Graph Linear Convolution Pooling for Learning in Incomplete High-Dimensional Data Supplementary File

Fanghui Bi, Tiantian He, *Member, IEEE*, Yew Soon Ong, *Fellow, IEEE*, and Xin Luo, *Senior Member, IEEE*

This is the supplementary file for the paper entitled "Graph Linear Convolution Pooling for Learning in Incomplete High-Dimensional Data". The proofs, additional tables and figures are put into this file and cited by the paper.

I. Proofs

A. Proof of Theorem 1

To prove ***Theorem* 1**, two directions of the iff conditions should be considered. If the conditions that S_1=S_2=S and $\kappa\cdot\sum_{y=x,y\in X_1} g_{c_1,y}\big/\sqrt{W(y)}=\sum_{y=x,y\in X_2} g_{c_2,y}\big/\sqrt{W(y)}$ are given, for $\kappa=\sqrt{W(c_2)/W(c_1)}$ and $x\in S$. According to (6), we have:

$$\begin{cases} h(c_i,X_i)=\sum\limits_{x\in X_i}\hat{g}_{c_i x}x, \\ \hat{g}_{c_i x}=\dfrac{g_{c_i,x}}{\sqrt{W(c_i)\cdot W(x)}}. \end{cases} \tag{S1}$$

Given (S1), we derive:

$$\begin{cases} h(c_1,X_1)=\sum\limits_{x\in X_1}\hat{g}_{c_1,x}x=\sum\limits_{x\in X_1}\dfrac{g_{c_1,x}}{\sqrt{W(c_1)\cdot W(x)}}x, \\ h(c_2,X_2)=\sum\limits_{x\in X_2}\hat{g}_{c_2,x}x=\sum\limits_{x\in X_2}\dfrac{g_{c_2,x}}{\sqrt{W(c_2)\cdot W(x)}}x. \end{cases} \tag{S2}$$

With the condition that S_1=S_2=S, we have:

$$h(c_1,X_1)-h(c_2,X_2)=\sum_{x\in S}\left[\sum_{y=x,y\in X_1}\frac{g_{c_1,y}}{\sqrt{W(c_1)\cdot W(y)}}-\sum_{y=x,y\in X_2}\frac{g_{c_2,y}}{\sqrt{W(c_2)\cdot W(y)}}\right]\cdot x. \tag{S3}$$

Given $\kappa\cdot\sum_{y=x,y\in X_1} g_{c_1,y}\big/\sqrt{W(y)}=\sum_{y=x,y\in X_2} g_{c_2,y}\big/\sqrt{W(y)}$, for $\kappa=\sqrt{W(c_2)/W(c_1)}$, based on (S3), we directly have $h(c_1, X_1)=h(c_2, X_2)$.

If the conditions that $h(c_1, X_1)=h(c_2, X_2)$, we can prove that the conditions mentioned in ***Theorem* 1** are necessary by showing the contradictions while they are not satisfied. Given $h(c_1, X_1)=h(c_2, X_2)$, we have:

$$h(c_1,X_1)-h(c_2,X_2)=\sum_{x\in X_1}\frac{g_{c_1,x}}{\sqrt{W(c_1)\cdot W(x)}}x-\sum_{x\in X_2}\frac{g_{c_2,x}}{\sqrt{W(c_2)\cdot W(x)}}x=0. \tag{S4}$$

First, we assume $S_1\neq S_2$ for all $X_1, X_2\in\mathcal{X}$, the following equations are achieved:

$$\begin{aligned} &h(c_1,X_1)-h(c_2,X_2) \\ &=\sum_{x\in S_1\cap S_2}\left[\sum_{y=x,y\in X_1}\frac{g_{c_1,y}}{\sqrt{W(c_1)\cdot W(y)}}-\sum_{y=x,y\in X_2}\frac{g_{c_2,y}}{\sqrt{W(c_2)\cdot W(y)}}\right]\cdot x \\ &\quad+\sum_{x\in S_1\setminus S_2}\sum_{y=x,y\in X_1}\frac{g_{c_1,y}}{\sqrt{W(c_1)\cdot W(y)}}\cdot x-\sum_{x\in S_2\setminus S_1}\sum_{y=x,y\in X_2}\frac{g_{c_2,y}}{\sqrt{W(c_2)\cdot W(y)}}\cdot x=0. \end{aligned} \tag{S5}$$

Since (S5) holds for any x, we could define a function $f(\cdot)$ as:

$$x=\begin{cases} f(x), \text{ for } x\in S_1\cap S_2; \\ f(x)-1, \text{ for } x\in S_1\setminus S_2; \\ f(x)+1, \text{ for } x\in S_2\setminus S_1. \end{cases} \tag{S6}$$

And if (S5) holds, we also infer that:

$$
\begin{aligned}
&h(c_1, X_1) - h(c_2, X_2) \\
&= \sum_{x \in S_1 \cap S_2} \left[\sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} - \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \right] \cdot f(x) \\
&+ \sum_{x \in S_1 \setminus S_2} \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} \cdot f(x) - \sum_{x \in S_2 \setminus S_1} \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \cdot f(x) = 0.
\end{aligned} \tag{S7}
$$

By substituting (S6) into (S7), we infer:

$$
\begin{aligned}
&h(c_1, X_1) - h(c_2, X_2) \\
&= \sum_{x \in S_1 \cap S_2} \left[\sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} - \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \right] \cdot x \\
&+ \sum_{x \in S_1 \setminus S_2} \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} \cdot (x+1) - \sum_{x \in S_2 \setminus S_1} \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \cdot (x-1) = 0.
\end{aligned} \tag{S8}
$$

As (S5) is equal to (S8), we have:

$$
\begin{aligned}
&h(c_1, X_1) - h(c_2, X_2) \\
&= \sum_{x \in S_1 \cap S_2} \left[\sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} - \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \right] \cdot x \\
&+ \sum_{x \in S_1 \setminus S_2} \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} \cdot x - \sum_{x \in S_2 \setminus S_1} \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \cdot x \\
&+ \sum_{x \in S_1 \setminus S_2} \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} - \sum_{x \in S_2 \setminus S_1} \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \\
&= \sum_{x \in S_1 \setminus S_2} \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} + \sum_{x \in S_2 \setminus S_1} \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} = 0.
\end{aligned} \tag{S9}
$$

Since the terms in the above summation operators are positive, i.e., (S9) cannot hold obviously. Thus, the assumption that $S_1 \neq S_2$ is false. Thus, given $h(c_1, X_1)=h(c_2, X_2)$, we have $S_1=S_2$.

Furthermore, based on $S_1=S_2=S$, we have the following inference:

$$
\sum_{x \in S_1 \setminus S_2} \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} \cdot x - \sum_{x \in S_2 \setminus S_1} \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \cdot x = 0. \tag{S10}
$$

Hence, according to (S5) and (S10), we have:

$$
h(c_1, X_1) - h(c_2, X_2) = \sum_{x \in S} \left[\sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} - \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} \right] \cdot x = 0. \tag{S11}
$$

Obviously, each term in the above summation is equal to zero:

$$
\sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1) \cdot W(y)}} - \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2) \cdot W(y)}} = 0. \tag{S12}
$$

Hence, we obtain:

$$
\sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(c_1)} \cdot \sqrt{W(y)}} - \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(c_2)} \cdot \sqrt{W(y)}} = \frac{1}{\sqrt{W(c_1)}} \cdot \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(y)}} - \frac{1}{\sqrt{W(c_2)}} \cdot \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(y)}} = 0. \tag{S13}
$$

Eq. (S13) can be rewritten as:

$$
\sqrt{\frac{W(c_2)}{W(c_1)}} \cdot \sum_{y=x, y \in X_1} \frac{g_{c_1,y}}{\sqrt{W(y)}} = \sum_{y=x, y \in X_2} \frac{g_{c_2,y}}{\sqrt{W(y)}}. \tag{S14}
$$

We further set $\kappa = \sqrt{W(c_2)/W(c_1)}$, we have $\kappa \cdot \sum_{y=x, y \in X_1} g_{c_1,y} \Big/ \sqrt{W(y)} = \sum_{y=x, y \in X_2} g_{c_2,y} \Big/ \sqrt{W(y)}$, for $x \in S$. Therefore, based on these inferences, ***Theorem*** **1** holds.□

B. Proof of Corollary 1

Following ***Theorem* 1**, the pooling function using the strategy in (14) can be denoted as $p(c, X^{(1)}, X^{(2)},\ldots, X^{(L)})=(\alpha+\varepsilon/|X|)\cdot c+\sum_{l=\{1\sim L\}, x\in X^{(l)}} h(c, x)$, c, $X^{(1)}, X^{(2)},\ldots, X^{(L)}\in\mathcal{X}$, where $|X^{(1)}|=|X^{(2)}|=\ldots=|X^{(L)}|=|X|$. According to ***Theorem* 1**, it is seen that when the condition that $X_1^{(l)}=\{S, \mu_1\}$, $X_2^{(l)}=\{S, \mu_2\}$, and $\kappa\cdot\sum_{y=x,y\in X_1} g_{c_1,y}\big/\sqrt{W(y)}=\sum_{y=x,y\in X_2} g_{c_2,y}\big/\sqrt{W(y)}$, for $\kappa=\sqrt{W(c_2)/W(c_1)}$, $x\in S$, and $l=\{1\sim L\}$ is fulfilled, $h(c_1, X_1^{(l)})-h(c_2, X_1^{(l)})=0$, for $l=\{1\sim L\}$, i.e., the aggregation function in (6) cannot distinguish different graph structures. To prove ***Corollary* 1**, it should be proved that $\mathcal{T}$ can correctly distinguish all different structures that the aggregation function in (6) fails previously. To do so, two cases require to be considered.

(1)$c_1\neq c_2$.

Given $X_1^{(l)}=\{S, \mu_1\}$, $X_2^{(l)}=\{S, \mu_2\}$, and $\kappa\cdot\sum_{y=x,y\in X_1} g_{c_1,y}\big/\sqrt{W(y)}=\sum_{y=x,y\in X_2} g_{c_2,y}\big/\sqrt{W(y)}$, for $\kappa=\sqrt{W(c_2)/W(c_1)}$, $x\in S$, and $l=\{1\sim L\}$, we have $h(c_1, X_1^{(l)})-h(c_2, X_2^{(l)})=0$, for $l=\{1\sim L\}$ based on ***Theorem* 1**. Hence, we have $p(c_1, X_1^{(1)}, X_1^{(2)},\ldots, X_1^{(L)})-p(c_2, X_2^{(1)}, X_2^{(2)},\ldots, X_2^{(L)})=(\alpha+\varepsilon/|X_1|)\cdot c_1-(\alpha+\varepsilon/|X_2|)\cdot c_2$. As $c_1\neq c_2$, $p(c_1, X_1^{(1)}, X_1^{(2)},\ldots, X_1^{(L)})\neq p(c_2, X_2^{(1)}, X_2^{(2)},\ldots, X_2^{(L)})$ is obvious.

(2)$c_1=c_2$.

