Supplementary Information for "*A Multitask Network Robustness Analysis System Based on the Graph Isomorphism Network Model*"

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I. Abbreviations

Abbreviations of Algorithms:

GIN-MAS: Graph Isomorphism Network-based Multitask Analysis System
LFR [1]: Learning Feature Representation
RP [2]: Robustness Predictor
SPP [3]: Spatial Pyramid Pooling
GCN [4]: Graph Convolutional Network
MLP: Multi-Layer Perceptron
KNN [5]: k-Nearest Neighbours
LR [6]: Linear Regression
DT [7]: Decision Tree
RF [8]: Random Forest

Abbreviations of Attack Strategies:

TAR: maximum degree-TARgeted node-removal attack
RND: Random NoDe-removal attack

II. Tables: Comparison on Nine Synthetic Networks

Tables S1–S9 show prediction errors obtained by GIN-MAS, LFR, RP, SPP, GCN, MLP, KNN, LR, DT, and RF, on nine synthetic networks. An integer in parentheses indicates the rank of the method for robustness measure; an asterisk '*' denotes that the corresponding method is statistically inferior to GIN-MAS, while an approximation '≈' indicates no statistical difference between the corresponding method and GIN-MAS, according to the Kruskal-Wallis H-test.

Table S1: For BA (Barabási–Albert) networks.

BA (*:69; ≈:3)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.012 (1)	0.039 (5,*)	0.070 (8,*)	0.043 (7,*)	0.130 (10,*)	0.043 (6,*)	0.034 (4,*)	0.091 (9,*)	0.033 (3,*)	0.029 (2,*)
		RND	0.015 (1)	0.020 (2,*)	0.046 (9,*)	0.027 (3,*)	0.071 (10,*)	0.037 (6,*)	0.036 (5,*)	0.044 (8,*)	0.038 (7,*)	0.031 (4,*)
	Connectivity Robustness	TAR	0.024 (1)	0.047 (4,*)	0.075 (8,*)	0.049 (5,*)	0.190 (9,*)	0.064 (7,*)	0.051 (6,*)	0.221 (10,*)	0.043 (3,*)	0.041 (2,*)
		RND	0.016 (1)	0.025 (7,*)	0.119 (9,*)	0.026 (8,*)	0.213 (10,*)	0.020 (4,*)	0.020 (3,*)	0.024 (6,*)	0.022 (5,*)	0.018 (2,≈)
Directed	Controllability Robustness	TAR	0.014 (1)	0.025 (2,*)	0.091 (4,*)	0.043 (3,*)	0.111 (6,*)	0.102 (5,*)	0.125 (7,*)	0.128 (8,*)	0.209 (10,*)	0.192 (9,*)
		RND	0.015 (1)	0.025 (2,*)	0.077 (8,*)	0.030 (3,*)	0.091 (10,*)	0.056 (6,*)	0.055 (5,*)	0.043 (4,*)	0.086 (9,*)	0.075 (7,*)
	Connectivity Robustness	TAR	0.024 (1)	0.059 (3,*)	0.065 (4,*)	0.046 (2,*)	0.246 (8,*)	0.136 (5,*)	0.139 (6,*)	0.193 (7,*)	0.267 (10,*)	0.261 (9,*)
		RND	0.017 (1)	0.020 (4,*)	0.120 (9,*)	0.034 (7,*)	0.223 (10,*)	0.021 (5,*)	0.018 (3,≈)	0.041 (8,*)	0.023 (6,*)	0.018 (2,≈)

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Table S2: For EH (extreme homogeneous) networks.

EH (*:59; ≈:10; +:3)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.009 (1)	0.011 (2,*)	0.054 (4,*)	0.045 (3,*)	0.073 (5,*)	0.090 (6,*)	0.104 (7,*)	0.161 (10,*)	0.140 (9,*)	0.140 (8,*)
		RND	0.008 (1)	0.009 (2,≈)	0.020 (4,*)	0.017 (3,*)	0.030 (7,*)	0.022 (5,*)	0.029 (6,*)	0.041 (10,*)	0.031 (9,*)	0.030 (8,*)
	Connectivity Robustness	TAR	0.016 (1)	0.106 (3,*)	0.138 (6,*)	0.057 (2,*)	0.271 (10,*)	0.123 (4,*)	0.136 (5,*)	0.196 (9,*)	0.169 (7,*)	0.177 (8,*)
		RND	0.016 (1)	0.023 (3,*)	0.121 (9,*)	0.019 (2,*)	0.227 (10,*)	0.024 (4,*)	0.033 (5,*)	0.033 (6,*)	0.037 (8,*)	0.034 (7,*)
Directed	Controllability Robustness	TAR	0.010 (4)	0.010 (2,≈)	0.118 (9,*)	0.073 (8,*)	0.052 (7,*)	0.026 (6,*)	0.009 (1,+)	0.131 (10,*)	0.013 (5,*)	0.010 (3,≈)
		RND	0.009 (3)	0.010 (4,≈)	0.050 (9,*)	0.028 (7,*)	0.034 (8,*)	0.017 (6,*)	0.009 (2,≈)	0.084 (10,*)	0.012 (5,*)	0.009 (1,≈)
	Connectivity Robustness	TAR	0.013 (3)	0.111 (7,*)	0.118 (8,*)	0.058 (6,*)	0.270 (10,*)	0.048 (5,*)	0.010 (1,+)	0.170 (9,*)	0.015 (4,≈)	0.012 (2,+)
		RND	0.015 (3)	0.016 (4,≈)	0.126 (9,*)	0.023 (7,*)	0.231 (10,*)	0.022 (6,*)	0.015 (2,≈)	0.034 (8,*)	0.020 (5,*)	0.015 (1,≈)

Table S3: For ER (Erdös-Rényi) networks.

ER (*:65; ≈:6; +:1)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.009 (1)	0.020 (3,*)	0.060 (9,*)	0.047 (8,*)	0.062 (10,*)	0.019 (2,*)	0.026 (5,*)	0.045 (7,*)	0.041 (6,*)	0.023 (4,*)
		RND	0.010 (1)	0.011 (3,*)	0.022 (9,*)	0.013 (6,*)	0.040 (10,*)	0.011 (2,≈)	0.012 (4,≈)	0.021 (8,*)	0.019 (7,*)	0.013 (5,*)
	Connectivity Robustness	TAR	0.021 (1)	0.087 (7,*)	0.130 (9,*)	0.083 (6,*)	0.226 (10,*)	0.048 (3,*)	0.053 (4,*)	0.095 (8,*)	0.067 (5,*)	0.048 (2,*)
		RND	0.016 (1)	0.023 (6,*)	0.114 (9,*)	0.022 (5,*)	0.215 (10,*)	0.019 (2,*)	0.021 (3,*)	0.024 (7,*)	0.027 (8,*)	0.022 (4,*)
Directed	Controllability Robustness	TAR	0.014 (1)	0.018 (2,*)	0.074 (10,*)	0.052 (7,*)	0.060 (9,*)	0.036 (4,*)	0.041 (5,*)	0.034 (3,*)	0.057 (8,*)	0.050 (6,*)
		RND	0.013 (1)	0.019 (3,*)	0.048 (9,*)	0.029 (7,*)	0.051 (10,*)	0.016 (2,*)	0.020 (4,*)	0.035 (8,*)	0.026 (6,*)	0.022 (5,*)
	Connectivity Robustness	TAR	0.025 (2)	0.091 (7,*)	0.117 (9,*)	0.052 (5,*)	0.244 (10,*)	0.050 (4,*)	0.052 (6,*)	0.098 (8,*)	0.028 (3,≈)	0.023 (1,+)
		RND	0.017 (2)	0.018 (3,≈)	0.118 (9,*)	0.020 (5,*)	0.223 (10,*)	0.021 (6,*)	0.019 (4,≈)	0.040 (8,*)	0.022 (7,*)	0.017 (1,≈)

Table S4: For QS (q-snapback) networks.

