香港城市大學
City University of Hong Kong
電腦科學系
Department of Computer Science

Machine Learning for Combinatorial Optimization

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February 2, 2021

- Bengio, Yoshua, Andrea Lodi, and Antoine Prouvost. "**Machine learning for combinatorial optimization: a methodological tour d'horizon**." *European Journal of Operational Research* (2020).

Outline

1. Road Map
2. ML for Combinatorial Optimization
3. Conclusion

Outline

1. **Road Map**
2. ML for Combinatorial Optimization
3. Conclusion

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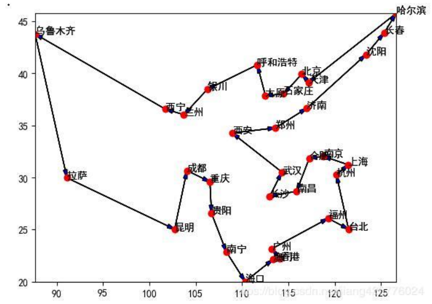
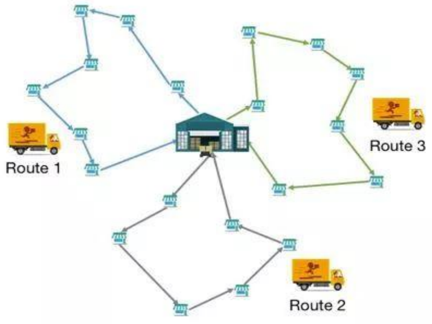
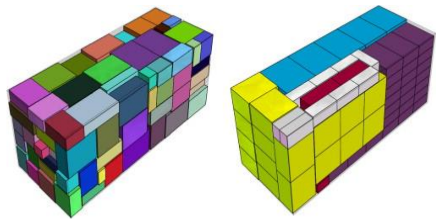
Combinatorial Optimization Problems