Similarly, we have $p(c_1, X_1^{(1)}, X_1^{(2)},\ldots, X_1^{(L)})-p(c_2, X_2^{(1)}, X_2^{(2)},\ldots, X_2^{(L)})=(\alpha+\varepsilon/|X_1|)\cdot c_1-(\alpha+\varepsilon/|X_2|)\cdot c_2$. Considering the condition that $c_1=c_2$, we thereby have the following inference:

$$p\left(c_1, X_1^{(1)}, X_1^{(2)},\ldots, X_1^{(L)}\right)-p\left(c_2, X_2^{(1)}, X_2^{(2)},\ldots, X_2^{(L)}\right)=\left(\alpha+\frac{\varepsilon}{|X_1|}\right)c-\left(\alpha+\frac{\varepsilon}{|X_2|}\right)c=\varepsilon\left(\frac{1}{|X_1|}-\frac{1}{|X_2|}\right)c, \tag{S15}$$

where $|X_1|=|N(c_1)|$ and $|X_2|=|N(c_2)|$. Since $|X_1|\neq|X_2|$, $p(c_1, X_1^{(1)}, X_1^{(2)},\ldots, X_1^{(L)})\neq p(c_2, X_2^{(1)}, X_2^{(2)},\ldots, X_2^{(L)})$, meaning that the locality-enhanced holistic pooling function $\mathcal{T}$ based on (6) and (14) can successfully distinguish the graph structures that solely utilizing the aggregation function in (6) fails to distinguish previously. Thus, ***Corollary* 1** holds.□

II. Supplementary Tables

A. Results of Comparison Experiments

The results of Tables SI-SVII have been discussed in Section V.B, whose details are as follows:

- Tables **SI-SII** record the RMSE and MAE of GLCPN;
- Tables **SIII-SIV** record the time cost in RMSE and MAE of GLCPN;
- Table **SV** reports the Friedman statistical results of all involved models;
- Tables **SVI-SVII** summarize the Wilcoxon signed-ranks test results.

TABLE SI

The RMSE and Win/Loss Counts of M1-16 on All Testing Cases.

No.	D1	D2	D3	D4	D5	D6	D7	D8	Win/Loss
M1	$0.1064_{\pm4.6E-5}$	$0.1375_{\pm7.6E-5}$	$0.1880_{\pm9.1E-2}$	$0.1352_{\pm3.1E-4}$	$0.5058_{\pm9.1E-2}$	$0.9384_{\pm9.0E-3}$	$1.0164_{\pm9.4E-3}$	$0.9979_{\pm3.1E-3}$	8/0
M2	$0.1117_{\pm1.4E-3}$	$0.1393_{\pm2.9E-3}$	$0.1438_{\pm2.4E-3}$	$0.1413_{\pm5.8E-4}$	$0.5129_{\pm4.0E-3}$	$0.8310_{\pm3.0E-2}$	$0.8650_{\pm1.5E-3}$	$0.8492_{\pm2.5E-3}$	8/0
M3	$0.0944_{\pm1.6E-4}$	$0.1284_{\pm9.2E-5}$	$0.1280_{\pm5.4E-4}$	$0.1276_{\pm2.4E-4}$	$0.4741_{\pm1.4E-2}$	$\mathbf{0.7931_{\pm2.7E-2}}$	$0.8385_{\pm8.2E-3}$	$0.8241_{\pm2.6E-2}$	7/1
M4	$0.0979_{\pm8.0E-5}$	$0.1337_{\pm3.7E-4}$	$0.1370_{\pm1.4E-3}$	$0.1417_{\pm2.2E-3}$	$0.6277_{\pm1.1E-2}$	$1.0414_{\pm2.0E-2}$	$1.0547_{\pm1.2E-2}$	$1.0315_{\pm1.8E-2}$	8/0
M5	$0.0894_{\pm6.2E-5}$	$0.1244_{\pm1.5E-4}$	$0.1187_{\pm3.3E-4}$	$0.1183_{\pm3.6E-4}$	$0.4673_{\pm1.6E-2}$	$0.8182_{\pm3.1E-2}$	$0.8348_{\pm9.1E-3}$	$0.8169_{\pm1.8E-2}$	8/0
M6	$0.0916_{\pm6.9E-5}$	$0.1266_{\pm3.3E-5}$	$0.1265_{\pm2.5E-4}$	$0.1241_{\pm2.9E-4}$	$0.4933_{\pm1.6E-2}$	$0.8725_{\pm2.7E-2}$	$0.8685_{\pm1.7E-2}$	$0.8441_{\pm1.7E-2}$	8/0
M7	$0.1089_{\pm1.1E-4}$	$0.1594_{\pm2.3E-4}$	$0.1495_{\pm3.9E-4}$	$0.1437_{\pm4.2E-4}$	$0.4636_{\pm1.7E-2}$	$0.8479_{\pm2.3E-2}$	$0.8461_{\pm9.3E-3}$	$0.8210_{\pm1.7E-2}$	8/0
M8	$0.0905_{\pm5.9E-5}$	$0.1246_{\pm1.0E-4}$	$0.1232_{\pm4.1E-4}$	$0.1222_{\pm2.7E-4}$	$0.4757_{\pm1.7E-2}$	$0.8430_{\pm3.2E-2}$	$0.8482_{\pm1.0E-2}$	$0.8229_{\pm1.9E-2}$	8/0
M9	$0.0894_{\pm5.7E-5}$	$0.1242_{\pm7.5E-5}$	$0.1185_{\pm3.4E-4}$	$0.1179_{\pm3.2E-4}$	$0.4698_{\pm1.7E-2}$	$0.8199_{\pm3.3E-2}$	$0.8361_{\pm9.2E-3}$	$0.8186_{\pm1.8E-2}$	8/0
M10	$0.0900_{\pm4.5E-5}$	$0.1252_{\pm1.8E-4}$	$0.1202_{\pm2.8E-4}$	$0.1200_{\pm2.9E-4}$	$0.4764_{\pm1.7E-2}$	$0.8517_{\pm3.3E-2}$	$0.8562_{\pm1.1E-2}$	$0.8286_{\pm1.7E-2}$	8/0
M11	$0.0992_{\pm1.0E-3}$	$0.1335_{\pm4.9E-4}$	$0.1299_{\pm2.1E-4}$	$0.1329_{\pm5.4E-4}$	$0.4972_{\pm1.6E-2}$	$0.8551_{\pm3.5E-2}$	$0.8695_{\pm1.1E-2}$	$0.8498_{\pm1.9E-2}$	8/0
M12	$0.0995_{\pm3.1E-5}$	$0.1313_{\pm1.4E-4}$	$0.1271_{\pm3.5E-4}$	$0.1267_{\pm3.4E-4}$	$0.4744_{\pm1.7E-2}$	$0.8261_{\pm3.2E-2}$	$0.8383_{\pm9.6E-3}$	$0.8178_{\pm1.8E-2}$	8/0
M13	$0.0918_{\pm1.6E-4}$	$0.1271_{\pm9.3E-5}$	$0.1247_{\pm2.4E-4}$	$0.1220_{\pm2.7E-4}$	$0.4756_{\pm1.8E-2}$	$0.8712_{\pm3.4E-2}$	$0.8692_{\pm1.3E-2}$	$0.8356_{\pm1.8E-2}$	8/0
M14	$0.1330_{\pm1.1E-3}$	$0.1611_{\pm1.7E-3}$	$0.1682_{\pm1.3E-3}$	$0.1636_{\pm1.7E-3}$	$0.4823_{\pm1.7E-2}$	$0.8255_{\pm3.2E-2}$	$0.8455_{\pm9.1E-3}$	$0.8242_{\pm1.7E-2}$	8/0
M15	$0.0929_{\pm2.7E-5}$	$0.1284_{\pm5.2E-5}$	$0.1324_{\pm4.6E-4}$	$0.1284_{\pm2.6E-4}$	$0.4751_{\pm1.8E-2}$	$0.8343_{\pm3.3E-2}$	$0.8451_{\pm1.0E-2}$	$0.8235_{\pm1.8E-2}$	8/0
M16	$\mathbf{0.0876_{\pm6.3E-5}}$	$\mathbf{0.1229_{\pm9.7E-5}}$	$\mathbf{0.1161_{\pm3.7E-4}}$	$\mathbf{0.1164_{\pm2.8E-4}}$	$\mathbf{0.4527_{\pm1.7E-2}}$	$0.8159_{\pm3.0E-2}$	$\mathbf{0.8281_{\pm8.7E-3}}$	$\mathbf{0.8015_{\pm1.8E-2}}$	—

TABLE SII

The MAE and Win/Loss Counts of M1-16 on All Testing Cases.

