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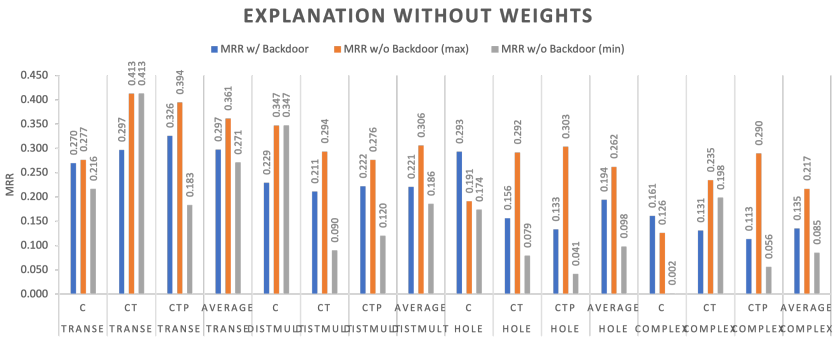
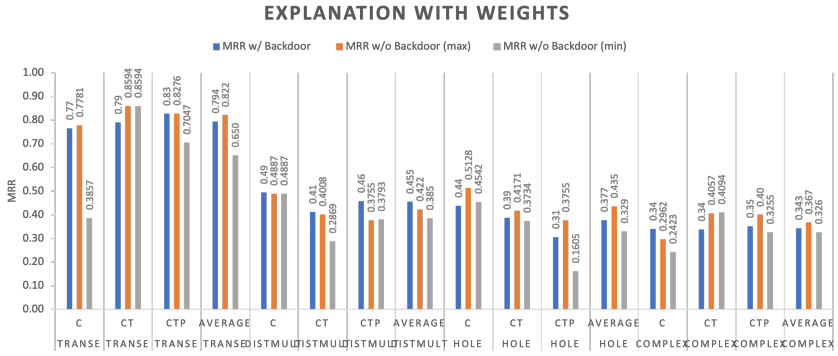
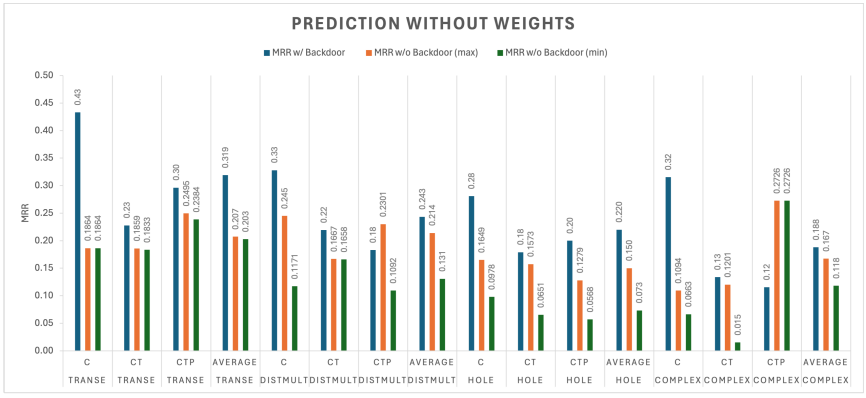
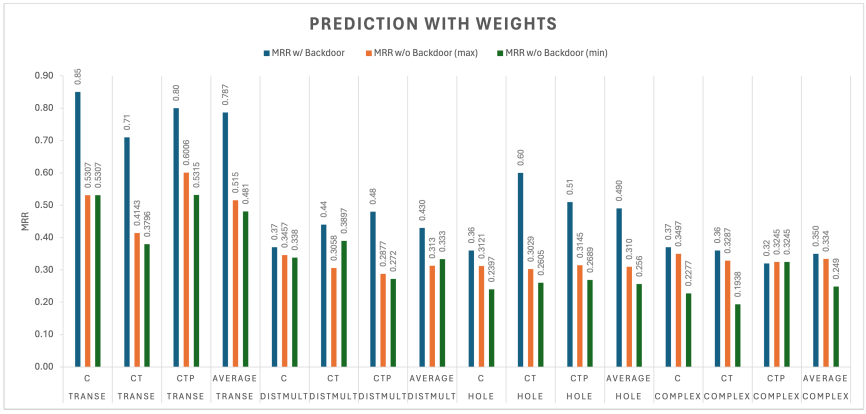
A Figures









B Hyper-parameters

Hyperparameters for Back2CausalDisco for its six trained KGE models

KG subgraph structure Optimizer Params	Model	Batches Count	Seed	Epochs	K	Eta	Loss	Regularizer	Regularizer Params	Optimizer
C {"lr": 0.005419994971545206}	TransE	100	0	500	200	15	multiclass_nll	LP	{"p": 3, "lambda": 1e-05}	adam
{"lr": 0.009073539061895694}	DistMult	100	0	500	200	10	nll	LP	{"p": 1, "lambda": 1e-05}	adam
{"lr": 0.006804906722850427}	HolE	100	0	100	100	5	multiclass_nll	LP	{"p": 3, "lambda": 0.0001}	adam
{"lr": 0.006956062741769883}	ComplEx	100	0	500	100	5	nll	LP		adam
CT {"lr": 0.0003679829492941821}	TransE	100	0	500	100	15	multiclass_nll	LP	{"p": 1, "lambda": 0.0001}	adam
{"lr": 0.005470737872602935}	DistMult	100	0	300	200	15	nll			adam
{"lr": 0.007873013829029064}	HolE	100	0	200	200	15	nll			adam
{"lr": 0.0036637828383358027}	ComplEx	100	0	300	100	10	nll			adam
CTP {"lr": 0.0022465391625126744}	TransE	100	0	300	200	15	nll			adam
{"lr": 0.009050039489719481}	DistMult	100	0	300	200	10	nll			adam
{"lr": 0.002808066144674794}	HolE	100	0	500	200	15	multiclass_nll	LP	{"p": 3, "lambda": 0.0001}	adam
{"lr": 0.0031153621036914864}	ComplEx	100	0	100	100	10	nll	LP	{"p": 3, "lambda": 1e-05}	adam