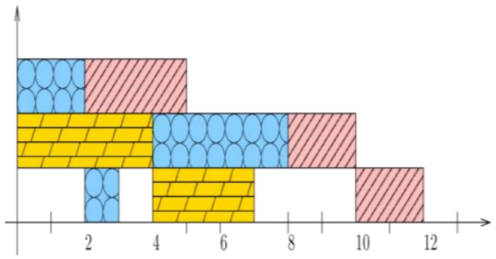
TSP



VRP

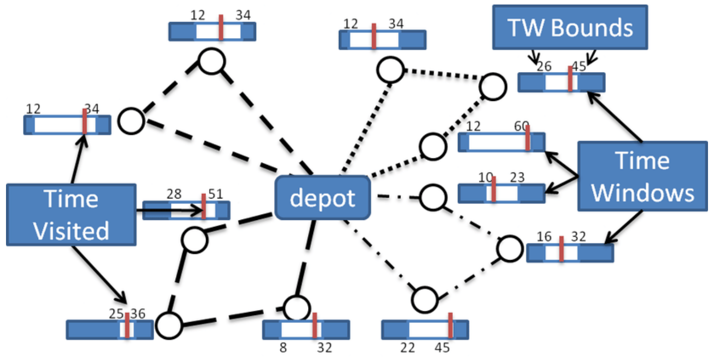


Bin Packing

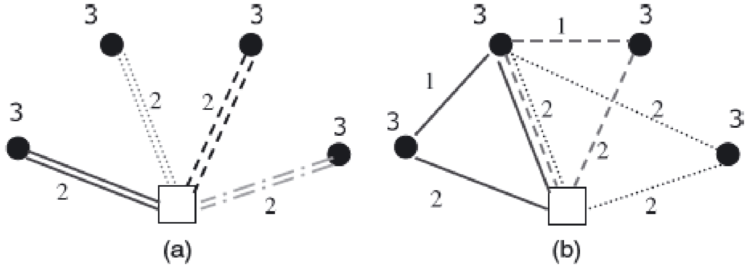


Scheduling

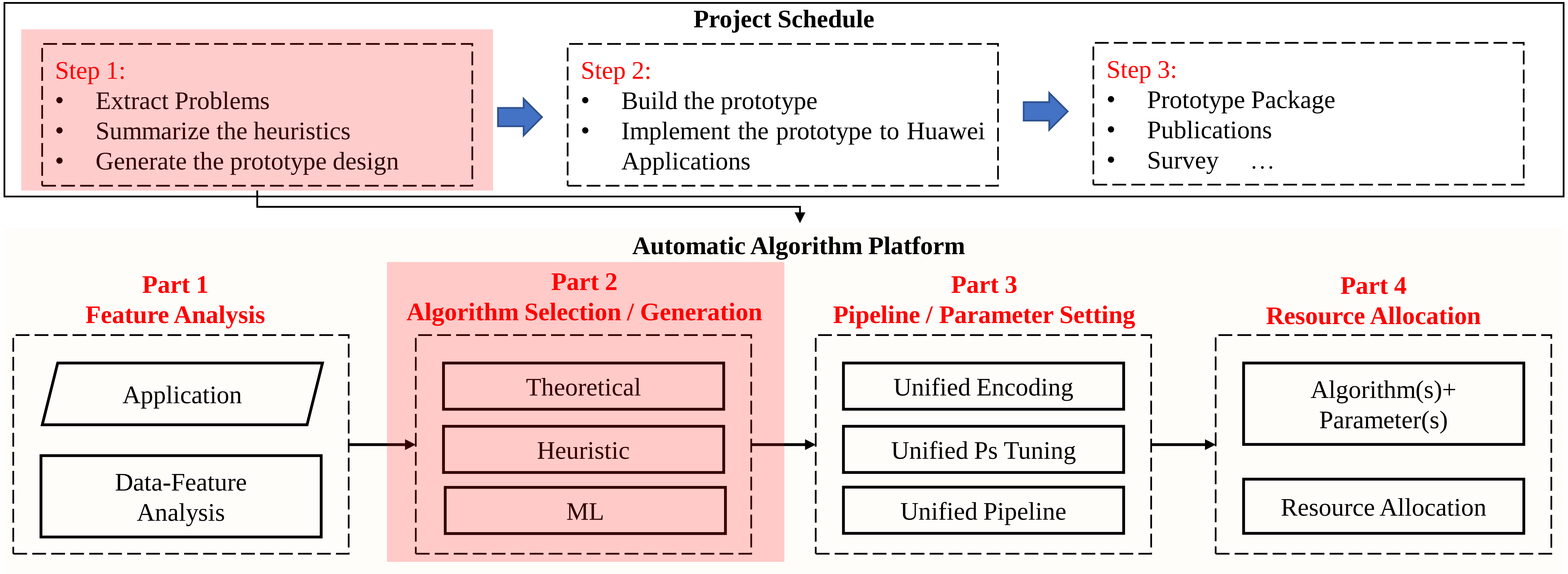
HuaWei Cases: VRP problems



- CVRP
- VRPB
- VRPTW
- SDVRP
- Applications



A fast design optimization method (platform) for VRP problems



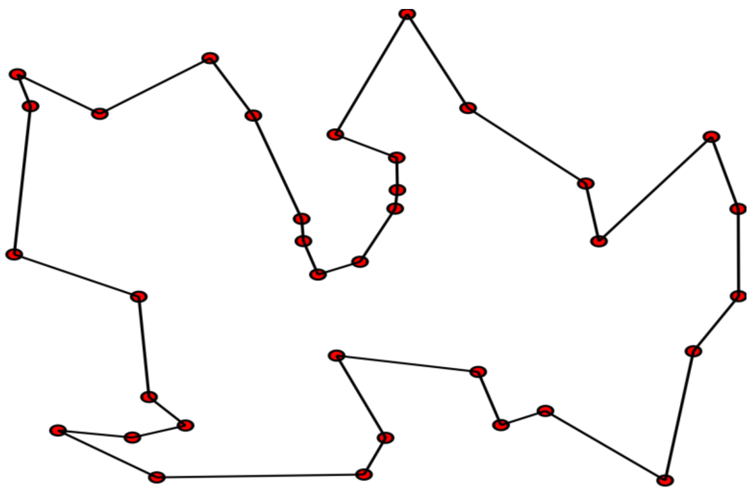
- **2021.1.19** Metaheuristics for Vehicle Routing Problems (Step 1 - Part 2)
- **2021.1.31** ML for Combinational Optimization (Step 1 - Part 2)

Outline

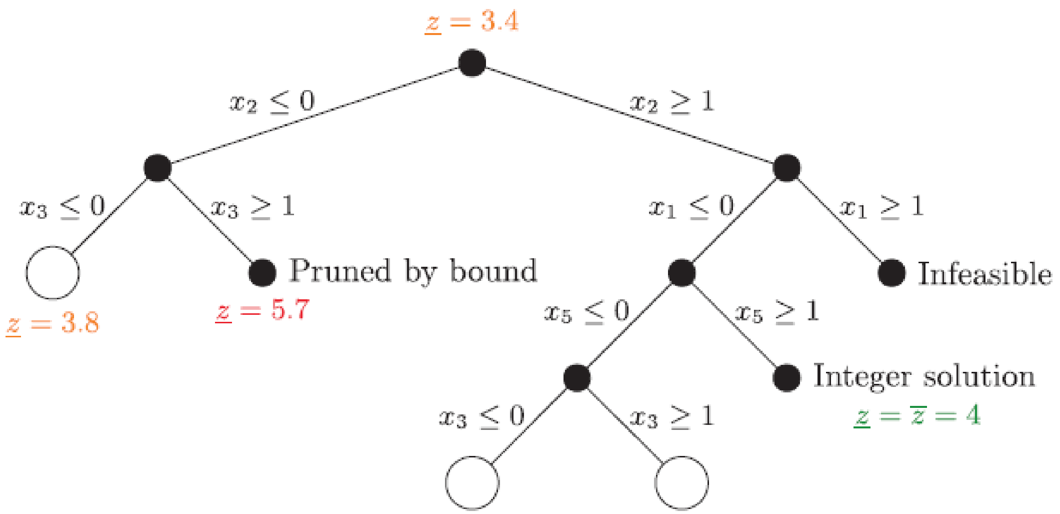
1. Road Map
2. **ML for Combinatorial Optimization**
3. Conclusion

ML for CO : **1) Preliminaries**

TSP problem

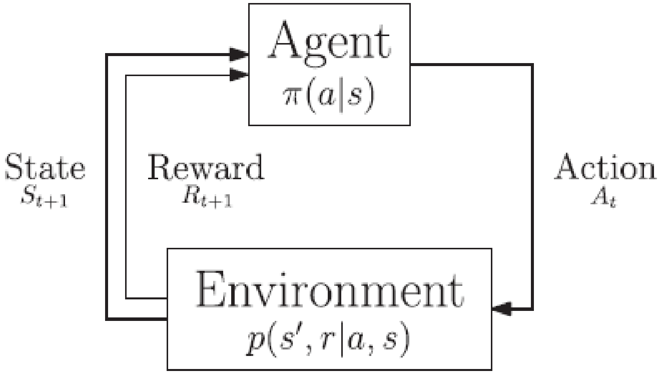


Branch-and-Bound

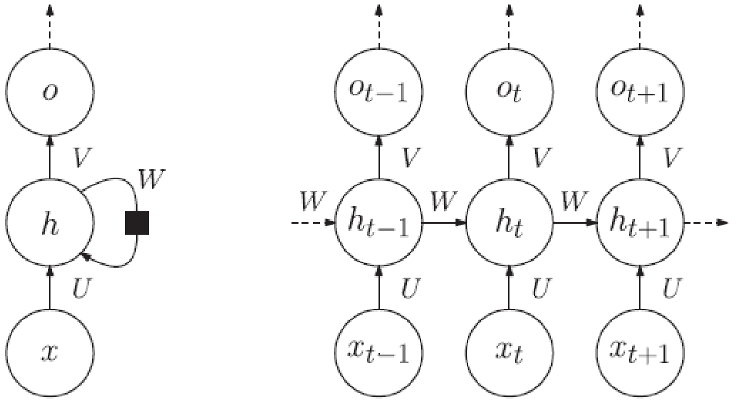


ML for CO : 1) Preliminaries

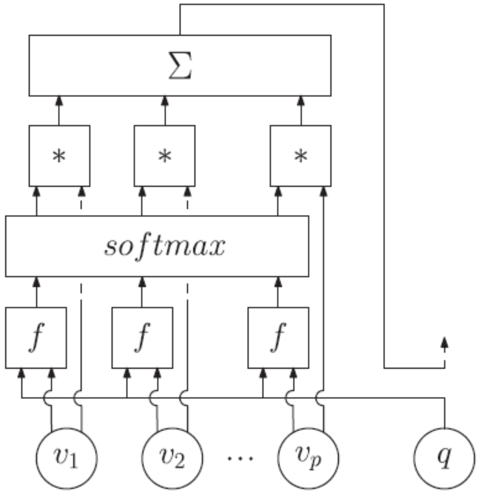
Reinforcement learning



Recurrent neural network



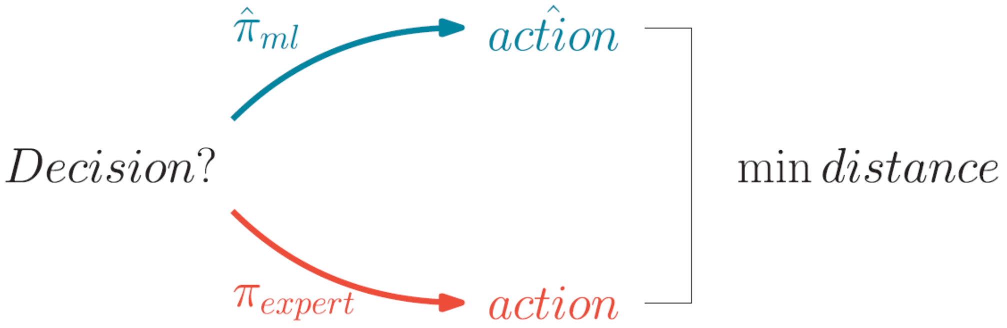
Attention mechanism



ML for CO : 2) Two strategies

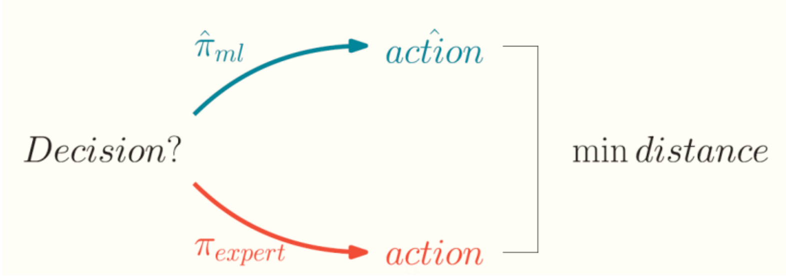
The policy is trained to reproduce the action of an expert policy by **minimizing some discrepancy in the action space**

