Appendix

Algorithm. The pseudocode formulation of the proposed GIL algorithm is given in Algorithm 1. We note that the presentation of the algorithm is independent of the specific MDP model used. Our specific formulation of an MDP model of the Maximal Independent Set (mIS) problem is given in Section 4.1.

Extended Results. We show an extended version of the results in Table 2, in which reported values are separated by the number of players n. We also include an additional analysis that evaluates the win rate percentage for each of the methods instead of average reward, since the average reward metric may be sensitive to outliers (i.e., game instances with abnormally large or small objective function values). This is shown in Table 3, with ties being broken randomly in case there is more than one winner. The full results of hyperparameter optimization are too expansive to report directly as tables, and have been included in the supplementary material in the `mcts_hyps.csv` and `il_hyps.csv` files for UCT and GIL respectively. For SA, the lowest tested value $\epsilon = 10$ of the simulated annealing rate was optimal across all settings tested (we did not explore lower values since the method would become significantly more expensive to run, and is already slow as shown in Figure 6).

Implementation. Our implementation is available at `https://github.com/VictorDarvariu/solving-graph-pgg` as Docker containers together with instructions that enable reproducing (up to hardware differences) all the results reported in the paper, including tables and figures. For complete instructions to reproduce the results, please consult the `README.md` file in the repository. We implement all approaches and baselines in Python using a variety of numerical and scientific computing packages [27, 25, 40, 43, 50]. For GIL, we use the PyTorch implementation of *structure2vec* provided by the original authors [14].

Data Availability. The provided implementation contains the necessary code and instructions to generate the synthetic data on which the experiments are carried out. Please consult the `README.md` file in the root of the repository.

Infrastructure and Runtimes. Experiments were carried out on an internal cluster of 8 machines, each equipped with 2 Intel Xeon E5-2630 v3 processors and 128GB RAM. On this infrastructure, the experiments reported in this paper took approximately 14 days to complete.

Algorithm 1 Graph Imitation Learning (GIL).

procedure GIL($\mathbf{G}^{train}, \mathbf{G}^{eval}$)
    $\Theta =$ INITPARAMS() ▷ Randomly initialize policy $\hat{\pi}$ and underlying GNN.
    $\mathcal{D} =$ COLLECTDATASET($\mathbf{G}^{train}$)
    while true **do**
        $b =$ SAMPLEBATCH($\mathcal{D}$)
        update Θ by SGD($b, \mathcal{L}$) ▷ See Equation 2 for loss term.
        CHECKSTOPPINGCRITERION($\hat{\pi}, \mathbf{G}^{eval}$) ▷ Validate performance on held-out set.
    return policy $\hat{\pi}$

procedure COLLECTDATASET($\mathbf{G}^{train}$)
    for G in $\mathbf{G}^{train}$ **do**
        $S_0 =$ INITSTATE(G)
        while $|\mathcal{A}(S_t)| > 0$ **do**
            $d =$ RUNMCTS(S_t) ▷ Collect a demonstration by MCTS policy π.
            $\mathcal{D} = \mathcal{D} \cup \{d\}$ ▷ Add demonstration to dataset.
            $A_t =$ ROBUSTCHILD(d)
            $S_{t+1} = \mathcal{P}(S_t, A_t)$ ▷ Apply deterministic transition model.
            $t+=1$
    return $\mathcal{D}$

procedure RUNMCTS(S)
    create root node v from S
    for $i = 0$ to n_{sims} **do**
        $v_l =$ TREEPOLICY(v)
        $R =$ RANDOMDEFAULTPOLICY(v_l)
        BACKUP(v_l, R) ▷ Backup reward (proportional to objective f).
    $\mathbf{v} = [\,]$
    for a in $\mathcal{A}(S)$ **do** ▷ Construct vector of visit counts for all actions.
        $\mathbf{v}$.append($C(S, a)$)
    return $(S, \mathcal{A}(S), n, \mathbf{v})$

Table 2: Mean rewards obtained by the methods split by cost setting, graph model, objective function, and number of players.

