

Configuring LLM-Generated Heuristics via Instance-Specific Deep Reinforcement Learning



universität
wien

Xiaowei Liu and Kevin Tierney

July 16, 2026

Department of Business Decisions and Analytics

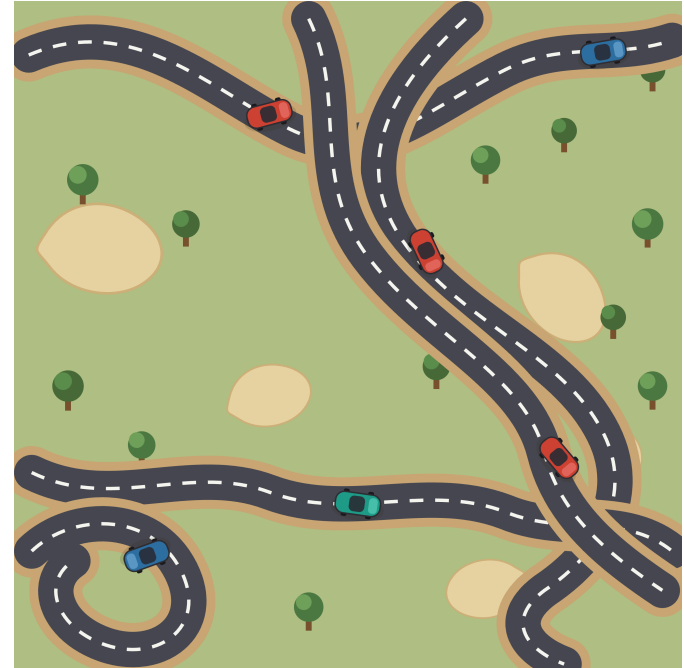
Automated Heuristic Discovery with VRPAgent

Background: Routing Problems

Vehicle Routing Problem (VRP)

Visit n customers with m vehicles such that

- each customer is visited exactly once
- the total travel cost is minimized.



Background: Routing Problems

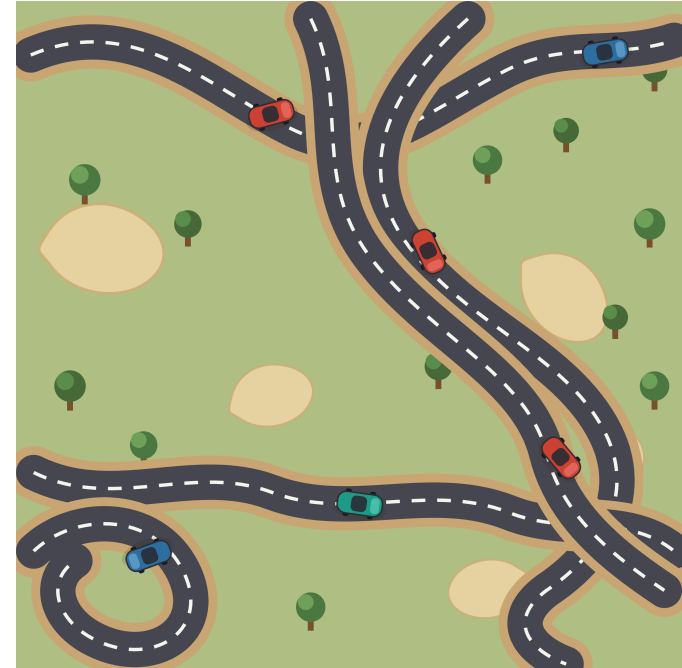
Vehicle Routing Problem (VRP)

Visit n customers with m vehicles such that

- each customer is visited exactly once
- the total travel cost is minimized.

And its variants:

- Capacitated VRP (CVRP)
- VRP with Time Windows (VRPTW)
- Prize-Collecting VRP (PCVRP)



Large Neighborhood Search (LNS)

The core idea of the LNS algorithm (Shaw, 1998) is to “**destroy and repair**”.

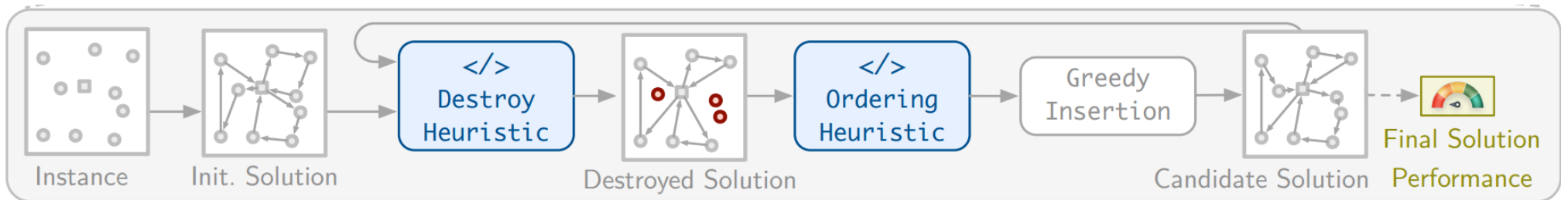
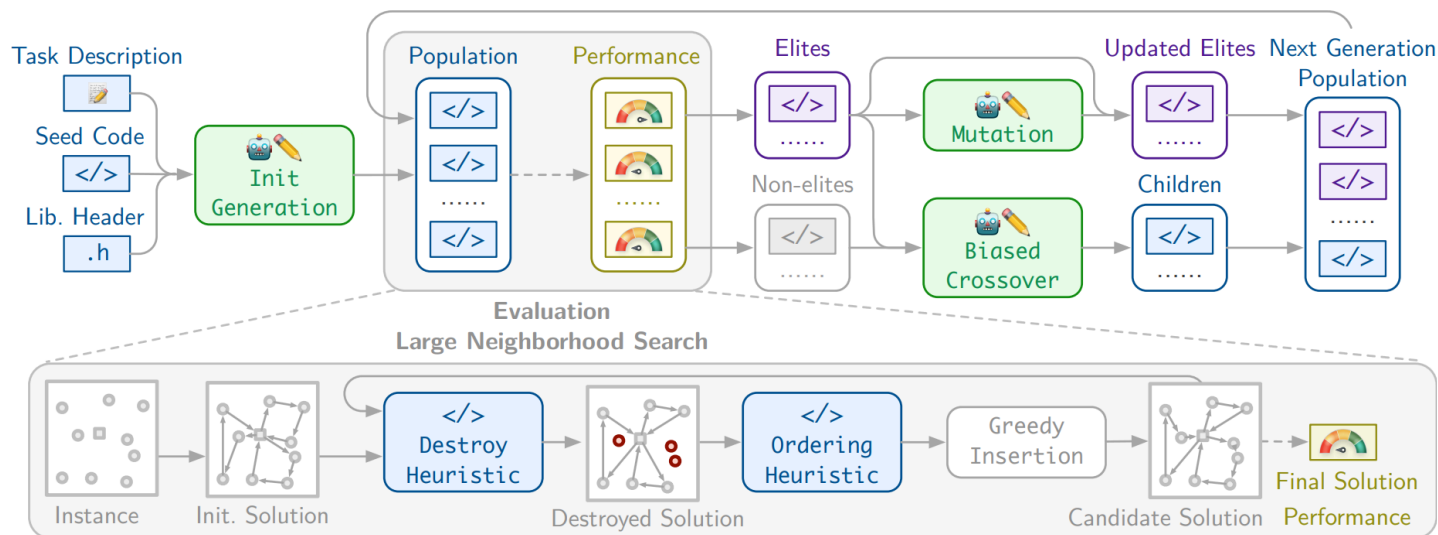


Figure adapted from (Hottung et al., 2025a)