- Demonstration

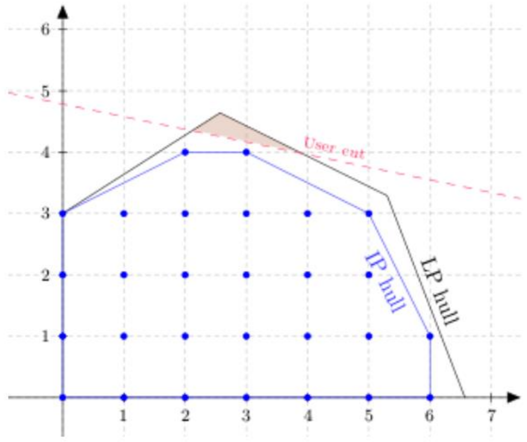


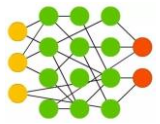
Learning through a reward signal, **maximizing the expected sum of future rewards** (the return) matters

- Experience



ML for CO : 2) Two strategies





neural network estimator

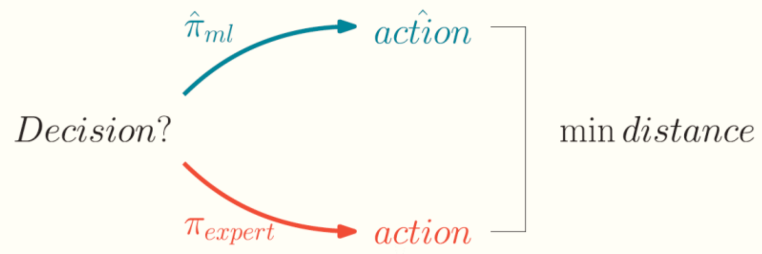
non-convex quadratic programming

iteratively add cutting planes

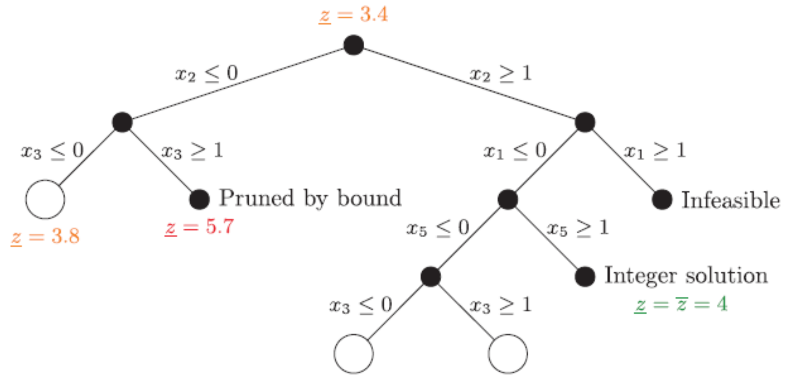
associated semidefinite programming relaxation

- Baltean-Lugojan, Radu, et al. *Selecting cutting planes for quadratic semidefinite outer-approximation via trained neural networks*. Technical Report, CPLEX Optimization, IBM, 2018.

use a **neural network** to approximate the **lower bound improvement** generated by tightening the current relaxation via cutting planes