c	**G**	f	n	Rand	TH	TLC	BR	PT	SA	UCT	GIL (ours)
HC	BA	F	15	0.757±0.005	0.814	0.785	0.753±0.006	0.797±0.016	0.825±0.001	**0.848**±0.000	0.845±0.001
			25	0.750±0.005	0.806	0.774	0.747±0.007	0.794±0.017	0.820±0.002	**0.842**±0.000	0.839±0.000
			50	0.742±0.007	0.797	0.773	0.741±0.005	0.788±0.016	0.811±0.001	**0.835**±0.000	0.832±0.001
			75	0.741±0.006	0.797	0.772	0.736±0.004	0.789±0.014	0.810±0.001	**0.831**±0.000	0.828±0.002
			100	0.737±0.005	0.796	0.767	0.732±0.004	0.787±0.012	0.808±0.001	**0.829**±0.000	0.826±0.001
		SW	15	0.708±0.007	0.793	0.738	0.702±0.009	0.763±0.020	0.806±0.001	**0.827**±0.000	0.825±0.000
			25	0.702±0.008	0.782	0.728	0.698±0.011	0.762±0.023	0.801±0.002	**0.820**±0.000	0.819±0.000
			50	0.694±0.010	0.774	0.726	0.691±0.007	0.756±0.021	0.791±0.001	**0.813**±0.000	0.811±0.000
			75	0.692±0.009	0.774	0.726	0.684±0.007	0.759±0.018	0.790±0.001	**0.809**±0.000	0.806±0.001
			100	0.688±0.008	0.774	0.720	0.680±0.007	0.757±0.016	0.788±0.001	**0.807**±0.001	0.804±0.001
	ER	F	15	0.806±0.004	0.839	0.861	0.807±0.002	0.839±0.007	0.849±0.002	**0.895**±0.000	0.892±0.001
			25	0.841±0.002	0.865	0.889	0.840±0.001	0.881±0.004	0.879±0.002	**0.925**±0.000	0.920±0.001
			50	0.893±0.001	0.909	0.934	0.892±0.001	0.930±0.001	0.924±0.001	**0.958**±0.000	0.954±0.000
			75	0.916±0.001	0.928	0.953	0.915±0.001	0.946±0.001	0.940±0.000	**0.970**±0.000	0.965±0.006
			100	0.930±0.001	0.940	0.962	0.930±0.001	0.957±0.001	0.951±0.001	**0.977**±0.000	0.969±0.011
		SW	15	0.782±0.004	0.823	0.841	0.782±0.001	0.820±0.008	0.836±0.002	**0.882**±0.000	0.878±0.001
			25	0.829±0.002	0.856	0.877	0.827±0.001	0.871±0.005	0.872±0.002	**0.918**±0.000	0.912±0.000
			50	0.887±0.001	0.905	0.931	0.887±0.001	0.927±0.002	0.921±0.001	**0.956**±0.000	0.948±0.002
			75	0.913±0.001	0.925	0.951	0.912±0.001	0.944±0.001	0.938±0.000	**0.969**±0.000	0.965±0.001
			100	0.928±0.001	0.939	0.960	0.928±0.001	0.955±0.001	0.950±0.001	**0.976**±0.000	0.971±0.002
	WS	F	15	0.818±0.007	0.817	0.868	0.814±0.005	0.833±0.007	0.848±0.006	**0.904**±0.002	0.903±0.000
			25	0.799±0.006	0.807	0.867	0.801±0.004	0.817±0.006	0.828±0.003	**0.891**±0.000	0.890±0.000
			50	0.801±0.002	0.805	0.864	0.801±0.003	0.819±0.005	0.830±0.001	**0.890**±0.000	**0.890**±0.000
			75	0.799±0.002	0.800	0.862	0.801±0.003	0.818±0.003	0.827±0.001	**0.886**±0.000	**0.886**±0.000
			100	0.800±0.001	0.802	0.863	0.801±0.002	0.818±0.004	0.828±0.001	0.887±0.000	**0.888**±0.000
		SW	15	0.795±0.009	0.797	0.850	0.790±0.006	0.811±0.008	0.832±0.008	**0.889**±0.002	0.888±0.000
			25	0.775±0.008	0.784	0.847	0.779±0.005	0.797±0.007	0.812±0.003	**0.875**±0.000	0.873±0.001
			50	0.778±0.003	0.784	0.845	0.780±0.005	0.799±0.005	0.815±0.001	**0.876**±0.000	0.875±0.000
			75	0.777±0.002	0.779	0.843	0.780±0.003	0.798±0.003	0.812±0.001	**0.871**±0.000	**0.871**±0.000
