CP 2024 GIRONA

Learning Lagrangian Multipliers for the Travelling Salesman Problem

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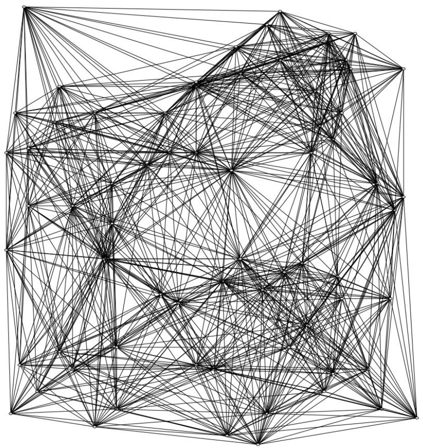
CANADA RESEARCH CHAIR IN HEALTHCARE ANALYTICS AND LOGISTICS HANALOG

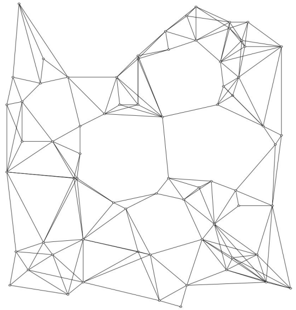
USC University of Southern California

POLYTECHNIQUE MONTRÉAL

Introduction

Improved Filtering for Weighted Circuit Constraints, (Benchimol P, van Hoeve WJ, Régin J-C, Rousseau L-M, Rueher R, 2012, *Constraints* 17:3, 205-233.)





- **WeightedCircuit constraint**: 1-tree relaxation for domain filtering and application to a Branch-and-Bound solver
- **Objective**: improving the 1-tree relaxation for the BnB solver

Plan

1. 1-tree and Held-Karp Relaxation
2. Proposed Approach
3. Application and Results

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Introduction: Travelling Salesman Problem (TSP)

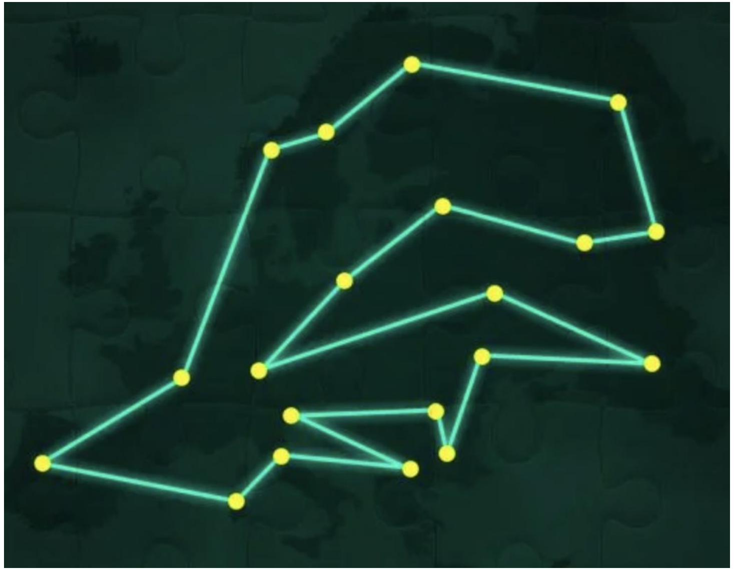
$$\min \sum_{e \in E} c_e x_e$$

$$\text{s. t.} \sum_{e \in \delta(v)} x_e = 2, \ \forall v \in V$$

$$\sum_{e \in E} x_e = |V|$$

$$\sum_{e \in S} x_e \leq |S| - 1, \ \forall S \text{ subtour of } G$$

$$x_e \in \{0, 1\}, \ \forall e \in E$$



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1. Minimize total tour cost

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3. The tour has the right length

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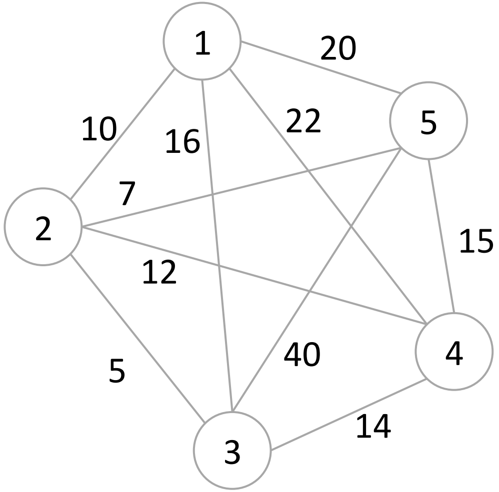
1. Minimize total tour cost
2. Each node is connected by 2 edges
3. The tour has the right length
4. No disconnected subtour is created

1-tree Relaxation

- A minimum *1-tree* T is a minimum spanning tree on G\{1}, to which {1} is connected back to T with 2 cheapest edges



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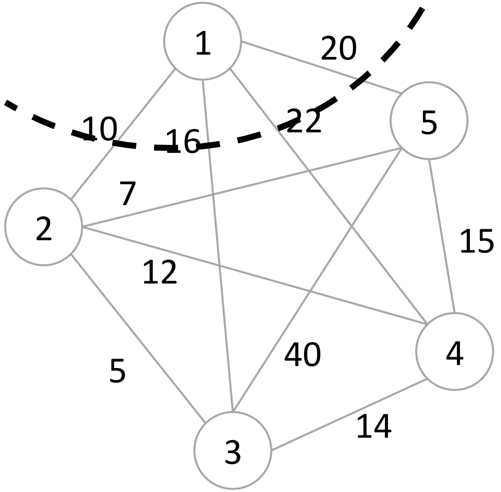

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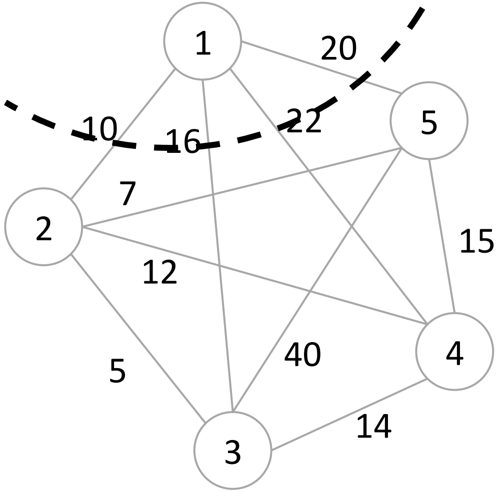