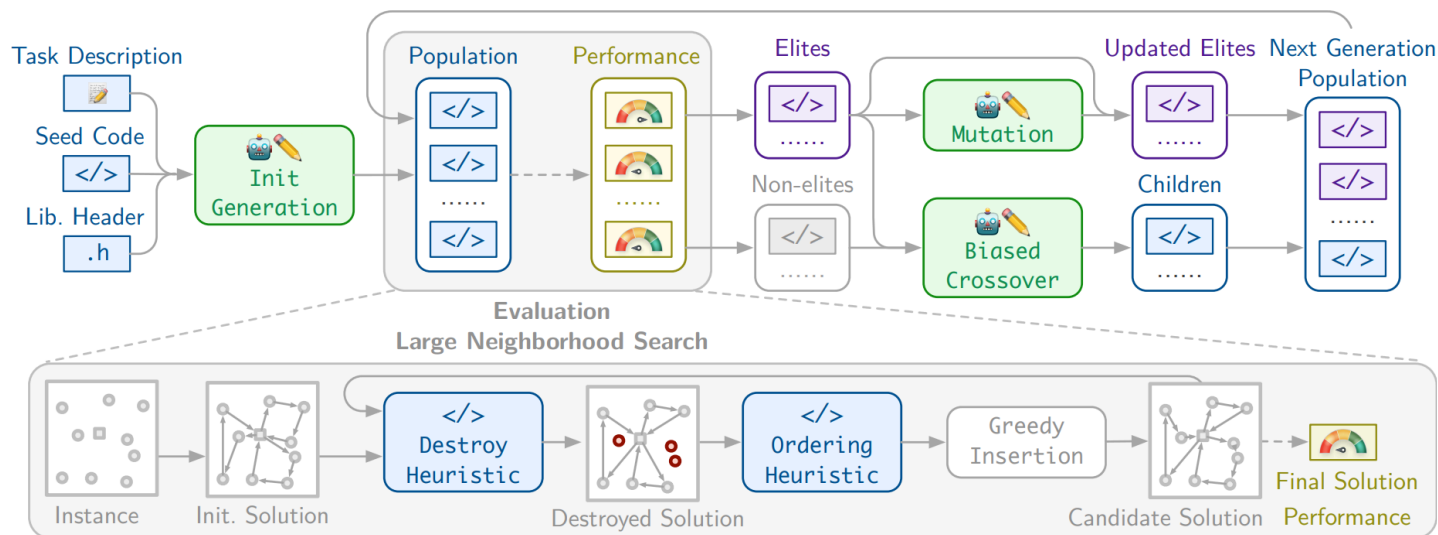
VRPAgent: Automated Heuristic Discovery by LLMs



VRPAgent pipeline overview. Figure adapted from (Hottung et al., 2025a)

1 Initial heuristics generation

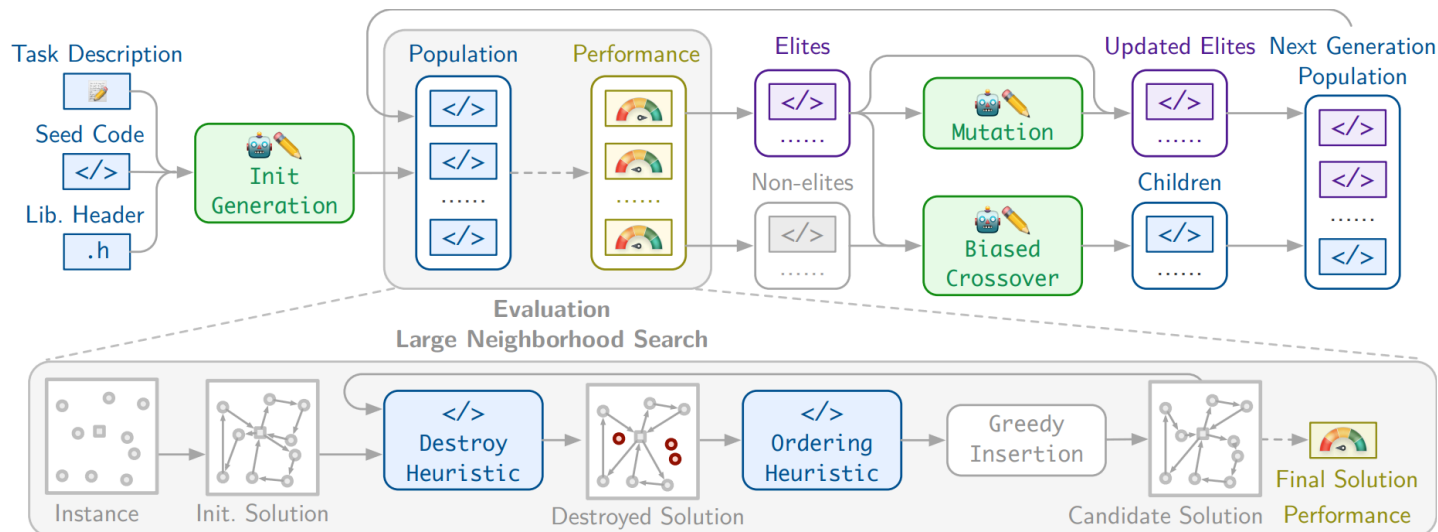
VRPAgent: Automated Heuristic Discovery by LLMs



VRPAgent pipeline overview. Figure adapted from (Hottung et al., 2025a)

1 Initial heuristics generation 2 Evaluation via LNS

VRPAgent: Automated Heuristic Discovery by LLMs

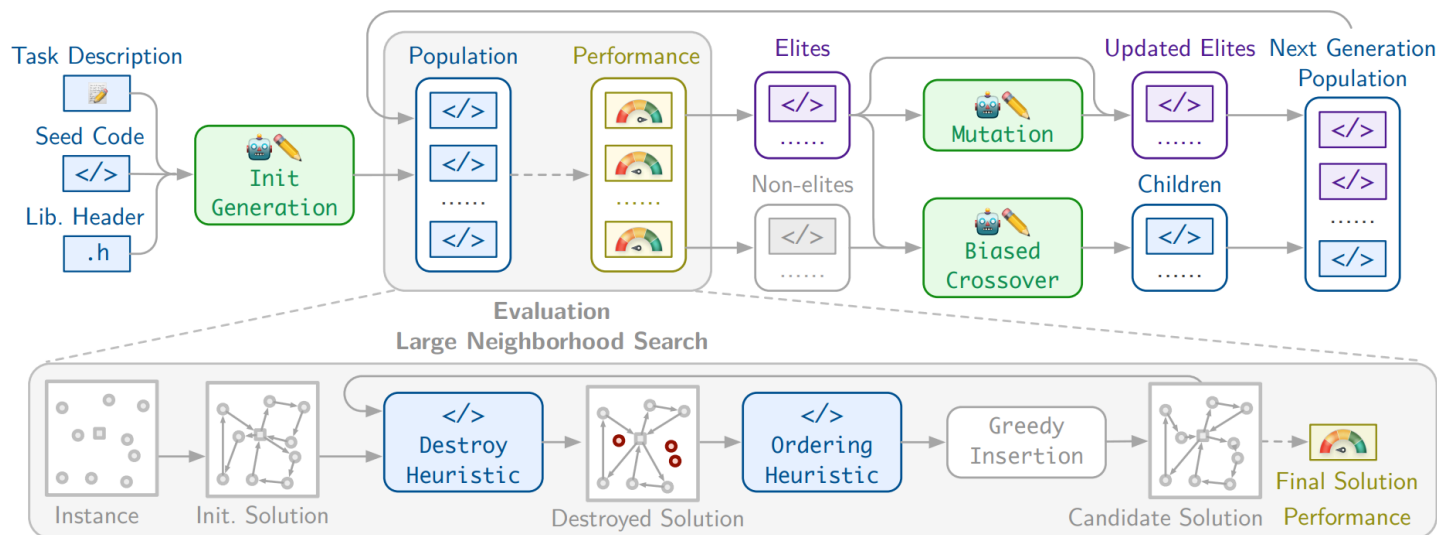


VRPAgent pipeline overview. Figure adapted from (Hottung et al., 2025a)

1 Initial heuristics generation 2 Evaluation via LNS 3 Genetic Algorithm

- Improve each elite via *mutation*
- *Crossover* of elites and non-elites

VRPAgent: Automated Heuristic Discovery by LLMs



VRPAgent pipeline overview. Figure adapted from (Hottung et al., 2025a)