			100	0.778±0.001	0.781	0.844	0.780±0.003	0.798±0.004	0.813±0.001	0.871±0.000	**0.872**±0.000
IC	BA	F	15	0.837±0.001	0.851	—	0.837±0.001	0.846±0.005	**0.855**±0.000	**0.855**±0.000	**0.855**±0.000
			25	0.835±0.001	0.845	—	0.835±0.000	0.844±0.006	0.851±0.000	**0.852**±0.000	0.850±0.000
			50	0.832±0.000	0.842	—	0.832±0.000	0.840±0.006	**0.848**±0.000	0.846±0.000	0.845±0.001
			75	0.832±0.001	0.841	—	0.832±0.001	0.839±0.005	**0.846**±0.000	0.843±0.000	0.843±0.001
			100	0.831±0.001	0.840	—	0.832±0.001	0.838±0.004	**0.844**±0.000	0.840±0.000	0.842±0.001
		SW	15	0.710±0.008	0.794	—	0.703±0.010	0.760±0.021	0.805±0.001	**0.807**±0.000	**0.807**±0.000
			25	0.702±0.009	0.779	—	0.698±0.010	0.759±0.023	0.799±0.001	**0.800**±0.000	**0.800**±0.000
			50	0.695±0.008	0.776	—	0.692±0.007	0.756±0.020	0.792±0.001	**0.793**±0.000	**0.793**±0.001
			75	0.689±0.009	0.774	—	0.682±0.006	0.756±0.017	0.789±0.001	**0.790**±0.000	**0.790**±0.001
			100	0.687±0.008	0.772	—	0.679±0.006	0.755±0.016	0.785±0.001	**0.786**±0.000	**0.786**±0.001
	ER	F	15	0.844±0.001	0.860	—	0.844±0.001	0.855±0.003	0.868±0.001	**0.873**±0.000	0.872±0.000
			25	0.865±0.001	0.880	—	0.864±0.001	0.881±0.001	0.892±0.001	**0.899**±0.000	0.898±0.001
			50	0.901±0.001	0.916	—	0.900±0.001	0.918±0.000	0.927±0.000	**0.932**±0.000	0.931±0.000
			75	0.921±0.000	0.931	—	0.921±0.000	0.935±0.000	0.943±0.000	**0.948**±0.000	0.943±0.006
			100	0.934±0.001	0.943	—	0.934±0.001	0.945±0.000	0.953±0.000	**0.957**±0.000	0.951±0.006
		SW	15	0.780±0.002	0.818	—	0.777±0.002	0.807±0.007	0.834±0.001	**0.843**±0.000	0.841±0.000
			25	0.829±0.002	0.855	—	0.827±0.001	0.856±0.002	0.873±0.001	**0.884**±0.000	0.882±0.001
			50	0.886±0.001	0.906	—	0.885±0.001	0.909±0.001	0.920±0.000	**0.926**±0.000	0.922±0.002
			75	0.912±0.001	0.925	—	0.912±0.001	0.930±0.000	0.939±0.000	**0.944**±0.000	0.942±0.002
			100	0.928±0.001	0.939	—	0.928±0.001	0.942±0.000	0.950±0.000	**0.954**±0.000	0.951±0.004
	WS	F	15	0.843±0.003	0.844	—	0.841±0.003	0.846±0.003	0.856±0.002	0.864±0.001	**0.865**±0.001
			25	0.841±0.002	0.843	—	0.843±0.002	0.848±0.002	0.856±0.001	0.861±0.000	**0.863**±0.000
			50	0.841±0.001	0.843	—	0.842±0.002	0.846±0.002	0.856±0.000	0.861±0.000	**0.864**±0.000
			75	0.841±0.000	0.842	—	0.842±0.001	0.847±0.001	0.856±0.000	0.861±0.000	**0.864**±0.000
			100	0.842±0.001	0.843	—	0.842±0.001	0.846±0.001	0.856±0.000	0.860±0.000	**0.864**±0.000
		SW	15	0.779±0.007	0.783	—	0.774±0.007	0.790±0.007	0.812±0.004	**0.829**±0.001	0.828±0.002
			25	0.775±0.006	0.781	—	0.782±0.006	0.794±0.006	0.812±0.002	0.823±0.000	**0.826**±0.000
			50	0.777±0.003	0.782	—	0.778±0.005	0.791±0.005	0.813±0.001	0.824±0.000	**0.829**±0.001
			75	0.777±0.001	0.780	—	0.780±0.003	0.792±0.003	0.812±0.001	0.822±0.000	**0.828**±0.001
			100	0.778±0.002	0.781	—	0.779±0.003	0.791±0.003	0.812±0.000	0.821±0.000	**0.828**±0.000