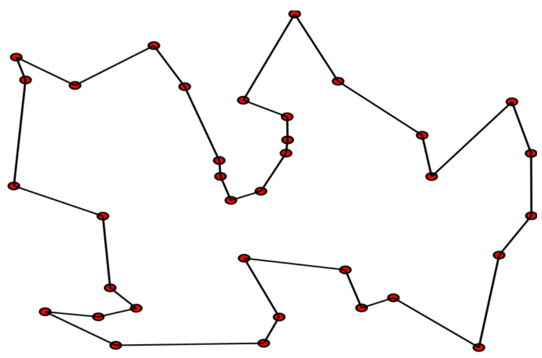


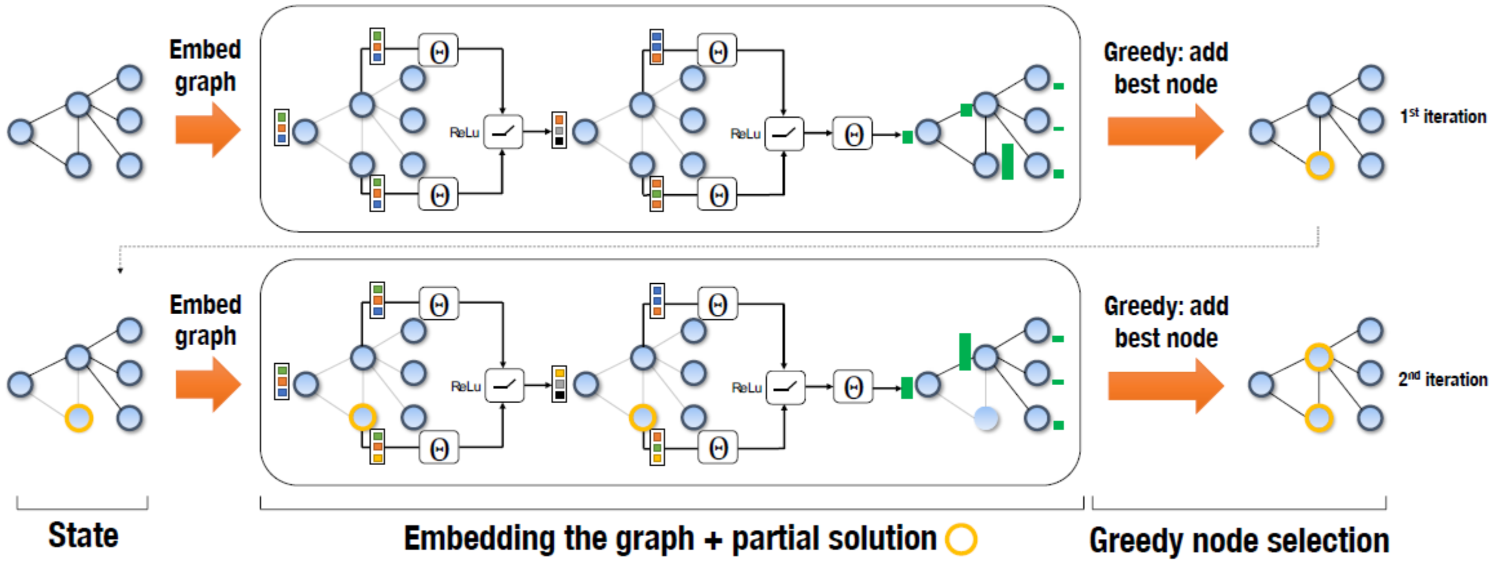
ML for CO : 2) Two strategies



- Alvarez, Alejandro Marcos, Quentin Louveaux, and Louis Wehenkel. "A supervised machine learning approach to variable branching in branch-and-bound." *In ecml*. 2014. → use a special type of **decision tree** to approximate **strong branching decisions** using supervised learning
- Khalil, Elias, et al. "Learning to branch in mixed integer programming." *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 30. No. 1. 2016. → a **linear model** is learned for every instance by using **strong branching at the top of the tree**
- Marcos Alvarez, Alejandro, Louis Wehenkel, and Quentin Louveaux. "Online learning for strong branching approximation in branch-and-bound." (2016). → **active fashion:** when the estimator is deemed unreliable, the algorithm falls back to true strong branching
- Gasse, Maxime, et al. "Exact combinatorial optimization with graph convolutional neural networks." *arXiv preprint arXiv:1906.01629* (2019). → use a **graph convolutional neural networks** **to** learn an offline approximation to strong branching

ML for CO : 2) Two strategies

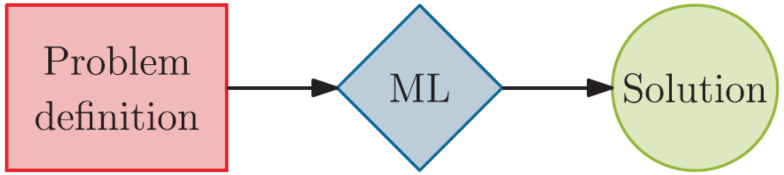




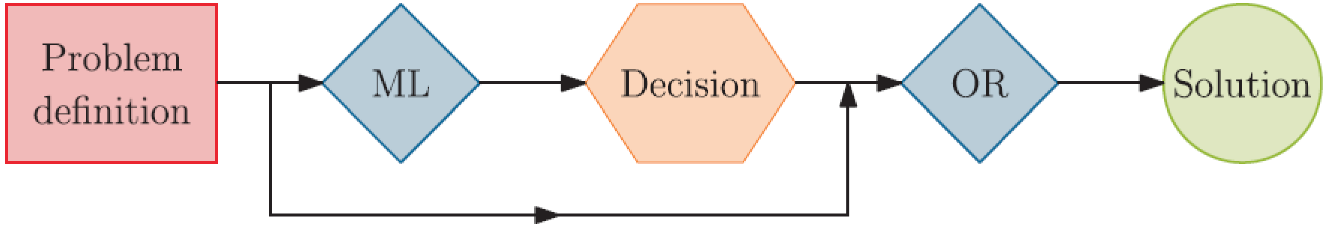
- Dai, Hanjun, et al. "Learning combinatorial optimization algorithms over graphs." *arXiv preprint arXiv:1704.01665* (2017). → build a **greedy heuristic framework**, where the **node selection policy** is learned using a graph neural network

ML for CO : 3) Algorithmic structure

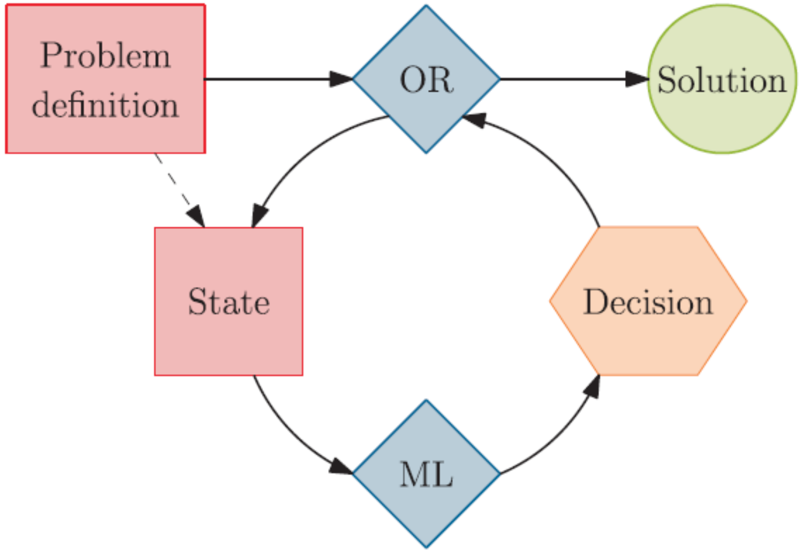
- End to end learning



- Learning to configure algorithms



- Machine learning alongside optimization algorithms



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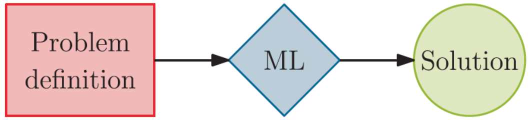
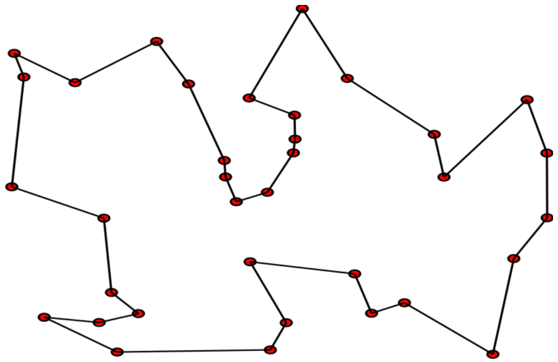
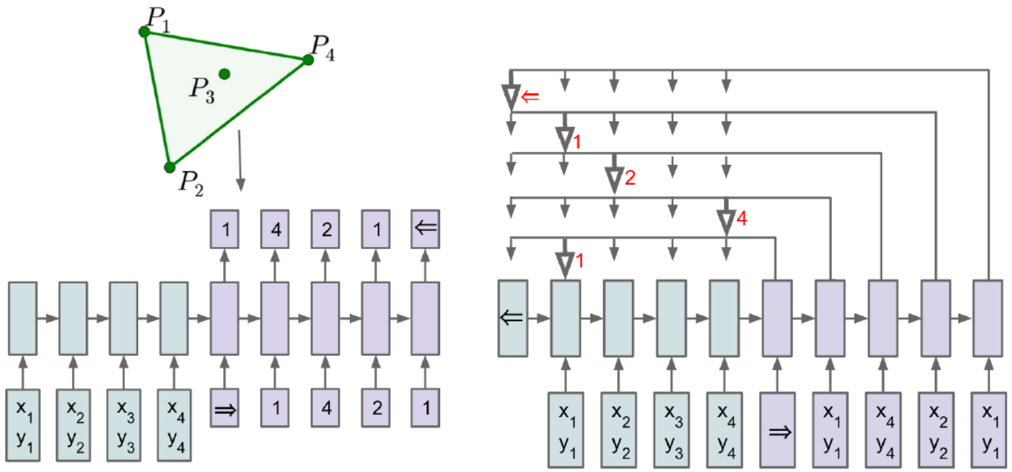