QS (*:63; ≈:8; +:1)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.009 (1)	0.017 (2,*)	0.028 (7,*)	0.021 (6,*)	0.056 (10,*)	0.019 (3,*)	0.021 (5,*)	0.044 (9,*)	0.040 (8,*)	0.019 (4,*)
		RND	0.009 (1)	0.010 (4,≈)	0.020 (8,*)	0.012 (6,*)	0.036 (10,*)	0.011 (5,*)	0.010 (3,≈)	0.028 (9,*)	0.013 (7,*)	0.010 (2,≈)
	Connectivity Robustness	TAR	0.017 (1)	0.088 (8,*)	0.102 (9,*)	0.030 (4,*)	0.233 (10,*)	0.033 (5,*)	0.023 (2,≈)	0.085 (7,*)	0.035 (6,*)	0.024 (3,*)
		RND	0.016 (1)	0.023 (7,*)	0.117 (9,*)	0.020 (5,*)	0.219 (10,*)	0.019 (2,*)	0.020 (3,*)	0.022 (6,*)	0.027 (8,*)	0.020 (4,*)
Directed	Controllability Robustness	TAR	0.013 (1)	0.016 (2,*)	0.055 (6,*)	0.029 (3,*)	0.080 (10,*)	0.052 (5,*)	0.058 (7,*)	0.051 (4,*)	0.076 (9,*)	0.071 (8,*)
		RND	0.015 (1)	0.017 (2,*)	0.055 (5,*)	0.019 (3,*)	0.076 (10,*)	0.067 (7,*)	0.066 (6,*)	0.054 (4,*)	0.075 (9,*)	0.072 (8,*)
	Connectivity Robustness	TAR	0.023 (1)	0.109 (9,*)	0.100 (8,*)	0.035 (2,*)	0.283 (10,*)	0.054 (4,*)	0.062 (6,*)	0.088 (7,*)	0.053 (3,*)	0.054 (5,*)
		RND	0.021 (2)	0.021 (4,≈)	0.122 (9,*)	0.021 (3,≈)	0.250 (10,*)	0.023 (5,≈)	0.020 (1,+)	0.040 (8,*)	0.030 (7,*)	0.023 (6,≈)

Table S5: For RH (random hexagon) networks.

RH (*:69; ≈:3)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.008 (1)	0.019 (2,*)	0.034 (4,*)	0.027 (3,*)	0.062 (9,*)	0.050 (5,*)	0.050 (6,*)	0.101 (10,*)	0.056 (8,*)	0.054 (7,*)
		RND	0.010 (1)	0.012 (2,*)	0.022 (8,*)	0.014 (3,*)	0.041 (9,*)	0.016 (6,*)	0.016 (5,*)	0.058 (10,*)	0.018 (7,*)	0.016 (4,*)
	Connectivity Robustness	TAR	0.021 (1)	0.080 (7,*)	0.089 (8,*)	0.045 (2,*)	0.220 (10,*)	0.074 (6,*)	0.051 (3,*)	0.128 (9,*)	0.056 (5,*)	0.055 (4,*)
		RND	0.015 (1)	0.023 (5,*)	0.115 (9,*)	0.024 (6,*)	0.211 (10,*)	0.023 (4,*)	0.021 (3,*)	0.025 (7,*)	0.027 (8,*)	0.021 (2,*)
Directed	Controllability Robustness	TAR	0.012 (1)	0.014 (2,*)	0.059 (4,*)	0.033 (3,*)	0.085 (5,*)	0.102 (7,*)	0.100 (6,*)	0.115 (10,*)	0.109 (8,*)	0.113 (9,*)
		RND	0.012 (1)	0.013 (2,≈)	0.045 (9,*)	0.018 (3,*)	0.049 (10,*)	0.022 (4,*)	0.025 (5,*)	0.030 (6,*)	0.034 (8,*)	0.030 (7,*)
	Connectivity Robustness	TAR	0.025 (1)	0.084 (3,*)	0.085 (4,*)	0.046 (2,*)	0.280 (10,*)	0.122 (8,*)	0.089 (5,*)	0.135 (9,*)	0.091 (6,*)	0.092 (7,*)
		RND	0.018 (2)	0.017 (1,≈)	0.118 (9,*)	0.020 (3,≈)	0.221 (10,*)	0.023 (5,*)	0.022 (4,*)	0.033 (8,*)	0.029 (7,*)	0.025 (6,*)

Table S6: For RT (random triangle) networks.

RT (*:72)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.010 (1)	0.026 (2,*)	0.045 (4,*)	0.029 (3,*)	0.080 (10,*)	0.067 (9,*)	0.053 (7,*)	0.061 (8,*)	0.051 (6,*)	0.048 (5,*)
		RND	0.011 (1)	0.014 (2,*)	0.025 (9,*)	0.016 (3,*)	0.043 (10,*)	0.021 (6,*)	0.021 (5,*)	0.023 (8,*)	0.023 (7,*)	0.020 (4,*)
	Connectivity Robustness	TAR	0.023 (1)	0.065 (3,*)	0.088 (4,*)	0.049 (2,*)	0.182 (10,*)	0.143 (8,*)	0.117 (6,*)	0.157 (9,*)	0.118 (7,*)	0.104 (5,*)
		RND	0.018 (1)	0.029 (6,*)	0.116 (9,*)	0.024 (2,*)	0.213 (10,*)	0.029 (7,*)	0.027 (5,*)	0.026 (3,*)	0.032 (8,*)	0.027 (4,*)
Directed	Controllability Robustness	TAR	0.011 (1)	0.022 (2,*)	0.079 (5,*)	0.039 (3,*)	0.064 (4,*)	0.112 (7,*)	0.116 (8,*)	0.086 (6,*)	0.141 (10,*)	0.133 (9,*)
		RND	0.014 (1)	0.020 (3,*)	0.050 (9,*)	0.020 (2,*)	0.052 (10,*)	0.027 (5,*)	0.025 (4,*)	0.033 (6,*)	0.045 (8,*)	0.036 (7,*)
	Connectivity Robustness	TAR	0.027 (1)	0.072 (3,*)	0.079 (4,*)	0.048 (2,*)	0.214 (10,*)	0.169 (7,*)	0.164 (6,*)	0.146 (5,*)	0.183 (9,*)	0.179 (8,*)
		RND	0.020 (1)	0.023 (2,*)	0.121 (9,*)	0.024 (3,*)	0.222 (10,*)	0.026 (4,*)	0.027 (5,*)	0.041 (8,*)	0.034 (7,*)	0.028 (6,*)

Table S7: For SF (generic scale-free) networks.

SF (*:46; ≈:11; +:15)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.041 (7)	0.105 (8,*)	0.209 (9,*)	0.039 (6,+)	0.311 (10,*)	0.019 (3,+)	0.018 (2,+)	0.037 (5,+)	0.022 (4,+)	0.018 (1,+)
		RND	0.020 (2)	0.050 (8,*)	0.123 (9,*)	0.025 (5,*)	0.247 (10,*)	0.020 (1,≈)	0.022 (4,*)	0.041 (7,*)	0.026 (6,*)	0.021 (3,≈)
	Connectivity Robustness	TAR	0.038 (7)	0.022 (4,+)	0.053 (8,*)	0.035 (6,+)	0.059 (9,*)	0.029 (5,+)	0.012 (1,+)	0.074 (10,*)	0.017 (3,+)	0.013 (2,+)
		RND	0.025 (1)	0.043 (8,*)	0.119 (9,*)	0.035 (6,*)	0.261 (10,*)	0.031 (3,*)	0.031 (4,*)	0.029 (2,≈)	0.038 (7,*)	0.031 (5,*)
Directed	Controllability Robustness	TAR	0.010 (1)	0.045 (7,*)	0.161 (9,*)	0.021 (6,*)	0.278 (10,*)	0.015 (4,*)	0.011 (3,≈)	0.051 (8,*)	0.016 (5,*)	0.011 (2,≈)
		RND	0.014 (2)	0.044 (8,*)	0.130 (9,*)	0.019 (5,*)	0.173 (10,*)	0.014 (4,≈)	0.014 (3,≈)	0.043 (7,*)	0.019 (6,*)	0.013 (1,≈)
	Connectivity Robustness	TAR	0.024 (4)	0.032 (6,≈)	0.044 (8,*)	0.043 (7,*)	0.142 (10,*)	0.030 (5,*)	0.014 (2,+)	0.111 (9,*)	0.019 (3,+)	0.014 (1,+)
		RND	0.029 (3)	0.046 (7,*)	0.141 (9,*)	0.054 (8,*)	0.270 (10,*)	0.031 (4,*)	0.028 (2,≈)	0.038 (6,*)	0.035 (5,*)	0.028 (1,≈)

Table S8: For SW-NW (Newman–Watts small-world) networks.