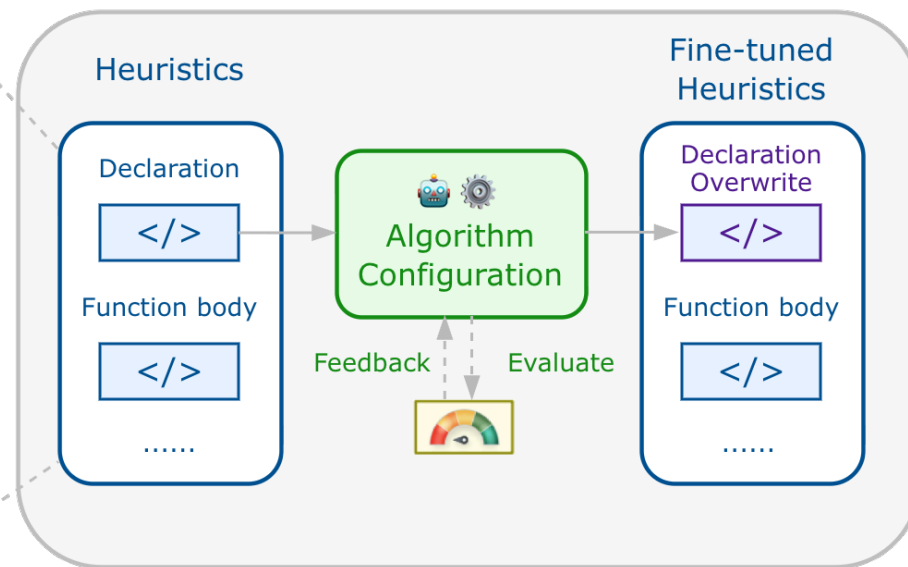
1 Initial heuristics generation **2** Evaluation via LNS **3** Genetic Algorithm **4** Re-evaluation

Heuristics Discovered by LLMs

```
// Customer selection function generated by LLM
std::vector<int> select_by_llm_1(const
Solution& sol) {
    const int MIN_CUSTOMERS_TO_REMOVE = 15;
    const int MAX_CUSTOMERS_TO_REMOVE = 25;
    //... Configurations definitions ...

    std::unordered_set<int> selectedCustomers;
    int numCustomersToRemove =
getRandomNumber(MIN_CUSTOMERS_TO_REMOVE,
MAX_CUSTOMERS_TO_REMOVE);
    //... Main code block logic ...

    return
std::vector<int>(selectedCustomers.begin(),
selectedCustomers.end());
}
```



Algorithm Configuration

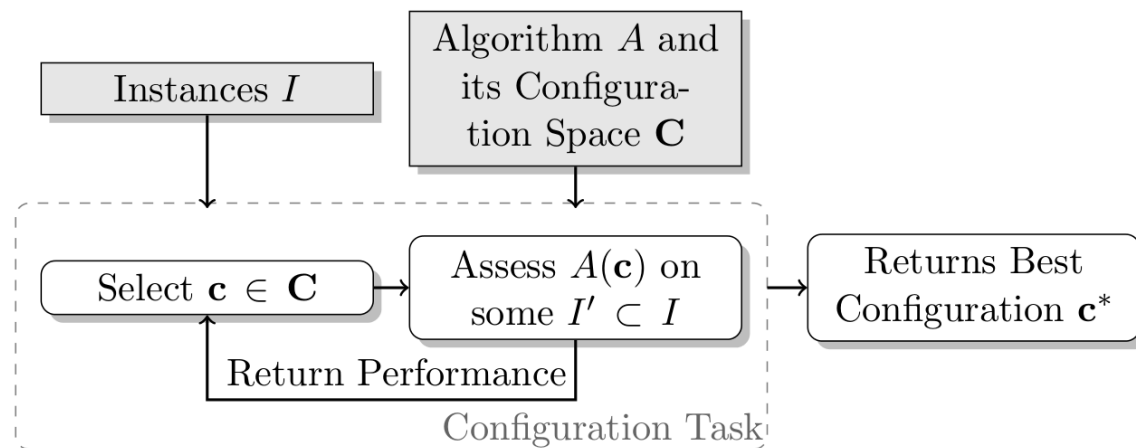


Figure 4. Workflow of Algorithm Configuration

Figure adapted from AutoML.org.

Examples of Parameters in Heuristics

- Float parameters

Example: `prob_tour_neighbor` and `prob_geo_neighbor`.

- Integer parameters

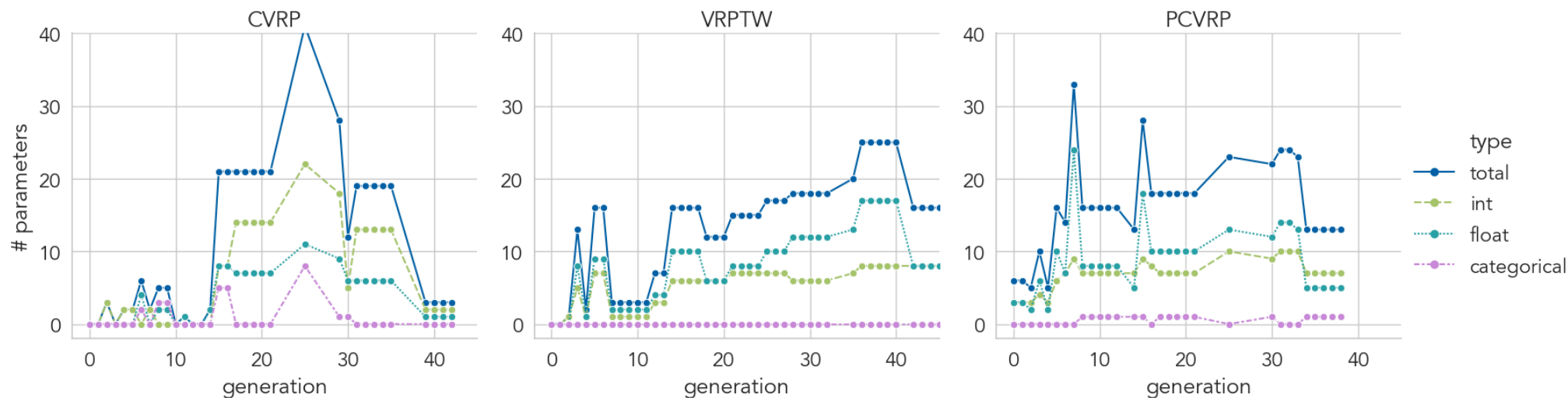
Example: `min_customers_to_remove` and `max_customers_to_remove`.

- “Categorical” parameters (discarded)

Most of them are dependencies, e.g., in the form of $y = x + 1$.

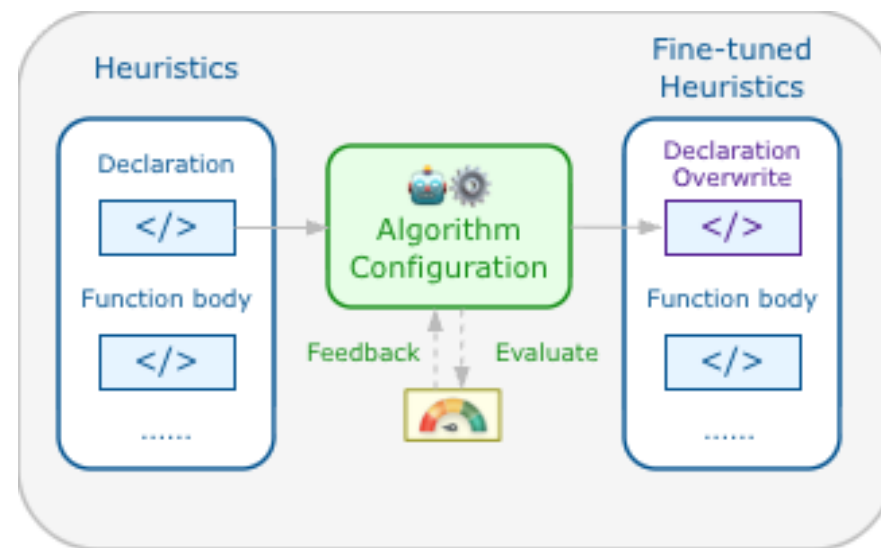
Examples of Parameters in Heuristics

The number of parameters increases in early generations and decreases later.