Table 3: Win rates (%) for the different methods.

c	**G**	f	n	Rand	TH	TLC	BR	PT	SA	UCT	GIL (ours)
HC	BA	F	15	1.800	1.000	0.400	0.900	17.100	9.300	**43.100**	26.400
			25	0.400	0.300	0.400	0.100	20.200	5.000	**47.900**	**25.700**
			50	0.000	0.000	0.000	0.000	12.900	2.300	**62.800**	22.000
			75	0.000	0.000	0.100	0.000	13.400	0.800	**66.400**	19.300
			100	0.000	0.000	0.000	0.000	11.200	0.700	**73.800**	14.300
		SW	15	1.800	0.700	0.400	0.900	18.400	12.000	**39.500**	26.300
			25	0.300	0.100	0.400	0.300	20.600	8.900	**41.500**	27.900
			50	0.100	0.000	0.000	0.000	14.900	3.600	**60.800**	20.600
			75	0.100	0.100	0.100	0.000	15.400	2.200	**62.600**	19.500
			100	0.000	0.000	0.000	0.000	13.000	2.000	**68.400**	16.600
	ER	F	15	0.900	0.100	1.100	0.900	7.700	5.200	**54.600**	29.500
			25	0.300	0.000	0.200	0.100	5.000	2.400	**64.800**	**27.200**
			50	0.000	0.000	0.600	0.000	3.100	0.900	**65.500**	29.900
			75	0.000	0.000	0.600	0.000	1.700	0.200	**64.400**	33.100
			100	0.000	0.000	0.300	0.000	1.200	0.400	**67.800**	30.300
		SW	15	0.800	0.200	1.100	0.600	7.300	5.700	**53.800**	30.500
			25	0.200	0.100	0.500	0.100	4.900	2.400	**60.600**	31.200
			50	0.000	0.000	0.800	0.000	2.700	1.500	**74.800**	20.200
			75	0.000	0.000	0.500	0.000	1.700	0.100	**69.000**	**28.700**
			100	0.000	0.000	0.200	0.000	1.400	0.000	**73.500**	24.900
	WS	F	15	0.300	0.000	0.800	0.200	0.700	3.100	**58.200**	36.700
			25	0.000	0.000	0.600	0.000	0.500	0.500	**57.200**	41.200
			50	0.000	0.000	0.100	0.000	0.000	0.000	**55.700**	44.200
			75	0.000	0.000	0.000	0.000	0.000	0.000	**50.700**	49.300
			100	0.000	0.000	0.000	0.000	0.000	0.000	43.700	**56.300**
		SW	15	0.600	0.000	0.700	0.300	0.900	3.100	**55.800**	38.600
			25	0.000	0.000	0.500	0.000	0.400	1.200	**61.600**	36.300
			50	0.000	0.000	0.000	0.000	0.000	0.000	**60.600**	39.400
			75	0.000	0.000	0.000	0.000	0.000	0.000	49.800	**50.200**
			100	0.000	0.000	0.000	0.000	0.000	0.000	47.200	**52.800**
IC	BA	F	15	4.500	1.400	—	3.100	18.200	24.700	**25.100**	23.000
			25	2.100	0.400	—	2.200	22.800	22.900	**31.700**	17.900
			50	0.400	1.200	—	0.600	21.400	**34.000**	25.400	17.000
			75	0.200	0.800	—	0.300	20.300	**40.200**	20.500	17.700
			100	0.000	0.100	—	0.100	21.700	**48.200**	14.900	15.000
		SW	15	1.900	1.800	—	1.600	19.200	24.200	25.600	**25.700**
			25	0.600	0.900	—	0.400	22.800	24.600	**27.200**	23.500
			50	0.100	0.600	—	0.000	21.200	24.300	**27.600**	26.200
			75	0.000	0.300	—	0.000	20.200	25.800	**25.100**	**28.600**
			100	0.000	0.000	—	0.000	21.500	24.500	25.300	**28.700**
	ER	F	15	2.300	1.000	—	2.400	9.600	20.300	**35.300**	29.100
			25	0.600	0.300	—	0.000	6.800	19.200	**39.600**	33.500
			50	0.000	0.100	—	0.000	1.900	17.000	**43.600**	37.400
			75	0.000	0.100	—	0.000	1.500	15.000	**57.200**	26.200
			100	0.000	0.100	—	0.000	0.500	14.000	**55.700**	29.700
		SW	15	2.300	0.800	—	1.700	10.000	19.600	**35.100**	30.500
			25	0.800	0.500	—	0.300	7.500	18.700	**42.100**	30.100
			50	0.200	0.400	—	0.100	3.800	18.500	**49.000**	28.000
			75	0.000	0.200	—	0.000	1.200	12.600	**49.600**	36.400
			100	0.000	0.100	—	0.000	0.700	13.100	**54.400**	**31.700**
	WS	F	15	1.200	0.000	—	0.200	1.500	12.800	37.500	**46.800**
			25	0.200	0.000	—	1.200	2.500	14.800	36.200	**45.100**
			50	0.000	0.000	—	0.000	0.100	3.700	**27.200**	**69.000**
			75	0.000	0.000	—	0.000	0.000	1.300	18.400	**80.300**
			100	0.000	0.000	—	0.000	0.000	0.400	9.700	**89.900**
		SW	15	0.700	0.100	—	1.000	2.300	15.400	**41.400**	39.100
			25	0.000	0.100	—	1.100	2.000	13.200	34.900	**48.700**
			50	0.000	0.000	—	0.000	0.100	2.800	**27.200**	**69.900**
			75	0.000	0.000	—	0.000	0.000	1.600	19.000	**79.400**
			100	0.000	0.000	—	0.000	0.000	0.600	12.000	**87.400**