SW-NW (*:68; ≈:4)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.008 (1)	0.011 (2,*)	0.018 (3,*)	0.020 (4,*)	0.047 (6,*)	0.051 (9,*)	0.050 (8,*)	0.058 (10,*)	0.049 (7,*)	0.047 (5,*)
		RND	0.008 (1)	0.009 (2,*)	0.017 (8,*)	0.011 (5,*)	0.028 (9,*)	0.012 (6,*)	0.010 (4,*)	0.043 (10,*)	0.012 (7,*)	0.009 (3,*)
	Connectivity Robustness	TAR	0.016 (1)	0.089 (7,*)	0.089 (8,*)	0.026 (2,*)	0.232 (10,*)	0.041 (6,*)	0.033 (4,*)	0.105 (9,*)	0.034 (5,*)	0.030 (3,*)
		RND	0.016 (1)	0.022 (6,*)	0.124 (9,*)	0.021 (5,*)	0.221 (10,*)	0.018 (4,*)	0.018 (3,*)	0.027 (8,*)	0.022 (7,*)	0.018 (2,≈)
Directed	Controllability Robustness	TAR	0.011 (1)	0.016 (3,*)	0.047 (10,*)	0.022 (4,*)	0.036 (7,*)	0.034 (6,*)	0.042 (9,*)	0.037 (8,*)	0.024 (5,*)	0.016 (2,*)
		RND	0.009 (1)	0.015 (4,*)	0.033 (9,*)	0.015 (5,*)	0.037 (10,*)	0.016 (6,*)	0.017 (7,*)	0.024 (8,*)	0.014 (3,*)	0.010 (2,≈)
	Connectivity Robustness	TAR	0.019 (1)	0.098 (9,*)	0.087 (8,*)	0.029 (4,*)	0.248 (10,*)	0.035 (6,*)	0.034 (5,*)	0.080 (7,*)	0.019 (2,*)	0.021 (3,≈)
		RND	0.016 (1)	0.019 (4,*)	0.125 (9,*)	0.022 (5,*)	0.230 (10,*)	0.023 (7,*)	0.019 (3,*)	0.042 (8,*)	0.022 (6,*)	0.017 (2,≈)

Table S9: For SW-WS (Watts–Strogatz small-world) networks.

SW-WS (*:67; ≈:3; +:2)			GIN-MAS	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Undirected	Controllability Robustness	TAR	0.008 (1)	0.013 (2,*)	0.029 (6,*)	0.022 (3,*)	0.047 (10,*)	0.032 (7,*)	0.024 (4,*)	0.038 (8,*)	0.039 (9,*)	0.027 (5,*)
		RND	0.008 (1)	0.009 (3,*)	0.016 (8,*)	0.011 (5,*)	0.031 (10,*)	0.012 (6,*)	0.010 (4,*)	0.030 (9,*)	0.014 (7,*)	0.009 (2,≈)
	Connectivity Robustness	TAR	0.016 (1)	0.091 (8,*)	0.092 (9,*)	0.025 (3,*)	0.236 (10,*)	0.032 (6,*)	0.025 (2,*)	0.085 (7,*)	0.032 (5,*)	0.027 (4,*)
		RND	0.015 (1)	0.023 (6,*)	0.122 (9,*)	0.021 (5,*)	0.222 (10,*)	0.017 (2,*)	0.018 (4,*)	0.027 (8,*)	0.024 (7,*)	0.017 (3,*)
Directed	Controllability Robustness	TAR	0.012 (1)	0.016 (2,*)	0.039 (10,*)	0.027 (6,*)	0.037 (9,*)	0.021 (3,*)	0.029 (8,*)	0.029 (7,*)	0.025 (5,*)	0.023 (4,*)
		RND	0.010 (1)	0.012 (2,*)	0.033 (9,*)	0.017 (7,*)	0.040 (10,*)	0.015 (5,*)	0.015 (4,*)	0.029 (8,*)	0.016 (6,*)	0.012 (3,*)
	Connectivity Robustness	TAR	0.020 (3)	0.097 (9,*)	0.088 (8,*)	0.028 (4,*)	0.245 (10,*)	0.034 (6,*)	0.032 (5,*)	0.071 (7,*)	0.019 (2,+)	0.017 (1,+)
		RND	0.017 (1)	0.019 (4,*)	0.123 (9,*)	0.021 (5,*)	0.230 (10,*)	0.022 (6,*)	0.019 (3,≈)	0.043 (8,*)	0.023 (7,*)	0.017 (2,≈)

Table S10: Overall prediction errors of GIN (*single task*), LFR, RP, SPP, GCN, MLP, KNN, LR, DT, and RF for measuring the 9 synthetic networks. Part (I): the training and test instances are taken from the same distributed data; Part (II): the training and test instances are taken from different distributed data. The value following '$\pm$' represents the standard deviation; an integer in parentheses indicates the rank of the method under a specific robustness metric; an asterisk '*' denotes that the corresponding method is statistically inferior to GIN, using the Kruskal-Wallis H-test.

