
Leader Reward for POMO-Based Neural Combinatorial Optimization

Chaoyang Wang
Fudan University
chaoyangwang22@m.fudan.edu.cn

Pengzhi Cheng
Fudan University
pzcheng23@m.fudan.edu.cn

Jingze Li
Fudan University
jingzeli20@fudan.edu.cn

Weiwei Sun
Fudan University
wwsun@fudan.edu.cn

Abstract

Deep neural networks based on reinforcement learning (RL) for solving combinatorial optimization (CO) problems are developing rapidly and have shown a tendency to approach or even outperform traditional solvers. However, existing methods overlook an important distinction: CO problems differ from other traditional problems in that they focus solely on the optimal solution provided by the model within a specific length of time, rather than considering the overall quality of all solutions generated by the model. In this paper, we propose Leader Reward and apply it during two different training phases of the Policy Optimization with Multiple Optima (POMO) [Kwon et al., 2020] model to enhance the model’s ability to generate optimal solutions. This approach is applicable to a variety of CO problems, such as the Traveling Salesman Problem (TSP), the Capacitated Vehicle Routing Problem (CVRP), and the Flexible Flow Shop Problem (FFSP), but also works well with other POMO-based models or inference phase’s strategies. We demonstrate that Leader Reward greatly improves the quality of the optimal solutions generated by the model. Specifically, we reduce the POMO’s gap to the optimum by more than 100 times on TSP100 with almost no additional computational overhead.

1 Introduction

Efficient methods for solving combinatorial optimization (CO) problems are widely used in industry, including in deliveries, vehicle routing, production scheduling processes, and other real-world scenarios, all of which hold significant value. However, many CO problems are NP-hard, which means they cannot be quickly solved to an optimal solution. Heuristic solvers such as LKH [Helsgaun, 2000, 2017] and HGS [Konstantakopoulos et al., 2022] have been proposed and are designed by experts based on domain knowledge tailored to specific problems. However, they are less efficient at solving larger-scale CO problems.

Recently, an increasing amount of work has been proposed that uses neural networks to solve CO problems like the Traveling Salesman Problem (TSP) and the Capacitated Vehicle Routing Problem (CVRP), namely Neural Combinatorial Optimization (NCO) [Bello et al., 2017]. These works mainly consist of methods based on supervised learning (SL) and reinforcement learning (RL). While SL-based methods require a large amount of labeled data, which is time-consuming for the solver to provide, RL-based methods are more attractive and promising. They not only do not rely on the expert’s domain knowledge and labeled datasets, but also are capable of providing high-quality approximate solutions in a short time.

One of the RL-based methods is the construction method, which utilizes transformer architecture [Vaswani et al., 2017] to generate solutions sequentially through a decoder. It computes the reward function and uses the REINFORCE algorithm [Williams, 1992] to train the model. POMO [Kwon et al., 2020] takes advantage of the symmetry in the CO problems. They solve the same CO problem from different perspectives and propose a new baseline suitable for the REINFORCE algorithm, which greatly reduces variance and improves the stability of training, making it one of the mainstream approaches. Several subsequent works have adopted it and, based on POMO, have optimized the performance of the inference phase or improved the model’s ability to generalize across distributions and scales. Some other works apply this approach to other CO problems like the flexible flow shop problem (FFSP) and the asymmetric traveling salesman problem (ATSP).

However, such a routine does not take the special aspects of the CO problem into account. For a given CO problem, it focuses only on the optimal solution among all the solutions provided by the model after a period of inference, regardless of the quality of the other solutions. Thus, a good NCO model should value the quality of the best solution (Leader) among all the solutions given, rather than the average quality of all solutions generated. Moreover, when the model repeatedly infers the same problem, it should be able to explore more new solutions, even if the average quality of the solutions produced by each inference might decrease as a result.

In this paper, we propose Leader Reward, which changes the advantage function in the REINFORCE algorithm, and we apply it to two different training phases to motivate the model for more exploration and to place greater emphasis on the leader solution. The implementation of Leader Reward is straightforward, requiring few modifications to POMO’s advantage function and training process. By leveraging the multi-perspective problem-solving properties of POMO, it effectively integrates with POMO-based models and other inference strategies such as Simulation-Guided Beam Search (SGBS) [Choo et al., 2022] and Efficient Active Search (EAS) [Hottung et al., 2022].

We demonstrate that Leader Reward provides a method to balance exploration and exploitation for POMO. Experimental results indicate that the leader solution often results from stochastic variation, suggesting it is an unbiased, correct, and under-explored direction for the model. We assess the effectiveness of Leader Reward across various CO problems, such as TSP, CVRP, and FFSP, as well as different POMO-based models like MVMoE [Zhou et al., 2024] and Omni-VRP [Zhou et al., 2023]. The results show that Leader Reward significantly enhances model performance with almost no additional computational overhead. Particularly, we reduce POMO’s gap to the optimum by more than 100 times on TSP100, a much greater improvement than that achieved by other studies.

2 Related work

Neural Combinatorial Optimization The initial attempt to solve CO problems using neural network methods was made by Vinyals et al. [2015]. They proposed the Pointer Network, which selects a member from the input sequence with a pointer and solved the problem of variable-size output dictionaries based on SL. As the model continuously constructs a complete solution from an initial point, it is known as the construction method. Bello et al. [2017] suggested using RL for training because SL requires optimal solutions of CO problems as labels. Whereas CO problems are mostly NP-hard and difficult to solve optimally, it is feasible to compute the quality of a solution and design a reward function. Kool et al. [2019] proposed AM which modified the model to include attention layers and used the REINFORCE algorithm to train the model, employing a simple greedy rollout as a baseline through the policy gradient. Kwon et al. [2020] exploited the symmetry in the CO solution representation and proposed POMO which forced the model to solve the same problem from different starting points and used the average of these solutions as the baseline in the REINFORCE algorithm. This approach directly reduces the high variance of different trajectories and improves the training speed and stability of RL.

There is another type of method based on improvement which starts with a random initial solution and iteratively improves it. L2I [Lu et al., 2020] learn to refine the solution with an operator. NeuRewriter [Chen and Tian, 2019] learns a strategy for selecting heuristics and rewrites the current solution. Some other works improve local search or refine strategies [Kim et al., 2021, Hudson et al., 2022, Xin et al., 2021, Ma et al., 2021, Zheng et al., 2023, Ma et al., 2023]. However, these methods are often limited by search efficiency and high time overhead of inference.

