10$ )	<b>0.976/0.979/0.982</b>	<b>0.896/0.960/0.964</b>	<b>0.950/0.952/0.955</b>	<b>0.939/0.941/0.943</b>	<b>0.912/0.912/0.913</b>

Figure 4. Approximation ratios of ZTop and ECO-DQN baselines (100 instances). ZTop’s results are in blue and the best results are in bold. ER and BA refer to two types of the random graphs.  $m$  represents the number of models used for the ensemble. The variable  $n$  on the left and top represents the number of vertices of the training set graphs and the test set graphs respectively. ZTopping ECO-DQN substantially improves the ECO-DQN and outperforms the conventional averaging ensemble method in all the cases.

the AM learning framework even with only 3 models. We also compare the AM (sampling) method with our ZTop using all (100) models and the results are showed in the bottom table. In most cases, our method can also outperform the AM (sampling) method with a considerably shorter time. In the CVRP ( $n = 100$ ) problem, we achieve the mean length of route 16.19 in 13.4 minutes while AM (sampling) requires 2 hours to achieve only 16.23. In the SPCTSP ( $n = 100$ ) problem, we achieve 6.11 in 8.4 minutes while REOPT (half) algorithm requires a substantially long time of 16 hours to achieves a poorer performance 6.16. We also observe that averaging ensemble method sometimes even decreases the performance, e.g., the objective drops from 31.21 to 31.20 in the OP ( $n = 100$ ) problem. Moreover, in most cases, averaging ensemble method only achieves minor improvements.

### 4.4. Graph Maximum Cut Problem

The graph maximum cut problem is a classical problem in graph theory. The cut of a graph is a partition of the vertex set into two complementary sets and the number of edges or the sum of edges’ weight between these two sets is denoted as the cut’s capacity. The maximum cut is the cut that has a maximum capacity.

We employ the state-of-the-art ECO-DQN (Barrett et al., 2020) as the learning framework for the maximum cut problem. ECO-DQN leverages reinforcement learning (Deep Q learning (Mnih et al., 2015)) to learn useful heuristics unsupervisedly. So, like the AM learning framework, we do not require any solution to train the model. The model architecture of ECO-DQN is Message Passing Neural Networks (MPNN) (Gilmer et al., 2017). It represents each vertex as an embedding. Several rounds of message passing update the vertices’ embeddings. The probability distribution over all the actions is computed through a readout function. The ECO-DQN proposes the *test-time exploration* concept where their policy is to improve a given solution instead of constructing a solution from scratch. Their original evaluation protocol is to generate 50 random solutions on the fly, employ the model to improve them and pick the best

one. We generate 50 random solutions in advance and ensure every method is improving the same 50 solutions. We select 50 models uniformly from the last quarter of training epochs. We evaluate the ensemble performance of 3, 5, and 10 models. We report the approximation ratio averaged over all the test instances.

**Approximation Ratio.** We consider two types of random graphs used in the original paper (Barrett et al., 2020). One is Erdős-Rényi (denoted as ER) (Erdos et al., 1960), and the other is Barabasi-Albert (denoted as BA) (Albert & Barabási, 2002) with the edge weights belong to  $\{0, 1, -1\}$ . We select two worst-performance cases of the original paper to show ZTopping can improve the ECO-DQN learning framework. One case is to train the model on ER ( $n = 20$ ) graphs and tested on ER ( $n = 20, 40, 60, 100, 200$ ) graphs where  $n$  refers to the number of vertices, the other is to train the model on BA graphs and tested on BA ( $n = 20, 40, 60, 100, 200$ ) graphs. The results are summarized in Fig 4, and ZTop substantially improves the performance of ECO-DQN in all the scenarios. Furthermore, we also observe a similar phenomenon as in the routing problems: the averaging ensemble method decreases the performance. The more models we used for the averaging ensemble, the lower performance it achieves. This phenomenon verifies our assumptions that the averaging ensemble may cancel out each heuristic’s contribution.

We show that ZTop can substantially improve the performance of the three learning approaches above. Moreover, the three learning approaches cover two of the most popular architectures: pointer network and s2v, and they also cover both weakly-supervised learning and reinforcement learning algorithms. The variety of these learning frameworks illustrate the universality of our ZTop method.