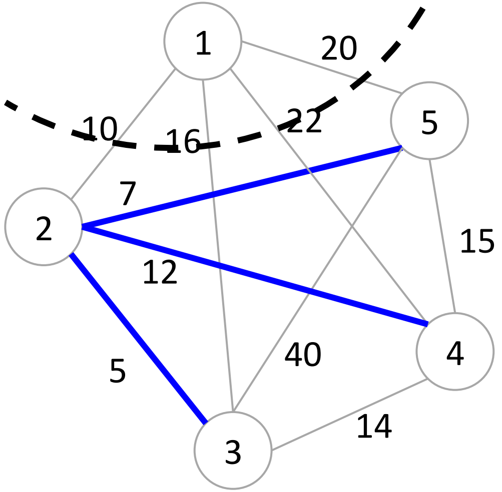

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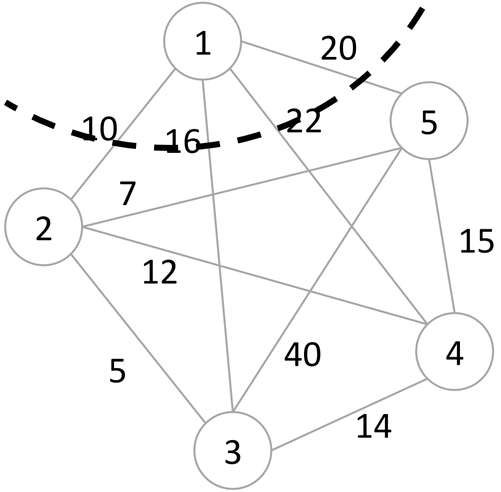
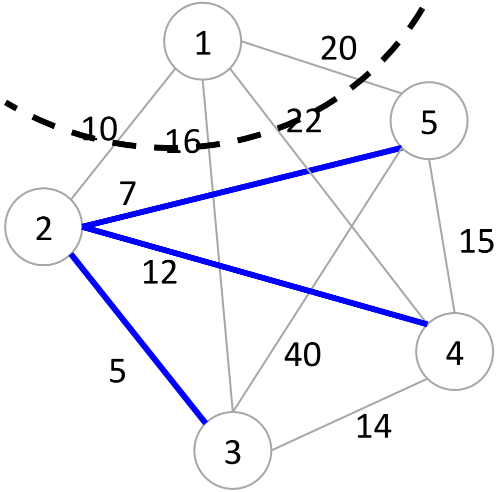
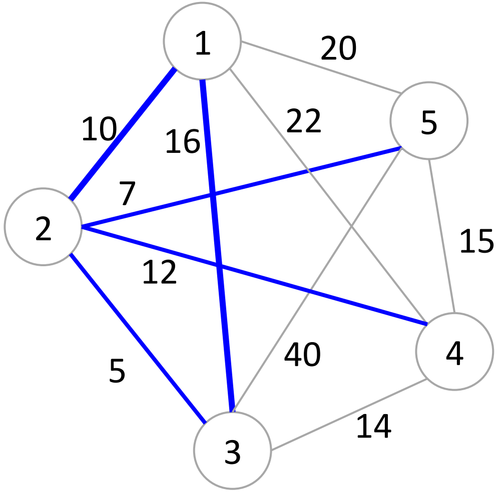






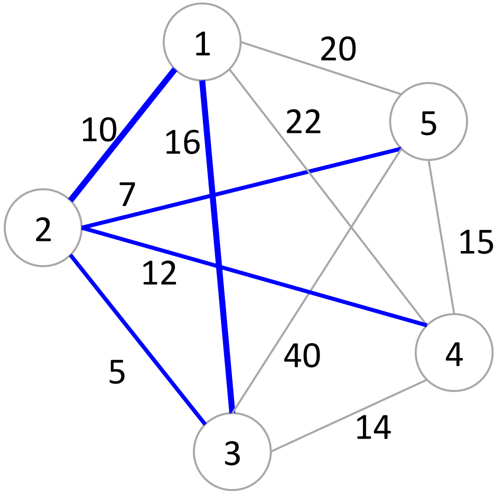
1-tree Relaxation

- A 1-tree is effectively the result of the **relaxation of the degree constraints** in the TSP model

$$
\begin{aligned}
\min \; & \sum_{e \in E} c_e x_e \\
\text{s. t.} \; & \cancel{\sum_{e \in \delta(v)} x_e = 2, \; \forall v \in V} \\
& \sum_{e \in E} x_e = |V| \\
& \sum_{e \in S} x_e \le |S| - 1, \; \forall S \text{ subtour of } G \\
& x_e \in \{0, 1\}, \; \forall e \in E
\end{aligned}
$$

1-tree Relaxation

- A tour is a 1-tree, and finding a minimum 1-tree is fast: **dual bound generation**



Bound: **50**

Held-Karp Relaxation

- The 1-tree can be tightened by Lagrangean relaxation, where **λ** penalizes the node degree violation

$$\begin{aligned} \min \sum_{e \in E} c_e x_e & \\ \text{s. t. } \cancel{\sum_{e \in \delta(v)} x_e = 2, \ \forall v \in V} & \\ \sum_{e \in E} x_e = |V| & \\ \sum_{e \in S} x_e \leq |S| - 1, \ \forall S \text{ subtour of } G & \\ x_e \in \{0,1\}, \ \forall e \in E & \end{aligned}$$

$$\begin{aligned} \min \sum_{e \in E} c_e x_e + \sum_{i \in V} \lambda_i \Big(\sum_{e \in \delta(i)} x_e - 2 \Big) & \\ \sum_{e \in E} x_e = |V| & \\ \sum_{e \in S} x_e \leq |S| - 1, \ \forall S \text{ subtour of } G & \\ x_e \in \{0,1\}, \ \forall e \in E & \end{aligned}$$