POMO-Based Methods As POMO is a very efficient construction method that can solve hundreds of instances in a few seconds, there has since been a lot of work either exploiting the symmetry of this solution representation or extending and optimizing POMO. Kwon et al. [2021] applied this symmetry in the CO problem to the MatNet model, making it useful for the FFSP problem and the ATSP problem as well. Sym-NCO [Kim et al., 2022] exploits symmetries such as rotational invariance and reflection invariance that can greatly improve the generalization of POMO. ELG-POMO [Gao et al., 2023] devises an auxiliary strategy for learning from local transferable topological features and integrates it with typical construction policies to improve the generality of the model through joint training. Omni-VRP [Zhou et al., 2023] proposed a generic meta-learning framework to simultaneously improve the generalization of models in terms of size and distribution and applied it to POMO.

Inference Phase Techniques There are many techniques applied to the inference phase as well. When a model is trained, these inference techniques can better help the model to find the optimal solution. Active Search [Bello et al., 2017] can help models to optimize the parameters of the pointer network using RL in the test phase. SGBS [Choo et al., 2022] is able to examine candidate solutions in a fixed-width tree search. Hottung et al. [2022] proposed to drastically reduce the time overhead by modifying only a fraction of the model parameters during RL training in the testing phase, known as EAS.

Our method is also based on the symmetry proposed by POMO, as we take advantage of the fact that POMO solves the same problem from different perspectives. This means that our method combines well with POMO-based methods, as well as lots of inference phase techniques, and is able to work together to improve the performance of the model.

3 Preliminary

Construction-based NCO method is to train a neural network π_θ with learnable weights θ . For a CO problem, the model π_θ can recursively generate a solution (or a trajectory) τ using sampling rollout or greedy rollout, denoted as $\tau \sim \pi_\theta$.

The probability that the model makes an action a in state s is denoted as $\pi_\theta(a|s)$, and the probability that the model generates a solution $\tau = (a_1, a_2, \dots, a_n)$ can be computed as $p_\theta(\tau|s) = \prod_{i=1}^n \pi_\theta(a_i|s_i)$. For each solution τ generated by the model, the reward for that solution can be computed by the reward function $R(\tau)$. Note that the reward is only given when the model has finished generating a solution. Given a problem instance s randomly generated from the problem distribution \mathcal{D} , we want to find the θ that maximize the reward $\arg \max_\theta \mathbb{E}_{\tau \sim \pi_\theta(s)}(R(\tau))$

We use the REINFORCE algorithm to learn the weight parameter θ of the model. Specifically, we need to maximize the objective function $\mathcal{L}(\theta) = \mathbb{E}_{\tau \sim \pi_\theta(s)}(R(\tau) - b)$, where $R(\tau) - b$ is the advantage function, and b is a baseline which is used to reduce the variance. We use the gradient ascent $\nabla_\theta \mathcal{L}(\theta) = (R(\tau) - b) \nabla_\theta \log p_\theta(\tau|s)$ to update the weight parameter θ of the model.

4 Methods

4.1 Leader Reward in the main training phase

Inspired by POMO, we will solve the same CO problem many times from different perspectives, e.g., the TSP problem will choose different points as starting points, and the FFSP problem will choose different orders for assigning work to the machines. One of the biggest differences between CO problems and other problems is that for a given specific problem, we will only focus on the best of all the solutions, and it does not matter how good the quality of the other solutions given by the model are, except for the best one. This means that the measure of whether a model is good or bad should not be the expected quality of all the solutions given by the model $\arg \max_\theta \mathbb{E}_{\tau \sim \pi_\theta(s)}(R(\tau))$, but the expected quality of the best solution after the model solves a particular CO problem multiple times $\arg \max_\theta \mathbb{E}_{\tau_1, \dots, \tau_n \sim \pi_\theta(s)} \max(R(\tau_1), R(\tau_2), \dots, R(\tau_n))$. The objective function $R(\tau) - b$ based on POMO does not allow the model to learn the importance of the leader solution.

We therefore propose the Leader Reward. Specifically, after rolling out a set of trajectories $\{\tau_1, \tau_2, \dots, \tau_n\}$ by sampling from the same problem s_i , we compute the new advantage function using the following method:

$$\mathcal{A}_{\text{Leader}_i}^j = \begin{cases} \alpha \times (R(\tau_i^j) - b_i) & \text{if } j = \arg \max_j (R(\tau_i^j) - b_i) \\ R(\tau_i^j) - b_i & \text{if } j \neq \arg \max_j (R(\tau_i^j) - b_i). \end{cases} \quad (1)$$

In Equation 1, $\alpha > 1$, which is a hyperparameter that controls the extra reward earned by the leader. We will take the average reward of all the trajectories sampled from the same problem as the baseline b_i , and then add an extra Leader Reward to the leader trajectory. To maximize the objective function $\mathcal{L}(\theta)$, we use a gradient ascent as follows:

$$\nabla_{\theta} \mathcal{L}(\theta) \leftarrow \frac{1}{BN} \sum_{i=1}^B \sum_{j=1}^N \mathcal{A}_{\text{Leader}_i}^j \nabla_{\theta} \log p_{\theta}(\tau_i^j | s_i), \quad (2)$$

where $\log p_{\theta}(\tau_i^j | s_i)$ represents the log probability of sampling the trajectory τ_i^j , B is the batch size, and N is the number of different trajectories sampling from the same problem. Algorithm 1 describes the pseudocode for applying Leader Reward to the training. It is worth noting that in practice, we divide the advantage value for all trajectories by α (line 7). Since the Adam optimizer is used, multiplying the advantage function by a constant value does not change the result. However, when α is large, there are some advantages to this approach, which we will explain in Section 4.2.