No.	D1	D2	D3	D4	D5	D6	D7	D8	Win/Loss
M1	$0.0710_{\pm5.2E-5}$	$0.0998_{\pm5.8E-5}$	$0.1429_{\pm8.7E-2}$	$0.0949_{\pm2.3E-4}$	$0.1997_{\pm4.0E-2}$	$0.4856_{\pm4.0E-3}$	$0.4557_{\pm5.1E-3}$	$0.4564_{\pm4.4E-3}$	8/0
M2	$0.0698_{\pm1.1E-3}$	$0.0992_{\pm2.0E-3}$	$0.0918_{\pm2.2E-3}$	$0.0917_{\pm5.4E-4}$	$0.2367_{\pm6.8E-3}$	$0.4471_{\pm1.3E-2}$	$0.4151_{\pm4.7E-3}$	$0.4018_{\pm3.2E-3}$	8/0
M3	$0.0644_{\pm7.5E-4}$	$0.0950_{\pm6.1E-4}$	$0.0954_{\pm1.6E-3}$	$0.0907_{\pm4.4E-4}$	$0.2231_{\pm3.9E-3}$	$0.4536_{\pm2.0E-2}$	$0.4291_{\pm5.2E-3}$	$0.4057_{\pm1.2E-2}$	8/0
M4	$0.0672_{\pm1.7E-4}$	$0.0987_{\pm3.3E-4}$	$0.1007_{\pm1.3E-3}$	$0.1003_{\pm1.9E-3}$	$0.3002_{\pm6.7E-3}$	$0.7225_{\pm1.0E-2}$	$0.6819_{\pm1.2E-2}$	$0.6546_{\pm1.1E-2}$	8/0
M5	$0.0584_{\pm5.2E-5}$	$0.0898_{\pm8.9E-5}$	$0.0839_{\pm1.9E-4}$	$0.0818_{\pm1.7E-4}$	$0.1813_{\pm3.6E-3}$	$0.3894_{\pm7.4E-3}$	$0.3629_{\pm4.1E-3}$	$0.3518_{\pm2.2E-3}$	8/0
M6	$0.0600_{\pm5.2E-5}$	$0.0916_{\pm3.7E-5}$	$0.0905_{\pm2.8E-4}$	$0.0870_{\pm2.8E-4}$	$0.2138_{\pm3.3E-3}$	$0.4471_{\pm8.9E-3}$	$0.4002_{\pm8.9E-3}$	$0.3858_{\pm2.6E-3}$	8/0
M7	$0.0726_{\pm6.7E-5}$	$0.1181_{\pm1.1E-4}$	$0.1088_{\pm3.0E-4}$	$0.1029_{\pm2.7E-4}$	$0.1724_{\pm3.5E-3}$	$0.4020_{\pm6.8E-3}$	$0.3610_{\pm3.9E-3}$	$0.3437_{\pm2.1E-3}$	8/0
M8	$0.0594_{\pm3.9E-5}$	$0.0899_{\pm4.2E-5}$	$0.0876_{\pm2.1E-4}$	$0.0851_{\pm1.4E-4}$	$0.1856_{\pm3.6E-3}$	$0.3984_{\pm8.4E-3}$	$0.3612_{\pm4.0E-3}$	$0.3489_{\pm1.7E-3}$	8/0
M9	$0.0583_{\pm4.6E-5}$	$0.0896_{\pm4.6E-5}$	$0.0837_{\pm2.1E-4}$	$0.0813_{\pm1.3E-4}$	$0.1815_{\pm3.7E-3}$	$0.3870_{\pm7.8E-3}$	$0.3612_{\pm4.1E-3}$	$0.3508_{\pm1.7E-3}$	8/0
M10	$0.0592_{\pm7.9E-5}$	$0.0904_{\pm8.4E-5}$	$0.0849_{\pm1.8E-4}$	$0.0831_{\pm1.4E-4}$	$0.1833_{\pm3.9E-3}$	$0.4083_{\pm9.2E-3}$	$0.3646_{\pm4.6E-3}$	$0.3488_{\pm2.0E-3}$	8/0
M11	$0.0642_{\pm7.6E-4}$	$0.0931_{\pm4.7E-4}$	$0.0940_{\pm2.4E-4}$	$0.0939_{\pm3.2E-4}$	$0.2148_{\pm2.8E-3}$	$0.4287_{\pm9.5E-3}$	$0.3859_{\pm4.5E-3}$	$0.3681_{\pm3.7E-3}$	8/0
M12	$0.0681_{\pm2.9E-5}$	$0.0951_{\pm7.6E-5}$	$0.0906_{\pm2.0E-4}$	$0.0895_{\pm1.6E-4}$	$0.1921_{\pm3.5E-3}$	$0.3942_{\pm8.2E-3}$	$0.3647_{\pm4.1E-3}$	$0.3540_{\pm1.8E-3}$	8/0
M13	$0.0603_{\pm1.2E-4}$	$0.0922_{\pm7.3E-5}$	$0.0890_{\pm8.7E-5}$	$0.0849_{\pm1.5E-4}$	$0.1758_{\pm3.7E-3}$	$0.4100_{\pm9.5E-3}$	$0.3632_{\pm3.8E-3}$	$0.3454_{\pm2.5E-3}$	8/0
M14	$0.0903_{\pm8.8E-4}$	$0.1121_{\pm4.5E-4}$	$0.1175_{\pm2.1E-3}$	$0.1208_{\pm2.4E-3}$	$0.2052_{\pm3.9E-3}$	$0.4036_{\pm7.5E-3}$	$0.3762_{\pm3.9E-3}$	$0.3640_{\pm1.7E-3}$	8/0
M15	$0.0613_{\pm1.3E-5}$	$0.0932_{\pm7.1E-5}$	$0.0957_{\pm2.8E-4}$	$0.0907_{\pm1.8E-4}$	$0.1845_{\pm3.9E-3}$	$0.3933_{\pm8.2E-3}$	$0.3609_{\pm4.1E-3}$	$0.3508_{\pm2.0E-3}$	8/0
M16	$\mathbf{0.0569_{\pm3.6E-5}}$	$\mathbf{0.0882_{\pm8.3E-5}}$	$\mathbf{0.0810_{\pm3.2E-4}}$	$\mathbf{0.0800_{\pm9.7E-5}}$	$\mathbf{0.1628_{\pm3.7E-3}}$	$\mathbf{0.3709_{\pm8.9E-3}}$	$\mathbf{0.3340_{\pm3.5E-3}}$	$\mathbf{0.3200_{\pm2.4E-3}}$	—

TABLE SIII

The Training Time Cost in RMSE (Sec.) and Win/Loss Counts of M1-16 on All Testing Cases.

No.	D1	D2	D3	D4	D5	D6	D7	D8	Win/Loss
M1	$23639_{\pm3281.13}$	$15262_{\pm2313.04}$	$3784_{\pm1328.82}$	$2847_{\pm888.49}$	$3124_{\pm1319.35}$	$705_{\pm42.48}$	$2485_{\pm516.66}$	$3041_{\pm843.18}$	8/0
M2	$86717_{\pm8762.90}$	$100478_{\pm34208.66}$	$16636_{\pm5717.27}$	$21886_{\pm775.19}$	$19_{\pm0.28}$	$9_{\pm1.63}$	$36_{\pm0.28}$	$61_{\pm13.49}$	8/0
M3	$111765_{\pm25822.30}$	$53694_{\pm8577.76}$	$7264_{\pm2205.15}$	$3598_{\pm2076.02}$	$24_{\pm3.35}$	$17_{\pm2.33}$	$51_{\pm4.53}$	$77_{\pm12.26}$	8/0
M4	$27007_{\pm2315.49}$	$15677_{\pm1372.02}$	$2394_{\pm232.15}$	$1801_{\pm168.76}$	$180_{\pm97.91}$	$7_{\pm1.26}$	$14_{\pm3.72}$	$21_{\pm5.98}$	8/0
M5	$86409_{\pm4060.43}$	$47689_{\pm2030.77}$	$6504_{\pm91.71}$	$3641_{\pm79.94}$	$291_{\pm18.47}$	$39_{\pm2.60}$	$140_{\pm11.96}$	$270_{\pm46.18}$	8/0
M6	$23776_{\pm382.51}$	$12475_{\pm346.35}$	$\mathbf{812_{\pm12.78}}$	$522_{\pm12.12}$	$56_{\pm35.34}$	$16_{\pm7.04}$	$24_{\pm5.96}$	$36_{\pm1.19}$	7/1
M7	$80054_{\pm9638.93}$	$29526_{\pm807.53}$	$4109_{\pm152.29}$	$2698_{\pm41.52}$	$110_{\pm2.65}$	$18_{\pm1.68}$	$206_{\pm269.24}$	$133_{\pm18.17}$	8/0
M8	$27716_{\pm332.19}$	$16827_{\pm11.01}$	$1909_{\pm36.29}$	$1024_{\pm17.55}$	$60_{\pm2.82}$	$15_{\pm0.64}$	$45_{\pm2.21}$	$77_{\pm9.62}$	8/0
M9	$80932_{\pm622.02}$	$47631_{\pm210.16}$	$6386_{\pm68.83}$	$3507_{\pm47.87}$	$299_{\pm24.09}$	$38_{\pm1.41}$	$126_{\pm9.59}$	$213_{\pm62.21}$	8/0
M10	$40161_{\pm3369.92}$	$15008_{\pm148.85}$	$2706_{\pm74.28}$	$1274_{\pm3.51}$	$140_{\pm13.83}$	$29_{\pm2.40}$	$69_{\pm6.52}$	$105_{\pm13.40}$	8/0
M11	$31986_{\pm9000.12}$	$13559_{\pm1278.28}$	$2148_{\pm458.26}$	$1307_{\pm119.87}$	$98_{\pm3.94}$	$36_{\pm2.25}$	$69_{\pm4.48}$	$92_{\pm6.29}$	8/0
M12	$23748_{\pm1717.06}$	$15310_{\pm697.19}$	$5418_{\pm537.70}$	$\mathbf{218_{\pm315.74}}$	$44_{\pm3.44}$	$8_{\pm0.64}$	$25_{\pm2.68}$	$44_{\pm8.21}$	7/1
M13	$29599_{\pm322.72}$	$14960_{\pm598.34}$	$1793_{\pm48.35}$	$962_{\pm26.48}$	$91_{\pm3.36}$	$43_{\pm1.99}$	$91_{\pm3.42}$	$134_{\pm3.75}$	8/0
M14	$64241_{\pm20949.85}$	$37383_{\pm16126.03}$	$6290_{\pm2004.81}$	$4118_{\pm758.49}$	$123_{\pm8.32}$	$16_{\pm1.57}$	$96_{\pm3.01}$	$230_{\pm29.74}$	8/0
M15	$41094_{\pm218.09}$	$22592_{\pm278.36}$	$3390_{\pm42.10}$	$1900_{\pm27.05}$	$65_{\pm2.76}$	$28_{\pm1.30}$	$54_{\pm2.22}$	$75_{\pm4.14}$	8/0
M16	$\mathbf{18053_{\pm805.84}}$	$\mathbf{10682_{\pm1625.76}}$	$1243_{\pm328.76}$	$337_{\pm50.30}$	$\mathbf{10_{\pm0.66}}$	$\mathbf{5_{\pm0.36}}$	$\mathbf{14_{\pm0.32}}$	$\mathbf{19_{\pm1.52}}$	—

TABLE SIV

THE TRAINING TIME COST IN MAE (SEC.) AND WIN/LOSS COUNTS OF M1-16 ON ALL TESTING CASES.