Held-Karp Relaxation

- This is equivalent to modifying the edge costs

$$\min \sum_{e\in E} c_e x_e + \sum_{i\in V} \lambda_i \Big(\sum_{e\in\delta(i)} x_e - 2 \Big) \longrightarrow \min \sum_{e\in E} \underline{(c_e + \lambda_{e_1} + \lambda_{e_2})} x_e$$

$$\sum_{e\in E} x_e = |V| \qquad \sum_{e\in E} x_e = |V|$$

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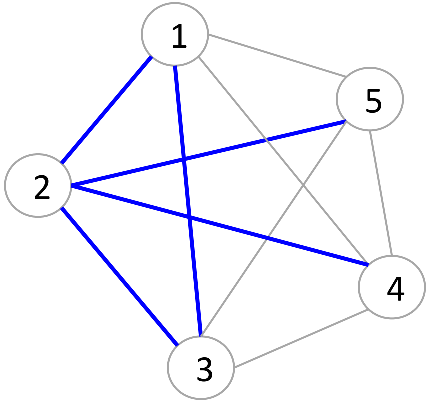
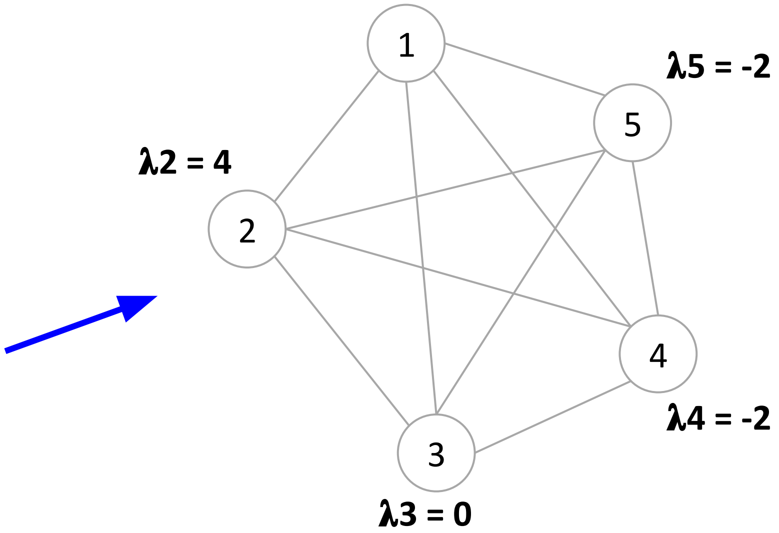
Held-Karp Relaxation

- **If T is a tour,** then LB = TSP value, else
- **Iterative factors update** for bound tightening:
  a. positive for degrees > 2 to discourage selected edges,
  b. negative for degrees = 1,
  c. 0 for degrees = 2

Bound: **50**

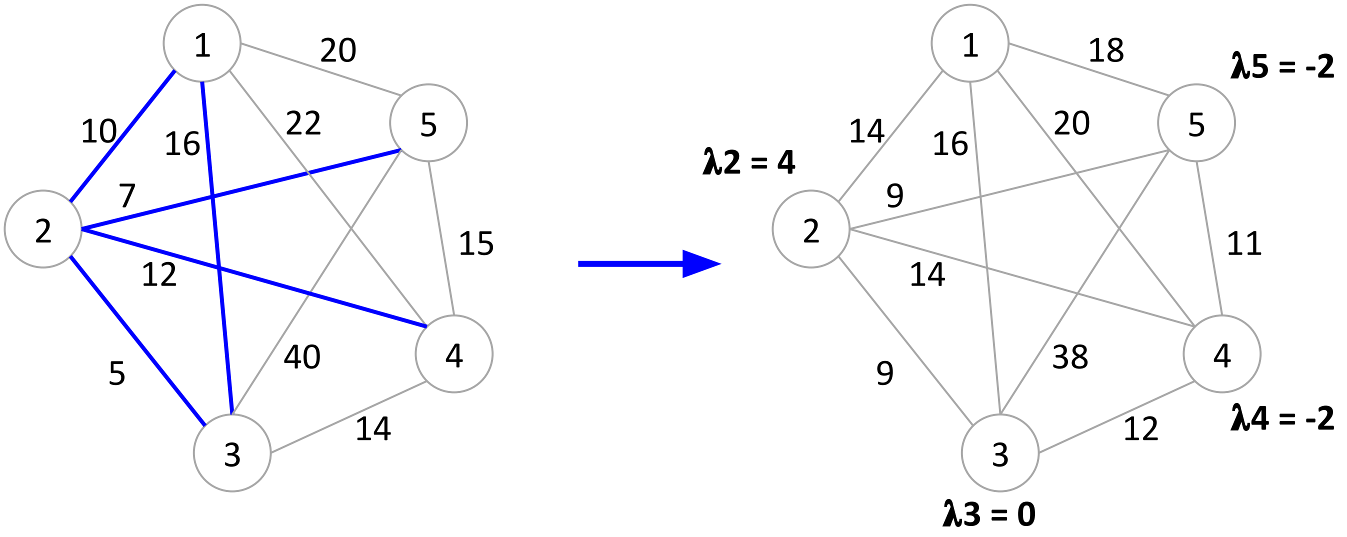




Held-Karp Relaxation

- Adding factors on the nodes modifies the minimum 1-tree but not the optimal tour

Bound: **50**



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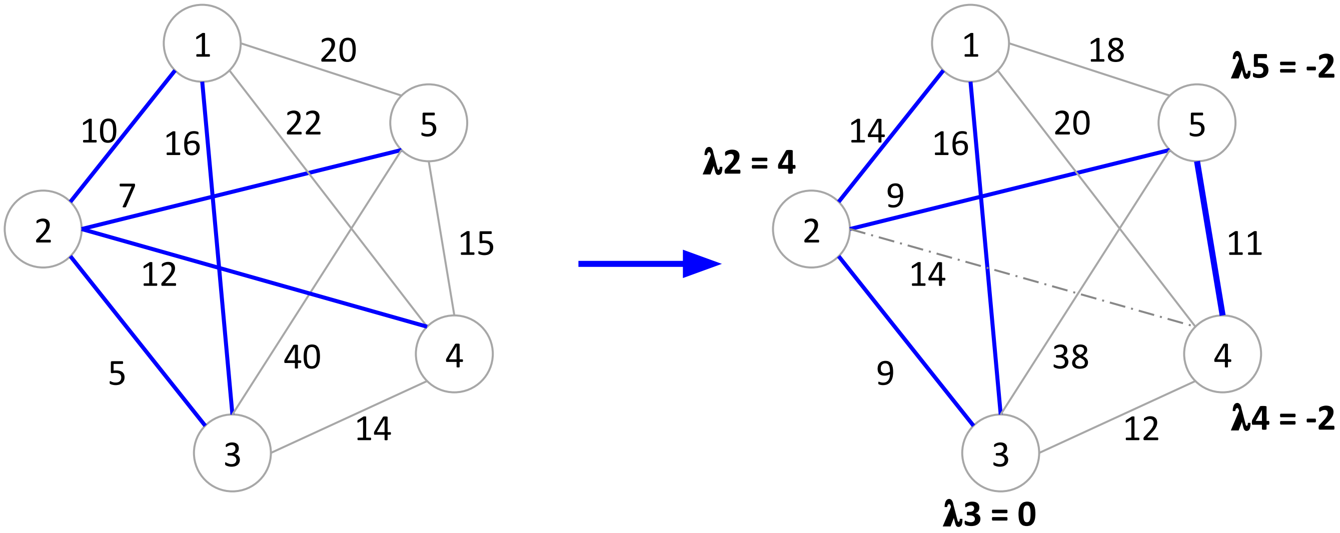