Tested Data	Robustness Measure			GIN	LFR	RP	SPP	GCN	MLP	KNN	LR	DT	RF
Part (I) Within Range (WR)	Undirected	Controllability Robustness ($\mathcal{Q}_\mathcal{T}$)	TAR	0.008 $\pm$0.004 (1)	0.021 $\pm$0.018 (2,*)	0.072 $\pm$0.033 (9,*)	0.024 $\pm$0.017 (3,*)	0.171 $\pm$0.075 (10,*)	0.038 $\pm$0.024 (6,*)	0.034 $\pm$0.032 (4,*)	0.061 $\pm$0.037 (8,*)	0.041 $\pm$0.040 (7,*)	0.036 $\pm$0.034 (5,*)
			RND	0.018 $\pm$0.007 (1)	0.022 $\pm$0.012 (2,*)	0.046 $\pm$0.031 (9,*)	0.022 $\pm$0.010 (3,*)	0.087 $\pm$0.066 (10,*)	0.024 $\pm$0.012 (4,*)	0.025 $\pm$0.014 (6,*)	0.040 $\pm$0.020 (8,*)	0.030 $\pm$0.016 (7,*)	0.024 $\pm$0.013 (5,*)
		Connectivity Robustness ($\mathcal{P}_\mathcal{T}$)	TAR	0.015 $\pm$0.003 (1)	0.052 $\pm$0.025 (7,*)	0.064 $\pm$0.029 (8,*)	0.031 $\pm$0.019 (2,*)	0.138 $\pm$0.056 (10,*)	0.044 $\pm$0.031 (6,*)	0.036 $\pm$0.039 (3,*)	0.083 $\pm$0.037 (9,*)	0.041 $\pm$0.046 (5,*)	0.038 $\pm$0.040 (4,*)
			RND	0.024 $\pm$0.015 (1)	0.032 $\pm$0.019 (6,*)	0.113 $\pm$0.017 (9,*)	0.030 $\pm$0.017 (3,*)	0.202 $\pm$0.017 (10,*)	0.028 $\pm$0.016 (2,*)	0.030 $\pm$0.017 (5,*)	0.032 $\pm$0.016 (7,*)	0.036 $\pm$0.021 (8,*)	0.030 $\pm$0.017 (4,*)
	Undirected	Controllability Robustness ($\mathcal{Q}_\mathcal{T}$)	TAR	0.009 $\pm$0.005 (1)	0.015 $\pm$0.008 (2,*)	0.083 $\pm$0.032 (10,*)	0.029 $\pm$0.021 (3,*)	0.082 $\pm$0.039 (9,*)	0.046 $\pm$0.035 (4,*)	0.047 $\pm$0.045 (5,*)	0.060 $\pm$0.041 (8,*)	0.058 $\pm$0.059 (7,*)	0.054 $\pm$0.055 (6,*)
			RND	0.016 $\pm$0.006 (1)	0.022 $\pm$0.012 (2,*)	0.065 $\pm$0.029 (9,*)	0.024 $\pm$0.011 (3,*)	0.089 $\pm$0.037 (10,*)	0.029 $\pm$0.019 (4,*)	0.030 $\pm$0.022 (5,*)	0.041 $\pm$0.024 (8,*)	0.039 $\pm$0.030 (7,*)	0.033 $\pm$0.026 (6,*)
		Connectivity Robustness ($\mathcal{P}_\mathcal{T}$)	TAR	0.018 $\pm$0.005 (1)	0.065 $\pm$0.028 (7,*)	0.068 $\pm$0.029 (8,*)	0.033 $\pm$0.017 (2,*)	0.181 $\pm$0.055 (10,*)	0.056 $\pm$0.040 (6,*)	0.048 $\pm$0.047 (3,*)	0.090 $\pm$0.038 (9,*)	0.054 $\pm$0.063 (5,*)	0.053 $\pm$0.061 (4,*)
			RND	0.025 $\pm$0.016 (1)	0.029 $\pm$0.019 (4,*)	0.116 $\pm$0.015 (9,*)	0.033 $\pm$0.020 (6,*)	0.211 $\pm$0.018 (10,*)	0.029 $\pm$0.014 (5,*)	0.027 $\pm$0.017 (3,*)	0.043 $\pm$0.017 (8,*)	0.035 $\pm$0.022 (7,*)	0.027 $\pm$0.017 (2,*)
Part (II) Out of Range (OR)	Undirected	Controllability Robustness ($\mathcal{Q}_\mathcal{T}$)	TAR	0.010 $\pm$0.015 (1)	0.064 $\pm$0.073 (7,*)	0.128 $\pm$0.071 (8,*)	0.037 $\pm$0.028 (2,*)	0.172 $\pm$0.076 (9,*)	0.056 $\pm$0.037 (6,*)	0.040 $\pm$0.040 (3,*)	0.222 $\pm$0.184 (10,*)	0.050 $\pm$0.050 (5,*)	0.043 $\pm$0.043 (4,*)
			RND	0.021 $\pm$0.015 (1)	0.043 $\pm$0.043 (7,*)	0.085 $\pm$0.054 (8,*)	0.032 $\pm$0.020 (5,*)	0.087 $\pm$0.063 (9,*)	0.029 $\pm$0.019 (4,*)	0.029 $\pm$0.021 (3,*)	0.186 $\pm$0.144 (10,*)	0.035 $\pm$0.022 (6,*)	0.027 $\pm$0.020 (2,*)
		Connectivity Robustness ($\mathcal{P}_\mathcal{T}$)	TAR	0.020 $\pm$0.017 (1)	0.093 $\pm$0.051 (7,*)	0.162 $\pm$0.118 (9,*)	0.047 $\pm$0.029 (3,*)	0.142 $\pm$0.056 (8,*)	0.065 $\pm$0.045 (6,*)	0.045 $\pm$0.046 (2,*)	0.251 $\pm$0.192 (10,*)	0.054 $\pm$0.056 (5,*)	0.050 $\pm$0.049 (4,*)
			RND	0.029 $\pm$0.031 (1)	0.054 $\pm$0.044 (7,*)	0.161 $\pm$0.057 (9,*)	0.045 $\pm$0.025 (5,*)	0.206 $\pm$0.023 (10,*)	0.049 $\pm$0.032 (6,*)	0.035 $\pm$0.032 (3,*)	0.143 $\pm$0.109 (8,*)	0.044 $\pm$0.036 (4,*)	0.033 $\pm$0.032 (2,*)
	Directed	Controllability Robustness ($\mathcal{Q}_\mathcal{T}$)	TAR	0.011 $\pm$0.012 (1)	0.055 $\pm$0.065 (6,*)	0.164 $\pm$0.088 (10,*)	0.046 $\pm$0.034 (5,*)	0.084 $\pm$0.041 (8,*)	0.056 $\pm$0.036 (7,*)	0.040 $\pm$0.036 (2,*)	0.154 $\pm$0.112 (9,*)	0.046 $\pm$0.049 (4,*)	0.041 $\pm$0.043 (3,*)
			RND	0.019 $\pm$0.012 (1)	0.048 $\pm$0.041 (7,*)	0.120 $\pm$0.063 (10,*)	0.038 $\pm$0.023 (5,*)	0.092 $\pm$0.038 (8,*)	0.034 $\pm$0.021 (2,*)	0.034 $\pm$0.024 (3,*)	0.117 $\pm$0.077 (9,*)	0.041 $\pm$0.030 (6,*)	0.035 $\pm$0.027 (4,*)
		Connectivity Robustness ($\mathcal{P}_\mathcal{T}$)	TAR	0.023 $\pm$0.020 (1)	0.104 $\pm$0.061 (7,*)	0.148 $\pm$0.104 (8,*)	0.056 $\pm$0.037 (5,*)	0.193 $\pm$0.059 (9,*)	0.071 $\pm$0.037 (6,*)	0.047 $\pm$0.041 (2,*)	0.320 $\pm$0.243 (10,*)	0.052 $\pm$0.057 (4,*)	0.048 $\pm$0.050 (3,*)
			RND	0.030 $\pm$0.028 (1)	0.049 $\pm$0.041 (7,*)	0.155 $\pm$0.046 (9,*)	0.049 $\pm$0.031 (6,*)	0.215 $\pm$0.022 (10,*)	0.048 $\pm$0.030 (5,*)	0.033 $\pm$0.029 (3,*)	0.142 $\pm$0.099 (8,*)	0.041 $\pm$0.033 (4,*)	0.032 $\pm$0.029 (2,*)

Table S11: Detailed runtime comparison for GIN-MAS, LFR, RP, SPP, LFR, MLP, KNN, LR, DT, and RF against network size changes (Unit: Second).

Network Size		1000	2000	3000	4000	5000	6000	7000	8000	9000	10000
GNN	GIN-MAS	0.0028	0.0026	0.0028	0.0030	0.0032	0.0035	0.0035	0.0038	0.0041	0.0043
	GCN	0.0612	0.1226	0.1772	0.2662	0.2832	0.3499	0.3786	0.4876	0.5263	0.6838
CNN	LFR	2.7729	8.1911	18.5060	36.4061	57.5839	85.0764	116.3463	163.0242	205.2720	271.3228
	RP	0.0255	0.0297	0.0286	0.0290	0.0301	0.0288	0.0300	0.0298	0.0291	0.0305
	SPP	0.0235	0.0277	0.0305	0.0261	0.0271	0.0288	0.0296	0.0305	0.0311	0.0355
ML	MLP	0.0223	0.0567	0.1078	0.1679	0.2325	0.3172	0.4120	0.5531	0.6624	0.8264
	KNN	0.0215	0.0564	0.1097	0.1677	0.2339	0.3221	0.4131	0.5537	0.6627	0.8345
	LR	0.0212	0.0562	0.1077	0.1666	0.2319	0.3183	0.4140	0.5535	0.6651	0.8314
	DT	0.0216	0.0564	0.1083	0.1679	0.2341	0.3216	0.4093	0.5366	0.6467	0.8080
	RF	0.0219	0.0587	0.1095	0.1574	0.2321	0.3160	0.4099	0.5489	0.6529	0.8189

Table S12: [*Undirected Networks + Controllability Robustness*] Prediction errors obtained by GIN-MAS, LFR, RP, SPP, GCN, MLP, KNN, LR, DT, and RF, on the 'Out-of-Range' (OR) networks. The training data are drawn from the synthetic networks of sizes $N \in [700, 1300]$, while the test data are from that of sizes $N \in [200, 700)$ and $N \in (700, 1800]$. An integer in parentheses indicates the rank of the method for robustness measure; an asterisk '*' denotes that the corresponding method is statistically inferior to GIN-MAS, using the Kruskal-Wallis H-test.