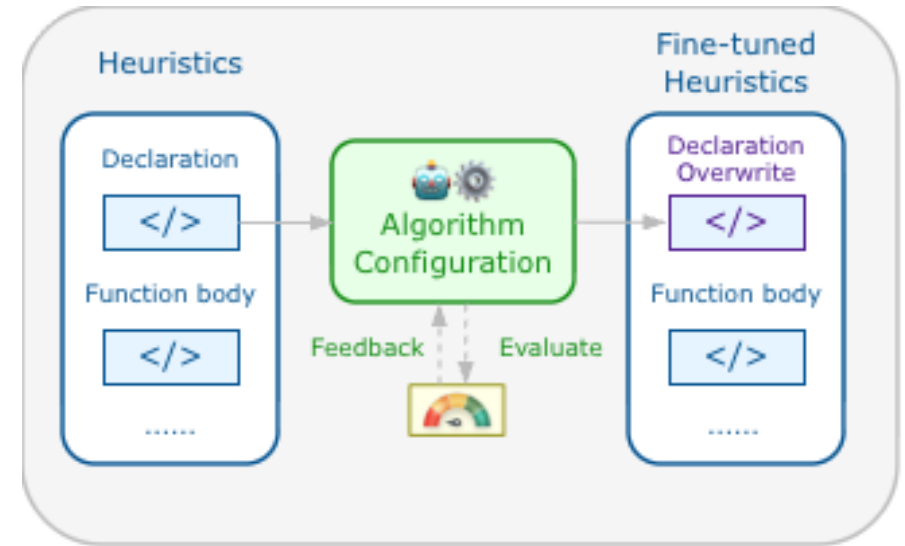
Configuration Setup

- Configurator: We use the **irace** package (López-Ibáñez et al., 2016) with a total budget of **3500** experiments on **256** training instances (never fully utilized).



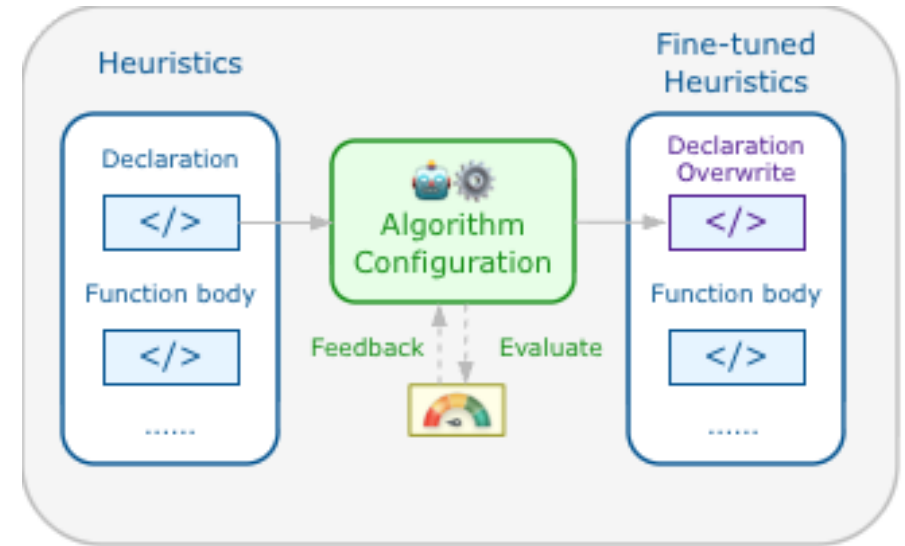
Configuration Setup

- Configurator: We use the **irace** package (López-Ibáñez et al., 2016) with a total budget of **3500** experiments on **256** training instances (never fully utilized).
- On average, it takes ~11 hours (VRPTW) and ~20 hours (CVRP and PCVRP) to fine-tune.
- * Each LNS search takes **20** seconds and **irace** can use **16** cores.



Configuration Setup

- Configurator: We use the **irace** package (López-Ibáñez et al., 2016) with a total budget of **3500** experiments on **256** training instances (never fully utilized).
- On average, it takes ~11 hours (VRPTW) and ~20 hours (CVRP and PCVRP) to fine-tune.
- Finally, we evaluate on 64 training + 64 testing instances (500 customers).



Can LLM-generated heuristics be fine-tuned?

Can LLM-generated heuristics be fine-tuned?

Yes.

Can LLM-generated heuristics be fine-tuned?

Yes.

Can the best discovered LLM-generated heuristics be fine-tuned?

Can LLM-generated heuristics be fine-tuned?

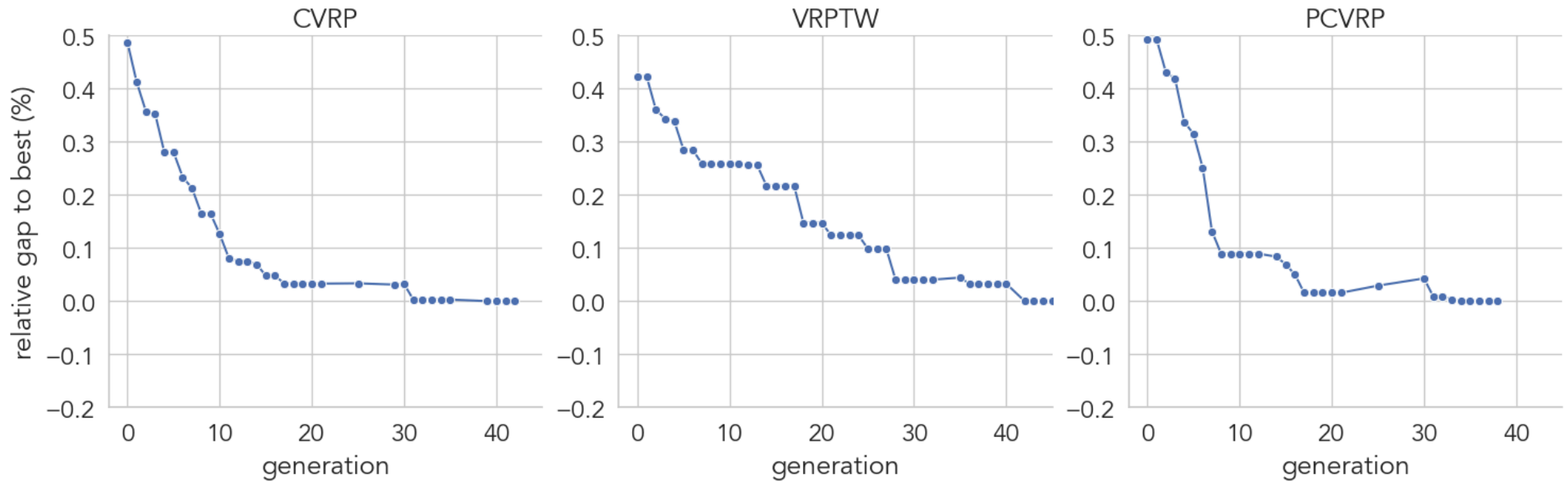
Yes.

Can the best discovered LLM-generated heuristics be fine-tuned?

Yes.

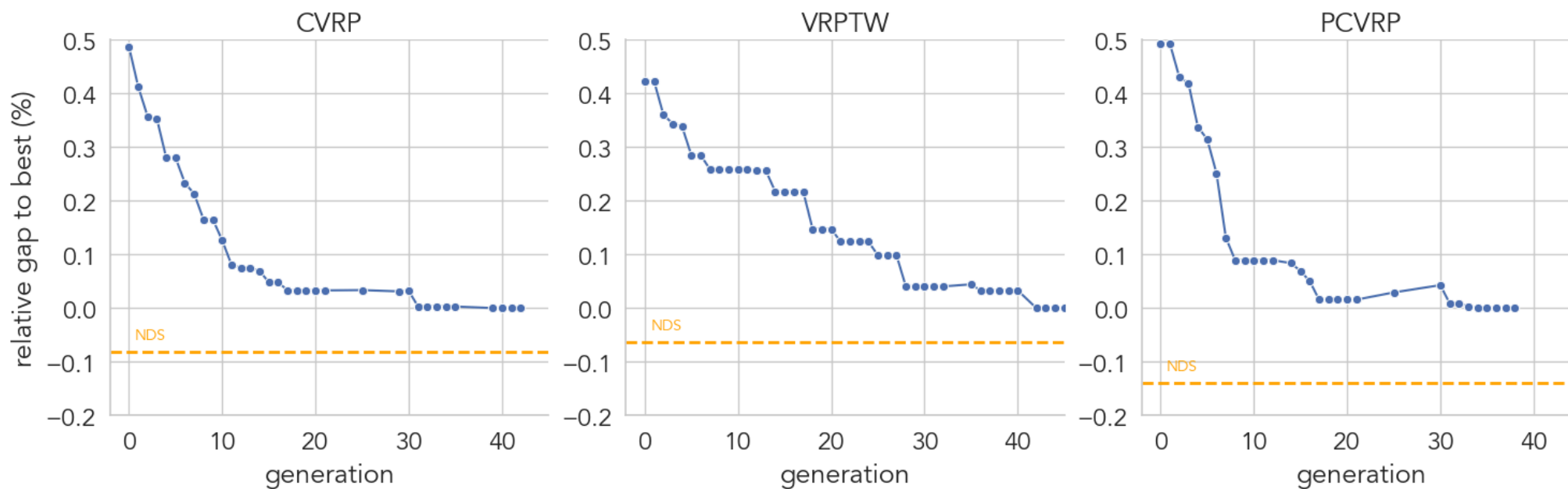
Fine-tuning Best Heuristics

* “Best”: Evaluated on 64 instances, see (Hottung et al., 2025a).