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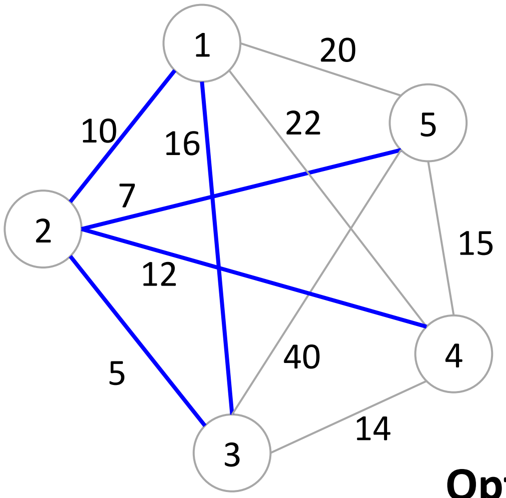
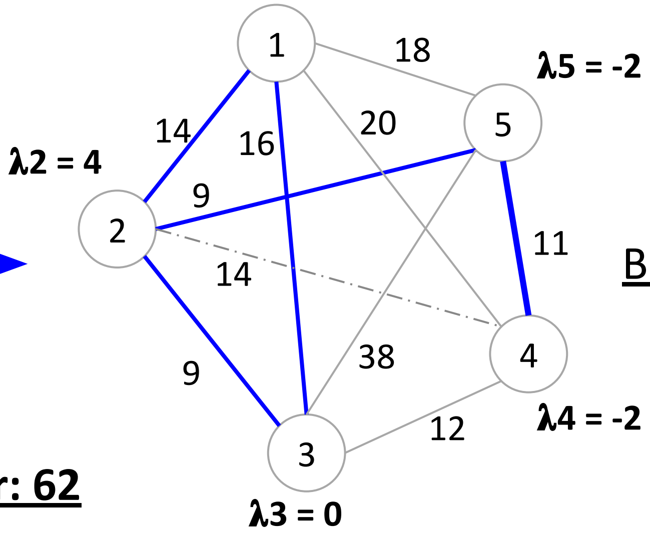


