## I. Supplementary for Convergence and Performance

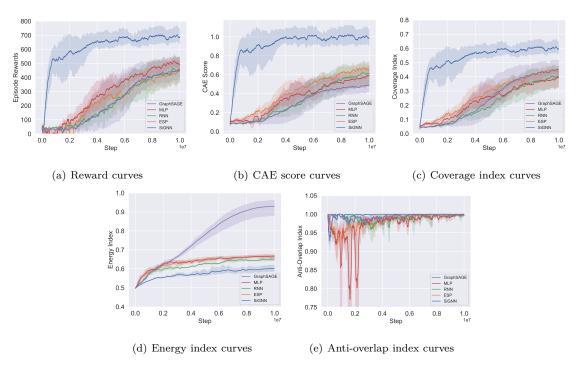


Fig. 1. The curves of rewards, CAE scores and corresponding indexes for scenario with global observation.

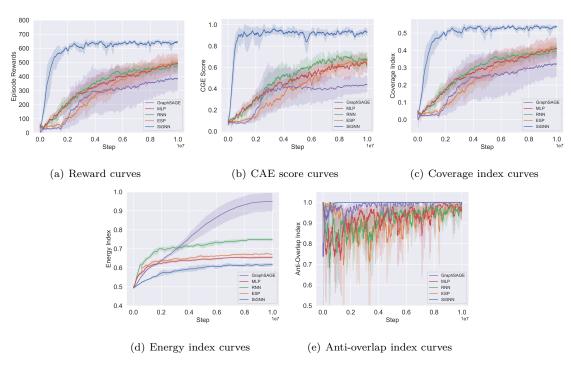


Fig. 2. The curves of rewards, CAE scores and corresponding indexes for scenario with  $R_{\rm obs}=70.$ 

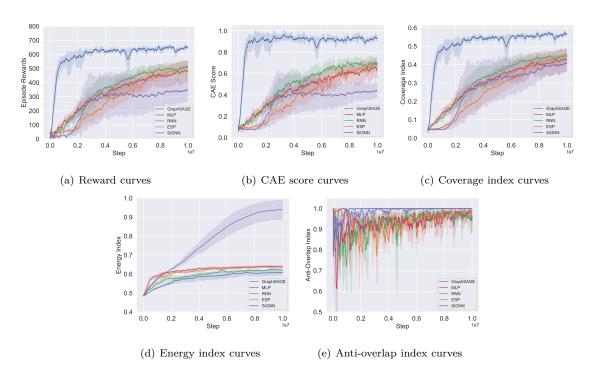


Fig. 3. The curves of rewards, CAE scores and corresponding indexes for scenario with  $R_{\rm obs}=50.$ 

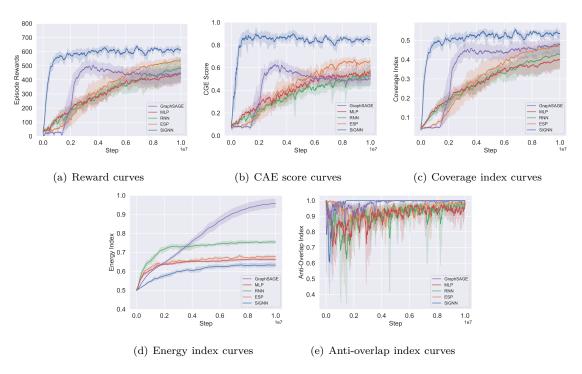


Fig. 4. The curves of rewards, CAE scores and corresponding indexes for scenario with  $R_{\rm obs}=30.$ 

## II. Supplementary for Comparison among Learning-based Approaches

 $\label{eq:TABLEI} \mbox{TABLE I}$  Metric Performance under Global Observation

Algorithm	CAE Score	Coverage Index	Energy Index	Anti-Overlap Index
GraphSAGE	$0.4861 \pm 0.1105$	$0.4495 \pm 0.0716$	$0.9299 \pm 0.0543$	$0.3998 \pm 0.0979$
MLP	$0.5866 \pm 0.1165$	$0.3921 \pm 0.0759$	$0.6632 \pm 0.0111$	$0.9975 \pm 0.0027$
RNN	$0.6129 \pm 0.1552$	$0.3998 \pm 0.0979$	$0.6478 \pm 0.0084$	$0.9972 \pm 0.0027$
ESP	$0.6428 \pm 0.0739$	$0.4332 \pm 0.0488$	$0.6689 \pm 0.0119$	$0.9883 \pm 0.0028$
$\operatorname{SiGNN}$	$\bf 0.9852 \pm 0.1104$	$\bf 0.5947 \pm 0.0563$	$0.6008 \pm 0.0209$	$0.9999 \pm 0.0001$