Range of Tested Network Size N		$[200, 300]$	$[300, 400]$	$[400, 500]$	$[500, 600]$	$[600, 700]$	$[1300, 1400]$	$[1400, 1500]$	$[1500, 1600]$	$[1600, 1700]$	$[1700, 1800]$
TAR	GIN-MAS	0.020 (1)	0.017 (1)	0.016 (1)	0.014 (1)	0.014 (1)	0.012 (1)	0.013 (1)	0.013 (1)	0.013 (1)	0.014 (1)
	LFR	0.133 (9,*)	0.143 (9,*)	0.115 (8,*)	0.095 (7,*)	0.061 (7,*)	0.034 (3,*)	0.043 (4,*)	0.052 (5,*)	0.059 (7,*)	0.066 (7,*)
	RP	0.317 (10,*)	0.253 (10,*)	0.193 (10,*)	0.131 (9,*)	0.080 (8,*)	0.068 (8,*)	0.078 (8,*)	0.089 (8,*)	0.102 (9,*)	0.112 (9,*)
	SPP	0.079 (2,*)	0.072 (3,*)	0.052 (2,*)	0.044 (2,*)	0.038 (2,*)	0.033 (2,*)	0.035 (2,*)	0.038 (2,*)	0.043 (3,*)	0.047 (3,*)
	GCN	0.100 (8,*)	0.099 (7,*)	0.099 (7,*)	0.098 (8,*)	0.097 (9,*)	0.097 (9,*)	0.096 (9,*)	0.098 (9,*)	0.097 (8,*)	0.097 (8,*)
	MLP	0.097 (7,*)	0.079 (5,*)	0.076 (5,*)	0.061 (5,*)	0.052 (5,*)	0.057 (7,*)	0.059 (7,*)	0.055 (6,*)	0.059 (6,*)	0.058 (6,*)
	KNN	0.091 (3,*)	0.072 (2,*)	0.070 (3,*)	0.049 (3,*)	0.042 (3,*)	0.035 (4,*)	0.036 (3,*)	0.047 (4,*)	0.037 (2,*)	0.041 (2,*)
	LR	0.093 (5,*)	0.106 (8,*)	0.151 (9,*)	0.177 (10,*)	0.190 (10,*)	0.436 (10,*)	0.453 (10,*)	0.465 (10,*)	0.485 (10,*)	0.495 (10,*)
	DT	0.095 (6,*)	0.085 (6,*)	0.082 (6,*)	0.067 (6,*)	0.061 (6,*)	0.056 (6,*)	0.056 (6,*)	0.056 (7,*)	0.055 (5,*)	0.057 (5,*)
	RF	0.092 (4,*)	0.077 (4,*)	0.073 (4,*)	0.058 (4,*)	0.050 (4,*)	0.044 (5,*)	0.047 (5,*)	0.047 (3,*)	0.047 (4,*)	0.047 (4,*)
RND	GIN-MAS	0.025 (1)	0.020 (1)	0.017 (1)	0.014 (1)	0.013 (1)	0.009 (1)	0.009 (1)	0.009 (1)	0.009 (1)	0.009 (1)
	LFR	0.070 (9,*)	0.064 (9,*)	0.052 (7,*)	0.040 (7,*)	0.027 (7,*)	0.018 (4,*)	0.021 (6,*)	0.025 (7,*)	0.029 (7,*)	0.032 (7,*)
	RP	0.178 (10,*)	0.129 (10,*)	0.086 (9,*)	0.061 (8,*)	0.044 (8,*)	0.042 (8,*)	0.047 (8,*)	0.052 (8,*)	0.057 (8,*)	0.060 (8,*)
	SPP	0.032 (3,*)	0.033 (6,*)	0.026 (5,*)	0.024 (4,*)	0.021 (3,*)	0.018 (5,*)	0.019 (4,*)	0.023 (6,*)	0.027 (6,*)	0.031 (6,*)
	GCN	0.058 (8,*)	0.059 (8,*)	0.061 (8,*)	0.061 (9,*)	0.061 (9,*)	0.063 (9,*)	0.063 (9,*)	0.063 (9,*)	0.065 (9,*)	0.065 (9,*)
	MLP	0.030 (2,*)	0.027 (3,*)	0.025 (4,*)	0.025 (5,*)	0.022 (5,*)	0.020 (6,*)	0.020 (5,*)	0.020 (4,*)	0.021 (4,*)	0.021 (4,*)
	KNN	0.034 (5,*)	0.027 (4,*)	0.024 (3,*)	0.021 (2,*)	0.021 (4,*)	0.016 (3,*)	0.018 (3,*)	0.018 (3,*)	0.018 (3,*)	0.019 (3,*)
	LR	0.049 (7,*)	0.046 (7,*)	0.121 (10,*)	0.129 (10,*)	0.161 (10,*)	0.300 (10,*)	0.305 (10,*)	0.315 (10,*)	0.318 (10,*)	0.333 (10,*)
	DT	0.035 (6,*)	0.029 (5,*)	0.026 (6,*)	0.026 (6,*)	0.023 (6,*)	0.020 (7,*)	0.022 (7,*)	0.021 (5,*)	0.022 (5,*)	0.023 (5,*)
	RF	0.033 (4,*)	0.026 (2,*)	0.023 (2,*)	0.022 (3,*)	0.020 (2,*)	0.015 (2,*)	0.016 (2,*)	0.017 (2,*)	0.017 (2,*)	0.017 (2,*)

Table S13: [*Undirected Networks + Connectivity Robustness*] Prediction errors obtained by GIN-MAS, LFR, RP, SPP, GCN, MLP, KNN, LR, DT, and RF, on the 'Out-of-Range' (OR) networks. The training data are drawn from the synthetic networks of sizes $N \in [700, 1300]$, while the test data are from that of sizes $N \in [200, 700)$ and $N \in (700, 1800]$. An integer in parentheses indicates the rank of the method for robustness measure; an asterisk '*' denotes that the corresponding method is statistically inferior to GIN-MAS, using the Kruskal-Wallis H-test.