No.	D1	D2	D3	D4	D5	D6	D7	D8	Win/Loss
M1	$23721_{\pm 3496.87}$	$15111_{\pm 2262.50}$	$3546_{\pm 1292.37}$	$2993_{\pm 970.69}$	$3291_{\pm 1367.57}$	$717_{\pm 32.25}$	$2477_{\pm 515.63}$	$3059_{\pm 836.57}$	8/0
M2	$86846_{\pm 8947.68}$	$85208_{\pm 37758.77}$	$17226_{\pm 4821.14}$	$21905_{\pm 790.42}$	$571_{\pm 80.59}$	$11_{\pm 2.98}$	$57_{\pm 19.28}$	$75_{\pm 13.74}$	8/0
M3	$54936_{\pm 13745.18}$	$17854_{\pm 5042.50}$	$2543_{\pm 242.30}$	$2248_{\pm 876.67}$	$32_{\pm 5.97}$	$23_{\pm 3.85}$	$64_{\pm 5.28}$	$97_{\pm 14.80}$	8/0
M4	$28132_{\pm 3352.69}$	$14422_{\pm 1371.31}$	$2242_{\pm 159.11}$	$1834_{\pm 123.43}$	$335_{\pm 41.57}$	$8_{\pm 1.95}$	$19_{\pm 4.85}$	$29_{\pm 6.76}$	8/0
M5	$78178_{\pm 3396.68}$	$43853_{\pm 1915.68}$	$5763_{\pm 122.28}$	$3500_{\pm 78.80}$	$293_{\pm 15.35}$	$47_{\pm 5.34}$	$206_{\pm 7.42}$	$435_{\pm 30.94}$	8/0
M6	$20161_{\pm 818.08}$	$10973_{\pm 459.04}$	$\mathbf{712_{\pm 41.90}}$	$491_{\pm 20.89}$	$30_{\pm 4.12}$	$19_{\pm 9.76}$	$19_{\pm 3.09}$	$27_{\pm 3.61}$	7/1
M7	$102976_{\pm 10275.42}$	$23993_{\pm 212.93}$	$2487_{\pm 84.92}$	$2433_{\pm 38.51}$	$95_{\pm 6.41}$	$21_{\pm 1.64}$	$198_{\pm 209.61}$	$182_{\pm 7.46}$	8/0
M8	$25686_{\pm 760.97}$	$15297_{\pm 485.69}$	$1681_{\pm 32.21}$	$973_{\pm 22.12}$	$64_{\pm 2.17}$	$13_{\pm 0.71}$	$39_{\pm 3.85}$	$78_{\pm 6.25}$	8/0
M9	$74130_{\pm 997.08}$	$43757_{\pm 289.41}$	$5758_{\pm 92.65}$	$3394_{\pm 34.17}$	$320_{\pm 11.69}$	$53_{\pm 3.67}$	$213_{\pm 13.72}$	$417_{\pm 20.05}$	8/0
M10	$36989_{\pm 2171.40}$	$13019_{\pm 360.84}$	$2285_{\pm 71.03}$	$1200_{\pm 42.06}$	$152_{\pm 16.69}$	$27_{\pm 1.92}$	$74_{\pm 9.68}$	$141_{\pm 17.84}$	8/0
M11	$25744_{\pm 5430.47}$	$20815_{\pm 5353.89}$	$1801_{\pm 294.71}$	$1317_{\pm 137.64}$	$64_{\pm 4.11}$	$25_{\pm 0.66}$	$44_{\pm 2.60}$	$56_{\pm 2.80}$	8/0
M12	$21000_{\pm 1241.13}$	$13453_{\pm 556.08}$	$4944_{\pm 899.33}$	$2100_{\pm 256.52}$	$49_{\pm 2.66}$	$6_{\pm 0.59}$	$23_{\pm 2.97}$	$47_{\pm 7.44}$	8/0
M13	$27687_{\pm 845.58}$	$12942_{\pm 614.46}$	$1549_{\pm 56.24}$	$846_{\pm 23.25}$	$79_{\pm 1.85}$	$37_{\pm 1.22}$	$82_{\pm 3.54}$	$130_{\pm 1.91}$	8/0
M14	$24117_{\pm 7551.16}$	$12243_{\pm 3910.36}$	$1103_{\pm 625.83}$	$791_{\pm 335.47}$	$77_{\pm 16.68}$	$20_{\pm 4.30}$	$100_{\pm 17.31}$	$204_{\pm 35.47}$	8/0
M15	$40326_{\pm 463.23}$	$20638_{\pm 204.73}$	$2982_{\pm 23.92}$	$1731_{\pm 23.45}$	$59_{\pm 1.03}$	$21_{\pm 0.68}$	$39_{\pm 3.49}$	$65_{\pm 3.94}$	8/0
M16	$\mathbf{14200_{\pm 1727.31}}$	$\mathbf{8362_{\pm 1621.56}}$	$728_{\pm 136.53}$	$\mathbf{440_{\pm 133.24}}$	$\mathbf{6_{\pm 0.01}}$	$\mathbf{3_{\pm 0.18}}$	$\mathbf{9_{\pm 0.40}}$	$\mathbf{11_{\pm 0.60}}$	—

TABLE SV

RESULTS OF THE FRIEDMAN TEST IN ESTIMATION ACCURACY (RMSE AND MAE) AND EFFICIENCY (CONVERGING TIME IN RMSE AND MAE).

No.	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16
Accuracy*	14.06	12.53	9.43	14.13	3.41	9.41	9.81	6.03	3.10	6.38	11.31	8.00	7.38	12.25	7.72	**1.06**
Efficiency**	12.06	11.00	9.90	6.25	14.19	2.94	11.34	6.16	13.56	8.91	7.75	5.19	7.94	9.22	8.38	**1.22**

** High F-rank denotes low RMSE/MAE; ** High F-rank denotes low time cost to converge.*

TABLE SVI

RESULTS OF THE WILCOXON SIGNED-RANKS TEST IN RMSE AND MAE CORRESPONDING TO TABLES S8, S9, AND S12.

Comparison	*R*+*	*R*–	*p*-value**
M16 vs M1	136	0	**2.41E-4**
M16 vs M2	136	0	**2.41E-4**
M16 vs M3	124	12	**2.05E-3**
M16 vs M4	136	0	**2.41E-4**
M16 vs M5	136	0	**2.41E-4**
M16 vs M6	136	0	**2.41E-4**
M16 vs M7	136	0	**2.41E-4**
M16 vs M8	136	0	**2.41E-4**
M16 vs M9	136	0	**2.41E-4**
M16 vs M10	136	0	**2.41E-4**
M16 vs M11	136	0	**2.41E-4**
M16 vs M12	136	0	**2.41E-4**
M16 vs M13	136	0	**2.41E-4**
M16 vs M14	136	0	**2.41E-4**
M16 vs M15	136	0	**2.41E-4**

** For M16, higher R+ values indicate higher estimation accuracy; ** With the significance level of 0.1, the accepted hypotheses are highlighted.*

TABLE SVII

RESULTS OF THE WILCOXON SIGNED-RANKS TEST ON CONVERGING TIME IN RMSE AND MAE CORRESPONDING TO TABLES S10, S11, AND S12.

Comparison	*R*+*	*R*–	*p*-value**
M16 vs M1	136	0	**2.41E-4**
M16 vs M2	136	0	**2.41E-4**
M16 vs M3	136	0	**2.41E-4**
M16 vs M4	120	16	**3.05E-3**
M16 vs M5	136	0	**2.41E-4**
M16 vs M6	119	17	**4.48E-3**
M16 vs M7	136	0	**2.41E-4**
M16 vs M8	136	0	**2.41E-4**
M16 vs M9	136	0	**2.41E-4**
M16 vs M10	136	0	**2.41E-4**
M16 vs M11	136	0	**2.41E-4**
M16 vs M12	127	9	**1.24E-3**
M16 vs M13	136	0	**2.41E-4**
M16 vs M14	136	0	**2.41E-4**
M16 vs M15	136	0	**2.41E-4**

** For M16, higher R+ values indicate higher computational efficiency; ** With the significance level of 0.1, the accepted hypotheses are highlighted.*

B. Results of Hyperparameter Sensitivity Test

- Table **SVIII** (discussed in Section V.C) summarizes the suggested hyperparameter settings of GLCPN.

TABLE SVIII
SUGGESTED HYPERPARAMETER SETTINGS OF GLCPN.

Learning Rate	L_2 Regularization Coefficient	Batch Size	L	K	α
1e-2	1e-4	2^{11}	3	64	0.1

C. Results of Ablation Studies

- Tables **SIX-SX** (discussed in Section V.D.i) summarize the training and validation errors (RMSE and MAE) of GLCPN and its several variants, including GLCPN-MF, GLCPN-A&T, GLCPN-A, and GLCPN-T;
- Tables **SXI-SXII** (discussed in Section V.D.ii) record the RMSE, MAE, training epochs, time cost per epoch, and total time cost of GLCPN and its variants, including GLCPN-B and GLCPN-AT;
- Tables **SXIII-SXIV** (discussed in Section V.D.iii) present the RMSE and MAE of GLCPN and its variants, including GLCPN-S, GLCPN-SS, GLCPN-M, and GLCPN-C.

TABLE SIX
THE TRAINING AND VALIDATION RMSE OF GLCPN-MF, GLCPN-A&T, GLCPN-A, GLCPN-T, AND GLCPN ON D1-8.

No.		D1	D2	D3	D4	D5	D6	D7	D8
Training RMSE	GLCPN-MF	**0.0627±3.4E-5**	0.0990±5.6E-5	**0.0701±7.6E-4**	**0.0695±5.8E-3**	**0.2180±2.2E-2**	**0.3729±3.7E-2**	**0.4610±2.3E-2**	**0.4985±4.0E-2**
	GLCPN-A&T	0.0654±9.1E-4	0.1007±1.3E-3	0.0752±1.3E-3	0.0791±1.7E-3	0.4022±1.3E-2	0.6534±4.3E-2	0.8138±1.1E-2	0.7741±6.3E-2
	GLCPN-A	0.0713±5.1E-5	0.0957±6.5E-4	0.0873±8.0E-5	0.0774±2.2E-4	0.2691±1.4E-2	0.6571±2.9E-2	0.7264±1.4E-2	0.7624±2.3E-2
	GLCPN-T	0.0692±1.5E-3	0.1022±1.8E-3	0.1009±2.5E-2	0.0931±2.6E-3	0.4432±3.0E-2	0.6819±3.1E-2	0.8024±1.0E-2	0.8054±1.3E-2
	GLCPN	0.0711±5.0E-5	**0.0951±4.9E-4**	0.0866±9.3E-5	0.0758±3.3E-4	0.2615±1.9E-2	0.5423±1.9E-2	0.5958±2.8E-2	0.6009±3.5E-2
Validation RMSE	GLCPN-MF	0.0865±6.1E-5	0.1232±1.5E-4	0.1195±2.2E-4	0.1174±2.4E-4	0.4585±8.4E-3	0.8622±3.1E-2	0.8902±5.6E-2	0.8859±5.7E-2
	GLCPN-A&T	0.0840±4.8E-4	0.1210±1.4E-4	0.1141±2.7E-4	0.1143±3.4E-4	0.4470±1.0E-2	**0.7601±2.2E-2**	0.8381±5.1E-2	0.8612±5.8E-2
	GLCPN-A	0.0835±6.1E-5	0.1195±7.7E-5	0.1125±4.2E-4	0.1118±4.6E-4	0.4393±9.5E-3	0.7640±2.6E-2	0.8466±5.0E-2	0.8676±5.8E-2
	GLCPN-T	0.0883±4.8E-4	0.1247±3.0E-4	0.1284±9.8E-3	0.1233±4.8E-4	0.4509±9.4E-3	0.7604±2.3E-2	0.8419±4.9E-2	0.8694±5.6E-2
	GLCPN	**0.0831±5.0E-5**	**0.1195±3.9E-5**	**0.1119±3.6E-4**	**0.1112±4.3E-4**	**0.4273±8.1E-3**	0.7674±2.9E-2	**0.8272±5.2E-2**	**0.8388±5.7E-2**

MF stands for matrix factorization, i.e., no graph convolution; A stands for the nonlinear activation; and T stands for the feature transformation.

TABLE SX
THE TRAINING AND VALIDATION RMSE OF GLCPN-MF, GLCPN-A&T, GLCPN-A, GLCPN-T, AND GLCPN ON D1-8.