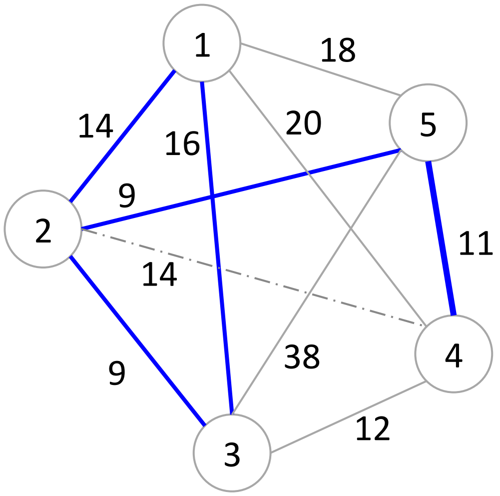


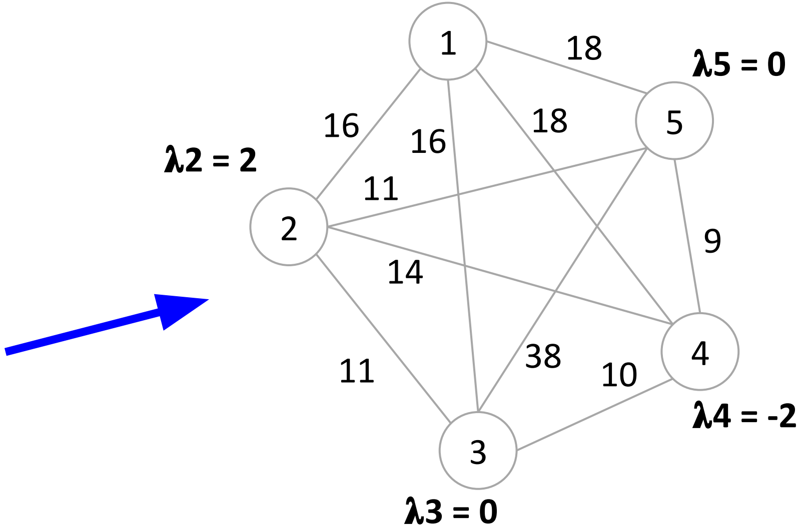
Bound: 59

Optimal tour: 62

Held-Karp Relaxation

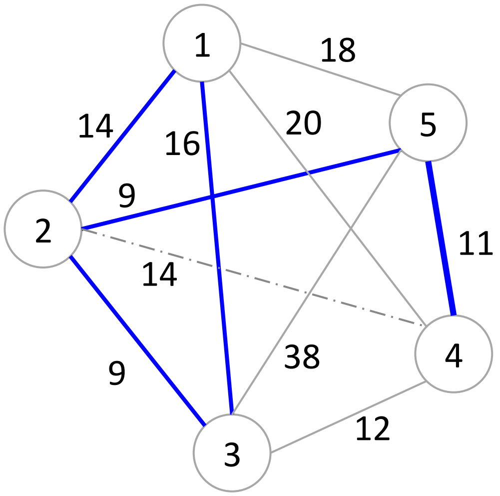
Bound: **59**

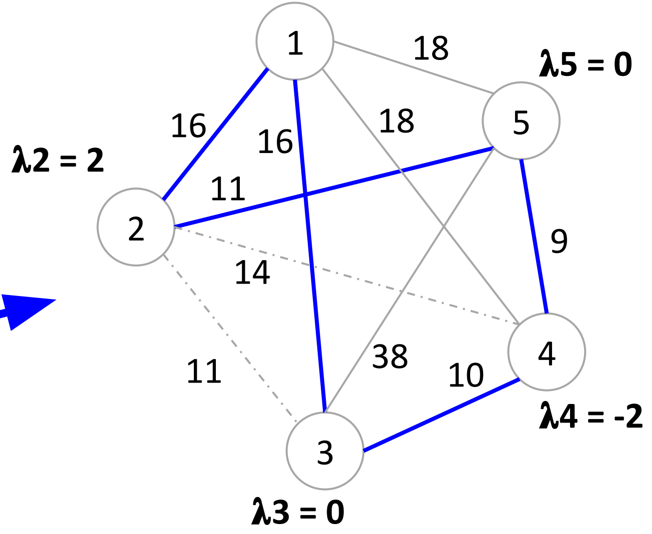




Held-Karp Relaxation

Bound: **59**





Bound: **62**

Plan

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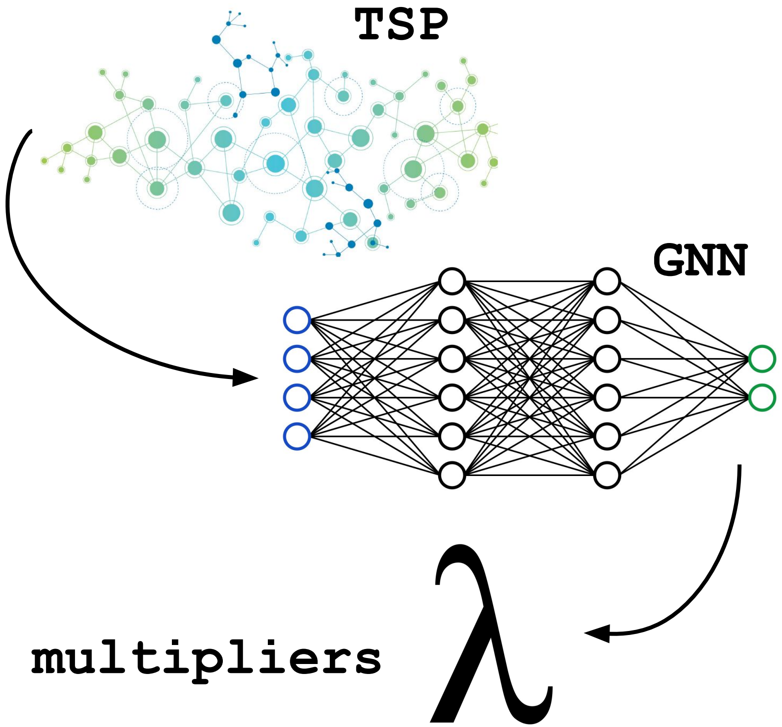
Proposed Approach

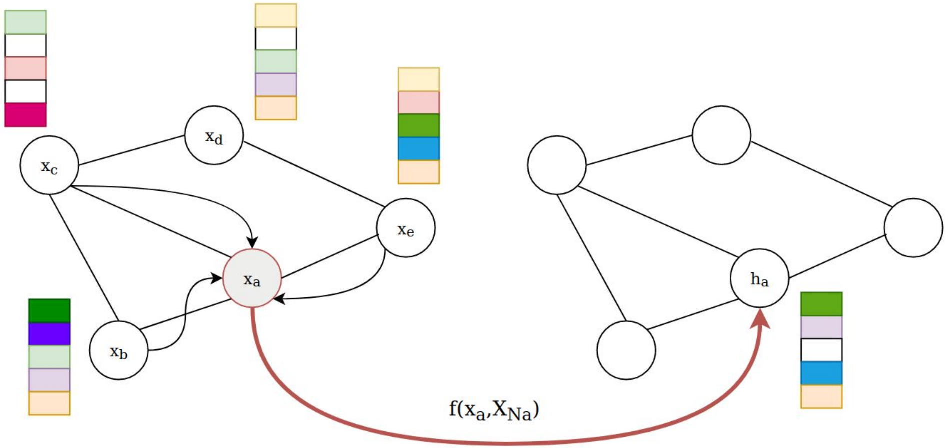
- Predicting the **Lagrangian Multipliers** to kickstart the Lagrangian relaxation

- Leverage the graph structure of the TSP by using **graph neural networks (GNN)** for the multipliers inference



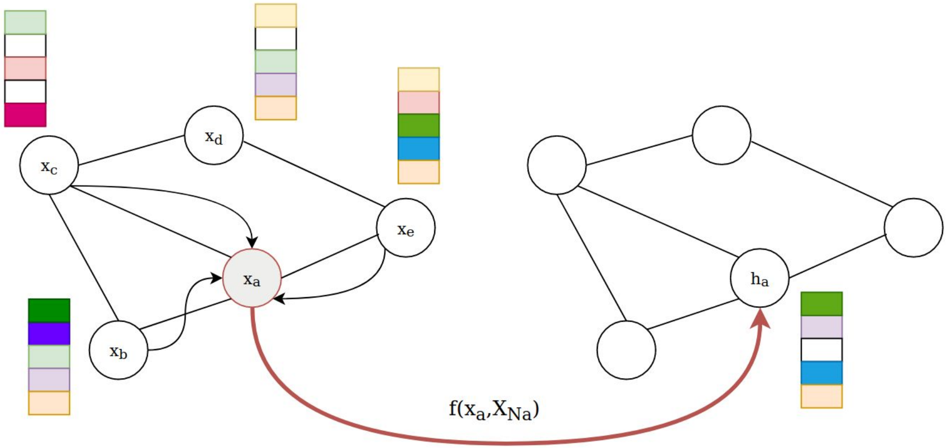
Graph Neural Networks

- **Graph Neural Networks** (GNNs) process graph-structured data:
    - **Node Representation:** GNNs learn to represent nodes based on their features and their neighbors'
    - **Message Passing:** Iterative process where nodes update their states by exchanging information with adjacent nodes



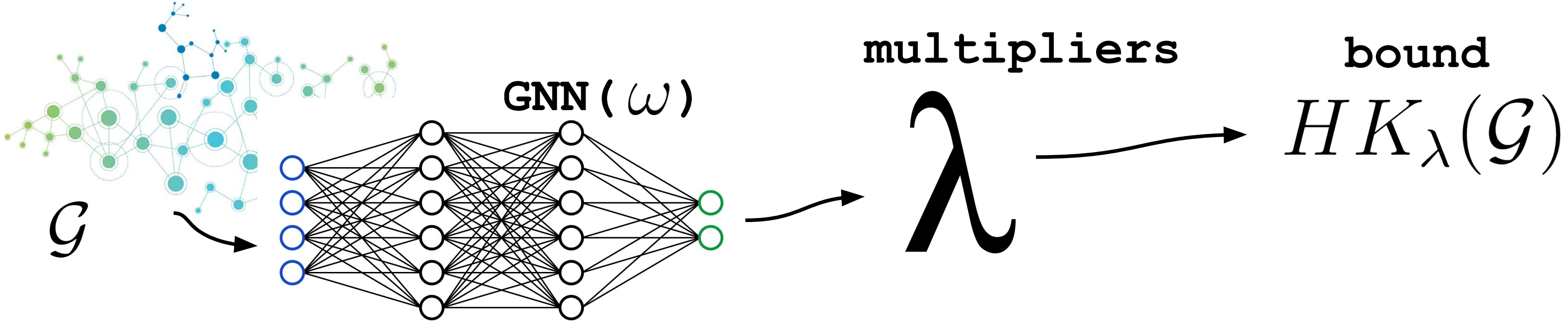
Graph Neural Networks

- **GNNs for TSP:**
  - **TSP graph structure:** GNNs handle the **features** and **variable size** of TSP representations
  - **Multipliers generation:** GNNs capture complex dependencies and patterns in the graph, aiding in better optimization