Range of Tested Network Size N		$[200, 300]$	$[300, 400]$	$[400, 500]$	$[500, 600]$	$[600, 700]$	$[1300, 1400]$	$[1400, 1500]$	$[1500, 1600]$	$[1600, 1700]$	$[1700, 1800]$
TAR	GIN-MAS	0.044 (1)	0.032 (1)	0.028 (1)	0.025 (1)	0.023 (1)	0.021 (1)	0.022 (1)	0.022 (1)	0.023 (1)	0.024 (1)
	LFR	0.231 (9,*)	0.216 (8,*)	0.191 (7,*)	0.160 (7,*)	0.110 (7,*)	0.081 (6,*)	0.093 (7,*)	0.107 (7,*)	0.116 (7,*)	0.125 (7,*)
	RP	0.499 (10,*)	0.421 (10,*)	0.352 (10,*)	0.257 (10,*)	0.131 (8,*)	0.108 (8,*)	0.129 (8,*)	0.149 (8,*)	0.165 (8,*)	0.184 (8,*)
	SPP	0.121 (5,*)	0.099 (5,*)	0.079 (2,*)	0.059 (2,*)	0.051 (2,*)	0.046 (2,*)	0.052 (3,*)	0.057 (2,*)	0.064 (5,*)	0.071 (5,*)
	GCN	0.227 (8,*)	0.217 (9,*)	0.212 (9,*)	0.211 (8,*)	0.208 (9,*)	0.203 (9,*)	0.204 (9,*)	0.204 (9,*)	0.203 (9,*)	0.204 (9,*)
	MLP	0.124 (6,*)	0.097 (4,*)	0.094 (5,*)	0.079 (5,*)	0.073 (6,*)	0.092 (7,*)	0.092 (6,*)	0.091 (6,*)	0.096 (6,*)	0.096 (6,*)
	KNN	0.113 (3,*)	0.091 (2,*)	0.088 (4,*)	0.062 (3,*)	0.054 (3,*)	0.047 (3,*)	0.046 (2,*)	0.063 (3,*)	0.048 (2,*)	0.054 (2,*)
	LR	0.138 (7,*)	0.157 (7,*)	0.205 (8,*)	0.227 (9,*)	0.239 (10,*)	0.523 (10,*)	0.542 (10,*)	0.549 (10,*)	0.577 (10,*)	0.587 (10,*)
	DT	0.114 (4,*)	0.100 (6,*)	0.097 (6,*)	0.080 (6,*)	0.069 (5,*)	0.065 (5,*)	0.064 (5,*)	0.070 (5,*)	0.060 (4,*)	0.069 (4,*)
	RF	0.110 (2,*)	0.091 (3,*)	0.088 (3,*)	0.070 (4,*)	0.063 (4,*)	0.057 (4,*)	0.060 (4,*)	0.063 (4,*)	0.060 (3,*)	0.062 (3,*)
RND	GIN-MAS	0.037 (1)	0.024 (1)	0.023 (1)	0.021 (1)	0.020 (1)	0.015 (1)	0.015 (1)	0.015 (1)	0.015 (1)	0.014 (1)
	LFR	0.086 (8,*)	0.067 (8,*)	0.059 (7,*)	0.051 (7,*)	0.039 (7,*)	0.026 (4,*)	0.030 (5,*)	0.032 (5,*)	0.036 (5,*)	0.038 (5,*)
	RP	0.273 (10,*)	0.225 (9,*)	0.192 (9,*)	0.160 (9,*)	0.132 (9,*)	0.131 (8,*)	0.138 (8,*)	0.146 (8,*)	0.152 (8,*)	0.158 (8,*)
	SPP	0.053 (7,*)	0.047 (7,*)	0.039 (6,*)	0.031 (4,*)	0.026 (4,*)	0.027 (5,*)	0.029 (4,*)	0.034 (6,*)	0.038 (6,*)	0.043 (6,*)
	GCN	0.233 (9,*)	0.225 (10,*)	0.224 (10,*)	0.224 (10,*)	0.223 (10,*)	0.221 (10,*)	0.221 (10,*)	0.222 (9,*)	0.221 (9,*)	0.221 (9,*)
	MLP	0.043 (4,*)	0.032 (4,*)	0.037 (5,*)	0.037 (6,*)	0.038 (6,*)	0.048 (7,*)	0.048 (7,*)	0.049 (7,*)	0.049 (7,*)	0.051 (7,*)
	KNN	0.042 (3,*)	0.030 (3,*)	0.028 (3,*)	0.025 (2,*)	0.026 (3,*)	0.021 (3,*)	0.022 (3,*)	0.021 (3,*)	0.022 (3,*)	0.021 (3,*)
	LR	0.044 (5,*)	0.036 (6,*)	0.089 (8,*)	0.098 (8,*)	0.107 (8,*)	0.216 (9,*)	0.220 (9,*)	0.224 (10,*)	0.227 (10,*)	0.240 (10,*)
	DT	0.046 (6,*)	0.034 (5,*)	0.033 (4,*)	0.033 (5,*)	0.031 (5,*)	0.028 (6,*)	0.030 (6,*)	0.029 (4,*)	0.028 (4,*)	0.030 (4,*)
	RF	0.042 (2,*)	0.029 (2,*)	0.027 (2,*)	0.026 (3,*)	0.025 (2,*)	0.020 (2,*)	0.021 (2,*)	0.020 (2,*)	0.020 (2,*)	0.020 (2,*)

Table S14: [*Directed Networks + Controllability Robustness*] Prediction errors obtained by GIN-MAS, LFR, RP, SPP, GCN, MLP, KNN, LR, DT, and RF, on the 'Out-of-Range' (OR) networks. The training data are drawn from the synthetic networks of sizes $N \in [700, 1300]$, while the test data are from that of sizes $N \in [200, 700)$ and $N \in (700, 1800]$. An integer in parentheses indicates the rank of the method for robustness measure; an asterisk '*' denotes that the corresponding method is statistically inferior to GIN-MAS, using the Kruskal-Wallis H-test.

Range of Tested Network Size N		$[200, 300]$	$[300, 400]$	$[400, 500]$	$[500, 600]$	$[600, 700]$	$[1300, 1400]$	$[1400, 1500]$	$[1500, 1600]$	$[1600, 1700]$	$[1700, 1800]$
TAR	GIN-MAS	0.025 (1)	0.020 (1)	0.017 (1)	0.015 (1)	0.014 (1)	0.010 (1)	0.011 (1)	0.011 (1)	0.011 (1)	0.011 (1)
	LFR	0.168 (9,*)	0.150 (9,*)	0.111 (8,*)	0.084 (7,*)	0.047 (3,*)	0.022 (2,*)	0.026 (2,*)	0.031 (2,*)	0.035 (2,*)	0.039 (2,*)
	RP	0.383 (10,*)	0.323 (10,*)	0.256 (10,*)	0.191 (10,*)	0.123 (9,*)	0.099 (9,*)	0.111 (9,*)	0.124 (9,*)	0.133 (9,*)	0.144 (9,*)
	SPP	0.101 (8,*)	0.081 (6,*)	0.065 (5,*)	0.051 (5,*)	0.046 (2,*)	0.041 (3,*)	0.044 (3,*)	0.046 (3,*)	0.052 (5,*)	0.056 (5,*)
	GCN	0.098 (7,*)	0.094 (8,*)	0.091 (7,*)	0.088 (8,*)	0.088 (8,*)	0.088 (8,*)	0.088 (8,*)	0.089 (8,*)	0.091 (8,*)	0.091 (8,*)
	MLP	0.064 (2,*)	0.053 (2,*)	0.077 (6,*)	0.052 (6,*)	0.054 (5,*)	0.079 (7,*)	0.052 (5,*)	0.085 (7,*)	0.068 (7,*)	0.061 (7,*)
	KNN	0.065 (3,*)	0.053 (3,*)	0.061 (4,*)	0.048 (4,*)	0.054 (4,*)	0.047 (5,*)	0.050 (4,*)	0.050 (5,*)	0.044 (3,*)	0.045 (3,*)
	LR	0.071 (5,*)	0.086 (7,*)	0.116 (9,*)	0.117 (9,*)	0.160 (10,*)	0.243 (10,*)	0.259 (10,*)	0.262 (10,*)	0.277 (10,*)	0.278 (10,*)
	DT	0.075 (6,*)	0.062 (5,*)	0.058 (3,*)	0.044 (3,*)	0.072 (7,*)	0.051 (6,*)	0.069 (7,*)	0.052 (6,*)	0.055 (6,*)	0.059 (6,*)
	RF	0.069 (4,*)	0.057 (4,*)	0.054 (2,*)	0.038 (2,*)	0.067 (6,*)	0.046 (4,*)	0.061 (6,*)	0.046 (4,*)	0.049 (4,*)	0.053 (4,*)
RND	GIN-MAS	0.026 (1)	0.022 (1)	0.018 (1)	0.016 (1)	0.015 (1)	0.011 (1)	0.011 (1)	0.010 (1)	0.010 (1)	0.010 (1)
	LFR	0.104 (9,*)	0.080 (9,*)	0.070 (8,*)	0.061 (7,*)	0.040 (7,*)	0.020 (2,*)	0.023 (3,*)	0.026 (5,*)	0.028 (2,*)	0.031 (5,*)
	RP	0.219 (10,*)	0.189 (10,*)	0.149 (10,*)	0.113 (10,*)	0.078 (9,*)	0.071 (9,*)	0.081 (9,*)	0.090 (9,*)	0.100 (9,*)	0.108 (9,*)
	SPP	0.068 (7,*)	0.058 (6,*)	0.040 (6,*)	0.032 (6,*)	0.027 (2,*)	0.021 (3,*)	0.023 (2,*)	0.025 (2,*)	0.030 (4,*)	0.034 (6,*)
	GCN	0.072 (8,*)	0.070 (8,*)	0.069 (7,*)	0.068 (8,*)	0.068 (8,*)	0.069 (8,*)	0.068 (8,*)	0.068 (8,*)	0.068 (8,*)	0.068 (8,*)
	MLP	0.043 (3,*)	0.037 (3,*)	0.036 (4,*)	0.029 (3,*)	0.033 (5,*)	0.027 (4,*)	0.026 (4,*)	0.026 (4,*)	0.029 (3,*)	0.029 (3,*)
	KNN	0.044 (4,*)	0.037 (4,*)	0.036 (3,*)	0.029 (4,*)	0.033 (4,*)	0.029 (5,*)	0.028 (5,*)	0.025 (3,*)	0.036 (5,*)	0.024 (2,*)
	LR	0.055 (6,*)	0.064 (7,*)	0.089 (9,*)	0.083 (9,*)	0.128 (10,*)	0.173 (10,*)	0.172 (10,*)	0.181 (10,*)	0.208 (10,*)	0.164 (10,*)
	DT	0.046 (5,*)	0.041 (5,*)	0.039 (5,*)	0.031 (5,*)	0.033 (6,*)	0.039 (7,*)	0.037 (7,*)	0.036 (7,*)	0.045 (7,*)	0.035 (7,*)
	RF	0.042 (2,*)	0.037 (2,*)	0.034 (2,*)	0.025 (2,*)	0.029 (3,*)	0.037 (6,*)	0.034 (6,*)	0.032 (6,*)	0.041 (6,*)	0.029 (4,*)