### 4.5. Multi-Label Classification

Multi-label classification (MLC) is the problem of assigning a set of labels to a given object. MLC can be viewed as a combinatorial classification problem, since the potential MLC’s label set is the powerset of the set of single labels.

## ZTop: Zero Training Overhead Portfolios

Metrics		Single LaMP	ZTopping LaMP (m=5/10/15)	Single HotVAE	ZTopping HotVAE (m=5/10/15)
Bibtex (k = 159)	ebF1	0.4375	0.4393/0.4474/ <b>0.451</b>	0.4596	0.4741/0.4786/ <b>0.4818</b>
	miF1	0.4633	0.4686/0.4751/ <b>0.4778</b>	0.4755	0.498/0.4992/ <b>0.5028</b>
	maF1	0.3789	0.3763/0.3867/ <b>0.3867</b>	0.3835	<b>0.4013</b> /0.4008/0.3979
Reuters (k = 90)	ebF1	0.9008	0.9098/0.9128/ <b>0.9153</b>	0.9091	0.9178/0.9207/ <b>0.9214</b>
	miF1	0.8855	0.8934/0.8954/ <b>0.8969</b>	0.884	0.9/0.9004/ <b>0.9013</b>
	maF1	0.5589	0.5629/0.5777/ <b>0.5802</b>	0.5831	<b>0.6194</b> /0.6181/0.5932
Delicious (k = 983)	ebF1	0.3469	0.3597/0.3616/ <b>0.3625</b>	N/A	N/A
	miF1	0.3582	0.3707/0.3732/ <b>0.3745</b>	N/A	N/A
	maF1	0.2012	0.2044/0.2054/ <b>0.2061</b>	N/A	N/A
Yeast (k = 14)	ebF1	0.638	0.6372/0.6394/ <b>0.6421</b>	0.6468	0.6511/0.6516/ <b>0.6519</b>
	miF1	0.6473	0.6474/0.6489/ <b>0.6505</b>	0.6576	0.6605/ <b>0.6622</b> /0.6615
	maF1	0.4713	0.4774/ <b>0.4783</b> /0.4772	<b>0.462</b>	0.461/0.4607/0.4584

Figure 5. **Multi-label classification.** The performance of **ZTop** and LaMP/HotVAE on different datasets. **ZTop**’s results are in blue and the best result for each dataset is in bold.  $m$  is the number of models used for the ensemble.  $k$  is the number of labels. We report ebF1, miF1 and maF1 scores of these approaches. We observe that **ZTop** significantly improves single LaMP or HotVAE on all the datasets except for Yeast. **ZTop** only improves slightly on Yeast since the dataset is relatively simple, with only 14 labels.

MLC is typically a supervised problem, with no obvious unsupervised metric to identify the best model at test time. The MLC models from the same training trajectory are not as heterogeneous as those learned for more standard CO problems, such as TSP or Sudoku. Thus, different MLC models may focus on the object’s different label subsets and therefore an averaging ensemble method is a good strategy. So, **ZTop** selects top validation performance models and averages their outputs, in contrast to other CO problems with well defined unsupervised metrics.

We tested **ZTop** on the two top state-of-the-art learning approaches for MLC, Label Message Passing (LaMP) (Lanchantin et al., 2019) and Higher Order correlation VAE (HotVAE) (Zhao et al., 2021) and on four datasets: Bibtex (Katakis et al., 2008), Reuters (Lewis et al., 2004), Delicious (Bi & Kwok, 2013) and Yeast (Nakai & Kanehisa, 1992). **ZTop** trains a single MLC architecture and selects  $n$  models with the lowest validation losses. **ZTop** runs inference with the  $n$  models and averages their sigmoid scores for the final prediction probabilities. We consider **ZTop** ensembles with 5, 10, and 15 models. To our knowledge, there are no other deep learning ensemble methods for MLC.