ML for CO : 3) Algorithmic structure





(a) Sequence-to-Sequence (b) Ptr-Net

- Vinyals, Oriol, Meire Fortunato, and Navdeep Jaitly. "Pointer networks." arXiv preprint arXiv:1506.03134 (2015). → **recurrent neural network** and an **attention mechanism** are used
- Bello, Irwan, et al. "Neural combinatorial optimization with reinforcement learning." arXiv preprint arXiv:1611.09940 (2016). → pointer network and reinforcement learning
- Nazari, Mohammadreza, et al. "Reinforcement learning for solving the vehicle routing problem." arXiv preprint arXiv:1802.04240 (2018). → pointer network and reinforcement learning on VRP

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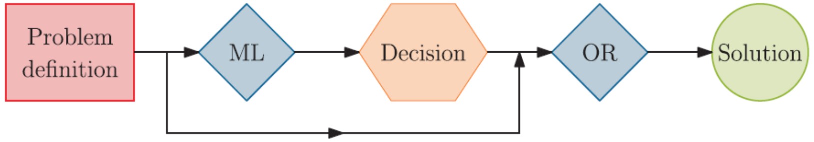
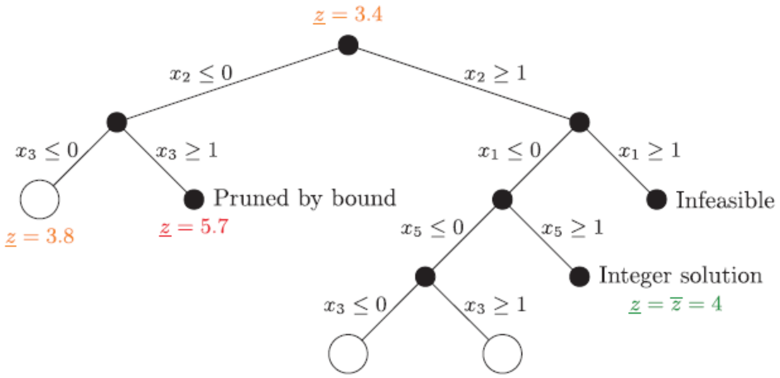
Learning to configure algorithms



ML for CO : 3) Algorithmic structure



- Bonami, P., Lodi, A., & Zarpellon, G. (2018). Learning a Classification of Mixed-Integer Quadratic Programming Problems. In Integration of constraint programming, artificial intelligence, and operations research . In Lecture Notes in Computer Science (pp. 595–604). → use different **machine learning** methods to **decide if linearizing the problem will solve faster**
- Kruber, M., Lübbecke, M. E., & Parmentier, A. (2017). Learning When to Use a Decomposition. In Integration of AI and OR techniques in constraint programming . In Lecture Notes in Computer Science (pp. 202–210) → use **machine learning** on mixed-integer linear programming instances to estimate **if Dantzig-Wolf decomposition is effective**
- Ansótegui, C. , Heymann, B. , Pon, J. , Sellmann, M. , & Tierney, K. (2019). Hyper-Reactive Tabu Search for MaxSAT. In R. Battiti, M. Brunato, I. Kotsireas, & P. M. Pardalos (Eds.), Learning and intelligent optimization . In Lecture Notes in Computer Science (pp. 309–325). Cham: Springer International Publishing .

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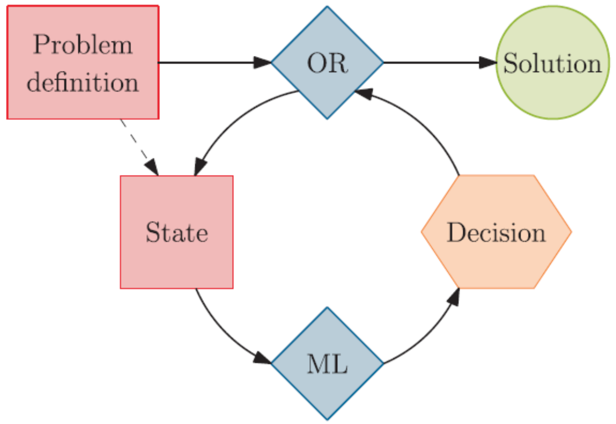
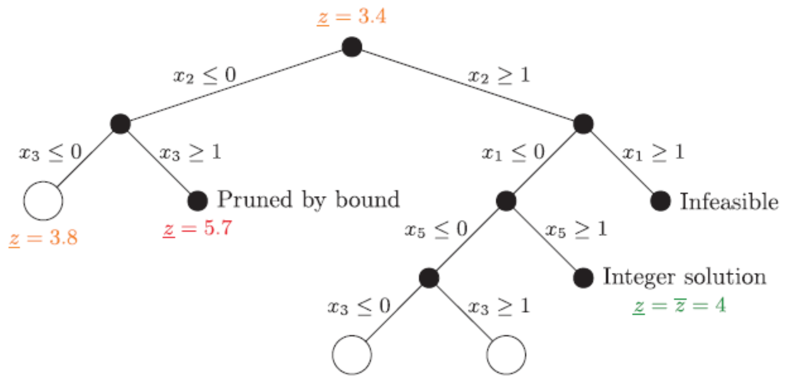
Machine learning alongside optimization algorithms



ML for CO : 3) Algorithmic structure



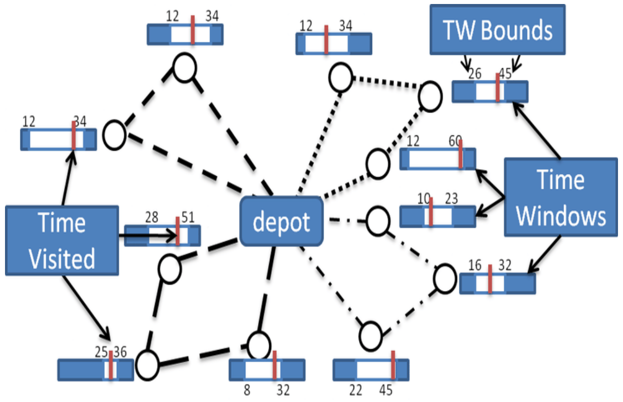
- ❑ Khalil, Elias B., et al. "Learning to Run Heuristics in Tree Search." IJCAI. 2017.
- ❑ Hottung, André, Shunji Tanaka, and Kevin Tierney. "Deep learning assisted heuristic tree search for the container pre-marshalling problem." Computers & Operations Research 113 (2020): 104781.