 $\label{eq:table_II} \text{Metric Performance under } R_{\text{obs}} = 70$ 

Algorithm	CAE Score	Coverage Index	Energy Index	Anti-Overlap Index
GraphSAGE	$0.4379 \pm 0.0893$	$0.3220 \pm 0.0893$	$0.9505 \pm 0.0579$	$0.9895 \pm 0.0235$
MLP	$0.6213 \pm 0.0936$	$0.4121 \pm 0.0741$	$0.6551 \pm 0.0054$	$0.9816 \pm 0.0257$
RNN	$0.6817 \pm 0.0810$	$0.4032 \pm 0.0355$	$0.7479 \pm 0.0079$	$0.9602 \pm 0.0498$
ESP	$0.6363 \pm 0.0471$	$0.4024 \pm 0.0355$	$0.6713 \pm 0.0017$	$0.9511 \pm 0.0490$
SiGNN	$0.8728 \pm 0.0376$	$0.5380 \pm 0.0078$	$0.6164 \pm 0.0097$	$1.0000 \pm 0.0000$

 $\label{eq:table_interpolation} \text{TABLE III}$  Metric Performance under  $R_{\text{obs}} = 50$ 

Algorithm	CAE Score	Coverage Index	Energy Index	Anti-Overlap Index
GraphSAGE	$0.4379 \pm 0.0893$	$0.4065 \pm 0.0537$	$0.9387 \pm 0.0645$	$0.9985 \pm 0.0015$
MLP	$0.6313 \pm 0.0936$	$0.4304 \pm 0.0752$	$0.6382 \pm 0.0084$	$0.9420 \pm 0.0673$
RNN	$0.7017 \pm 0.0810$	$0.4529 \pm 0.0528$	$0.6208 \pm 0.0047$	$0.9635 \pm 0.0528$
ESP	$0.6663 \pm 0.0471$	$0.4439 \pm 0.0142$	$0.6373 \pm 0.0053$	$0.9572 \pm 0.0691$
SiGNN	$0.9313 \pm 0.0376$	$0.5655 \pm 0.0109$	$0.6078 \pm 0.0181$	$1.0000 \pm 0.0000$

 $\label{eq:table_interpolation} \text{TABLE IV}$  Metric Performance under  $R_{\text{obs}} = 30$ 

Algorithm	CAE Score	Coverage Index	Energy Index	Anti-Overlap Index
${\bf GraphSAGE}$	$0.4997 \pm 0.0619$	$0.4802 \pm 0.0523$	$0.9562 \pm 0.0274$	$0.9932 \pm 0.0150$
MLP	$0.5201 \pm 0.0887$	$0.4001 \pm 0.0613$	$0.6631 \pm 0.0090$	$0.9794 \pm 0.0245$
RNN	$0.5340 \pm 0.1114$	$0.4269 \pm 0.0794$	$0.7542 \pm 0.0097$	$0.9760 \pm 0.0218$
ESP	$0.6587 \pm 0.0442$	$0.4713 \pm 0.0287$	$0.6769 \pm 0.0085$	$0.9891 \pm 0.0157$
SiGNN	$\bf 0.8444 \pm 0.0286$	$0.5340 \pm 0.0197$	$\bf 0.6324 \pm 0.0143$	$1.0000 \pm 0.0000$

## III. Supplementary for Scalability

 $\label{eq:table_V} \text{TABLE V}$  Scalability Performance under Partial Observation  $R_{\text{obs}} = 70$ 