**F1 scores.** We report three kinds of F1 scores: ebF1, miF1 and maF1 scores. The main results are summarized in Fig. 5. We can observe that **ZTopping** LaMP/HotVAE can significantly improve the LaMP/HotVAE on all the datasets except for Yeast. Yeast is a simple dataset with only 14 potential labels, so **ZTop** can only improve a little on that dataset.

### 4.6. Ablation Study

Herein we show how close **ZTop** ( $k$  models) is to the optimal  $k$ -model ensemble, computed by enumerating all possible

$k$ -model combinations, out of the top 100 validation models.

Problem	n = 20	n = 50	n = 100
	Approximation Ratio		
TSP	99.99	99.96	99.99
CVRP	99.93	99.95	99.99
SDVRP	99.98	99.99	99.99
OP (distance)	99.87	99.93	99.99
PCTSP	99.96	99.96	99.96
SPCTSP	99.96	98.97	99.99

Figure 6. The approximation ratio of performance between **ZTop** (3 best validation models wrt  $\phi$ ) and the optimal 3 models (out of top 100 validation models).  $n$  = number of graph vertices.

We only consider ensembles of size 3 since enumerating all the combinations requires considerable time. We compute the optimal 3-model ensemble (out of the top 100 validation models), for the different routing problems. The approximation ratios (Fig 6) are close to 1, the worst case is 98.97, which shows how **ZTop**’s strategy is near-optimal, given the top 100 validation models, implicitly selecting good and diverse models (heuristics) for these combinatorial problems.

## 5. Conclusion

We introduce the Zero Training Overhead Portfolio (**ZTop**) method, a simple yet effective model selection and ensemble mechanism to select a set of diverse models for learning to solve combinatorial problems. We demonstrate how **ZTopping** substantially improves the current state of the art deep learning frameworks on the hardest unique-solution Sudokus, a series of routing problems, the graph maximum cut problem, and multi-label classification.

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## References

- Abe, K., Xu, Z., Sato, I., and Sugiyama, M. Solving np-hard problems on graphs with extended alphago zero. *arXiv preprint arXiv:1905.11623*, 2019.
- Albert, R. and Barabási, A.-L. Statistical mechanics of complex networks. *Reviews of modern physics*, 74(1):47, 2002.
- Balas, E. The prize collecting traveling salesman problem. *Networks*, 19(6):621–636, 1989.
- Barrett, T., Clements, W., Foerster, J., and Lvovsky, A. Exploratory combinatorial optimization with reinforcement learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pp. 3243–3250, 2020.
- Bello, I., Pham, H., Le, Q. V., Norouzi, M., and Bengio, S. Neural combinatorial optimization with reinforcement learning. *arXiv preprint arXiv:1611.09940*, 2016.
- Bengio, Y., Lodi, A., and Prouvost, A. Machine learning for combinatorial optimization: a methodological tour d’horizon. *European Journal of Operational Research*, 2020.
- Bi, W. and Kwok, J. Efficient multi-label classification with many labels. In Dasgupta, S. and McAllester, D. (eds.), *Proceedings of the 30th International Conference on Machine Learning*, volume 28 of *Proceedings of Machine Learning Research*, pp. 405–413, Atlanta, Georgia, USA, 17–19 Jun 2013. PMLR. URL <http://proceedings.mlr.press/v28/bi13.html>.
- Biere, A. and Fröhlich, A. Evaluating CDCL restart schemes. In Berre, D. L. and Järvisalo, M. (eds.), *Proceedings of Pragmatics of SAT 2015, Austin, Texas, USA, September 23, 2015 / Pragmatics of SAT 2018, Oxford, UK, July 7, 2018*, volume 59 of *EPiC Series in Computing*, pp. 1–17. EasyChair, 2018.
- Buciluă, C., Caruana, R., and Niculescu-Mizil, A. Model compression. In *Proceedings of the 12th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 535–541, 2006.
- Chen, D., Bai, Y., Zhao, W., Ament, S., Gregoire, J., and Gomes, C. Deep reasoning networks for unsupervised pattern de-mixing with constraint reasoning. In *International Conference on Machine Learning*, pp. 1500–1509. PMLR, 2020.
- Dai, H., Dai, B., and Song, L. Discriminative embeddings of latent variable models for structured data. In *International conference on machine learning*, pp. 2702–2711, 2016.
- Deudon, M., Cournut, P., Lacoste, A., Adulyasak, Y., and Rousseau, L.-M. Learning heuristics for the tsp by policy gradient. In *International conference on the integration of constraint programming, artificial intelligence, and operations research*, pp. 170–181. Springer, 2018.
- Dick, T., Wong, E., and Dann, C. How many random restarts are enough. Technical report, Technical report, 2014.
- Erdos, P., Rényi, A., et al. On the evolution of random graphs. *Publ. Math. Inst. Hung. Acad. Sci.*, 5(1):17–60, 1960.
- Gagliolo, M. and Schmidhuber, J. Learning restart strategies. In *IJCAI*, pp. 792–797, 2007.
- Gilmer, J., Schoenholz, S. S., Riley, P. F., Vinyals, O., and Dahl, G. E. Neural message passing for quantum chemistry. In *International Conference on Machine Learning*, pp. 1263–1272. PMLR, 2017.
- Golden, B. L., Levy, L., and Vohra, R. The orienteering problem. *Naval Research Logistics (NRL)*, 34(3):307–318, 1987.
- Gomes, C. P. and Selman, B. Algorithm portfolios. *Artificial Intelligence*, 126(1-2):43–62, 2001.
- Gomes, C. P., Selman, B., Kautz, H., et al. Boosting combinatorial search through randomization. *AAAI/IAAI*, 98: 431–437, 1998.
- Gomes, C. P., Selman, B., Crato, N., and Kautz, H. Heavy-tailed phenomena in satisfiability and constraint satisfaction problems. *Journal of automated reasoning*, 24(1-2): 67–100, 2000.
- Gotmare, A., Keskar, N. S., Xiong, C., and Socher, R. A closer look at deep learning heuristics: Learning rate restarts, warmup and distillation. *arXiv preprint arXiv:1810.13243*, 2018.
- Han, B., Sim, J., and Adam, H. Branchout: Regularization for online ensemble tracking with convolutional neural networks. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, July 2017.
- Hinton, G., Vinyals, O., and Dean, J. Distilling the knowledge in a neural network. *arXiv preprint arXiv:1503.02531*, 2015.
- Hochreiter, S. and Schmidhuber, J. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.