No.		D1	D2	D3	D4	D5	D6	D7	D8
Training MAE	GLCPN-MF	**0.0427±1.8E-4**	0.0730±3.7E-4	**0.0535±4.7E-4**	**0.0482±7.3E-4**	0.0821±6.1E-3	**0.1266±7.0E-3**	**0.1623±7.4E-3**	**0.1715±1.3E-3**
	GLCPN-A&T	0.0445±1.1E-4	0.0732±2.1E-4	0.0543±7.1E-4	0.0556±1.6E-3	0.1553±8.3E-3	0.3173±1.0E-2	0.3235±3.1E-2	0.3146±2.6E-2
	GLCPN-A	0.0460±7.4E-5	**0.0694±6.5E-4**	0.0603±4.1E-4	0.0525±3.3E-4	**0.0748±1.2E-3**	0.3253±6.2E-3	0.3327±6.0E-3	0.3394±6.5E-3
	GLCPN-T	0.0471±1.8E-3	0.0755±1.5E-3	0.0726±1.7E-2	0.0659±1.7E-3	0.1693±8.2E-3	0.3327±1.5E-2	0.3458±2.6E-2	0.3355±2.1E-2
	GLCPN	0.0456±7.9E-5	0.0699±8.3E-4	0.0593±2.5E-4	0.0512±1.1E-4	0.0886±4.4E-3	0.2447±1.6E-2	0.1999±1.3E-2	0.2098±1.7E-2
Validation MAE	GLCPN-MF	0.0563±3.2E-5	0.0891±1.2E-4	0.0848±1.4E-4	0.0780±5.6E-3	0.1726±7.9E-4	0.4262±6.8E-3	0.3626±1.1E-2	0.3400±6.6E-3
	GLCPN-A&T	0.0543±7.2E-5	0.0867±2.3E-4	0.0802±1.8E-4	0.0786±2.0E-4	0.1846±3.9E-3	0.3799±3.6E-3	0.3594±7.6E-3	0.3467±9.0E-3
	GLCPN-A	0.0532±7.6E-5	0.0858±5.6E-5	0.0771±3.3E-4	0.0755±1.7E-4	0.1688±1.5E-3	0.3812±3.8E-3	0.3721±7.7E-3	0.3608±6.5E-3
	GLCPN-T	0.0576±6.4E-4	0.0902±1.3E-4	0.0923±8.2E-3	0.0859±3.5E-4	0.1911±1.9E-3	0.3836±4.1E-3	0.3655±6.9E-3	0.3642±9.1E-3
	GLCPN	**0.0527±6.0E-5**	**0.0857±3.0E-5**	**0.0763±2.7E-4**	**0.0749±2.2E-4**	**0.1595±1.6E-4**	**0.3686±5.3E-3**	**0.3422±9.1E-3**	**0.3286±5.5E-3**

MF stands for matrix factorization, i.e., no graph convolution; A stands for the nonlinear activation; and T stands for the feature transformation.

TABLE SXI
THE RMSE, TRAINING EPOCHS, TIME COST PER EPOCH (SEC.), AND TOTAL TIME COST (SEC.) OF GLCPN-B, GLCPN-AT, AND GLCPN ON D1-8.

No.		D1	D2	D3	D4	D5	D6	D7	D8
RMSE	GLCPN-B	0.1135±9.5E-5	0.1392±8.6E-4	0.1142±3.8E-4	0.1125±3.4E-4	0.4325±9.0E-3	0.7734±2.7E-2	0.8376±5.2E-2	0.8502±5.8E-2
	GLCPN-AT	**0.1112±1.8E-4**	0.1370±3.3E-3	0.1266±7.7E-4	0.1235±5.9E-4	0.4328±9.4E-3	0.7782±3.0E-2	0.8481±5.1E-2	0.8630±5.6E-2
	GLCPN	0.1115±9.9E-5	**0.1363±3.0E-3**	**0.1119±3.6E-4**	**0.1112±4.3E-4**	**0.4273±8.1E-3**	**0.7674±2.9E-2**	**0.8272±5.2E-2**	**0.8388±5.7E-2**
Epochs	GLCPN-B	71±30.16	**85±12.76**	115±10.34	**100±6.26**	17±0.98	39±4.77	21±2.73	17±1.96
	GLCPN-AT	88±26.53	128±21.67	123±3.67	114±9.22	17±1.17	32±6.36	12±0.75	10±2.50
	GLCPN	**71±30.16**	86±14.12	**104±10.35**	114±19.96	**12±1.36**	**28±1.96**	**12±1.94**	**10±1.47**
Time Cost Per Epoch	GLCPN-B	35±0.08	22±0.32	28±0.05	15±0.07	0.96±0.01	0.24±0.00	1.09±0.00	2.13±0.01
	GLCPN-AT	183±0.59	109±0.21	107±0.17	55±0.75	3.54±0.05	0.97±0.01	3.56±0.06	6.85±0.20
	GLCPN	**35±0.40**	**22±0.28**	**28±0.13**	**15±0.09**	**0.96±0.01**	**0.24±0.00**	**1.09±0.01**	**2.13±0.01**
Total Time Cost	GLCPN-B	2531±1074.25	1891±296.56	3264±289.51	**1472±90.81**	16±1.10	9±1.12	22±2.92	37±4.10
	GLCPN-AT	16102±4888.56	13992±2354.94	13103±373.16	6351±553.40	59±3.90	31±0.04	42±2.85	71±16.57
	GLCPN	**2497±1060.24**	**1880±292.48**	**2966±302.48**	1681±303.08	**11±1.35**	**7±0.43**	**13±2.15**	**21±3.17**

B stands for the binary adjacency matrix; and AT stands for the self-attention mechanism.

TABLE SXII

THE MAE, TRAINING EPOCHS, TIME COST PER EPOCH (SEC.), AND TOTAL TIME COST (SEC.) OF GLCPN-B, GLCPN-AT, AND GLCPN ON D1-8.

No.		D1	D2	D3	D4	D5	D6	D7	D8
MAE	**GLCPN-B**	$0.0736_{\pm 5.4E-5}$	$0.0987_{\pm 5.6E-4}$	$0.0780_{\pm 2.4E-4}$	$0.0761_{\pm 1.5E-4}$	$0.1667_{\pm 4.8E-4}$	$0.3759_{\pm 5.1E-3}$	$0.3536_{\pm 8.2E-3}$	$0.3398_{\pm 6.1E-3}$
	GLCPN-AT	$0.0738_{\pm 1.5E-4}$	$0.0991_{\pm 2.3E-3}$	$0.0892_{\pm 5.0E-4}$	$0.0854_{\pm 4.6E-4}$	$0.1637_{\pm 9.5E-4}$	$0.3782_{\pm 5.6E-3}$	$0.3651_{\pm 9.0E\text{\_}3}$	$0.3508_{\pm 5.7E-3}$
	GLCPN	**$0.0721_{\pm 6.7E-5}$**	**$0.0971_{\pm 1.3E-3}$**	**$0.0763_{\pm 2.7E-4}$**	**$0.0749_{\pm 2.2E-4}$**	**$0.1595_{\pm 1.6E-4}$**	**$0.3686_{\pm 5.3E-3}$**	**$0.3422_{\pm 9.1E-3}$**	**$0.3286_{\pm 5.5E-3}$**
Epochs	**GLCPN-B**	$54_{\pm 8.15}$	$52_{\pm 12.60}$	**$71_{\pm 13.16}$**	**$89_{\pm 12.19}$**	$12_{\pm 1.33}$	$60_{\pm 8.57}$	$31_{\pm 1.26}$	$19_{\pm 1.96}$
	GLCPN-AT	**$42_{\pm 12.58}$**	**$37_{\pm 10.79}$**	$107_{\pm 8.14}$	$107_{\pm 10.57}$	$15_{\pm 0.89}$	$37_{\pm 3.08}$	**$12_{\pm 1.10}$**	**$9_{\pm 3.20}$**
	GLCPN	$50_{\pm 12.09}$	$56_{\pm 9.68}$	$75_{\pm 12.27}$	$146_{\pm 15.77}$	**$11_{\pm 0.75}$**	**$27_{\pm 6.31}$**	$20_{\pm 3.01}$	$12_{\pm 2.04}$
Time Cost Per Epoch	**GLCPN-B**	$35_{\pm 0.09}$	$22_{\pm 0.33}$	$29_{\pm 0.09}$	$15_{\pm 0.08}$	$0.96_{\pm 0.01}$	$0.24_{\pm 0.00}$	$1.09_{\pm 0.00}$	$2.13_{\pm 0.01}$
	GLCPN-AT	$183_{\pm 0.61}$	$109_{\pm 0.56}$	$107_{\pm 0.10}$	$56_{\pm 0.76}$	$3.55_{\pm 0.05}$	$0.97_{\pm 0.01}$	$3.56_{\pm 0.07}$	$6.85_{\pm 0.18}$
	GLCPN	**$35_{\pm 0.40}$**	**$22_{\pm 0.32}$**	**$29_{\pm 0.19}$**	**$15_{\pm 0.08}$**	**$0.96_{\pm 0.01}$**	**$0.24_{\pm 0.00}$**	**$1.09_{\pm 0.01}$**	**$2.13_{\pm 0.01}$**
Total Time Cost	**GLCPN-B**	$1923_{\pm 287.08}$	**$1172_{\pm 295.15}$**	**$2018_{\pm 369.88}$**	**$1312_{\pm 179.24}$**	$12_{\pm 1.19}$	$15_{\pm 2.21}$	$34_{\pm 1.28}$	$40_{\pm 4.12}$
	GLCPN-AT	$7626_{\pm 2289.23}$	$4053_{\pm 1191.31}$	$11493_{\pm 874.54}$	$5932_{\pm 611.35}$	$53_{\pm 2.80}$	$36_{\pm 0.03}$	$43_{\pm 3.22}$	$65_{\pm 22.74}$
	GLCPN	**$1744_{\pm 412.10}$**	$1242_{\pm 198.53}$	$2140_{\pm 340.74}$	$2137_{\pm 221.26}$	**$10_{\pm 0.75}$**	**$6_{\pm 1.47}$**	**$22_{\pm 3.36}$**	**$25_{\pm 4.41}$**

B stands for the binary adjacency matrix; and AT stands for the self-attention mechanism.

TABLE SXIII

THE RMSE OF GLCPN-S, GLCPN-SS, GLCPN-M, GLCPN-C, AND GLCPN ON D1-8.