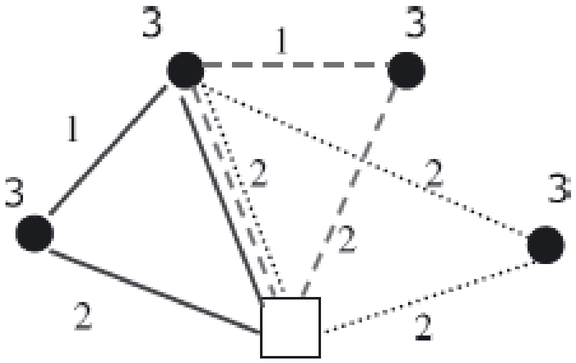
build **an machine learning model** to predict **whether or not running a given heuristic will yield a better solution** than the best

ML for CO : 4) Learning objective

- ***Multi-instance formulation***
- *Surrogate objectives*
- *On generalization*
- *Single instance learning*
- *Fine tuning and meta-learning*
- *Other metrics*

$$\min_{a \in \{a_1, a_2\}} \mathbb{E}_{i \sim P}\, m(i, a). \Rightarrow \min_{a \in \{a_1, a_2\}} \sum_{i \in D_{train}} \frac{1}{|D_{train}|} m(i, a).$$



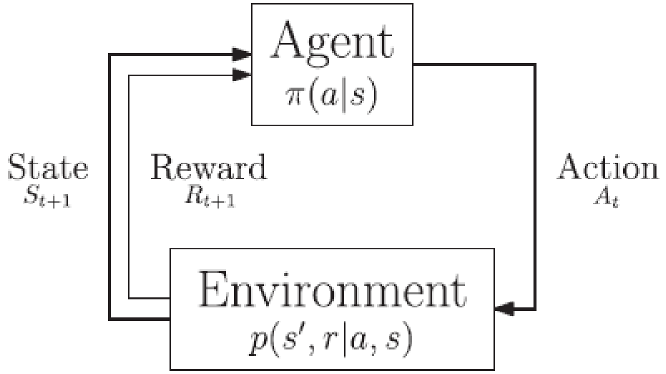


(b)

ML for CO : 4) Learning objective

- *Multi-instance formulation*
- ***Surrogate objectives***
- *On generalization*
- *Single instance learning*
- *Fine tuning and meta-learning*
- *Other metrics*

This sparse reward setting is challenging for reinforcement learning algorithms, and one might want to design a surrogate reward signal to encourage intermediate accomplishments.



❑ Gasse, Maxime, et al. "Exact combinatorial optimization with graph convolutional neural networks." arXiv preprint arXiv:1906.01629 (2019).

ML for CO : 4) Learning objective

- *Multi-instance formulation*
- *Surrogate objectives*
- ***On generalization***
- *Single instance learning*
- *Fine tuning and meta-learning*
- *Other metrics*

learned on a finite set of instances to perform well (generalize) to any "*real-world* "mixed-integer linear programming instance.

- From small to large
- From one to different problems
- From simple to complex

❑ Khalil, Elias, et al. "Learning to branch in mixed integer programming." Proceedings of the AAAI Conference on Artificial Intelligence. Vol. 30. No. 1. 2016.

ML for CO : 4) Learning objective

- *Multi-instance formulation*
- *Surrogate objectives*
- *On generalization*
- ***<u>Single instance learning</u>***
- *Fine tuning and meta-learning*
- *Other metrics*

starting the timer at the beginning of learning and competing with other solvers to get the solution the fastest

the model still needs to generalize to **<u>unseen states of the algorithm</u>**

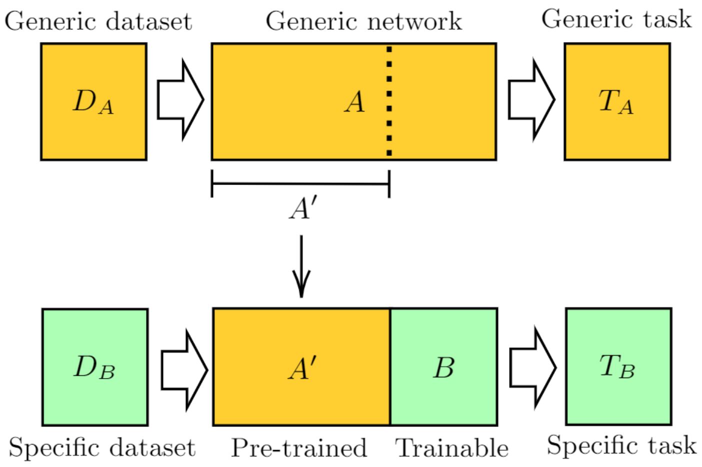
❑ Khalil, Elias, et al. "Learning to branch in mixed integer programming." Proceedings of the AAAI Conference on Artificial Intelligence. Vol. 30. No. 1. 2016.

ML for CO : 4) Learning objective

- *Multi-instance formulation*
- *Surrogate objectives*
- *On generalization*
- *Single instance learning*
- ***Fine tuning and meta-learning***
- *Other metrics*

Transfer learning / Multi-task learning

Meta-learning:
the inner loop trains the parameters of a model on the training set which are themselves optimized in an outer loop in a way that depends on meta-parameters

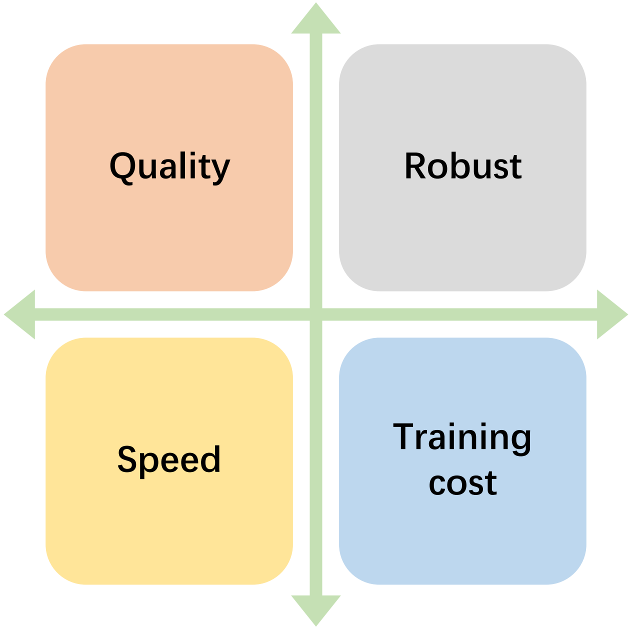


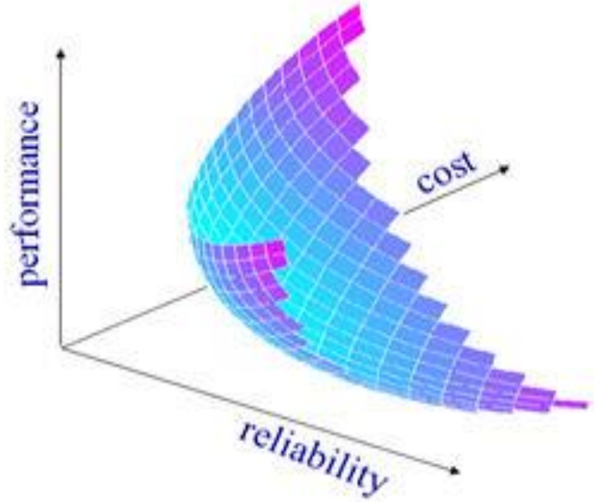
❑ Fitzgerald, Tadhg, et al. "React: Real-time algorithm configuration through tournaments." Seventh Annual Symposium on Combinatorial Search. 2014.