Algorithm 1 Applying Leader Reward in the main training phase

Input: model parameter θ , batch size B , problem distribution \mathcal{D} , number of starting nodes N , number of training steps T , Leader Reward multiplier α

- 1: **for** $step = 1$ to T **do**
- 2: **for** $i = 1$ to B **do**
- 3: $s_i \leftarrow \text{SampleInstance}(\mathcal{D})$
- 4: $\{a_i^1, a_i^2, \dots, a_i^N\} \leftarrow \text{SelectStartNodes}(s_i)$
- 5: $\tau_i^j \leftarrow \text{SampleRollout}(a_i^j, s_i, \pi_{\theta}) \quad \forall j \in \{1, \dots, N\}$
- 6: $b_i \leftarrow \frac{1}{N} \sum_{j=1}^N R(\tau_i^j)$
- 7: $\mathcal{A}_{\text{Leader}_i}^j \leftarrow \frac{1}{\alpha} (R(\tau_i^j) - b_i) \quad \forall j \in \{1, \dots, N\}$
- 8: $l_i^* \leftarrow \arg \max_j (R(\tau_i^j) - b_i) \quad \forall j \in \{1, \dots, N\}$
- 9: $\mathcal{A}_{\text{Leader}_i}^{l_i^*} \leftarrow (R(\tau_i^{l_i^*}) - b_i)$
- 10: **end for**
- 11: $\nabla_{\theta} \mathcal{L}(\theta) \leftarrow \frac{1}{BN} \sum_{i=1}^B \sum_{j=1}^N \mathcal{A}_{\text{Leader}_i}^j \nabla_{\theta} \log p_{\theta}(\tau_i^j | s_i) \quad \forall i \in \{1, \dots, B\}, \forall j \in \{1, \dots, N\}$
- 12: $\theta \leftarrow \text{Adam}(\theta, \nabla_{\theta} \mathcal{L}(\theta))$
- 13: **end for**

Output: trained model parameter θ

In Figure 1, we show the log probability of generating the leader trajectory and the maximum log probability of 100 trajectories for each TSP100 problem during the training phase. The log probability of the leader trajectory is much smaller than the maximum log probability, implying that it is a low-probability event generated by random sampling and that the model has not yet sufficiently explored it. We also show the results after adding the Leader Reward (LR) during training, which remain the same. This is because all the datasets are randomly generated during the training phase, so no data is reused, thus reducing the risk of overfitting.

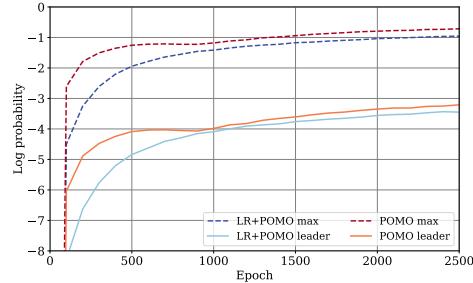


Figure 1: Log probability curve during the training phase.

Proposition 1. Consider one of the steps during the generation of the solution for the model. Let s be the state given by the environment at this step, and a_i be each action the model can take under the state. Let π_θ be the neural network whose parameters are θ and learning rate is γ . The probability of each action model can take $\pi_\theta(a_i|s)$ is calculated from the softmax function $\sigma(z_i) = e^{z_i} / (\sum_j e^{z_j})$ where z_i represents the score for each decision calculated by the model. The entropy $H(p)$ of a probability distribution p over n actions is given by $H(p) = -\sum_{i=1}^n p_i \log(p_i)$. Assume a^* is the leader action and $\pi_\theta(a^*|s) < -\frac{1}{n} \sum_i \pi_\theta(a_i|s)$, and the new entropy is $H(p')$ after giving the leader an extra reward r . Then $H(p') > H(p)$.

See Appendix A for the proof. Therefore, Leader Reward is also a way to increase exploration and control the model's balance between exploration and exploitation by adjusting the size of the value of α . In RL, exploration is crucial for effectively learning how to navigate an environment and make optimal decisions. It can help the model discover new strategies as well as handle sparse rewards. Some traditional methods, such as the Epsilon-Greedy Algorithm [Sutton and Barto, 2018] will use a hyperparameter ϵ to make the model explore randomly with a certain small probability, but the directions explored in this randomized exploration may be sometimes good, sometimes bad. However, the Leader Reward will guide the model in the right direction, as the leader trajectory derived from multiple rollouts of the same problem is a solution free of fluctuations and bias, as well as a new direction not fully explored by the model. This means that the quality of the model's exploration will be higher than traditional methods.

4.2 Leader Reward in the final training phase

The distinction in CO problems, which focuses solely on the quality of the optimal solution, not only alters the metrics for evaluating model performance but also modifies the strategies employed by models during inference. When assessing a model's inferential capabilities, we usually consider the model's performance across various inference time durations and tailor our method to meet the demands of real-world scenarios. If enough time is available for inference, allowing the model to generate numerous trajectories through sampling rollout, a model that explores diverse potential paths and generates varied solutions will outperform others. Conversely, if the model is afforded only a limited number of attempts or even just a single try at solving a problem due to time constraints, a more robust model is probabilistically favored to provide a reasonably good approximate solution.

Algorithm 2 Applying Leader Reward in the final training phase

Input: learning rate γ , model parameter θ , batch size B , problem distribution \mathcal{D} , number of starting nodes N , number of training steps T' , Leader Reward multiplier α

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1: for  $step = 1$  to  $T'$  do
2:   for  $i = 1$  to  $B$  do
3:      $s_i \leftarrow \text{SampleInstance}(\mathcal{D})$ 
4:      $\{a_i^1, a_i^2, \dots, a_i^N\} \leftarrow \text{SelectStartNodes}(s_i)$ 
5:      $\tau_i^j \leftarrow \text{SampleRollout}(a_i^j, s_i, \pi_\theta) \quad \forall j \in \{1, \dots, N\}$ 
6:      $b_i \leftarrow \frac{1}{N} \sum_{j=1}^N R(\tau_i^j)$ 
7:      $l_i^* \leftarrow \arg \max_j (R(\tau_i^j) - b_i) \quad \forall j \in \{1, \dots, N\}$ 
8:      $\mathcal{A}_{\text{Leader}_i}^{l_i^*} \leftarrow (R(\tau_i^{l_i^*}) - b_i)$ 
9:   end for
10:   $\nabla_\theta \mathcal{L}(\theta) \leftarrow \frac{1}{BN} \sum_{i=1}^B \sum_{j=1}^N \mathcal{A}_{\text{Leader}_i}^j \nabla_\theta \log p_\theta(\tau_i^j | s_i) \quad \forall i \in \{1, \dots, B\}, \forall j \in \{1, \dots, N\}$ 
11:   $\theta \leftarrow \text{Adam}(\theta, \nabla_\theta \mathcal{L}(\theta), \gamma)$ 
12: end for

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Output: trained model parameter θ

As mentioned in Section 4.1, applying different values of α during training alters the extent to which the model explores, leading to a final model that tends towards being either aggressive or conservative. This approach can also be employed in the final training phase. Hence, we propose Algorithm 2, a method based on Leader Reward, to adjust the conservativeness of the model. This algorithm could enhance the model's aggressiveness by setting $\alpha = +\infty$ and balance the specific degrees of aggression and conservatism by adjusting the learning rate γ , ensuring the model converges to an

appropriate state. It just requires a small amount of training time, converging in just 100 epochs on TSP100, which is approximately one-thirtieth of the entire training process.