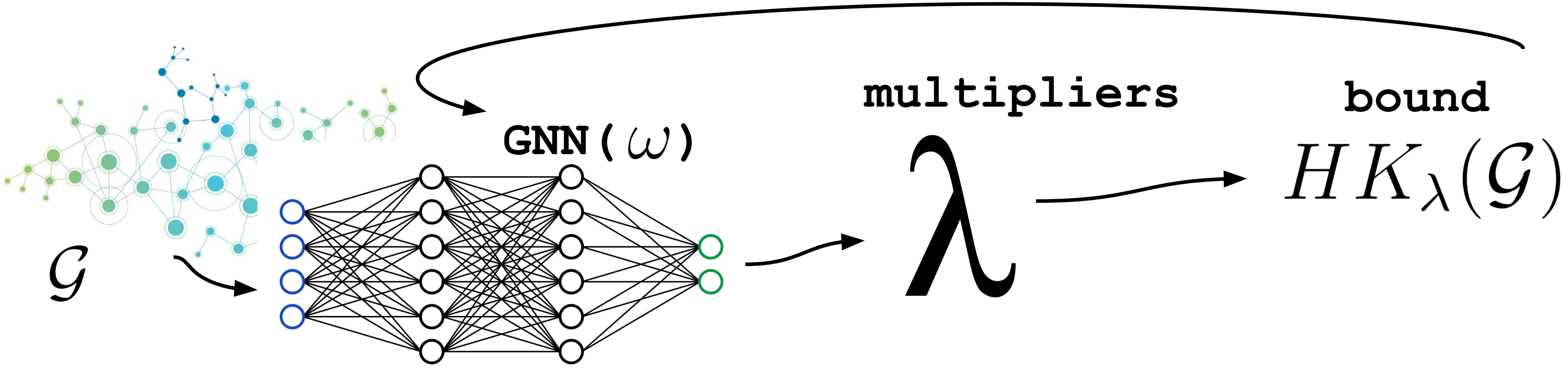
Learning Approach

- **Self-supervised Learning** for the **prediction of Lagrangian Multipliers:**
  - A GNN with parameters ω is used to predict Lagrangian multipliers,
  - the GNN is trained by computing the gradient on the bound



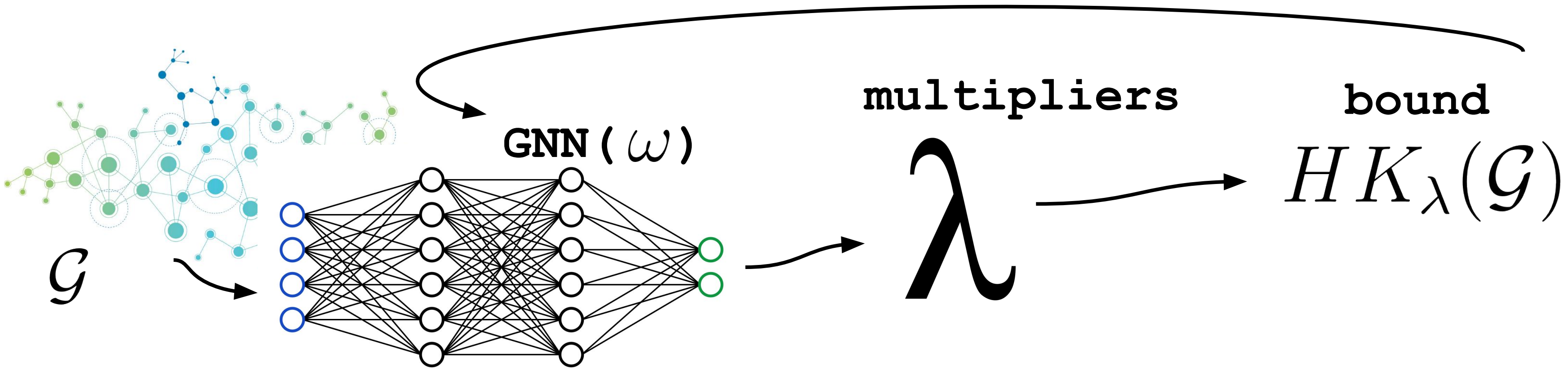
Learning Approach

$$\frac{\partial HK_\lambda(\mathcal{G})}{\partial \omega}$$



Learning Approach

$$\frac{\partial HK_\lambda(\mathcal{G})}{\partial \omega} = \frac{\partial HK_\lambda(\mathcal{G})}{\partial \lambda} \times \frac{\partial \lambda}{\partial \omega}$$



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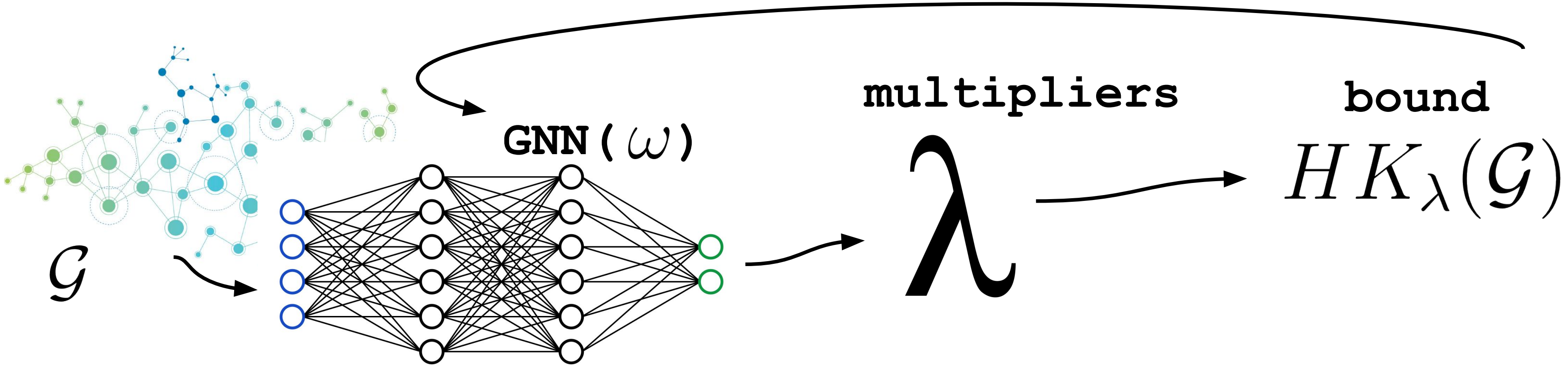
GNN backprop



