APPENDIX

A. Trip node features

A list of 23 features extracted from complex operational constraints for each trip node in graph represention is given as Table I.

TABLE I
THE DESCRIPTION OF FEATURES IN GRAPH REPRESENTION

Type	Feature	Description
Chain granularity	exp_trip_cnt	Expect trip cnt in one chain.
	max_work_time	Maximum working time in one chain.
	$cum\_runtime\_range$	Lower and upper bound of cumulative runtimes in one chain.
Trip granularity	$departure\_direction$	One hot encoding of departure direction for each trip.
	$trip\_index$	Index of each trip in its corresponding chain.
	$departure\_time\_range$	Lower and upper bound of departure time for each trip.
	$departure\_order\_range$	Lower and upper bound of departure order for each trip.
	$runtime\_stats$	Statistics of running time for each trip. (Max, min, mean, and median)
	$headway\_lower\_stats$	Statistics of headway's lower bound for each trip. (Max, min, mean, and median)
	$headway\_upper\_stats$	Statistics of headway's upper bound for each trip. (Max, min, mean, and median)

TABLE II
SOME BASIC INFORMATION OF THE TWO-WAY BUS LINE

Operational constraints	"up" bus line	"down" bus line
total number of trips	86	86
operation period	06:00 - 21:30	06:30 - 22:00
global max headway	20min	20min
peak periods and corresponding max headways	08:00 - 09:00, 7min 17:00 - 18:30, 7min	08:30 - 09:30, 7min 17:10 - 18:40, 7min
running time of each period	06:00 - 06:30, 27min 06:30 - 08:00, 31min 08:00 - 09:30, 36min 09:30 - 16:00, 29min 16:00 - 17:00, 31min 17:00 - 18:30, 34min 18:30 - 20:00, 31min 20:00 - 21:31, 28min	06:30 - 08:10, 28min 08:10 - 09:40, 35min 09:40 - 16:00, 29min 16:00 - 17:10, 31min 17:10 - 18:40, 34min 18:40 - 22:01, 27min
lunch break and dinner break	lunch break, 10:30 - 12:30, 30min dinner break, 17:00 - 20:00, 20min	

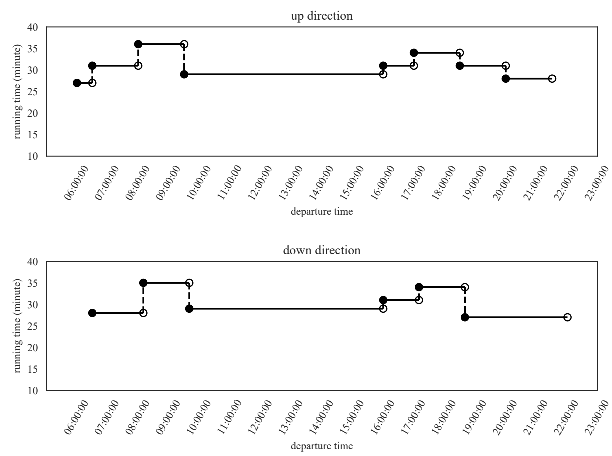

Fig. 1. The step-like running times for each direction.

B. Case study

Here we demonstrate the effectiveness of our proposed baseline and GCN-based methodology through a real-life case. We choose a typical two-way bus line which carries over 5 thousands passengers per day, from a big city of eastern China. Table II shows some basic information of the case and the step-like running times for each direction are further displayed in Fig. 1.

The detailed requirements of each chain given by schedulers is shown in Table III, we can see that the schedulers are accustomed to name different types of chains according to their key attributes, e.g, "short chain" means chains with less number of trips compared to that of "long chain".

Based on these parameters of the case, we formulate the problem into an MILP instance and solve the obtained instance using both a baseline approach with a time limit of 20 minutes (abbreviated as Baseline_20min) and a GCN-based approach with a time limit of 16 minutes (abbreviated as GCN_16min). The instance is highly complicated with over 10 thousands variables and over 20 thousands constraints. Note that it may takes hours or even days to find the optimal solution, while in practice a suboptimal solution is usually sufficient. And for humans, solving such a problem by hand is extremely difficult, even professional schedulers would spend 1 or 2 days to obtain a rough plan which may have conflicts in details and would not want to change it in the next six months.