Figure 2 shows the gap between the solutions generated by the model and the optimal solution when applying Algorithm 2 to solve the same problem by sampling multiple times. It is observed that this algorithm results in a decline in the average quality of solutions produced by the model, as the gap of the solution provided by the model escalates from 2.13% to 8.52% when solving the problem just once. This escalation occurs because, when a model solves the same problem only a limited number of times, the emphasis is on the average quality of solutions it provides. Conversely, as the model solves the same problem more frequently, a more aggressive model becomes advantageous.

Given that POMO leverages the symmetry of solution representations and data augmentation, POMO-based methods typically involve solving the same problem a large number of times during the inference phase. Taking the TSP100 as an example, these methods will sample the same problem 800 times. This algorithm is designed to leverage POMO’s capability of repeated problem-solving, enhancing the model’s aggressiveness at the expense of deteriorating the average solution quality. The trade-off aims to improve the probability of generating high-quality, optimal solutions.

4.3 Leader Reward + SGBS + EAS

As POMO is a highly efficient construction method, recently numerous improvements have been made to enhance its performance. One such improvement is SGBS + EAS, an optimization strategy tailored for the POMO’s inference phase. Our method can also be applied to the inference phase and works well with SGBS + EAS, further reducing the gap between the model’s solution and the optimum.

SGBS is an inference phase technique that enhances the quality of solutions generated by the POMO model. During the solution generation process, it produces $\beta \times (\gamma - 1)$ directions at each step, and retains the best β among them through a greedy rollout mechanism. This method aims to generate the best β solutions at the same time, thereby improving the quality of the solutions generated by the model. Such an algorithm, capable of efficiently producing multiple solutions, enables us to attain a superior solution within a short inference time while also emphasizing the exploratory performance of the model. In contrast to the previous practice of pursuing a single greedy rollout to obtain a nearly approximate solution, we now, with the efficient inference strategy of SGBS, prefer the model to capitalize on the greater opportunities provided by SGBS to fully explore the potential of other solutions.

EAS is a method that trains on a test set by using POMO’s pre-trained model and updates the parameters during testing to enhance performance. It leverages the fact that the problem only requires an optimal solution and, given sufficient inference time, allows for tuning the model during this period. EAS accelerates the training process by updating only a subset of parameters. Since EAS involves training on a test set, it can be integrated with the approach described in Section 4.1. This integration treats EAS as the main training phase and uses Leader Rewards to guide the model in a correct new direction during training.

SGBS and EAS collaborate in a way that SGBS assists EAS by sharing incumbent solutions. SGBS helps EAS escape local optima by discovering superior solutions through efficient generative methods that leverage new paths explored by EAS during training. This method alternates between EAS and SGBS in sequence. However, SGBS has a significant time overhead, as one iteration of SGBS(4,4) on CVRP100 takes about 6 times longer than one iteration of EAS, and one iteration of SGBS(10,10) on TSP100 takes about 20 times longer than one iteration of EAS, which makes this strategy less viable when training time is limited. Experimentally, we found that increasing the number of iterations of

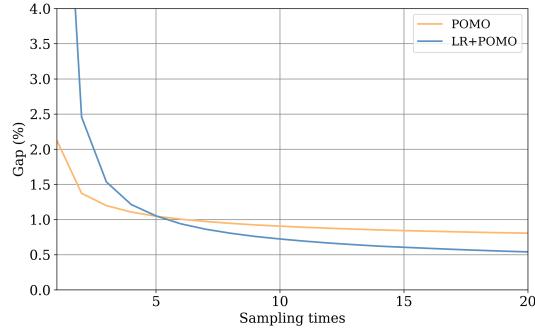


Figure 2: Gap of different sampling times on 10,000 instances of TSP100.

EAS improves model performance when time is limited, but at the expense of making the model more likely to fall into a local optimum and perform worse in the long term. However, since EAS operates in the testing phase, where time is precious, we believe that sacrificing a little long-term performance for a reduction in short-term performance is worthwhile.

There are also lots of other works based on POMO, such as MatNet, Omni-VRP, and MVMoE. Our approach is an optimization of the POMO training approach, and we find that it simultaneously benefits these POMO-based models. The experimental results are shown in Section 5. This demonstrates the generalizability of our approach.

5 Experiments

The training and testing were conducted on a single Nvidia RTX 4090 GPU. To evaluate the effectiveness of Leader Reward (abbreviated as LR in the table), we modified POMO (MIT license) [Kwon et al., 2020] and assessed its performance on the TSP and CVRP problems. We also applied our method to MatNet (MIT license) [Kwon et al., 2021] and tested its performance on the FFSP problem to show our method’s applicability to models that utilize the symmetric representation of solutions in POMO. Since the SGBS+EAS optimization is relevant to all three problems, we also evaluated the performance after implementing SGBS+EAS (MIT license) [Choo et al., 2022] in the inference phase. To further demonstrate the applicability of our method to other POMO-based models, we tested Leader Reward on two additional models, MVMoE (MIT license) [Zhou et al., 2024] and Omni-VRP (MIT license) [Zhou et al., 2023]. The results can be found in Appendix D. We also tested the performance of Leader Reward on the realistic datasets TSPLib [Reinelt, 1991] and CVRPLib [Uchoa et al., 2017]; details of these tests can be found in Appendix E. As some of the results in the table were obtained from different hardware (v3-8 TPU or Nvidia A100 GPUs), we’ve marked their time consumption with * for a fair comparison.

TSP The TSP problem can be considered one of the benchmark problems among CO problems, and many NCO models are tested for performance on the TSP problem. In the TSP, there are multiple points in a two-dimensional space, and the distance between any two points is measured using Euclidean distance. The goal is to find the minimal distance required to start from any one point, pass through each point exactly once, and return to the starting point. To maintain consistency with previous experiments, we used the test set generated by Choo et al. [2022]. Specifically, 10,000 instances of TSP100 were generated using the random seed 1234, and 1,000 instances each of TSP150 and TSP200 were generated using the random seed 1235.