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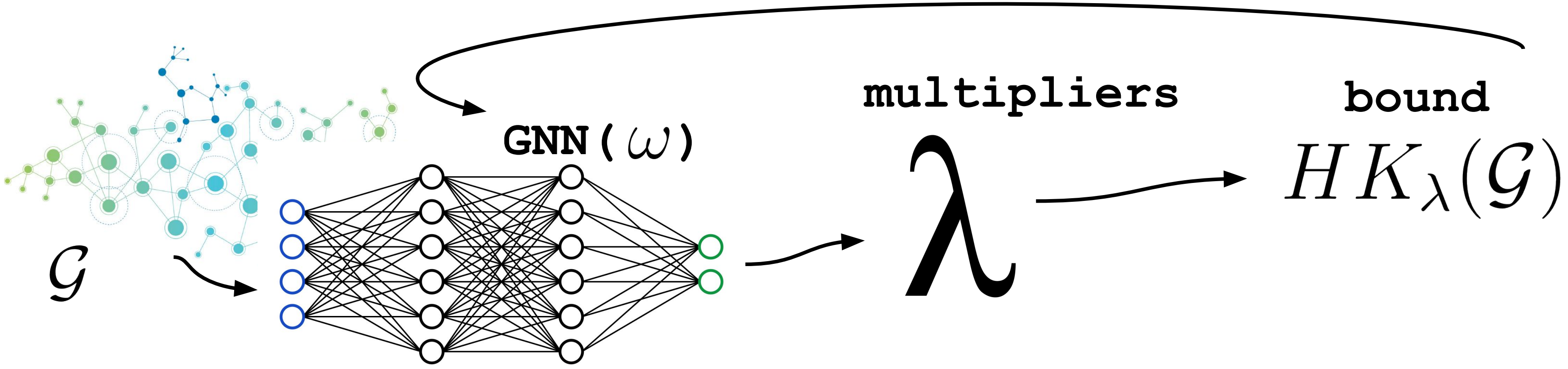
HK multipliers update

GNN backprop



Held-Karp multipliers update

$$\frac{\partial HK_\lambda(\mathcal{G})}{\partial \omega} = \frac{\partial HK_\lambda(\mathcal{G})}{\partial \lambda} \times \frac{\partial \lambda}{\partial \omega}$$

Held-Karp relaxation

$$\min \sum_{e \in E} c_e x_e + \sum_{i \in V} \lambda_i \Big(\sum_{e \in \delta(i)} x_e - 2 \Big) \longrightarrow \frac{\partial \mathrm{HK}(.)}{\partial \lambda_i} = \sum_{e \in \delta(i)} x_e - 2$$

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HK multipliers update

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Training - Datasets

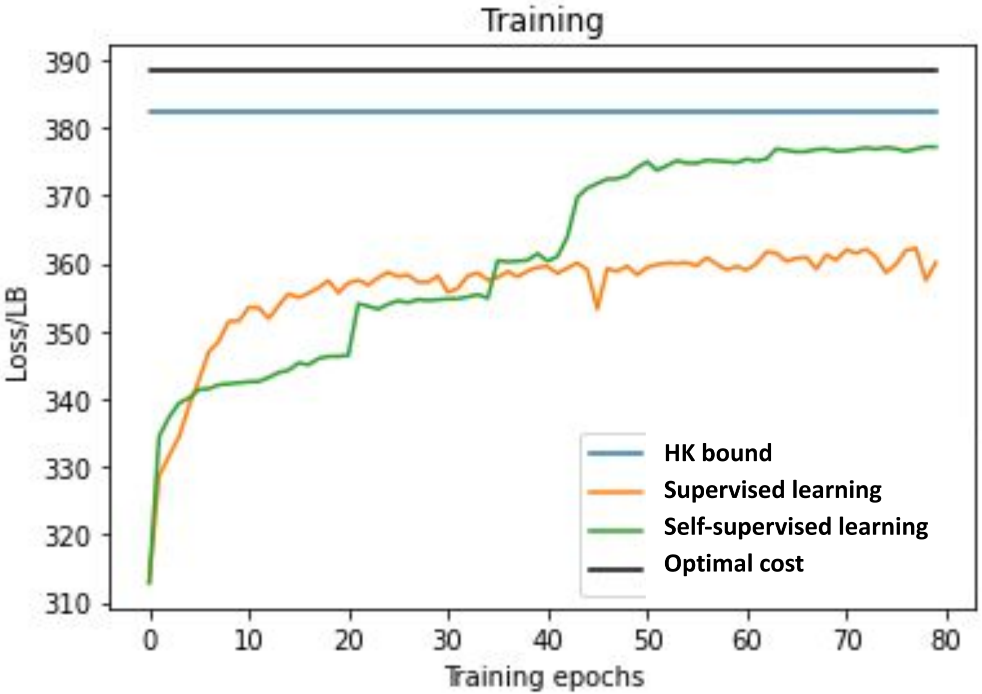
- Dataset randomly generated: **`Random`**, **`Clustered`** in sizes 100 and 200
- Existing dataset: **`Hard`**

- **Training set**: TSP instances + branch-and-bound subgraphs
- **Features**: distances and BnB state on *edges*, average/min distances on *nodes*

Training - Model and Baselines

- Baselines:
  - Optimal Solution,
  - HK Relaxation,
  - Supervised (graph attention network + fully-connected NN)
- Trained model:
  - Self-Supervised (graph attention network + fully-connected NN)

Training



Training
390
380
370
360
350
340
330
320
310
Loss/LB
0
10
20
30
40
50
60
70
80
Training epochs
HK bound
Supervised learning
Self-supervised learning
Optimal cost

Integration with Branch-and-Bound

- $HK_{\mathrm{GNN}_\omega}(\mathcal{G})$ provides a tight bound at each step of a BnB algorithm, enabling **pruning** and **filtering**
- Domain filtering: edges are **forced** or **excluded** from the solution based on replacement or insertion costs based on the 1-tree

Benchimol P, van Hoeve WJ, Régin J-C, Rousseau L-M, Rueher R, (2012), **Improved Filtering for Weighted Circuit Constraints**, *Constraints* 17:3, 205-233.