- Huang, G., Sun, Y., Liu, Z., Sedra, D., and Weinberger, K. Q. Deep networks with stochastic depth. In *European conference on computer vision*, pp. 646–661. Springer, 2016.
- Huang, G., Li, Y., Pleiss, G., Liu, Z., Hopcroft, J. E., and Weinberger, K. Q. Snapshot ensembles: Train 1, get m for free. *arXiv preprint arXiv:1704.00109*, 2017.
- Katakis, I., Tsoumakas, G., and Vlahavas, I. Multilabel text classification for automated tag suggestion. *ECML PKDD Discovery Challenge 2008*, pp. 75, 2008.
- Khalil, E., Dai, H., Zhang, Y., Dilkina, B., and Song, L. Learning combinatorial optimization algorithms over graphs. In *Advances in neural information processing systems*, pp. 6348–6358, 2017a.
- Khalil, E., Dai, H., Zhang, Y., Dilkina, B., and Song, L. Learning combinatorial optimization algorithms over graphs. In *Advances in neural information processing systems*, pp. 6348–6358, 2017b.
- Kocev, D., Vens, C., Struyf, J., and Džeroski, S. Ensembles of multi-objective decision trees. In *European conference on machine learning*, pp. 624–631. Springer, 2007.
- Kool, W., Van Hoof, H., and Welling, M. Attention, learn to solve routing problems! *arXiv preprint arXiv:1803.08475*, 2018.
- Krueger, D., Maharaj, T., Kramár, J., Pezeshki, M., Ballas, N., Ke, N. R., Goyal, A., Bengio, Y., Courville, A., and Pal, C. Zoneout: Regularizing rnns by randomly preserving hidden activations. *arXiv preprint arXiv:1606.01305*, 2016.
- Kurin, V., Godil, S., Whiteson, S., and Catanzaro, B. Improving sat solver heuristics with graph networks and reinforcement learning. *arXiv preprint arXiv:1909.11830*, 2019.
- lan, x., Zhu, X., and Gong, S. Knowledge distillation by on-the-fly native ensemble. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R. (eds.), *Advances in Neural Information Processing Systems*, volume 31, pp. 7517–7527. Curran Associates, Inc., 2018. URL <https://proceedings.neurips.cc/paper/2018/file/94ef7214c4a90790186e255304f8fd1f-Paper.pdf>.
- Lanchantin, J., Sekhon, A., and Qi, Y. Neural message passing for multi-label classification. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases*, pp. 138–163. Springer, 2019.
- Lewis, D. D., Yang, Y., Rose, T. G., and Li, F. Rcv1: A new benchmark collection for text categorization research. *Journal of machine learning research*, 5(Apr):361–397, 2004.
- Leyton-Brown, K., Nudelman, E., Andrew, G., McFadden, J., and Shoham, Y. A portfolio approach to algorithm selection. In *IJCAI*, volume 3, pp. 1542–1543, 2003.
- Loshchilov, I. and Hutter, F. Sgdr: Stochastic gradient descent with warm restarts. *arXiv preprint arXiv:1608.03983*, 2016.
- Lu, H., Zhang, X., and Yang, S. A learning-based iterative method for solving vehicle routing problems. In *International Conference on Learning Representations*, 2019.
- Mazyavkina, N., Sviridov, S., Ivanov, S., and Burnaev, E. Reinforcement learning for combinatorial optimization: A survey. *arXiv preprint arXiv:2003.03600*, 2020.
- McGuire, G., Tugemann, B., and Civario, G. There is no 16-clue sudoku: Solving the sudoku minimum number of clues problem. *CoRR*, abs/1201.0749, 2012. URL <http://arxiv.org/abs/1201.0749>.
- Mnih, V., Kavukcuoglu, K., Silver, D., Rusu, A. A., Veness, J., Bellemare, M. G., Graves, A., Riedmiller, M., Fidjeland, A. K., Ostrovski, G., et al. Human-level control through deep reinforcement learning. *nature*, 518(7540): 529–533, 2015.
- Nakai, K. and Kanehisa, M. A knowledge base for predicting protein localization sites in eukaryotic cells. *Genomics*, 14(4):897–911, 1992.
- Polikar, R. Ensemble based systems in decision making. *IEEE Circuits and systems magazine*, 6(3):21–45, 2006.
- Read, J., Pfahringer, B., and Holmes, G. Multi-label classification using ensembles of pruned sets. In *2008 eighth IEEE international conference on data mining*, pp. 995–1000. IEEE, 2008.
- Read, J., Pfahringer, B., Holmes, G., and Frank, E. Classifier chains for multi-label classification. *Machine learning*, 85(3):333, 2011.
- Rodriguez, J. J., Kuncheva, L. I., and Alonso, C. J. Rotation forest: A new classifier ensemble method. *IEEE transactions on pattern analysis and machine intelligence*, 28(10):1619–1630, 2006.
- Ross, I. M., Proulx, R. J., and Karpenko, M. Autonomous uav sensor planning, scheduling and maneuvering: An obstacle engagement technique. In *2019 American Control Conference (ACC)*, pp. 65–70. IEEE, 2019.