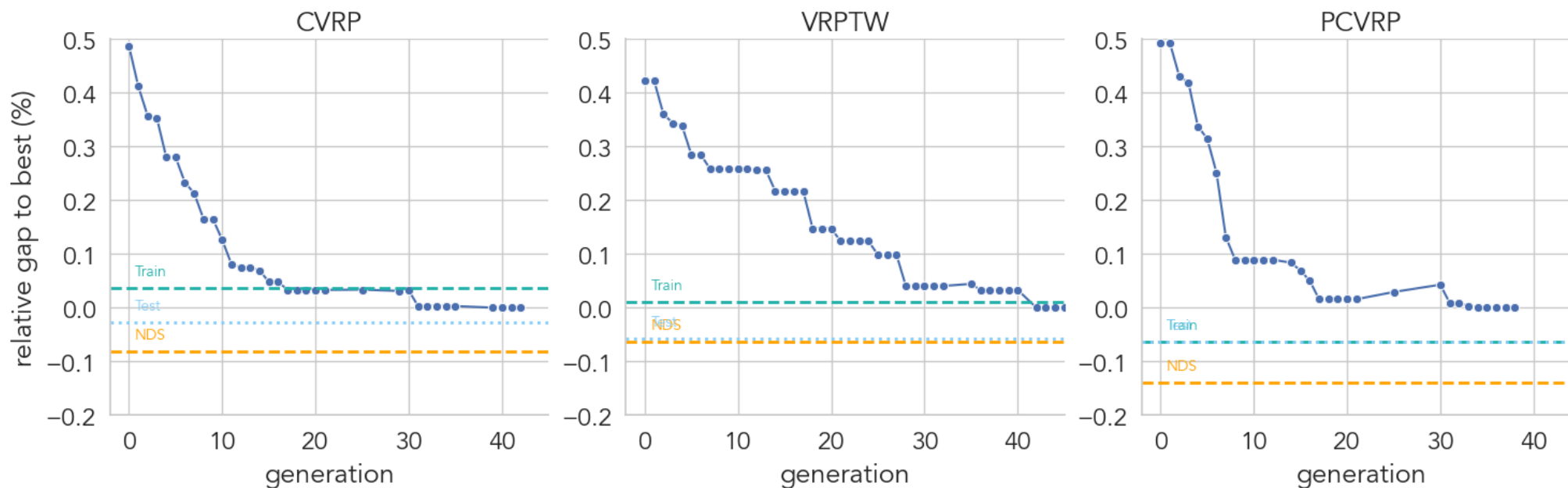
Fine-tuning Best Heuristics

*NDS: Neural Deconstruction Search baseline (Hottung et al., 2025b).



Fine-tuning Best Heuristics

*Train and Test: Fine-tuned parameters + best discovered heuristic function on training & testing instances



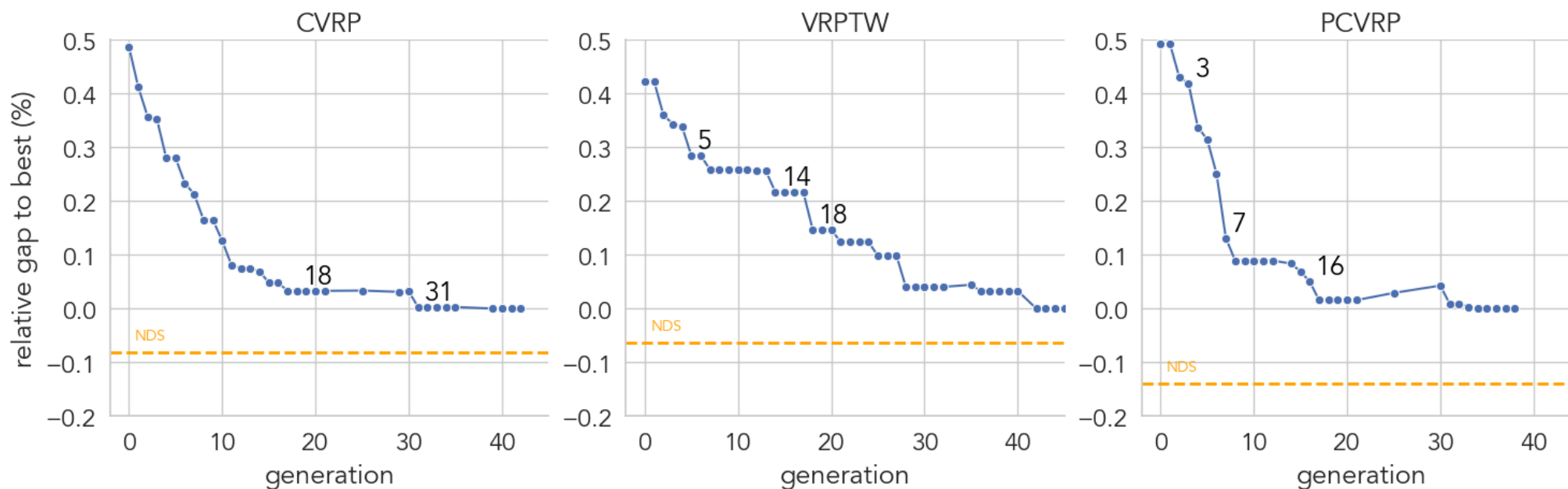
- The gaps are very *small*.
- However, even with fine-tuned parameters, the best discovered heuristic only approaches, but does not beat the NDS baseline.

Can early generations be tuned to beat later generations?

Can early generations be tuned to beat later generations?

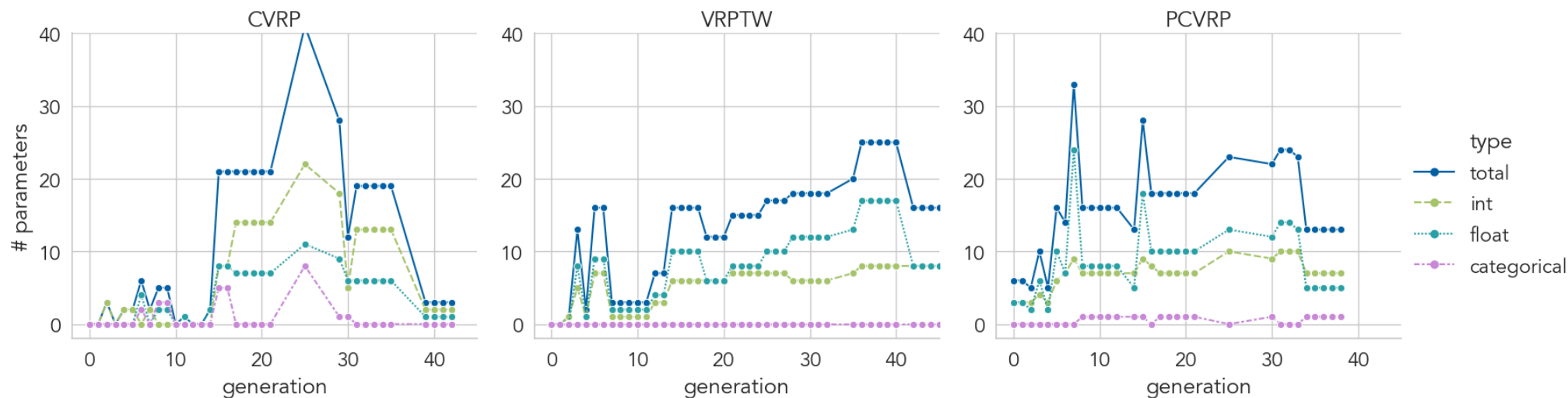
Well, it depends...