The vehicle scheduling results of Baseline_20min approach and GCN_16min approach are shown in Fig. 2 and Fig. 3 in the form of a Gantt chart, respectively. Blocks colored in green, blue, yellow and pink represent for up trips, down trips, lunch breaks and dinner breaks respectively. From these two figures we can find that the chains typed as "short chain" are automatically divided into two groups due

TABLE III
DETAILED REQUIREMENTS OF CHAINS GROUPED BY CHAIN TYPES

Chain type	Direction	Chain index	Number of trips	Max working time
"short chain"	up	1,2,3,4, 13,14,15	8	7 h
	down	5,6, 16,17	8	7 h
"long chain"	up	7,8,9	14	12 h
	down	10,11,12	14	12 h

to the restrictions of max working time and max headways of peak periods. Group 1 consisted of chain 1 to 6 could be named as "morning shift", which starts before 08:00 and ends before about 14:00, while group 2 consisted of chain 13 to 17 is often called "night shift", which starts after about 15:00 and ends after 20:00. The settings of "morning shift" and "night shift" happen to be consistent with traditional manual scheduling tricks, since they may be the only patterns to ensure the working time within 7 hours, but both of our two approaches could find them automatically without expert experience.

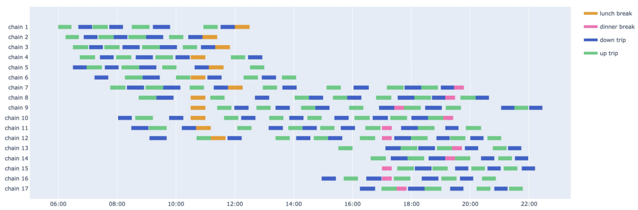

Fig. 2. Scheduling result of Baseline_20min approach in the form of a Gantt chart

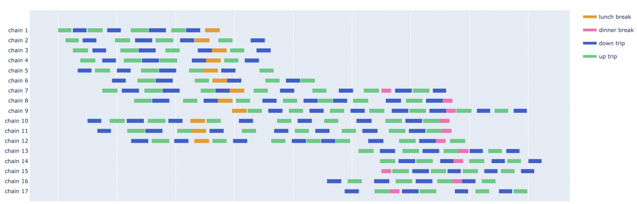

Fig. 3. Scheduling result of GCN_16min approach in the form of a Gantt chart

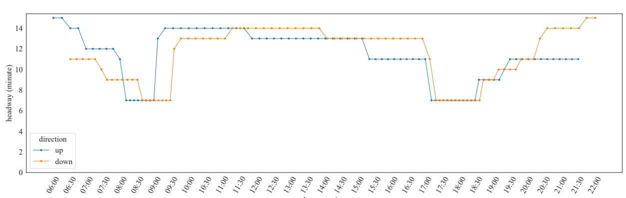

Fig. 4. The headways of the resulting timetables solved using Baseline_20min approach with an objective function value of 52.

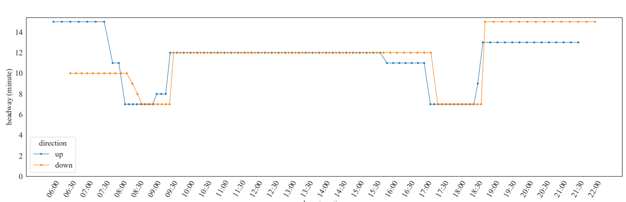

Fig. 5. The headways of the resulting timetables solved using GCN_16min approach with an objective function value of 45.

Fig. 4 and Fig. 5 respectively show the headways of the resulting timetable for two directions solved by two approaches, we can see that the max headway of each peak periods is strictly limited within 7 minutes according to the requirements. Both approaches are well enough for practical usages with regard to the smoothness of two timetables. In addition, the resulting timetable of GCN_16min approach is smoother than that of Baseline_20min approach, corresponding to GCN_16min approach obtaining a solution with a smaller objective function value.

In this case, the two permutation matrices contain a total of 14,792 binary variables, of which 4,212 variables (28.47%) have been fixed to 0 by our constructed GCN model. As a result, we achieve a 13.46% improvement in solution quality and a 20% reduction in solving time.