No.	D1	D2	D3	D4	D5	D6	D7	D8
GLCPN-S	$0.1331_{\pm 9.1E-5}$	$0.1660_{\pm 2.4E-4}$	$0.1677_{\pm 8.5E-4}$	$0.1593_{\pm 6.8E-4}$	$0.4418_{\pm 7.4E-3}$	$0.7816_{\pm 2.6E-2}$	$0.8445_{\pm 5.0E-2}$	$0.8593_{\pm 5.8E-2}$
GLCPN-SS	$0.0866_{\pm 3.4E-5}$	$0.1220_{\pm 2.5E-4}$	$0.1168_{\pm 3.0E-4}$	$0.1161_{\pm 5.8E-4}$	$0.4443_{\pm 9.2E-3}$	$0.7780_{\pm 2.6E-2}$	$0.8453_{\pm 4.8E-2}$	$0.8593_{\pm 5.4E-2}$
GLCPN-M	$0.0845_{\pm 6.9E-5}$	$0.1216_{\pm 9.7E-5}$	$0.1128_{\pm 2.3E-4}$	$0.1139_{\pm 4.8E-4}$	$0.4297_{\pm 7.7E-3}$	$0.7690_{\pm 2.9E-2}$	$0.8276_{\pm 5.1E-2}$	$0.8396_{\pm 5.7E-2}$
GLCPN-C	$0.0864_{\pm 8.6E-5}$	$0.1230_{\pm 9.5E-5}$	$0.1200_{\pm 2.9E-4}$	$0.1191_{\pm 4.9E-4}$	$0.4378_{\pm 8.8E-3}$	$0.7912_{\pm 2.9E-2}$	$0.8392_{\pm 5.2E-2}$	$0.8492_{\pm 5.8E-2}$
GLCPN	**$0.0831_{\pm 5.0E-5}$**	**$0.1195_{\pm 3.9E-5}$**	**$0.1119_{\pm 3.6E-4}$**	**$0.1112_{\pm 4.3E-4}$**	**$0.4273_{\pm 8.1E-3}$**	**$0.7674_{\pm 2.9E-2}$**	**$0.8272_{\pm 5.2E-2}$**	**$0.8388_{\pm 5.7E-2}$**

S stands for that a model only outputs the single final layer; SS stands for that a model only outputs the final layer but with self-loop message propagation; M stands for that a model outputs the mean of all the layers; and C stands for that a model concatenates the feature transformation.

TABLE SXIV

THE MAE OF GLCPN-S, GLCPN-SS, GLCPN-M, GLCPN-C, AND GLCPN ON D1-8.

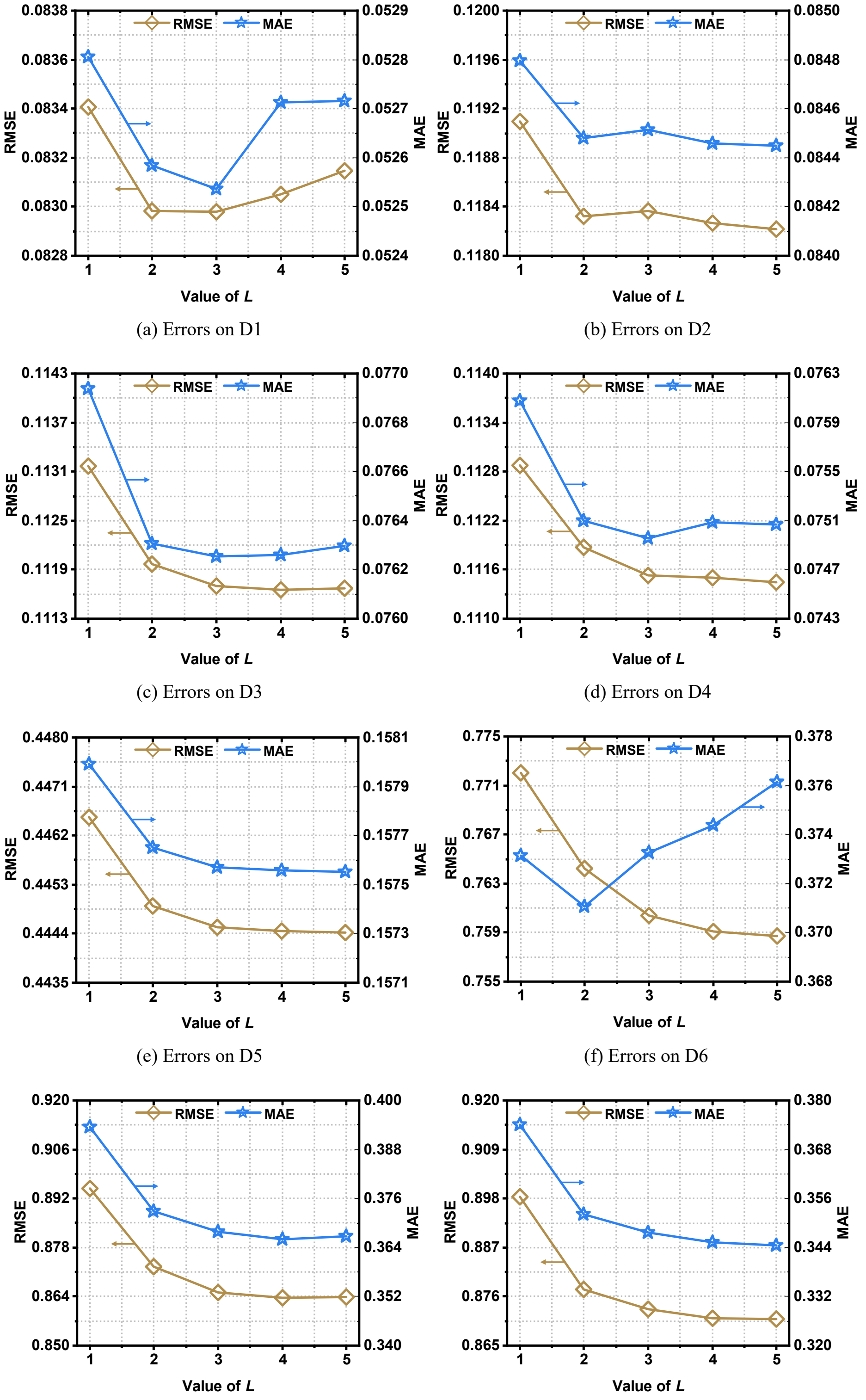
No.	D1	D2	D3	D4	D5	D6	D7	D8
GLCPN-S	$0.0909_{\pm 3.1E-4}$	$0.1187_{\pm 7.3E-4}$	$0.1152_{\pm 1.9E-3}$	$0.1123_{\pm 5.0E-4}$	$0.1812_{\pm 1.1E-3}$	$0.3905_{\pm 4.8E-3}$	$0.3705_{\pm 8.5E-3}$	$0.3594_{\pm 5.5E-3}$
GLCPN-SS	$0.0565_{\pm 7.2E-5}$	$0.0872_{\pm 7.8E-5}$	$0.0821_{\pm 1.8E-4}$	$0.0801_{\pm 2.4E-4}$	$0.1777_{\pm 1.7E-3}$	$0.3844_{\pm 7.2E-3}$	$0.3621_{\pm 5.6E-3}$	$0.3513_{\pm 1.2E-2}$
GLCPN-M	$0.0548_{\pm 6.3E-5}$	$0.0875_{\pm 7.7E-5}$	$0.0794_{\pm 1.7E-4}$	$0.0782_{\pm 2.0E-4}$	$0.1647_{\pm 6.7E-4}$	$0.3694_{\pm 6.0E-3}$	$0.3454_{\pm 8.9E-3}$	$0.3330_{\pm 5.3E-3}$
GLCPN-C	$0.0562_{\pm 8.0E-5}$	$0.0889_{\pm 8.6E-5}$	$0.0853_{\pm 1.8E-4}$	$0.0826_{\pm 2.6E-4}$	$0.1671_{\pm 1.1E-3}$	$0.3820_{\pm 5.4E-3}$	$0.3497_{\pm 8.8E-3}$	$0.3358_{\pm 5.4E-3}$
GLCPN	**$0.0527_{\pm 6.0E-5}$**	**$0.0857_{\pm 3.0E-5}$**	**$0.0763_{\pm 2.7E-4}$**	**$0.0749_{\pm 2.2E-4}$**	**$0.1595_{\pm 1.6E-4}$**	**$0.3686_{\pm 5.3E-3}$**	**$0.3422_{\pm 9.1E-3}$**	**$0.3286_{\pm 5.5E-3}$**

S stands for that a model only outputs the single final layer; SS stands for that a model only outputs the final layer but with self-loop message propagation; M stands for that a model outputs the mean of all the layers; and C stands for that a model concatenates the feature transformation.

III. SUPPLEMENTARY TABLES

The hyperparameter sensitivity test results have been drawn in Figs. S1-6, which are discussed in Section V.C. Their details are described as follows:

- Figs. **S1-2** plot the errors and epochs of GLCPN as L varies;
- Figs. **S3-4** plot the errors and epochs of GLCPN as K varies;
- Figs. **S5-6** plot the errors and epochs of GLCPN as α varies.



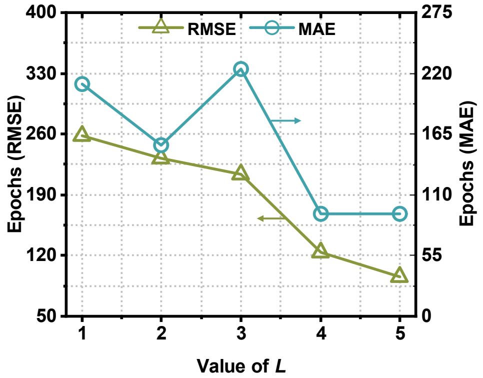
(a) Errors on D1 (b) Errors on D2

(c) Errors on D3 (d) Errors on D4

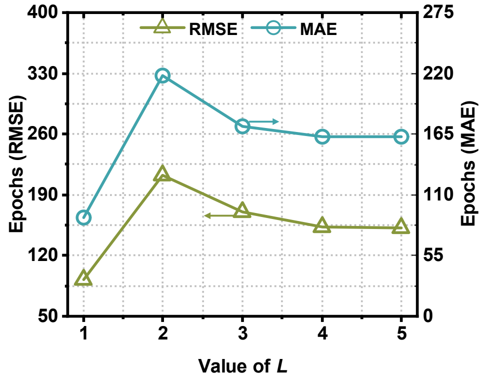
(e) Errors on D5 (f) Errors on D6

(g) Errors on D7 (h) Errors on D8

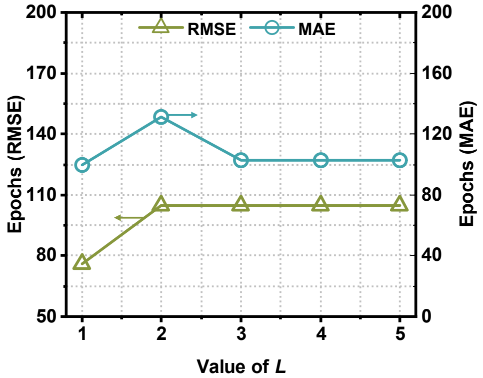
Fig. S1. Errors of GLCPN as L varies while other hyperparameters are being fixed on D1-8.