- Selsam, D., Lamm, M., Bünz, B., Liang, P., de Moura, L., and Dill, D. L. Learning a sat solver from single-bit supervision. *arXiv preprint arXiv:1802.03685*, 2018.
- Shen, Z., He, Z., and Xue, X. Meal: Multi-model ensemble via adversarial learning. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pp. 4886–4893, 2019.
- Singh, S., Hoiem, D., and Forsyth, D. Swapout: Learning an ensemble of deep architectures. In *Advances in neural information processing systems*, pp. 28–36, 2016.
- Song, J., Lanka, R., Yue, Y., and Ono, M. Co-training for policy learning. In *Uncertainty in Artificial Intelligence*, pp. 1191–1201. PMLR, 2020.
- Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research*, 15(1):1929–1958, 2014.
- Toth, P. and Vigo, D. *Vehicle routing: problems, methods, and applications*. SIAM, 2014.
- Tsoumakas, G., Katakis, I., and Vlahavas, I. Random k-labelsets for multilabel classification. *IEEE transactions on knowledge and data engineering*, 23(7):1079–1089, 2010.
- Vinyals, O., Fortunato, M., and Jaitly, N. Pointer networks. *Advances in neural information processing systems*, 28: 2692–2700, 2015.
- Wan, L., Zeiler, M., Zhang, S., Le Cun, Y., and Fergus, R. Regularization of neural networks using dropconnect. In *International conference on machine learning*, pp. 1058–1066, 2013.
- Wang, J., Yang, Y., Mao, J., Huang, Z., Huang, C., and Xu, W. Cnn-rnn: A unified framework for multi-label image classification. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 2285–2294, 2016.
- Williams, R. J. Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine learning*, 8(3-4):229–256, 1992.
- Xu, L., Hutter, F., Hoos, H. H., and Leyton-Brown, K. Satzilla: portfolio-based algorithm selection for sat. *Journal of artificial intelligence research*, 32:565–606, 2008.
- Zhang, W., Jiang, J., Shao, Y., and Cui, B. Efficient diversity-driven ensemble for deep neural networks. In *2020 IEEE 36th International Conference on Data Engineering (ICDE)*, pp. 73–84. IEEE, 2020.
- Zhao, W., Kong, S., Bai, J., Fink, D., and Gome, C. Hot-vae: Learning high-order label correlation for multi-label classification via attention-based variational autoencoders. In *Thirty-Fifth AAAI Conference on Artificial Intelligence*, 2021.
- Zhou, Z.-H., Wu, J., and Tang, W. Ensembling neural networks: many could be better than all. *Artificial intelligence*, 137(1-2):239–263, 2002.