Selecting Heuristics with Early Generations



Selecting Heuristics with Early Generations

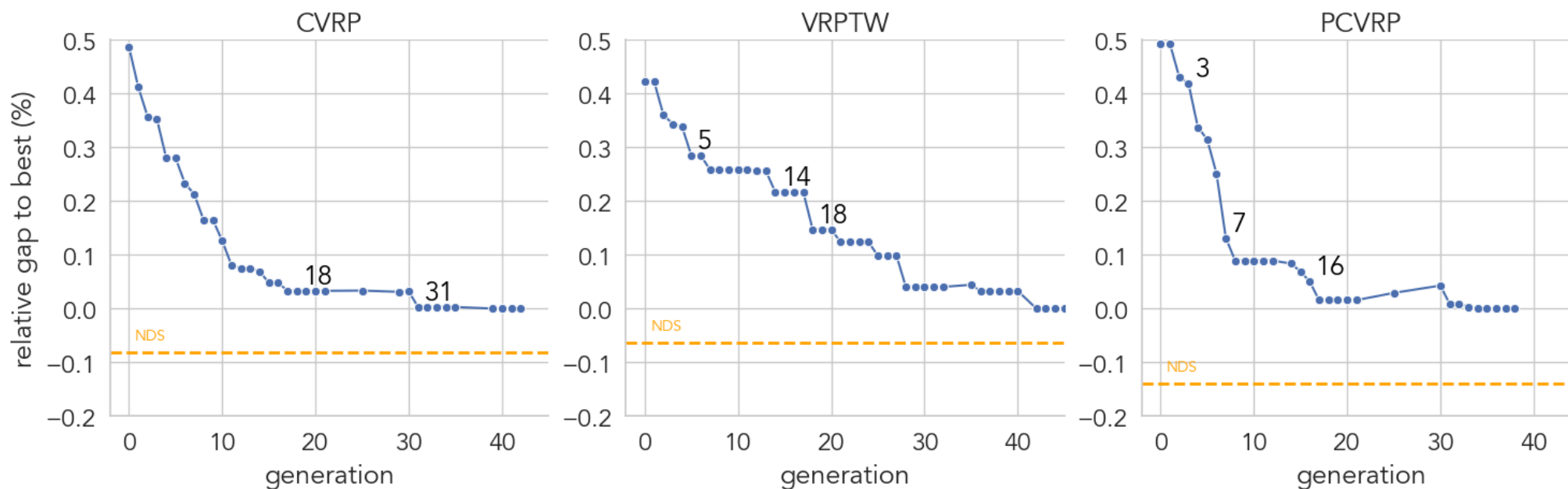
Recall the # parameters of the discovered heuristics.



Selecting Heuristics with Early Generations

Similar parameter structure (CVRP 18 vs. 31).

Different parameter structure (VRPTW and PCVRP).



Fine-tuning Heuristics with Early Generations

We take one run (seed 71) of **irace** and compare the fine-tuned heuristics against the best code with default parameters. Wilcoxon test p-values are reported ($\alpha = 0.05$).

Problem (dataset)	Heuristic	% Gaps to (best + default)	<i>p</i> -value	Significant?
CVRP (test)	gen 18	-0.056	0.126	N
CVRP (test)	gen 31	-0.068	0.066	N

Fine-tuning Heuristics with Early Generations

We take one run (seed 71) of **irace** and compare the fine-tuned heuristics against the best code with default parameters. Wilcoxon test p -values are reported ($\alpha = 0.05$).

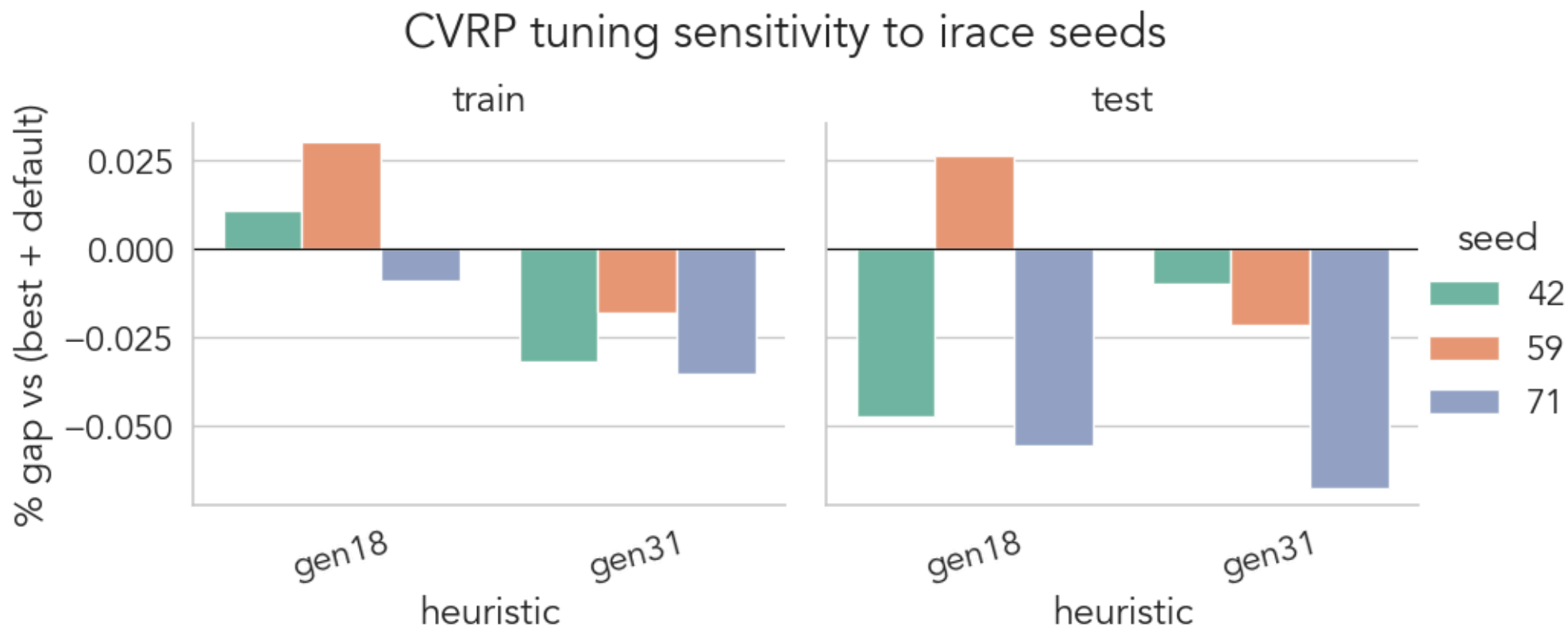
Problem (dataset)	Heuristic	% Gaps to (best + default)	p -value	Significant?
VRPTW (test)	gen 5	-0.008	-	-
VRPTW (test)	gen 14	0.063	-	-
VRPTW (test)	gen 18	0.135	-	-