We use the results of exact-solver Concorde [Cook et al., 2011] as a standard for comparison, and we also give the results of LKH3. For the NCO method, we give results for DPDP [Kool et al., 2022], COMPASS [Chalumeau et al., 2023], Poppy [Grinsztajn et al., 2023], and POMO. However, since our optimization is based on POMO, our main emphasis is on the magnitude of improvement in POMO. Just as POMO can be optimized using SGBS+EAS, we also present the results of combining Leader Reward with SGBS+EAS, as well as the results for different lengths of inference time.

As POMO trained a TSP100 model for a total of 3050 epochs, we also kept the overall training time consistent to ensure a fair comparison. Specifically, we use $\alpha = 40$ when applying Leader Reward in the main training phase and trained POMO for 2900 epochs, in the final training phase we set $\alpha = +\infty$ and the learning rate $\gamma = 5.5 \times 10^{-5}$ and trained for 100 epochs, and finally we set the learning rate to $\gamma = 5.5 \times 10^{-6}$ and trained for 50 epochs as an end. In the inference phase, we combined Leader Reward with SGBS+EAS. We selected the hyperparameters $\beta = 10$ and $\gamma = 10$ for SGBS. For EAS, we set the parameter of Leader Reward to $\alpha = 40$ and performed SGBS after every 20 EAS iterations.

Table 1 shows the performance of Leader Reward on the TSP problem. The result for LR+SGBS is not included in the table because we found that LR+SGBS+EAS performs better than LR+SGBS in terms of both time consumption and the gap. It can be found that Leader Reward can significantly improve the performance and generalization of the POMO model on the TSP. Specifically, Leader Reward reduces the POMO’s gap to the optimum by 10 times, and can be boosted up to 200 times when optimized with SGBS+EAS inference strategy. For generalization capabilities, Leader Reward can also reduce the gap by 97% and 84% on TSP150 and TSP200, respectively, which represents a huge improvement greater than that achieved by other studies.

Table 1: Experiment results on TSP

Method	Test (10K instances)			Generalization (1K instances)					
	TSP100		Time	TSP150		Time	TSP200		Time
	Cost	Gap		Cost	Gap		Cost	Gap	
Concorde	7.765	-	82m	9.346	-	17m	10.687	-	31m
LKH3	7.765	0.000%	8h	9.346	0.000%	99m	10.687	0.000%	3h
Poppy 16	7.770	0.07%	1m*	9.372	0.27%	20s*			
POMO	7.776	0.144%	1m	9.397	0.544%	14s	10.843	1.459%	31s
LR+POMO	7.766	0.014%	1m	9.364	0.193%	14s	10.792	0.985%	31s
POMO(sampling)	7.771	0.078%	3h*	9.378	0.355%	1h*	10.838	1.417%	3h*
DPDP	7.765	0.004%	2h*	9.434	0.937%	44m*	11.154	4.370%	74m*
COMPASS	7.765	0.002%	2h*	9.350	0.043%	32m*	10.723	0.337%	70m*
SGBS+EAS(short)	7.770	0.063%	37m	9.368	0.236%	11m	10.764	0.718%	29m
SGBS+EAS	7.768	0.045%	2h	9.359	0.142%	2h	10.739	0.484%	2h
LR+SGBS+EAS(short)	7.765	0.0007%	25m	9.347	0.009%	17m	10.701	0.133%	37m
LR+SGBS+EAS	7.765	0.0002%	2h	9.346	0.005%	2h	10.695	0.075%	2h

CVRP In the CVRP, multiple points are distributed across a two-dimensional space, each associated with a demand value. A vehicle may depart from the depot multiple times, pass through some of these points, and then return to the depot. The total demand of the points visited in each trip must not exceed the vehicle’s capacity. The goal is to find the shortest route that ensures each point is visited at least once.

We used the same test set setup as in the TSP problem, and we used the results of the heuristic solver HGS [Vidal et al., 2012, Vidal, 2022] as the baseline for comparison. For the training process, we used $\alpha = 10$ when applying Leader Reward in the main training phase and trained the POMO model for 28,500 epochs, and in the final training phase, we set $\alpha = +\infty$ and learning rate $\gamma = 5.5 \times 10^{-5}$ and reduced the learning rate to 0.2 times of the original after 1000 epochs and 1500 epochs. In the inference phase, we selected the hyperparameters $\beta = 4$ and $\gamma = 4$ for SGBS. For EAS, we set the parameter of Leader Reward to $\alpha = 10$ and performed SGBS after every 3 EAS iterations.

Table 2 displays the performance of Leader Reward on the CVRP problem. It is evident that Leader Reward enhances both the performance and generalization of the POMO model on this problem, reducing the gap by 35%, 27%, and 40% for CVRP100, CVRP150, and CVRP200, respectively.

FFSP To demonstrate the applicability of Leader Reward to models that leverage the symmetry of the solution representation, we also applied it to MatNet and tested the performance on the FFSP problem.

The FFSP problem is modeled on the production scheduling process in a real manufacturing application, where each job must be performed sequentially across S stages. Each stage has M types of machines, and each job takes a different amount of time on each machine. Within the same stage, it is only necessary to work on any one of the M types of machines. The goal of the problem is to find the shortest possible time required to complete all jobs.

To maintain consistency with previous experiments, we used $S = 3$ and $M = 4$, and the possible time required for each job was a random integer from 2 to 9. We used the test set generated by Kwon et al. [2021] and tested how the model performed with $N = \{20, 50, 100\}$ jobs. To ensure that the total training time is consistent, we chose $\alpha = \{4, 4, 2\}$ and trained MatNet for $\{50, 100, 150\}$ epochs, and then trained 30 and 20 epochs in the final training phase with learning rate $\gamma = 5.5 \times 10^{-5}$ and $\gamma = 5.5 \times 10^{-6}$. In the inference phase, we selected the hyperparameters $\beta = 5$ and $\gamma = 6$ for SGBS, and we performed SGBS after every 3 EAS iterations. We also give results for mixed-integer programming models CPLEX, and other heuristics methods.

Results in Table 3 show that the Leader Reward method outperforms both heuristic methods and NCO methods in solving the FFSP problem and significantly improves the performance of MatNet, demonstrating the effectiveness of our method for MatNet.