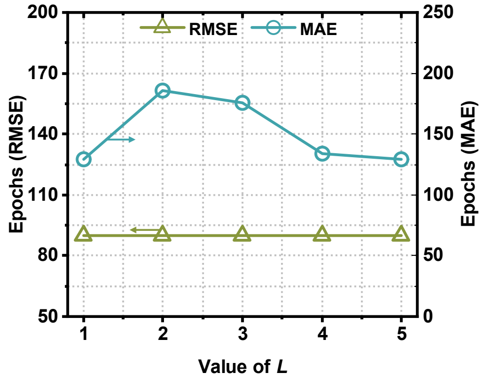
(a) Epochs on D1



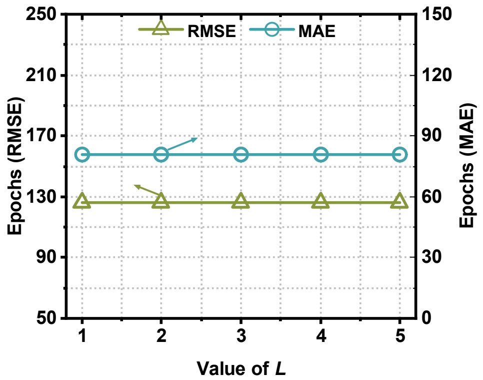
(b) Epochs on D2



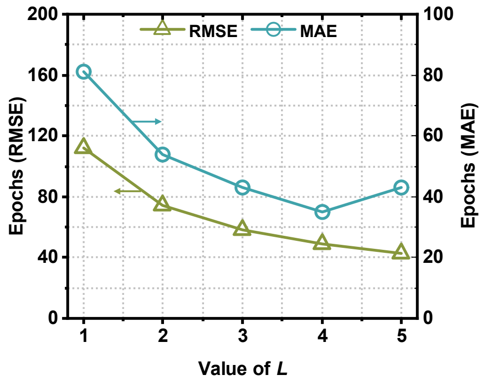
(c) Epochs on D3



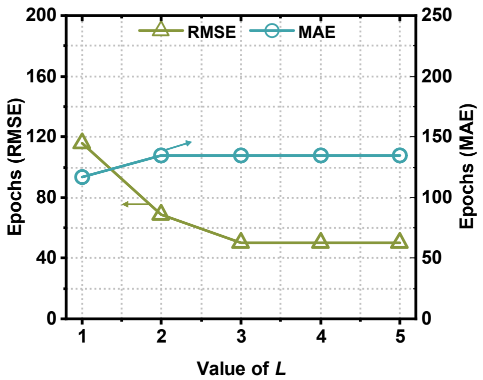
(d) Epochs on D4



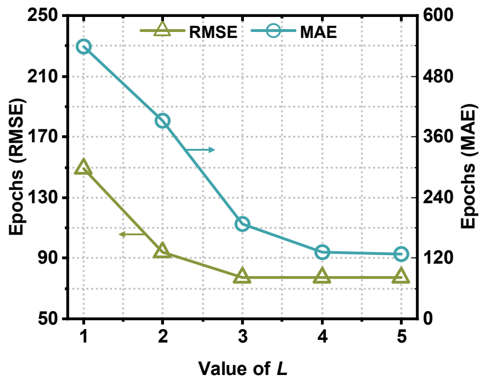
(e) Epochs on D5



(f) Epochs on D6

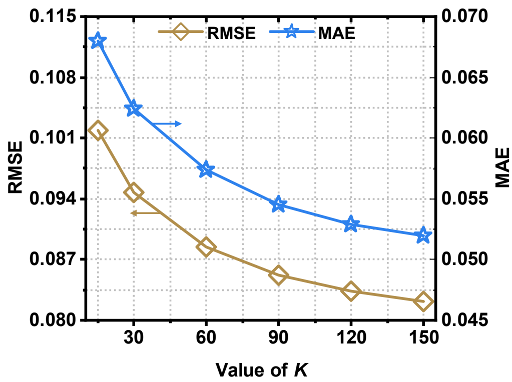


(g) Epochs on D7

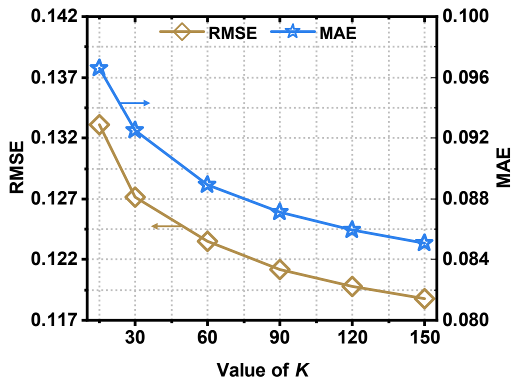


(h) Epochs on D8

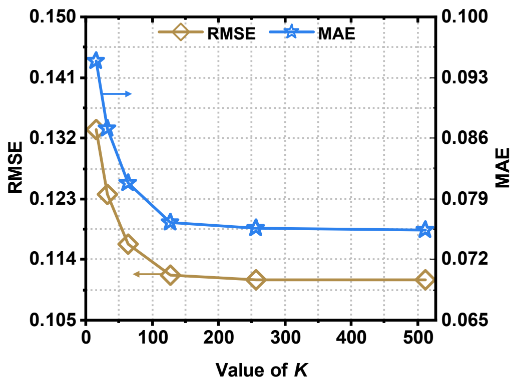
Fig. S2. Training epochs of GLCPN as L varies while other hyperparameters are being fixed on D1-8.