## 7. Appendix

is down, so we provide the link above.

### 7.1. Ablation Study

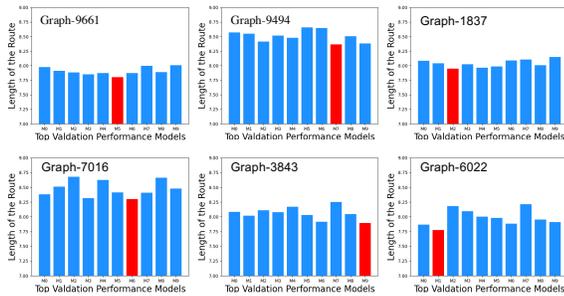


Figure 7. We randomly sample 6 graph instances from the validation set of the TSP-100 problem. We then test the top-10 validation models on these and report their results. One bar corresponds to one model. The red bar means this model performs the best.

We randomly sample 6 graphs from the 10,000 TSP-100 validation instances to show how different these models perform on the validation set. The top-10 validation models are tested on the 6 graphs, and we report their results in Fig. 7. The models are sorted on x-axis based on the validation performance, and the left first model is the best validation performance model. We can see that the best model of each graph instance is different. For each graph instance, the variance of models’ performance is also huge. This verifies our observations.

### 7.2. Traditional model selection workflow

---

#### Algorithm 2 Traditional model selection workflow

---

**Input:** Split Dataset  $D_{train}$ ,  $D_{val}$ ,  $D_{test}$ , performance metric  $\phi$   
**for** epoch= 1 **to**  $max\_epoch$  **do**  
    Train model on  $D_{train}$ .  
    Test model on  $D_{val}$  and record the best model  $M_{best}$ .  
**end for**  
Test model  $M_{best}$  on  $D_{test}$ .

---

We provide the traditional model selection workflow here. This can be compared with our **ZTop** workflow to show that we incur zero training overhead into the algorithm.

### 7.3. More details about the experiments settings

#### 7.3.1. SUDOKU

The 17-hint Sudoku data is public available through here <sup>1</sup>. This original site <sup>2</sup> maintained by the author Gordon Royle

<sup>1</sup><https://sites.google.com/site/dobrichev/sudoku-puzzle-collections>

<sup>2</sup><http://units.maths.uwa.edu.au/gordon/sudokumin.php>