Number	Steps	EGNN	MLP	RNN	ESP	Graphsage
	300k	$607.38\pm14.71$	$293.33 \pm 25.42$	$311.68 \pm 44.21$	$208.59 \pm 39.30$	$268.24 \pm 38.50$
5	1000k	$667.62 \pm 23.57$	$474.58 \pm 42.24$	$498.68 \pm 39.93$	$507.34 \pm 34.14$	$394.69 \pm 54.24$
10	300k	$424.53 \pm 19.85$	$7.83 \pm 38.26$	$37.69 \pm 38.89$	$7.57 \pm 31.23$	$-36.17 \pm 43.52$
10	1000k	$488.82 \pm 24.14$	$95.46 \pm 55.96$	$101.78 \pm 42.95$	$86.08 \pm 67.34$	$-335.17 \pm 88.26$
15	300k	$246.75 \pm 27.47$	$-245.42 \pm 32.58$	$-310.77 \pm 52.13$	$-92.52 \pm 35.62$	$-256.23 \pm 67.32$
15	1000k	$268.82 \pm 35.52$	$-81.04 \pm 52.62$	$26.52 \pm 58.76$	$24.56 \pm 67.73$	$-491.34 \pm 74.36$
20	300k	$35.77 \pm 63.15$	$-452.94 \pm 44.52$	$-295.15 \pm 38.46$	$-378.42 \pm 82.74$	$-378.18 \pm 62.52$
	1000k	$141.87 \pm 67.32$	$-623.17 \pm 50.70$	$-56.64 \pm 62.10$	$-174.42 \pm 104.42$	$-876.13 \pm 124.33$

 $\label{eq:table_VI} \text{TABLE VI}$  Scalability Performance under Partial Observation  $R_{\text{obs}} = 50$ 

Number	Steps	EGNN	MLP	RNN	ESP	Graphsage
_	300k	$619.76 \pm 26.43$	$286.22 \pm 32.60$	$331.68 \pm 44.21$	$198.59 \pm 29.30$	$288.24 \pm 38.50$
5	1000k	$649.61 \pm 26.11$	$489.38 \pm 52.24$	$517.68 \pm 29.90$	$501.34 \pm 34.14$	$364.69 \pm 54.24$
10	300k	$378.06 \pm 23.45$	$39.84\pm38.26$	$53.41 \pm 38.89$	$-6.62 \pm 51.92$	$-6.57 \pm 54.14$
10	1000k	$462.59 \pm 33.42$	$75.71 \pm 55.96$	$90.77\pm49.17$	$83.47 \pm 48.53$	$-235.17 \pm 78.42$
15	300k	$235.31 \pm 31.50$	$-202.66 \pm 41.68$	$-214.55 \pm 44.50$	$-104.39 \pm 67.43$	$-144.95 \pm 87.31$
15	1000k	$226.83 \pm 41.22$	$-58.44 \pm 60.13$	$43.01\pm69.55$	$55.68 \pm 41.77$	$-526.73 \pm 93.47$
20	300k	$50.68 \pm 37.32$	$-322.46 \pm 84.61$	$-336.59 \pm 52.36$	$-426.25 \pm 76.15$	$-558.18 \pm 95.12$
	1000k	$122.14 \pm 57.21$	$-378.82 \pm 76.32$	$-78.14 \pm 82.23$	$-118.54 \pm 45.50$	$-943.23 \pm 154.33$

 $\mbox{TABLE VII}$  Scalability Performance under Partial Observation  $R_{\rm obs}=30$ 

Number	Steps	EGNN	MLP	RNN	ESP	Graphsage
_	300k	$593.12 \pm 35.78$	$254.56 \pm 53.27$	$243.58 \pm 43.12$	$231.88 \pm 78.74$	$488.32 \pm 57.96$
5	1000k	$615.26 \pm 25.73$	$453.71 \pm 51.92$	$472.88 \pm 40.56$	$543.24 \pm 43.25$	$439.74 \pm 75.27$
10	300k	$394.88 \pm 32.12$	$43.83 \pm 47.59$	$49.99 \pm 39.24$	$34.98 \pm 62.81$	$-62.13 \pm 53.34$
10	1000k	$411.17 \pm 28.45$	$101.43 \pm 66.78$	$117.37 \pm 82.61$	$66.57 \pm 37.48$	$-171.87 \pm 69.14$
15	300k	$160.62 \pm 30.67$	$-215.73 \pm 50.45$	$-112.4 \pm 45.12$	$-154.59 \pm 68.34$	$-96.49 \pm 58.23$
15	1000k	$259.82 \pm 27.54$	$-141.24 \pm 59.87$	$20.05 \pm 70.29$	$23.09\pm40.12$	$-486.23 \pm 74.36$
20	300k	$70.93 \pm 46.78$	$-357.58 \pm 45.21$	$-278.35 \pm 53.87$	$-336.45 \pm 55.34$	$-376.38 \pm 62.78$
	1000k	$125.62 \pm 29.45$	$-288.76 \pm 51.34$	$-16.24 \pm 61.25$	$-78.34 \pm 86.12$	$-683.23 \pm 73.29$