* 1. **Variable vectorization**

Before embedding the optimization model into a CG framework to obtain the optimal solution, we will vectorize the variables used in Eq. (7), including the true travel time , the links *a*, the nodes *v*, the link travel time *t*a, the station waiting time *th v*, and the route choice probability *p*. After vectorization, the supervised tasks under the CG framework are constructed.

1. **The vectorization of the true travel time**

Based on the true travel time, as Eq.(4), its vectorized representation is shown as Eq. (8).

|  |  |
| --- | --- |
|  | **(8)** |

where *N* is the number of nodes, *h*∈*H* is the time interval, is the true travel time for the specific OD pair *rs* in the time interval *h*, is the vectorization of all OD pairs in all time intervals, in which is the number of all OD pairs.

1. **The vectorization of the links *a***

In this study, we assume that the walking time and in-vehicle time of the link *a* is independent of the time interval. Hence, and *ta* is not associated with the time interval *h*. Let *N*a be the number of all links, *N* is the number of nodes. The vectorization of the links in the *k* shortest paths of specific OD pair *rs* is shown as Eqs. (9)-(10). The vectorizations of the links in the *k* shortest paths of all OD pairs are shown as Eq. (11).

|  |  |
| --- | --- |
|  | **(9)** |
|  | **(11)** |

where is defined in Eq.(1), is the vectorization of the links in the *kth* shortest path of specific OD pair *rs*, whose elements are either 0 or 1, is the vectorization of the links in the *k* shortest paths of specific OD pair *rs*, is the vectorization of the links in the *k* shortest paths of all OD pairs, in which is the numbers of all OD pairs.

1. **The vectorization of the nodes *v***

In this study, we assume that the *th v* is associated with the time interval *h*. For the same route, there is a different *th v* in different time intervals. The *th v* is also associated with the direction of links. For the same station in the same time interval, there is different *.* Therefore, the coefficients of *th v* for the uplink and downlink areand , respectively. Let *Nv* be the node number considering the different directions. The vectorization of the waiting nodes in the *k* shortest paths of specific OD pair is shown as Eqs. (12)-(13). The vectorizations of the waiting nodes in the *k* shortest paths of all OD pairs are shown as Eq. (14).

|  |  |
| --- | --- |
|  | **(12)** |
|  | **(14)** |

where and are defined in Eq. (1), is the vectorization of the waiting nodes in the *kth*shortest path of specific OD pair, is the vectorization of the waiting nodes in the *k*shortest paths of specific OD pair， is the vectorization of the waiting nodes in the *k*shortest paths of all OD pairs, in which is the number of all OD pairs and *Nv* is the node number considering the different directions.

1. **The combined vectorization of the links *a* andthe nodes *v***

The links *a* andthe nodes *v* are further vectorized using ***B*** and ***M****h* as Eq. (15).

|  |  |
| --- | --- |
|  | **(15)** |

where is the combined vectorization of the links *a* andthe nodes *v*, in which is the number of all OD pairs, *Nv* is the node number considering the different directions, and *Na* is the number of all links.

1. **The vectorization of the link travel time *t*a**

The vectorization of the link travel time *t*a is shown as Eq. (16).

|  |  |
| --- | --- |
|  | **(16)** |

where is one of the decision variables, in which *a* represents all the links, including the walking links and in-vehicle links.

1. **The vectorization of the station waiting time *th v***

The vectorization of the station waiting time *th v* is shown as Eq. (17).

|  |  |
| --- | --- |
|  | **(17)** |

where is one of the decision variables, in which *v* represents all the nodes considering the different directions. It should be noticed that the *th v* is associated with the time interval *h* and the direction of the train.

1. **The combined vectorization of the link travel time *t*a and the station waiting time *th v***

The combined vectorization of the link travel time *t*a and the station waiting time *th v* is shown as Eq. (18).

|  |  |
| --- | --- |
|  | **(18)** |

where is the combined vectorization of the link travel time *t*a and the station waiting time *th v*, in which *Nv* is the node number considering the different directions, and *Na* is the number of all links.

1. **The vectorization of the route choice probability *p***

For the same OD pair, there is different travel time in different time intervals. Hence, for the same path of the OD pair *rs*, the probability is different in different time intervals. Therefore, the is associated with the time interval *h.* For the same time interval, the vectorization of the route choice probability is shown as Eq. (19).

|  |  |  |
| --- | --- | --- |
|  |  | **(19)** |

where , , is the number of all OD pairs.

The route choice probability in all time intervals is shown as Eq. (20).

|  |  |
| --- | --- |
|  | **(20)** |

where .

1. **Summary of all variable vectorizations**

The summary of all variable vectorizations is shown in Table 3.

**Table 3 Variable vectorization**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Variable | Scalar | Vector | Dimension | Type |
| True travel time |  |  |  | Dense |
| Links |  |  |  | Sparse |
| Nodes | 、 |  |  | Sparse |
| Links and nodes | 、、 |  |  | Sparse |
| Link travel time |  |  |  | Dense |
| Station  waiting time |  |  |  | Dense |
| Variable to be estimated | 、 |  |  | Dense |
| Route choice probability |  |  |  | Sparse |

1. **The vectorization of the optimization model**

Based on Table 3, the optimization model in Eq. (7) can be reformulated as Eq. (21).

|  |  |
| --- | --- |
| *s.t.* | **(21)** |

The main decision variable in the above optimization model is , including the link travel time (walking time when entering or exiting the station and in-vehicle time) and station waiting time (waiting time at origin station or transfer station). When the matrix is with full rank, there is the only solution for the optimization problem.