Table S15: [*Directed Networks + Connectivity Robustness*] Prediction errors obtained by GIN-MAS, LFR, RP, SPP, GCN, MLP, KNN, LR, DT, and RF, on the 'Out-of-Range' (OR) networks. The training data are drawn from the synthetic networks of sizes $N \in [700, 1300]$, while the test data are from that of sizes $N \in [200, 700)$ and $N \in (700, 1800]$. An integer in parentheses indicates the rank of the method for robustness measure; an asterisk '*' denotes that the corresponding method is statistically inferior to GIN-MAS, using the Kruskal-Wallis H-test.

Range of Tested Network Size N		$[200, 300]$	$[300, 400]$	$[400, 500]$	$[500, 600]$	$[600, 700]$	$[1300, 1400]$	$[1400, 1500]$	$[1500, 1600]$	$[1600, 1700]$	$[1700, 1800]$
TAR	GIN-MAS	0.048 (1)	0.036 (1)	0.031 (1)	0.028 (1)	0.026 (1)	0.021 (1)	0.020 (1)	0.021 (1)	0.020 (1)	0.020 (1)
	LFR	0.267 (8,*)	0.218 (8,*)	0.166 (7,*)	0.132 (7,*)	0.104 (7,*)	0.086 (6,*)	0.091 (6,*)	0.096 (6,*)	0.101 (7,*)	0.107 (7,*)
	RP	0.381 (10,*)	0.319 (10,*)	0.261 (9,*)	0.197 (8,*)	0.111 (8,*)	0.101 (8,*)	0.115 (8,*)	0.127 (8,*)	0.142 (8,*)	0.154 (8,*)
	SPP	0.148 (7,*)	0.122 (6,*)	0.083 (5,*)	0.064 (5,*)	0.054 (2,*)	0.043 (2,*)	0.044 (2,*)	0.048 (2,*)	0.055 (3,*)	0.061 (3,*)
	GCN	0.282 (9,*)	0.266 (9,*)	0.262 (10,*)	0.255 (10,*)	0.250 (9,*)	0.243 (9,*)	0.244 (9,*)	0.247 (9,*)	0.253 (9,*)	0.252 (9,*)
	MLP	0.085 (4,*)	0.074 (5,*)	0.086 (6,*)	0.077 (6,*)	0.086 (6,*)	0.098 (7,*)	0.097 (7,*)	0.102 (7,*)	0.100 (6,*)	0.100 (6,*)
	KNN	0.083 (3,*)	0.063 (3,*)	0.072 (4,*)	0.058 (4,*)	0.060 (3,*)	0.055 (3,*)	0.057 (3,*)	0.055 (3,*)	0.051 (2,*)	0.053 (2,*)
	LR	0.120 (6,*)	0.167 (7,*)	0.249 (8,*)	0.244 (9,*)	0.338 (10,*)	0.557 (10,*)	0.580 (10,*)	0.602 (10,*)	0.631 (10,*)	0.632 (10,*)
	DT	0.093 (5,*)	0.072 (4,*)	0.067 (3,*)	0.050 (3,*)	0.076 (5,*)	0.063 (5,*)	0.075 (5,*)	0.061 (5,*)	0.067 (5,*)	0.070 (5,*)
	RF	0.083 (2,*)	0.063 (2,*)	0.060 (2,*)	0.043 (2,=)	0.071 (4,*)	0.058 (4,*)	0.071 (4,*)	0.057 (4,*)	0.062 (4,*)	0.067 (4,*)
RND	GIN-MAS	0.036 (1)	0.028 (1)	0.026 (3)	0.023 (2)	0.022 (1)	0.017 (1)	0.016 (1)	0.016 (1)	0.016 (1)	0.016 (1)
	LFR	0.085 (8,*)	0.072 (8,*)	0.060 (7,*)	0.048 (7,*)	0.035 (6,*)	0.022 (4,*)	0.022 (4,*)	0.024 (4,*)	0.024 (4,*)	0.025 (4,*)
	RP	0.247 (10,*)	0.203 (9,*)	0.178 (9,*)	0.157 (9,*)	0.135 (9,*)	0.135 (8,*)	0.141 (8,*)	0.149 (8,*)	0.157 (8,*)	0.164 (8,*)
	SPP	0.059 (7,*)	0.058 (7,*)	0.045 (6,*)	0.037 (6,*)	0.032 (5,*)	0.030 (6,*)	0.031 (6,*)	0.036 (6,*)	0.042 (6,*)	0.047 (6,*)
	GCN	0.242 (9,*)	0.238 (10,*)	0.236 (10,*)	0.234 (10,*)	0.235 (10,*)	0.233 (10,*)	0.233 (10,*)	0.234 (10,*)	0.234 (10,*)	0.233 (10,*)
	MLP	0.040 (4,*)	0.033 (4,*)	0.033 (5,*)	0.032 (5,*)	0.036 (7,*)	0.049 (7,*)	0.047 (7,*)	0.052 (7,*)	0.052 (7,*)	0.048 (7,*)
	KNN	0.037 (2,=)	0.029 (2,=)	0.026 (2,=)	0.024 (3,=)	0.023 (3,=)	0.021 (2,*)	0.019 (2,*)	0.019 (2,*)	0.020 (2,*)	0.018 (2,*)
	LR	0.042 (6,*)	0.056 (6,*)	0.084 (8,*)	0.103 (8,*)	0.133 (8,*)	0.203 (9,*)	0.204 (9,*)	0.230 (9,*)	0.227 (9,*)	0.218 (9,*)
	DT	0.042 (5,*)	0.035 (5,*)	0.031 (4,*)	0.028 (4,*)	0.029 (4,*)	0.029 (5,*)	0.027 (5,*)	0.027 (5,*)	0.028 (5,*)	0.027 (5,*)
	RF	0.037 (3,=)	0.029 (3,=)	0.026 (1,=)	0.023 (1,+)	0.023 (2,=)	0.021 (3,*)	0.020 (3,*)	0.020 (3,*)	0.021 (3,*)	0.019 (3,*)

III. Figures: Comparison on the Ten Methods

Figures S1–S10 show the boxplot for the prediction errors obtained by GIN-MAS and the other nine methods. In the 'pure' mode (P), the training and test datasets are from either pure real-world networks (RWN) or synthetic networks (ER, QS, SF, or SW-NW). In the 'hybrid' mode (H), the training dataset consists of both real-world networks and synthetic networks.