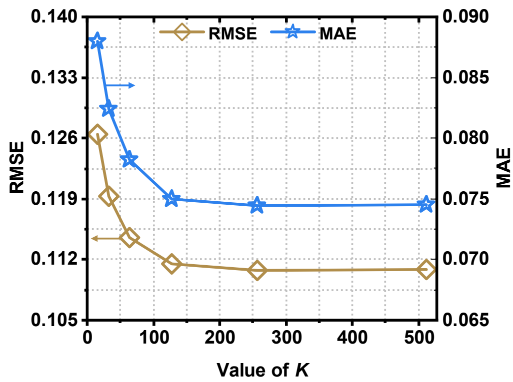
(a) Errors on D1



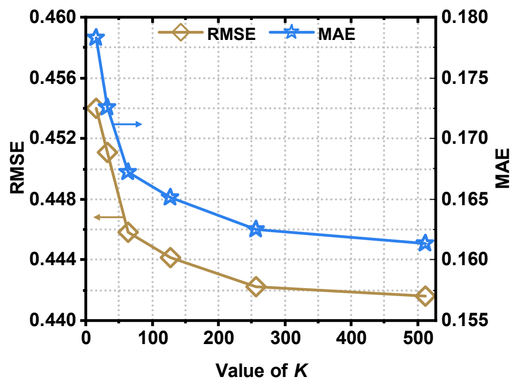
(b) Errors on D2



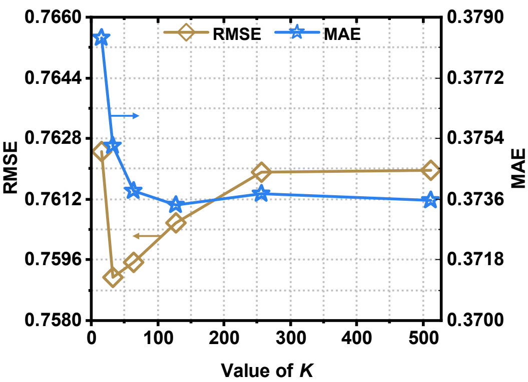
(c) Errors on D3



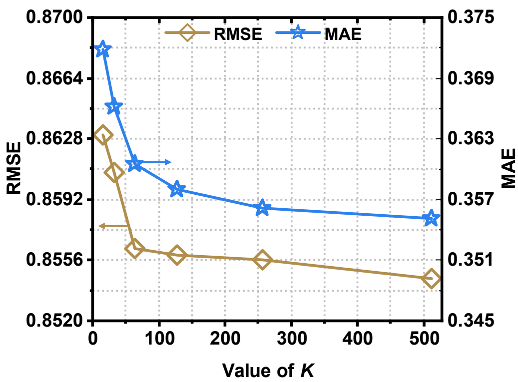
(d) Errors on D4



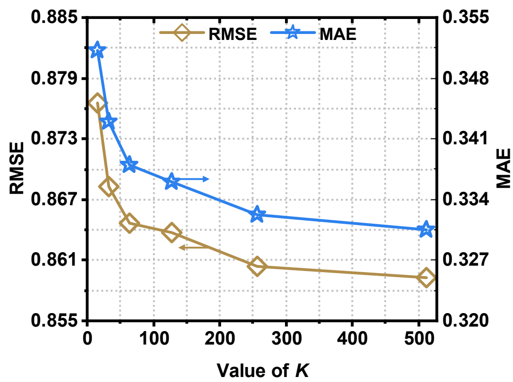
(e) Errors on D5



(f) Errors on D6

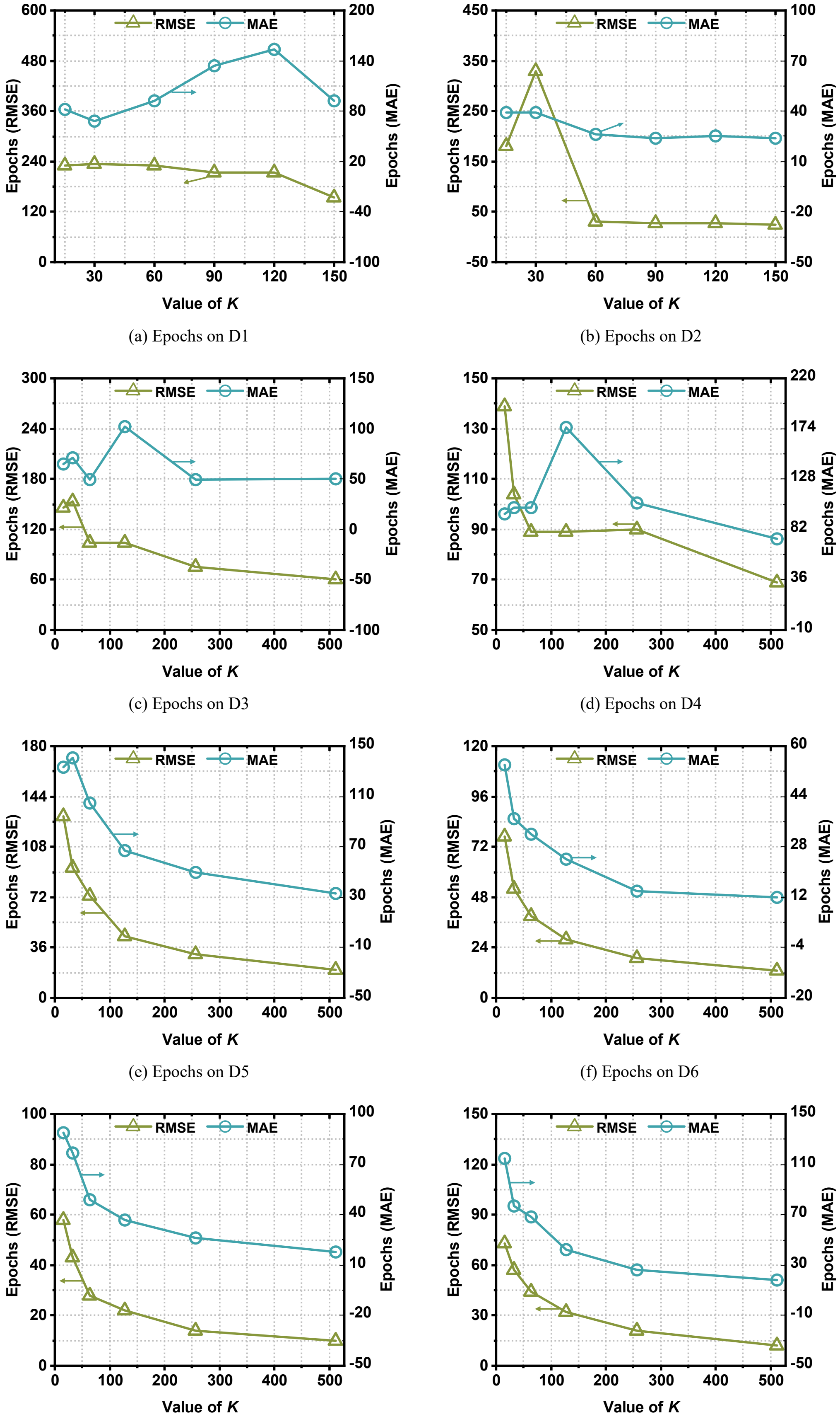


(g) Errors on D7



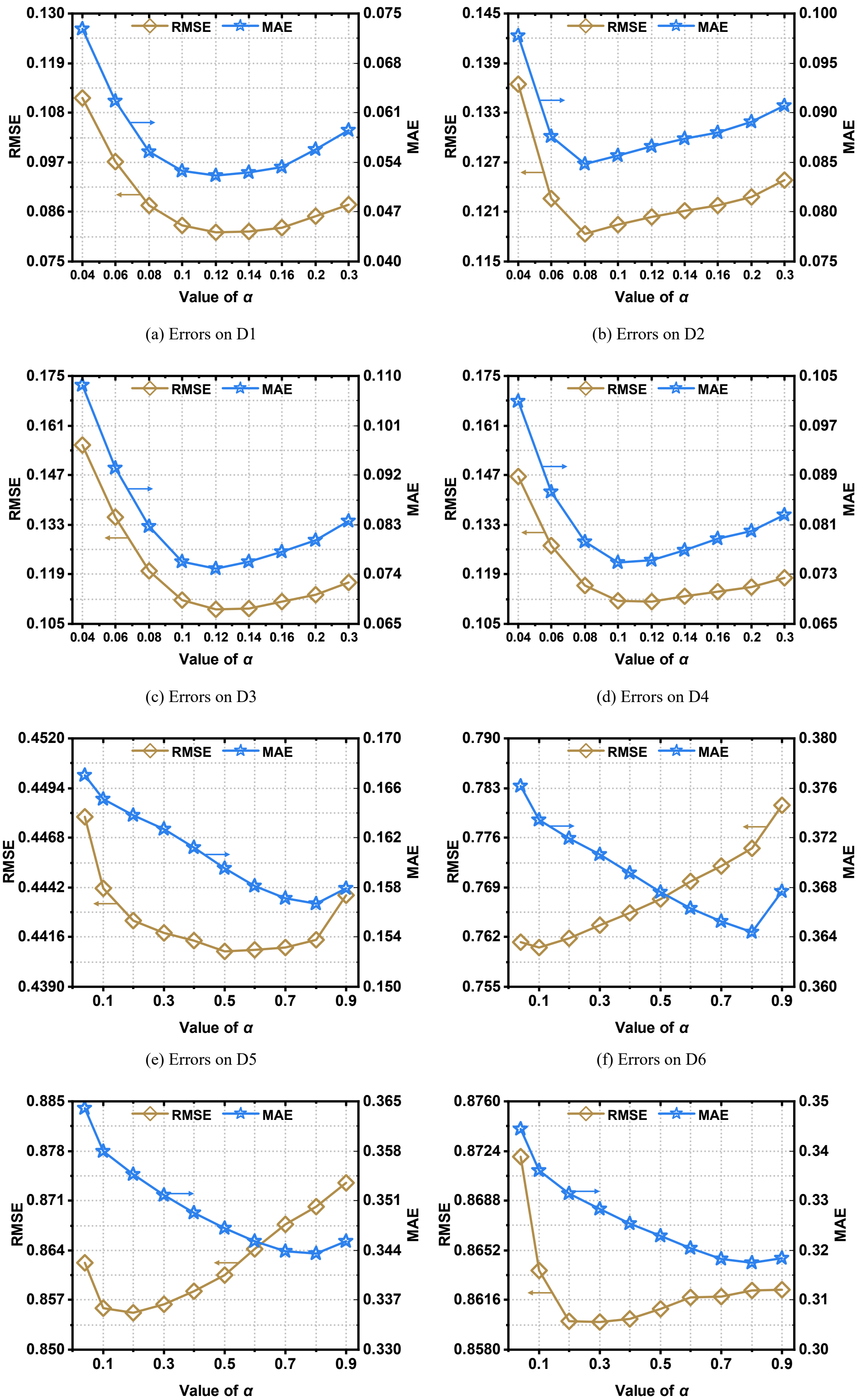
(h) Errors on D8

Fig. S3. Errors of GLCPN as *K* varies while other hyperparameters are being fixed on D1-8.



(a) Epochs on D1
(b) Epochs on D2
(c) Epochs on D3
(d) Epochs on D4
(e) Epochs on D5
(f) Epochs on D6
(g) Epochs on D7
(h) Epochs on D8

Fig. S4. Training epochs of GLCPN as *K* varies while other hyperparameters are being fixed on D1-8.



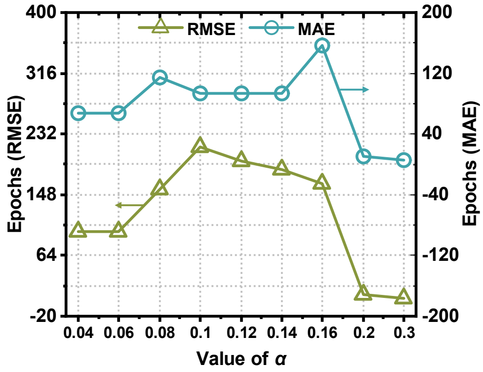
(a) Errors on D1 (b) Errors on D2

(c) Errors on D3 (d) Errors on D4

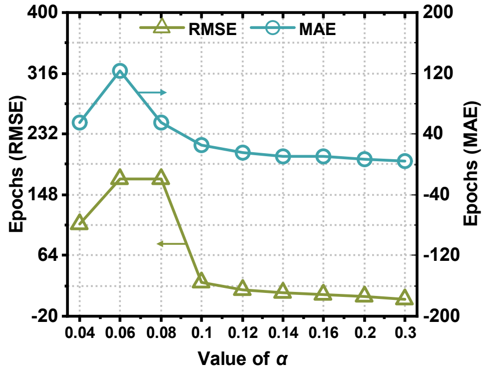
(e) Errors on D5 (f) Errors on D6

(g) Errors on D7 (h) Errors on D8

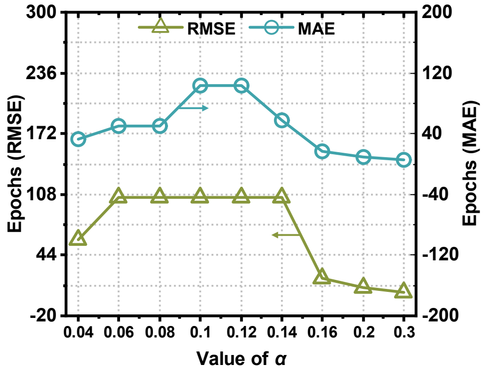
Fig. S5. Errors of GLCPN as α varies while other hyperparameters are being fixed on D1-8.



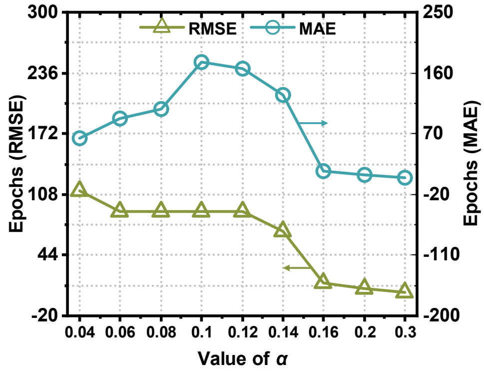
(a) Epochs on D1



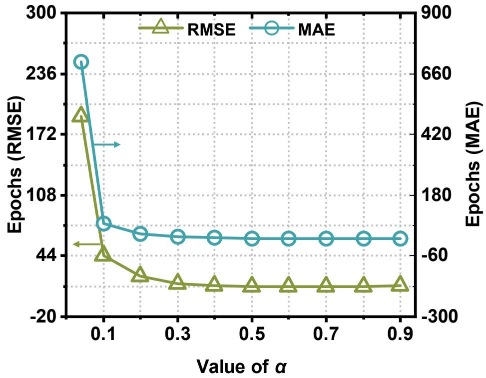
(b) Epochs on D2



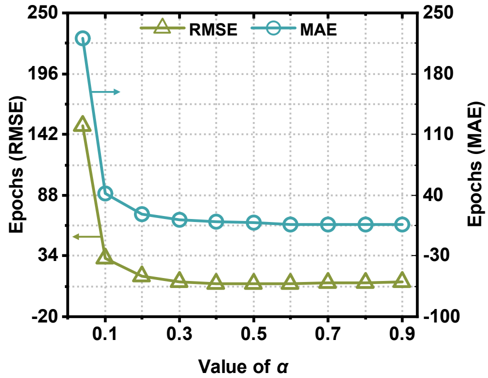
(c) Epochs on D3



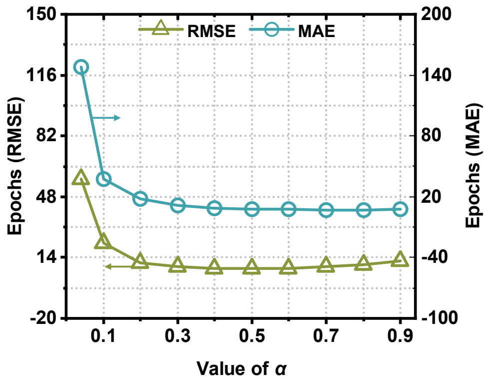
(d) Epochs on D4



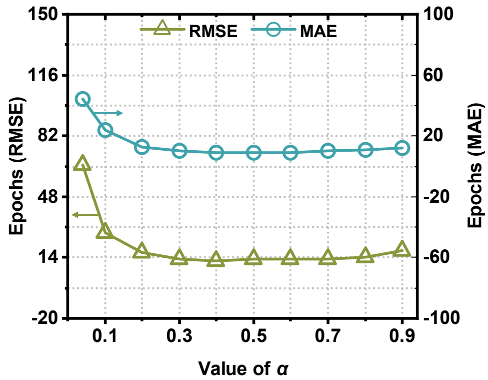
(e) Epochs on D5



(f) Epochs on D6



(g) Epochs on D7



(h) Epochs on D8

Fig. S6. Training epochs of GLCPN as α varies while other hyperparameters are being fixed on D1-8.