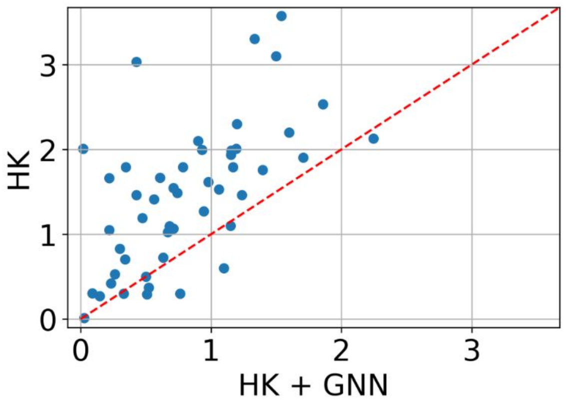
Integration with Branch-and-Bound

Practical considerations:

1. **Edges forced or excluded** from the solution modify the graph, which is **reflected in the features**
2. GNN-based multipliers generation is used in the **10 first nodes** of the BnB
3. **HK+GNN**: the trained GNN is used to bootstrap the multipliers generation

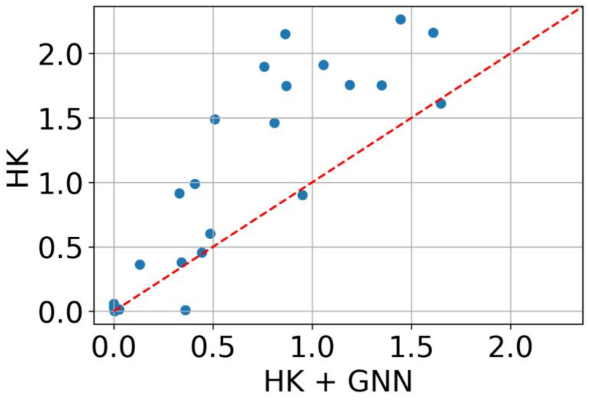
Experimental Results

- Compared to a BnB using HK alone, **HK+GNN** multiplier generation:
  - is 10% quicker in solving instances to optimality
  - reduces by 50% the optimality gap on timeout instances



(a) Results on Random200.

optimality gap in %



(b) Results on Clustered200.

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Configuration	Branch-and-bound with standard Held-Karp (HK)					Branch-and-bound with our approach (GNN + HK)				
	Time (sec.)	# solved (/50)	PDI	Filt. (%)	Opt. gap (%)	Time (sec.)	# solved (/50)	PDI	Filt. (%)	Opt. gap (%)
Random100	559	41/50	1127k	75.9	0.88					
Random200	1800	0/50	4.71m	67.8	1.82					
Clustered100	643	38/50	497k	17.7	0.19					
Clustered200	1800	0/50	922k	9.9	0.68					
Hard	1800	0/6	9.59M	6.4	0.32					

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Random200	1800	0/50	4.71m	67.8	1.82	1800				
Clustered100	643	38/50	497k	17.7	0.19	590 (- 8%)				
Clustered200	1800	0/50	922k	9.9	0.68	1800				
Hard	1800	0/6	9.59M	6.4	0.32	1800				

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Random200	1800	0/50	4.71m	67.8	1.82	1800	0/50 (+ 0%)			
Clustered100	643	38/50	497k	17.7	0.19	590 (- 8%)	40/50 (+ 5%)			
Clustered200	1800	0/50	922k	9.9	0.68	1800	0/50 (+ 0%)			
Hard	1800	0/6	9.59M	6.4	0.32	1800	0/6 (+ 0%)			

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Random200	1800	0/50	4.71m	67.8	1.82	1800	0/50 (+ 0%)	4.26m (- 10%)		
Clustered100	643	38/50	497k	17.7	0.19	590 (- 8%)	40/50 (+ 5%)	470k (- 5%)		
Clustered200	1800	0/50	922k	9.9	0.68	1800	0/50 (+ 0%)	690k (- 25%)		
Hard	1800	0/6	9.59M	6.4	0.32	1800	0/6 (+ 0%)	9.36M (- 2%)		

Experimental Results

- Compared to a BnB using HK alone, **HK+GNN** multiplier generation:
  - is 10% quicker in solving instances to optimality
  - reduces by 50% the optimality gap on timeout instances

Configuration	Branch-and-bound with standard Held-Karp (HK)					Branch-and-bound with our approach (GNN + HK)				
	Time (sec.)	# solved (/50)	PDI	Filt. (%)	Opt. gap (%)	Time (sec.)	# solved (/50)	PDI	Filt. (%)	Opt. gap (%)
Random100	559	41/50	1127k	75.9	0.88	497 (- 11%)	46/50 (+ 10%)	965k (- 14%)	77.7 (+ 2%)	
Random200	1800	0/50	4.71m	67.8	1.82	1800	0/50 (+ 0%)	4.26m (- 10%)	70.6 (+ 4%)	
Clustered100	643	38/50	497k	17.7	0.19	590 (- 8%)	40/50 (+ 5%)	470k (- 5%)	20.3 (+ 15%)	
Clustered200	1800	0/50	922k	9.9	0.68	1800	0/50 (+ 0%)	690k (- 25%)	12.6 (+27%)	
Hard	1800	0/6	9.59M	6.4	0.32	1800	0/6 (+ 0%)	9.36M (- 2%)	6.5 (+1%)	

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	Time (sec.)	# solved (/50)	PDI	Filt. (%)	Opt. gap (%)	Time (sec.)	# solved (/50)	PDI	Filt. (%)	Opt. gap (%)
Random100	559	41/50	1127k	75.9	0.88	497 (- 11%)	46/50 (+ 10%)	965k (- 14%)	77.7 (+ 2%)	0.48 (- 45%)
Random200	1800	0/50	4.71m	67.8	1.82	1800	0/50 (+ 0%)	4.26m (- 10%)	70.6 (+ 4%)	0.59 (- 68%)
Clustered100	643	38/50	497k	17.7	0.19	590 (- 8%)	40/50 (+ 5%)	470k (- 5%)	20.3 (+ 15%)	0.08 (- 58%)
Clustered200	1800	0/50	922k	9.9	0.68	1800	0/50 (+ 0%)	690k (- 25%)	12.6 (+27%)	0.38 (- 44%)
Hard	1800	0/6	9.59M	6.4	0.32	1800	0/6 (+ 0%)	9.36M (- 2%)	6.5 (+1%)	0.31 (- 3%)

Conclusion

- Introduction of a **self-supervised learning approach** using **GNNs** and **Held-Karp Lagrangian relaxation** to predict accurate Lagrangian multipliers

- The approach has potential applications for **more challenging TSP variants**, and **other Lagrangian relaxations**

- Limitations: **costly GNN** calls, best results when the graph distribution is known beforehand

Learning Lagrangian Multipliers for the TSP

Thanks!

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arxiv.org/abs/2312.14836