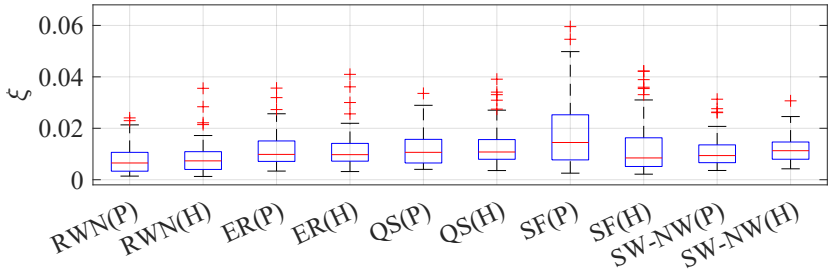

Fig. S1: GIN-MAS.

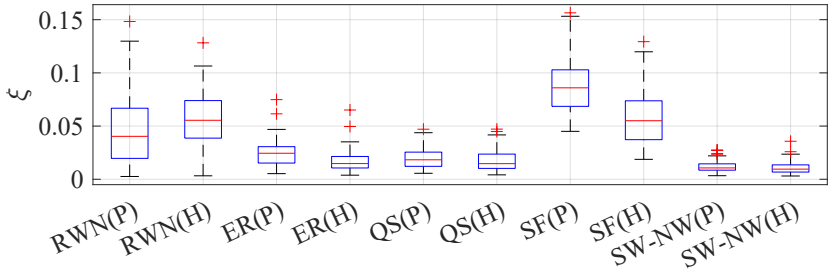

Fig. S2: LFR.

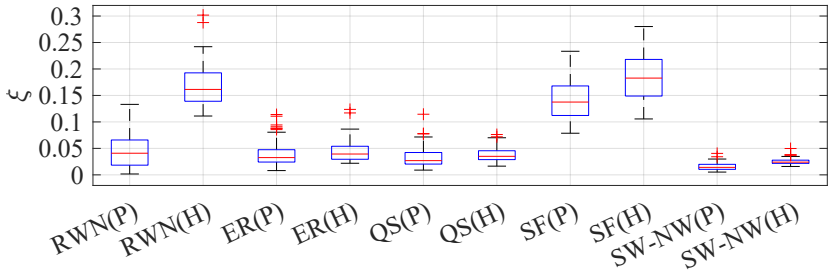

Fig. S3: RP.

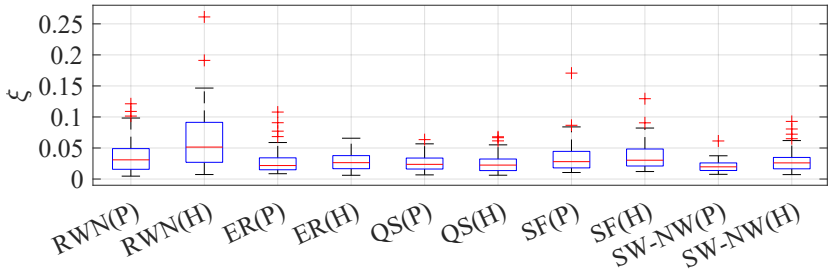

Fig. S4: SPP.

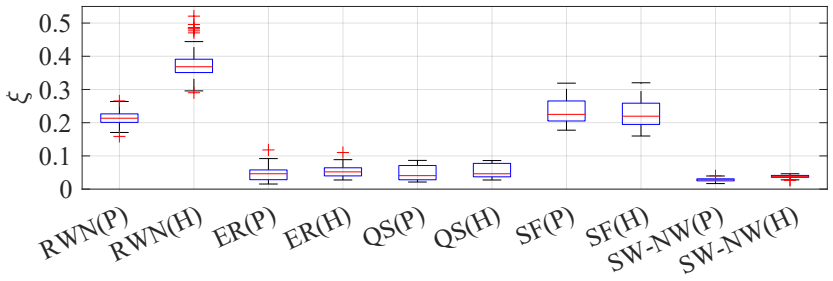

Fig. S5: GCN.

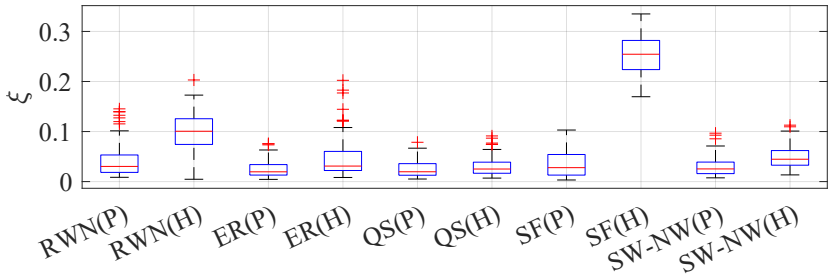

Fig. S6: MLP.

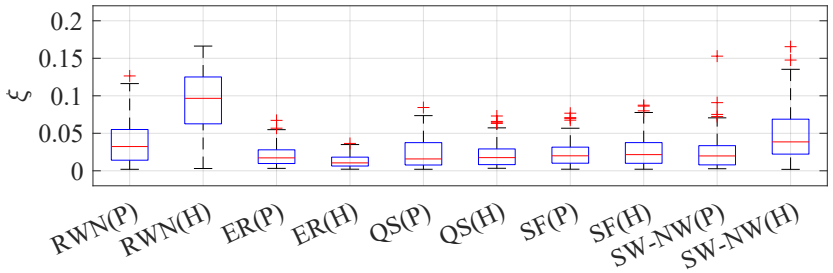

Fig. S7: KNN.

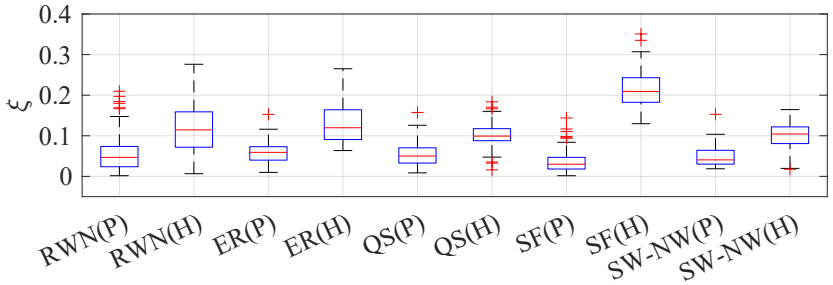

Fig. S8: LR.

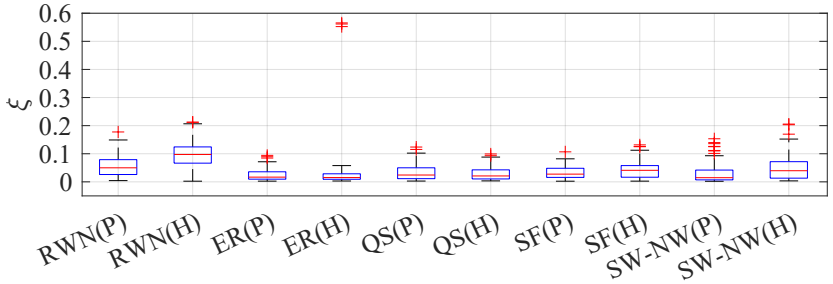

Fig. S9: DT.

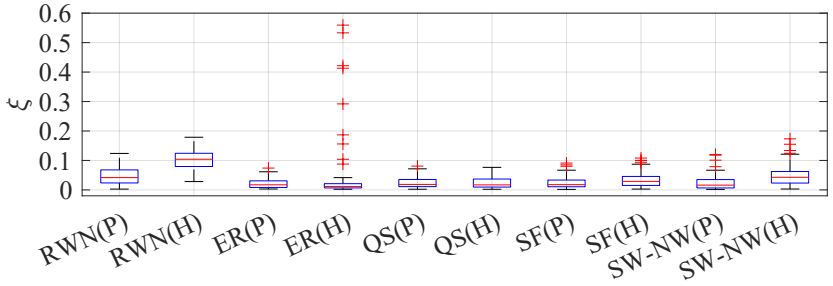

Fig. S10: RF.

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