Table 2: Experiment results on CVRP

Method	Test (10K instances)			Generalization (1K instances)					
	CVRP100			CVRP150			CVRP200		
	Cost	Gap	Time	Cost	Gap	Time	Cost	Gap	Time
HGS	15.563	-	24h	19.052	-	5h	21.755	-	9h
LKH3	15.646	0.532%	6d	19.222	0.891%	20h	22.003	1.138%	25h
Poppy 32	15.73	1.072%	5m*	19.50	2.350%	1m*			
POMO	15.754	1.228%	1m	19.686	3.324%	16s	23.057	5.983%	34s
LR+POMO	15.729	1.064%	1m	19.682	3.306%	16s	23.012	5.775%	34s
POMO(sampling)	15.663	0.641%	6h*	19.478	2.235%	2h*	23.176	6.530%	5h*
DPDP	15.627	0.410%	23h*	19.312	1.363%	5h*	22.263	2.333%	9h*
COMPASS(no aug)	15.594	0.198%	4h*	19.313	1.369%	2h*	22.462	3.248%	2h*
SGBS+EAS(short)	15.605	0.271%	2h	19.227	0.920%	1h	22.274	2.382%	3h
SGBS+EAS	15.587	0.152%	10h	19.154	0.532%	3h	22.109	1.626%	7h
LR+SGBS+EAS(short)	15.588	0.158%	2h	19.160	0.566%	1h	22.106	1.611%	3h
LR+SGBS+EAS	15.579	0.099%	10h	19.126	0.389%	3h	21.966	0.967%	7h

Table 3: Experiment results on FFSP (1K instances)

	FFSP20			FFSP50			FFSP100		
	Cost	Gap	Time	Cost	Gap	Time	Cost	Gap	Time
CPLEX(60s)	46.37	91.857%	17h	×			×		
CPLEX(600s)	36.56	51.268%	167h						
Genetic Algorithm	30.57	26.484%	56h	56.37	16.851%	128h	98.69	12.036%	232h
Particle Swarm Opt.	29.07	20.278%	104h	55.11	14.239%	208h	97.32	10.480%	384h
MatNet	25.392	5.060%	2m	49.600	2.817%	5m	89.745	1.881%	13m
LR+MatNet	25.232	4.398%	2m	49.363	2.326%	5m	89.207	1.270%	13m
MatNet(sampling)	24.60	1.783%	10h*	48.78	1.117%	20h*	88.95	0.979%	40h*
SGBS+EAS(short)	24.467	1.233%	3h	48.837	1.235%	6h	88.980	1.013%	10h
SGBS+EAS	24.250	0.335%	15h	48.519	0.576%	30h	88.568	0.545%	60h
LR+SGBS+EAS(short)	24.395	0.935%	3h	48.596	0.736%	6h	88.455	0.417%	10h
LR+SGBS+EAS	24.169	-	15h	48.241	-	30h	88.088	-	60h

6 Conclusion and Discussion

In this paper, we propose a new advantage function, Leader Reward, applicable to the POMO model and other models that leverage the symmetry of this solution representation. We analyze the specificity of the CO problem and apply Leader Reward during two different phases of training to improve models' performance. Experiments show that this method performs well on various CO problems (TSP, CVRP, FFSP) and with different POMO-based models (MatNet, Omni-VPR, MVMoE). It is capable of further improving the model's performance using inference strategies. Moreover, this performance enhancement incurs almost no additional computational overhead.

For potential societal impacts, we believe that the CO problem is closely related to practical challenges such as deliveries, vehicle routing, and production scheduling. With the development of NCO, models that provide solutions with greater accuracy and in less time can significantly enhance the efficiency of societal and productive activities. Therefore, we believe that the societal impacts of our work are mainly positive, with generally no negative societal impacts. In future work, we will attempt to dynamically adjust the parameter α in the Leader Reward, aiming to better integrate it with other models and inference strategies.

Our code for the experiments can be found in the supplementary material.

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A Proof

Proof. Assume there are n actions $\{z_1, z_2, \dots, z_n\}$ and the leader action is z_1 . The probability of each actions chosen by model $p_i = \sigma(z_i) = \frac{e^{z_i}}{\sum_{j=1}^n e^{z_j}}$ and $p_1 < -\frac{1}{n} \sum_i p_i$.

We have that

$$\frac{\partial p_i}{\partial z_j} = p_i \cdot (\delta_{ij} - p_j),$$

where δ_{ij} is the Kronecker delta. The entropy is calculate by $H(p) = -\sum_{i=1}^n p_i \log(p_i)$.

As the original proposition is equivalent to $\frac{\partial H(p)}{\partial z_1} > 0$, we have that

$$\begin{aligned} \frac{\partial H(p)}{\partial z_1} &= \sum_{i=1}^n \frac{\partial H(p)}{\partial p_i} \cdot \frac{\partial p_i}{\partial z_1} \\ &= \frac{\partial H(p)}{\partial p_1} \cdot \frac{\partial p_1}{\partial z_1} + \sum_{i=2}^n \frac{\partial H(p)}{\partial p_i} \cdot \frac{\partial p_i}{\partial z_1} \\ &= (-\ln p_1 - 1) \cdot p_1 \cdot (1 - p_1) + \sum_{i=2}^n (-\ln p_i - 1) \cdot p_i(-p_1) \\ &= p_1 \cdot (-\ln p_1 + \sum_{i=1}^n p_i \ln p_i) \\ &= p_1 \cdot (-\ln p_1 - H(p)). \end{aligned}$$

As the sum of the probabilities of all actions $p_1 + p_2 + \dots + p_n = 1$, we have that

$$\begin{aligned} \frac{\partial H(p)}{\partial z_1} &= p_1 \cdot (-\ln p_1 - H(p)) \\ &= p_1 \cdot (-(p_1 + p_2 + \dots + p_n) \cdot \ln p_1 - H(p)). \end{aligned}$$

The entropy $H(p)$ will be maximum if and only if $p_2 = p_3 = \dots = p_n = \frac{1-p_1}{n-1}$, which implies that

$$\begin{aligned} \frac{\partial H(p)}{\partial z_1} &= p_1 \cdot (-(p_1 + p_2 + \dots + p_n) \cdot \ln p_1 - H(p)) \\ &> p_1 \cdot (-(p_1 + p_2 + \dots + p_n) \cdot \ln p_1 + p_1 \ln p_1 + \frac{1-p_1}{n-1} \cdot \sum_{i=2}^n \ln \frac{1-p_1}{n-1}) \\ &= p_1 \cdot (-(p_1 + (n-1) \cdot \frac{1-p_1}{n-1}) \cdot \ln p_1 + p_1 \ln p_1 + \frac{1-p_1}{n-1} \cdot (n-1) \cdot \ln \frac{1-p_1}{n-1}) \\ &= p_1 \cdot (1-p_1) \cdot (\ln \frac{1-p_1}{n-1} - \ln p_1) > 0. \end{aligned}$$