ML for CO : 4) Learning objective

- *Multi-instance formulation*
- *Surrogate objectives*
- *On generalization*
- *Single instance learning*
- *Fine tuning and meta-learning*
- ***Other metrics***

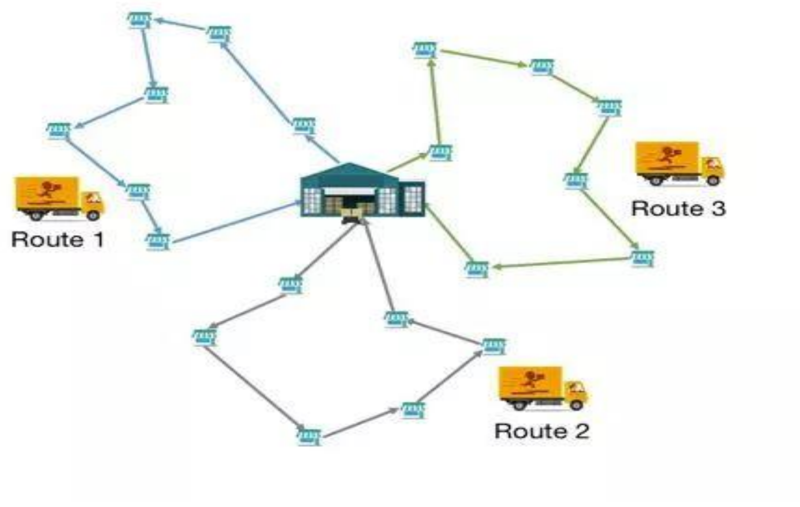
other metrics such as robustness, speed and training cost are important as well





ML for CO : 5) Challenges

- *Feasibility*
- *Modelling*
- *Scaling*
- *Data generation*



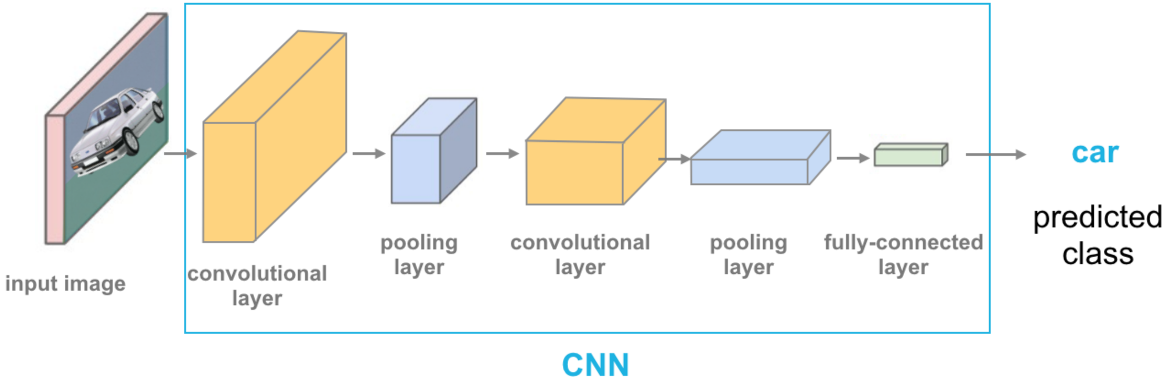
feasibility is not guaranteed

- how far the output is from the optimal solution
- if it respects the constraints of the problem

ML for CO : 5) Challenges

- *Feasibility*
- *Modelling*
- *Scaling*
- *Data generation*

In machine learning, we know prior for some problems, e.g., CNN

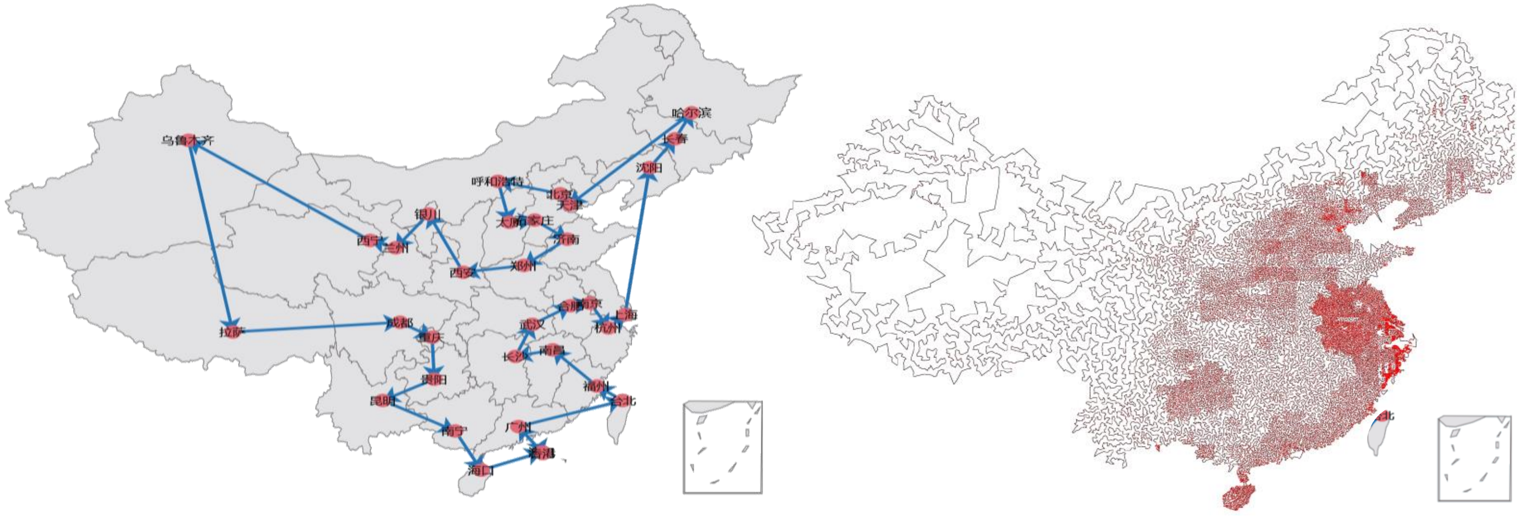


limited prior knowledge on using/choosing machine learning in combinatorial problems

- the optimization components of deep learning algorithms (say, modifications to stochastic gradient descent) could be different in combinatorial optimization context.