Fine-tuning Heuristics with Early Generations

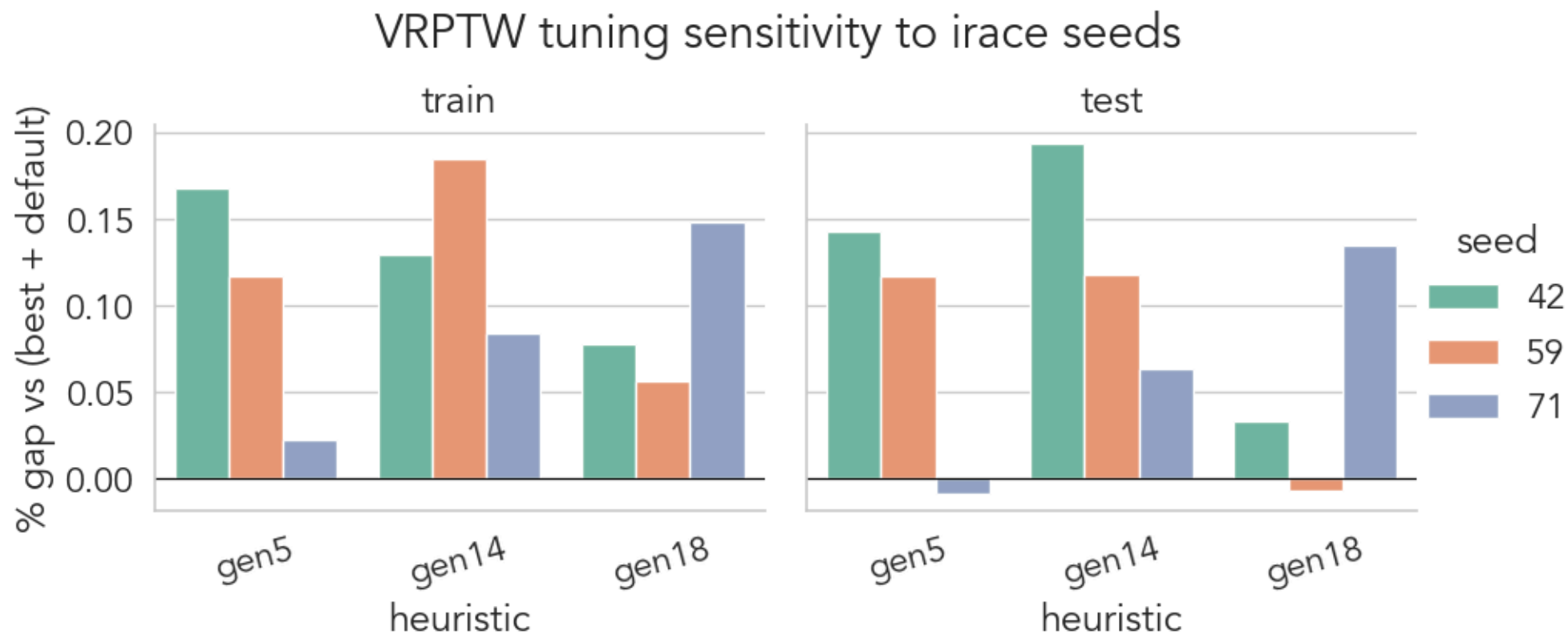
We take one run (seed 71) of **irace** and compare the fine-tuned heuristics against the best code with default parameters. Wilcoxon test p -values are reported ($\alpha = 0.05$).

Problem (dataset)	Heuristic	% Gaps to (best + default)	p -value	Significant?
PCVRP (test)	gen 3	0.254	-	-
PCVRP (test)	gen 7	-0.045	0.075	N
PCVRP (test)	gen 16	0.042	-	-

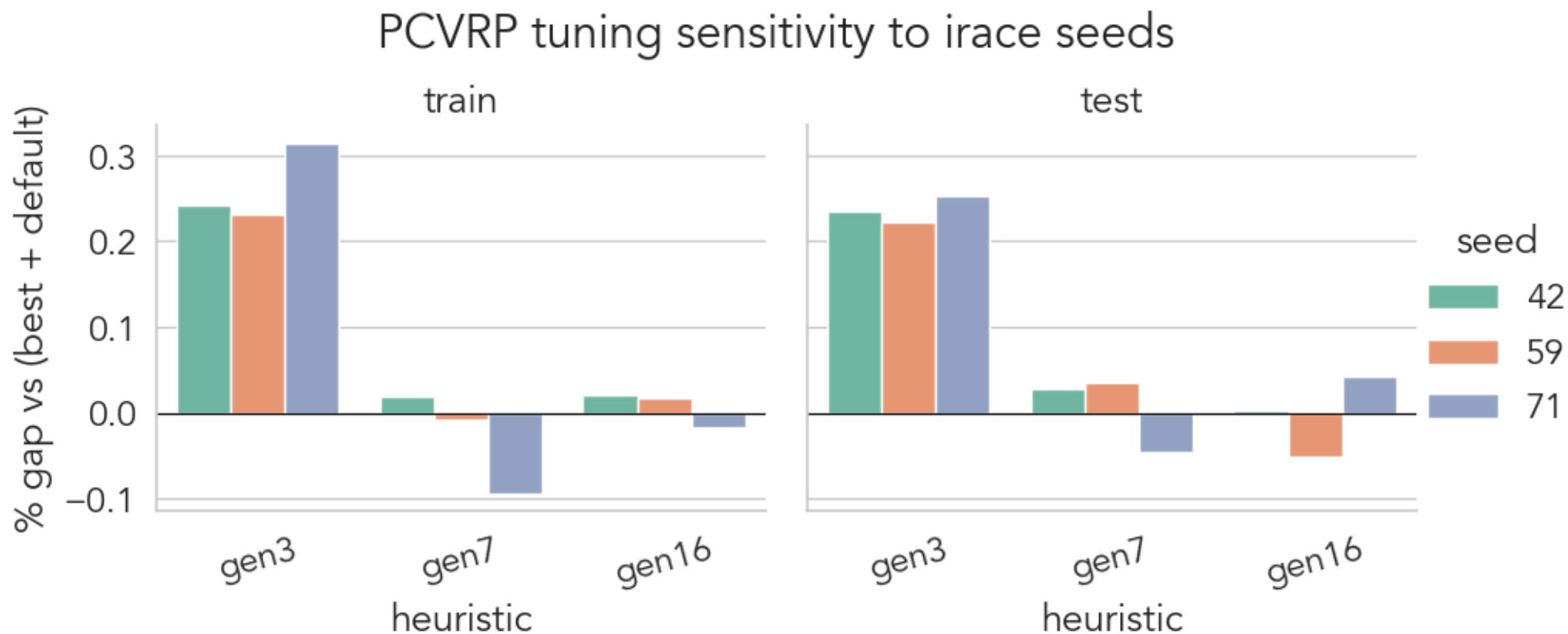
Sensitivity Analysis of irace Runs



Sensitivity Analysis of irace Runs



Sensitivity Analysis of irace Runs



Future work

Efficient Heuristic Discovery

Local LLM query:

-  
-    
-  

GA on instances:

-    
- 
-   

Efficient Heuristic Discovery

Local LLM query:

-  
-    
-  

GA on instances:

-    
- 
-   

LLM + GA:

-     
-    
-    

Efficient Heuristic Discovery

Local LLM query:

-  
-    
-  

RL training stage:

-   
-  
-   

GA on instances:

-    
- 
-   

After convergence:

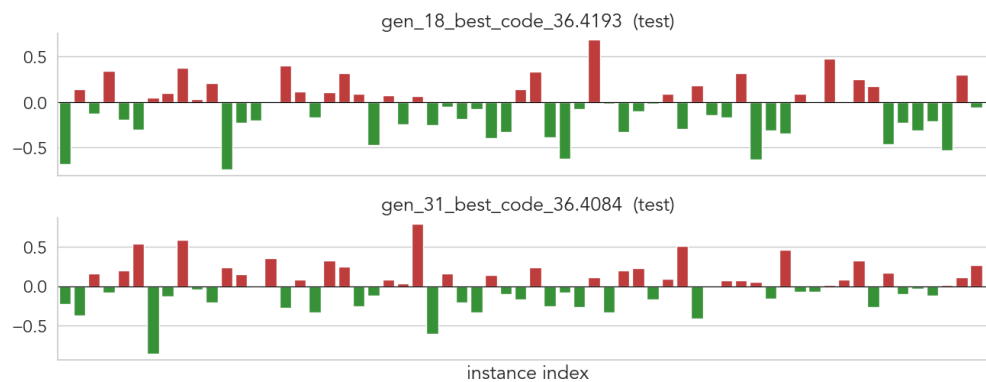
- 
-  
-  

LLM + GA:

-     
-    
-    

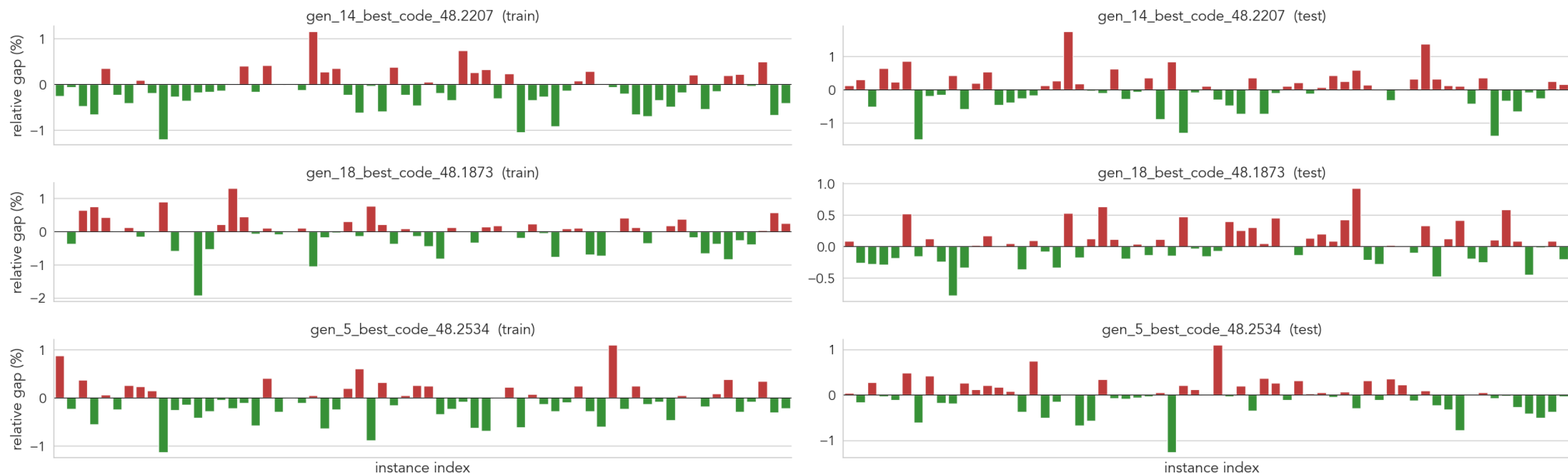
Instance-specific Algorithm Configuration

Paired per-sample difference - CVRP (seed 42)



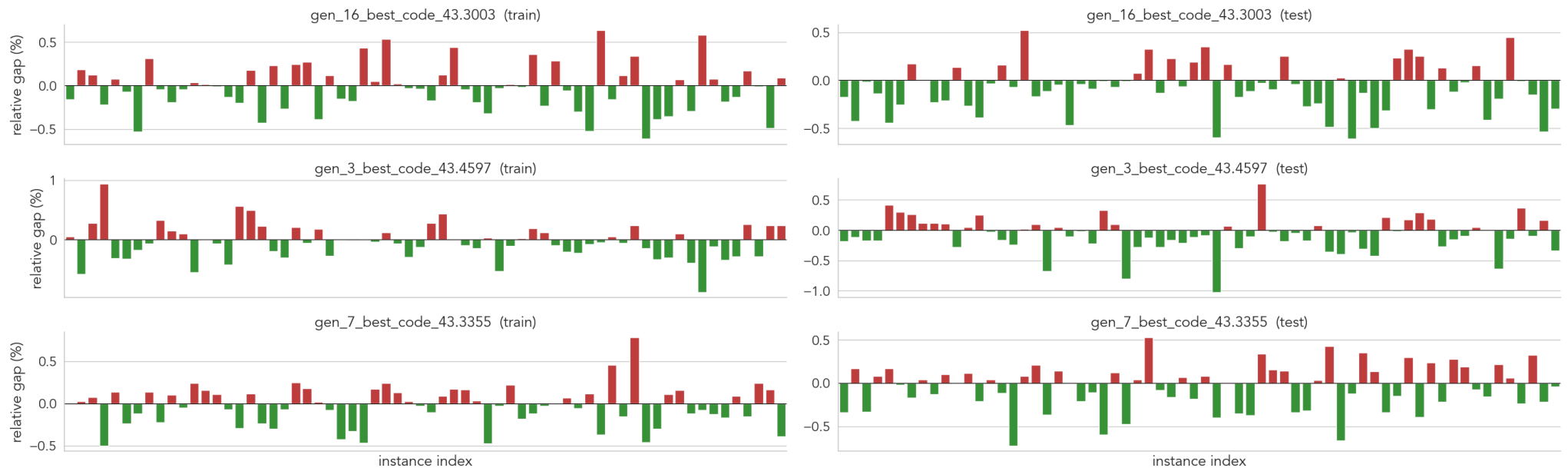
Instance-specific Algorithm Configuration

Paired per-sample difference - VRPTW (seed 42)



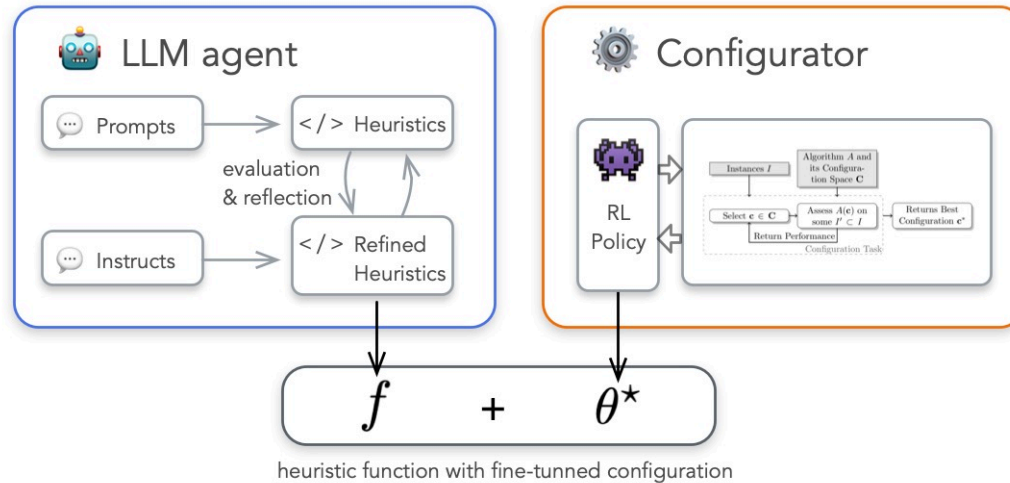
Instance-specific Algorithm Configuration

Paired per-sample difference - PCVRP (seed 42)



Instance-specific Algorithm Configuration

Using reinforcement learning (RL) for instance-specific algorithm configuration, e.g., OPTICAT (Schede et al., 2025).



Our research question is:

Can automated algorithm configuration for LLM-driven heuristic discovery achieve superior performance compared to the state-of-the-art,

Our research question is:

Can automated algorithm configuration for LLM-driven heuristic discovery achieve superior performance compared to the state-of-the-art, while addressing *transferability* and *generalization* of the parameter space?

Takeaways

1. Motivation: LLM-driven heuristic discovery with GA is powerful but costly.

Takeaways

1. Motivation: LLM-driven heuristic discovery with GA is powerful but costly.
2. Combining GA and AC may achieve better performance.
 - Early generations: ✗
 - “Middle” generations: ✓

1. Motivation: LLM-driven heuristic discovery with GA is powerful but costly.
2. Combining GA and AC may achieve better performance.
 - Early generations: ✗
 - “Middle” generations: ✓
3. Instance-specific deep RL may reduce the overall cost.

Special thanks to André Hottung for discussions.



VRPAgent/2510.07073



Slides/Personal site

- Hottung, A., Berto, F., Hua, C., Zepeda, N. G., Wetzel, D., Römer, M., Ye, H., Zago, D., Poli, M., Massaroli, S., Park, J., & Tierney, K. (2025a). VRPAgent: LLM-Driven Discovery of Heuristic Operators for Vehicle Routing Problems. *Arxiv*.
- Hottung, A., Wong-Chung, P., & Tierney, K. (2025b). Neural Deconstruction Search for Vehicle Routing Problems. *Transactions on Machine Learning Research*. <https://openreview.net/forum?id=bCmEP1Ltwq>
- López-Ibáñez, M., Dubois-Lacoste, J., Pérez Cáceres, L., Birattari, M., & Stützle, T. (2016). The irace package: Iterated racing for automatic algorithm configuration. *Operations Research Perspectives*, 3, 43–58. <https://doi.org/10.1016/j.orp.2016.09.002>
- Schede, E., Seiler, M., Tierney, K., & Trautmann, H. (2025). Deep reinforcement learning for instance-specific algorithm configuration. *GECCO*, 1190–1198.
- Shaw, P. (1998). Using Constraint Programming and Local Search Methods to Solve Vehicle Routing Problems. *CP*, 1520, 417–431.