□

B Hyperparameter Experiments

B.1 Hyperparameter for the main training phase

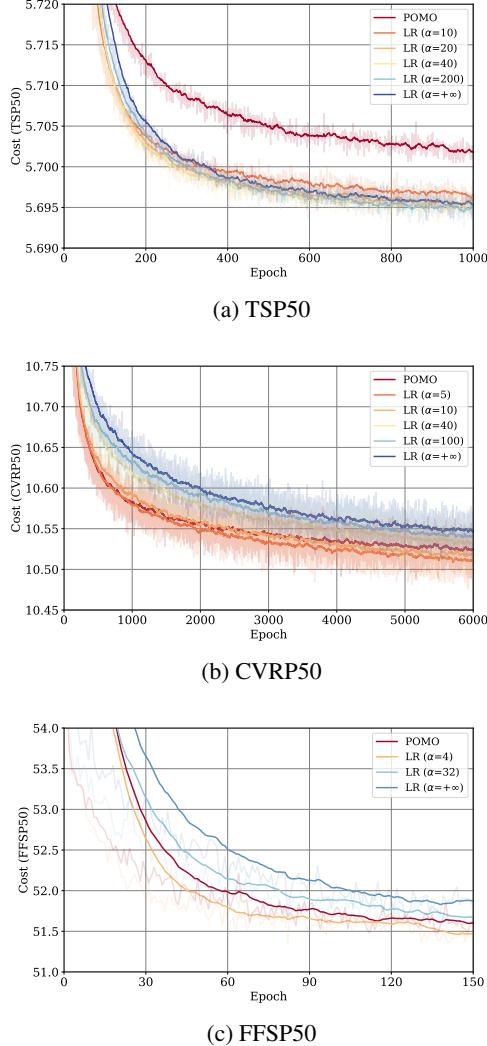


Figure 3: Comparison of learning curves when choosing different α for Leader Reward during the main training phase on the TSP, CVRP, and FFSP problem.

Figure 3 shows the learning curves on the TSP, CVRP, and FFSP problem in the case of using different α as a parameter for Leader Reward in the main training phase. As experiments on problems of size 100 would be too computationally expensive, we give the results for problems of size 50. In TSP, Leader Reward can give a large boost to POMO’s performance and is robust to the hyperparameter α . As α increases, the model gradually converges better, but there is a little negative lift when α is particularly large. In CVRP and FFSP, using too large an α will make the model perform worse instead. As we need to balance the exploration and exploitation of the model, a proper α will make the best use of Leader Reward’s performance.

We also notice that Poppy [Grinsztajn et al., 2023] proposed the policy gradient for populations, which is a little bit like setting $\alpha = +\infty$ in the Leader Reward when training only one population. However, as shown in the figure, this training method leads to poor model performance. Therefore, we consider poppy and Leader Reward to be two different methods, with the former emphasizing

performance improvement through large populations and the latter emphasizing making the model value the leader.

B.2 Hyperparameter for the final training phase

In this section, we test the results of applying Leader Reward to POMO only in the final training phase. Table 4 shows the expected value of the cost, the mean, and the variance of 100 trajectories sampled from the TSP100 problem when choosing different learning rates γ . The results show that our method has higher robustness to γ , as the costs drop dramatically (from 0.32% to about 0.11%) as long as γ is within a reasonable range.

It's worth noting that our method can significantly increase the variance of solutions (from about 0.05 to about 0.3) and ultimately improve the performance of the model, at the cost of reducing the average quality of the solution. Therefore, controlling γ within a reasonable range can maximize the performance of this method.

Table 4: Hyperparameter experiments of γ in the final training phase

Method	Cost(no aug.)	Gap	Mean (μ)	Variance (σ)
POMO	7.7891	0.316%	7.837	0.048
LR ($\gamma = 1 \times 10^{-5}$)	7.7739	0.121%	7.904	0.229
LR ($\gamma = 5.5 \times 10^{-5}$)	7.7726	0.104%	7.938	0.314
LR ($\gamma = 1 \times 10^{-4}$)	7.7728	0.106%	7.955	0.349
LR ($\gamma = 1.5 \times 10^{-4}$)	7.7733	0.113%	7.974	0.379

C Ablation Study

In order to demonstrate the effectiveness of Leader Reward in both phases, we further conduct an ablation study. Table 5 shows the cost and the gap in TSP, CVRP, and FFSP problems after removing some of the phases. The results show that both phases play a key role in improving the performance of the model.

Table 5: Ablation studies of LR

Method	TSP100		CVRP100		FFSP100	
	Cost	Gap	Cost	Gap	Cost	Gap
LR	7.766	0.014%	15.729	1.064%	89.207	1.270%
w/o main phase	7.766	0.025%	15.732	1.085%	89.294	1.369%
w/o final phase	7.768	0.040%	15.748	1.191%	89.406	1.496%
w/o both phase	7.776	0.144%	15.754	1.228%	89.745	1.881%

D Results on other POMO-based models

We further implement our method on MVMoE [Zhou et al., 2024] and Omni-VRP [Zhou et al., 2023]. We follow the default setting of the authors and the only change is applying Leader Reward to the advantage function during training. In both models, we set $\alpha = 5$ during the main phase and $\gamma = 5.5 \times 10^{-5}$ during the final phase. We also report the performance when the final phase is removed. As shown in Table 6 and Table 7, both phases bring significant improvement in performance.

Table 6: Performance on MVMoE ($N = 50$)

Problem	MVMoE		LR w/o final phase		LR	
	Cost	Gap	Cost	Gap	Cost	Gap
CVRP	10.427	0.890%	10.423	0.846%	10.416	0.785%
OVRP	6.657	2.418%	6.647	2.265%	6.625	1.937%
VRPB	8.167	1.495%	8.159	1.395%	8.149	1.275%
VRPL	10.501	0.087%	10.496	0.039%	10.486	-0.057%
VRPTW	15.000	3.412%	14.985	3.293%	14.955	3.088%
OVRPTW	8.964	3.217%	8.941	2.949%	8.916	2.662%
OVRPB	6.111	6.333%	6.093	6.016%	6.065	5.536%
OVRPL	6.653	2.502%	6.641	2.323%	6.624	2.053%
VRPBL	8.175	1.808%	8.162	1.655%	8.151	1.513%
VRPBTW	16.019	8.589%	15.986	8.364%	15.952	8.137%
VRPLTW	14.927	2.362%	14.913	2.253%	14.888	2.071%
OVRPBL	6.098	6.215%	6.077	5.856%	6.054	5.445%
OVRPBTW	9.490	9.350%	9.472	9.139%	9.449	8.877%
OVRPLTW	8.965	3.385%	8.942	3.125%	8.916	2.824%
VRPBLTW	15.941	8.748%	15.932	8.686%	15.897	8.448%
OVRPBTW	9.514	9.644%	9.484	9.298%	9.457	8.976%