ML for CO : 5) Challenges

- *Feasibility*
- *Modelling*
- *Scaling*
- *Data generation*

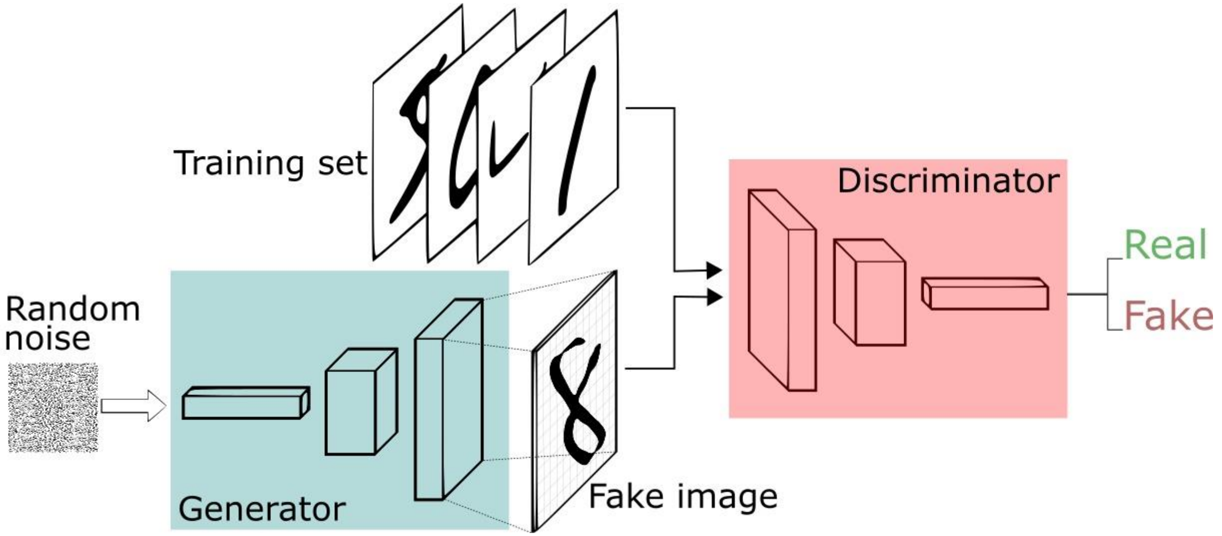


scaling to larger problems is challenging

- all of the papers tackling traveling salesman problem through machine learning and attempting to solve larger instances

ML for CO : 5) Challenges

- *Feasibility*
- *Modelling*
- *Scaling*
- *Data generation*



data generation is a subtle task

- generate more instances
- generate profitable instances
- generate target instances

Outline

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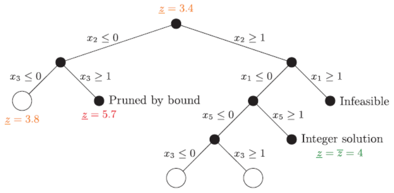
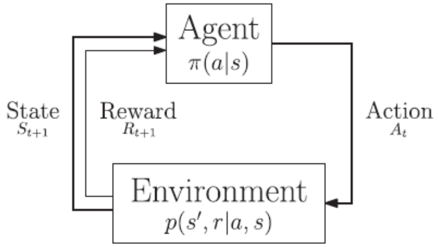
3. **Conclusion**

Conclusion

Combinatorial Optimization



Machine Learning



Two strategies
- demonstration
- experience

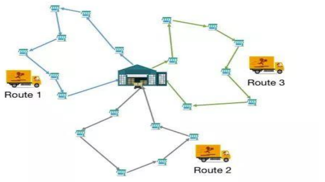
Algorithm Structure
- end to end
- configure
- alongside

Learning Objective
- generation
- ……

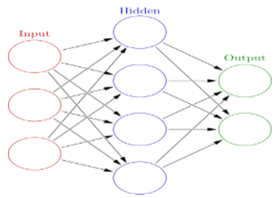
Methodology

Challenge

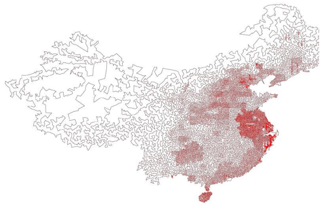
- *Feasibility*



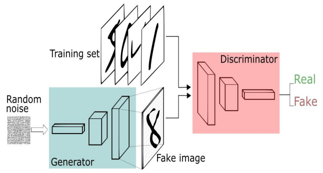
- *Modelling*

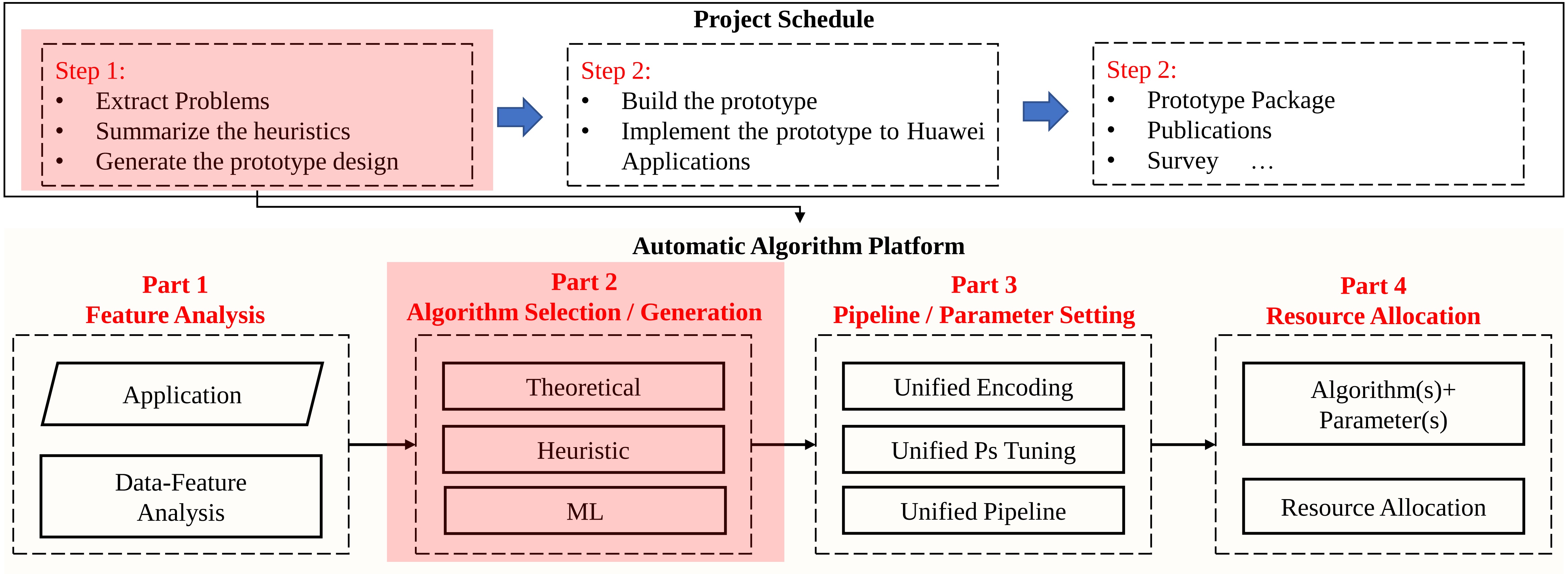


- *Scaling*



- *Data generation*





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Thanks!

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Date: February 1, 2021