Table 7: Performance on Omni-VRP (TSP, zero-shot)

(Size, Distribution)	Omni-VRP		LR w/o final phase		LR	
	Cost	Gap	Cost	Gap	Cost	Gap
(200, GM_2^5)	9.027	2.773%	8.991	2.353%	8.965	2.068%
(200, R)	8.372	2.124%	8.341	1.756%	8.329	1.610%
(200, E)	8.240	1.845%	8.216	1.546%	8.215	1.528%
(300, U)	13.400	3.442%	13.342	2.995%	13.329	2.892%
(300, GM_3^{10})	9.845	3.941%	9.797	3.439%	9.784	3.307%
(300, GM_7^{50})	5.787	2.714%	5.770	2.420%	5.761	2.257%
(300, R)	10.162	3.774%	10.114	3.287%	10.101	3.149%
(300, E)	9.801	3.384%	9.764	2.989%	9.765	3.007%
(500, R)	13.428	8.366%	13.356	7.788%	13.315	7.459%
(500, E)	12.672	7.996%	12.616	7.519%	12.589	7.286%
(1000, R)	20.374	19.214%	20.348	19.072%	20.101	17.625%
(1000, E)	18.575	18.629%	18.567	18.584%	18.397	17.502%

E Results on TSPLib and CVRPLib

This section gives a performance evaluation of our method on TSPLib [Reinelt, 1991] and CVRPLib [Uchoa et al., 2017], where we choose instances with size $N < 250$. Both POMO and our model are pre-trained on $N = 100$ and evaluated in Table 1 and Table 2. In this experiment, we report results under greedy strategy and instance augmentation. As shown below, our method outperforms POMO on both datasets. See Table 8 and Table 9.

Table 8: Performance comparison on TSPLib instances.

Instance	Optimal	POMO		LR+POMO	
		Cost	Gap	Cost	Gap
berlin52	7542	7545	0.04%	7544	0.03%
bier127	118282	128660	8.77%	120606	1.96%
ch130	6110	6120	0.16%	6117	0.11%
ch150	6528	6562	0.52%	6559	0.47%
d198	15780	18508	17.29%	18967	20.20%
eil101	629	641	1.91%	640	1.75%
eil51	426	430	0.94%	429	0.70%
eil76	538	544	1.12%	544	1.12%
kroA100	21282	21370	0.41%	21285	0.01%
kroA150	26524	26709	0.70%	26783	0.98%
kroA200	29368	29831	1.58%	30088	2.45%
kroB100	22141	22212	0.32%	22210	0.31%
kroB150	26130	26435	1.17%	26331	0.77%
kroB200	29437	29876	1.49%	30004	1.93%
kroC100	20749	20787	0.18%	20760	0.05%
kroD100	21294	21473	0.84%	21412	0.55%
kroE100	22068	22167	0.45%	22137	0.31%
lin105	14379	14454	0.52%	14419	0.28%
pr107	44303	44585	0.64%	44663	0.81%
pr124	59030	59246	0.37%	59075	0.08%
pr136	96772	97521	0.77%	97562	0.82%
pr144	58537	58802	0.45%	59403	1.48%
pr152	73682	74596	1.24%	75218	2.08%
pr226	80369	83281	3.62%	87103	8.38%
pr76	108159	108159	0.00%	108159	0.00%
rat195	2323	2512	8.14%	2432	4.69%
rat99	1211	1234	1.90%	1224	1.07%
rd100	7910	7910	0.00%	7910	0.00%
st70	675	677	0.30%	677	0.30%
ts225	126643	132623	4.72%	128711	1.63%
tsp225	3861	4111	6.48%	4093	6.01%
u159	42080	42480	0.95%	42460	0.90%
Avg Gap			2.12%		1.95%

Table 9: Performance comparison on CVRPLib instances.

Instance	Optimal	POMO		LR+POMO	
		Cost	Gap	Cost	Gap
X-n247-k50	37274	42420	13.81%	44217	18.63%
X-n242-k48	82751	89185	7.78%	89669	8.36%
X-n237-k14	27042	31272	15.64%	29363	8.58%
X-n233-k16	19230	21119	9.82%	20979	9.10%
X-n228-k23	25742	29354	14.03%	28758	11.72%
X-n223-k34	40437	43804	8.33%	43877	8.51%
X-n219-k73	117595	122208	3.92%	124756	6.09%
X-n214-k11	10856	11763	8.35%	11741	8.15%
X-n209-k16	30656	32399	5.69%	32410	5.72%
X-n204-k19	19565	20976	7.21%	21284	8.79%
X-n200-k36	58578	62102	6.02%	62272	6.31%
X-n195-k51	44225	50303	13.74%	49632	12.23%
X-n190-k8	16980	18067	6.40%	18389	8.30%
X-n186-k15	24145	25742	6.61%	25709	6.48%
X-n181-k23	25569	26978	5.51%	26606	4.06%
X-n176-k26	47812	52883	10.61%	52644	10.11%
X-n172-k51	45607	50356	10.41%	51538	13.00%
X-n167-k10	20557	21297	3.60%	21649	5.31%
X-n162-k11	14138	14985	5.99%	14969	5.88%
X-n157-k13	16876	18302	8.45%	17692	4.84%
X-n153-k22	21220	24356	14.78%	24050	13.34%
X-n148-k46	43448	47621	9.60%	47861	10.16%
X-n143-k7	15700	16380	4.33%	16533	5.31%
X-n139-k10	13590	14080	3.61%	13906	2.33%
X-n134-k13	10916	11315	3.66%	11334	3.83%
X-n129-k18	28940	29569	2.17%	29373	1.50%
X-n125-k30	55539	58421	5.19%	60122	8.25%
X-n120-k6	13332	14570	9.29%	13882	4.13%
X-n115-k10	12747	13878	8.87%	13351	4.74%
X-n110-k13	14971	15160	1.26%	15149	1.19%
X-n106-k14	26362	26967	2.29%	27423	4.02%
X-n101-k25	27591	29288	6.15%	29878	8.29%
Avg Gap			7.60%		7.41%

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