Table 3. Hyper-parameters for CausalKG-SufficientBackdoor for causal explanation for different subgraph structures and knowledge graph embedding models

KG subgraph structure	Model	Batches Count	Seed	Epochs	K	Eta	Loss	Regularizer	Optimizer
C	TransE	100	0	500	100	15	multiclass_nll	LP	adam
	DistMult	100	0	300	200	10	nll	LP	adam
	HolE	100	0	200	200	15	nll		adam
	ComplEx	100	0	500	200	15	nll		adam
CT	TransE	100	0	500	100	15	multiclass_nll	LP	adam
	DistMult	100	0	500	200	5	nll	LP	adam
	HolE	100	0	500	100	5	nll		adam
	ComplEx	100	0	300	200	15	nll		adam
CTP	TransE	100	0	300	100	5	multiclass_nll	LP	adam
	DistMult	100	0	300	100	15	multiclass_nll		adam
	HolE	100	0	500	100	5	nll		adam
	ComplEx	100	0	500	200	5	nll	LP	adam

Table 4. Hyper-parameters for CausalKG-SufficientBackdoor for causal prediction for different subgraph structures and knowledge graph embedding models

KG subgraph structure	Model	Batches Count	Seed	Epochs	K	Eta	Learning Rate
			C				
TransE	100	0	200	200	10	nll	0.003861276863411193
DistMult	100	0	500	200	10	nll	0.009073539061895694
HolE	100	0	500	200	15	multiclass_nll	0.002808066144674794
ComplEx	100	0	300	200	5	multiclass_nll	0.00023104489181310494
			CT				
TransE	100	0	500	100	15	multiclass_nll	0.0003679829492941821
DistMult	100	0	500	100	15	nll	0.0030317879554692347
HolE	100	0	500	200	15	nll	0.008303703454101804
ComplEx	100	0	500	100	15	nll	0.0030317879554692347
			CTP				
TransE	100	0	500	100	15	multiclass_nll	0.0003679829492941821
DistMult	100	0	500	200	15	nll	0.00964026132896019
HolE	100	0	300	200	10	nll	0.009050039489719481
ComplEx	100	0	500	200	5	nll	0.008411178371514666

Table 5. Hyper-parameters for CausalKG-BackdoorMaximum for causal explanation for different subgraph structures and knowledge graph embedding models

KG subgraph structure	Model	Batches Count	Seed	Epochs	K	Eta	Learning Rate
			C				
TransE	100	0	500	100	15	multiclass_nll	0.0003679829492941821
DistMult	100	0	500	100	5	nll	0.008926074507168386
HolE	100	0	300	200	15	nll	0.005470737872602935
ComplEx	100	0	300	200	10	nll	0.0010649400183823498
			CT				
TransE	100	0	200	100	5	multiclass_nll	0.0065626241383543605
DistMult	100	0	500	200	15	nll	0.009568416655679894
HolE	100	0	200	100	10	nll	0.009593928946448388
ComplEx	100	0	300	200	10	nll	0.0010649400183823498
			CTP				
TransE	100	0	500	100	15	multiclass_nll	0.0003679829492941821
DistMult	100	0	300	200	15	multiclass_nll	0.003988569481398215
HolE	100	0	200	200	15	nll	0.00823896555862303
ComplEx	100	0	500	200	5	nll	0.008411178371514666

Table 6. Hyper-parameters for CausalKG-BackdoorMaximum for causal prediction for different subgraph structures and knowledge graph embedding models

KG subgraph structure	Model	Batches	Count	Seed	Epochs	K	Eta	Learning Rate
			C					
	TransE	100	0	100	200	15	nll	0.007764913525398746
	DistMult	100	0	500	200	5	nll	0.008411178371514666
	HolE	100	0	100	200	5	nll	0.00870793645241166
	ComplEx	100	0	500	100	5	nll	0.006956062741769883
			CT					
	TransE	100	0	100	200	5	nll	0.00870793645241166
	DistMult	100	0	500	200	15	nll	0.00964026132896019
	HolE	100	0	100	200	5	nll	0.00870793645241166
	ComplEx	100	0	500	100	5	nll	0.008926074507168386
			CTP					
	TransE	100	0	200	200	15	nll	0.00823896555862303
	DistMult	100	0	500	200	15	nll	0.008303703454101804
	HolE	100	0	500	100	5	nll	0.009595749370048702
	ComplEx	100	0	300	100	5	nll	0.00259421578363632

Table 7. Hyper-parameters for CausalKG-WithBackdoor for causal explanation for different subgraph structures and knowledge graph embedding models

KG subgraph structure	Model	Batches	Count	Seed	Epochs	K	Eta	Learning Rate
			C					
	TransE	100	0	500	100	15	multiclass_nll	0.0003679829492941821
	DistMult	100	0	500	200	15	nll	0.008303703454101804
	HolE	100	0	500	200	15	nll	0.00964026132896019
	ComplEx	100	0	500	200	10	nll	0.009073539061895694
			CT					
	TransE	100	0	300	200	15	nll	0.005470737872602935
	DistMult	100	0	500	100	5	nll	0.008926074507168386
	HolE	100	0	500	100	5	multiclass_nll	0.0035189816388993367
	ComplEx	100	0	500	200	5	nll	0.008411178371514666
			CTP					
	TransE	100	0	100	200	5	nll	0.004716476651277433
	DistMult	100	0	100	200	5	nll	0.0022117885759380717
	HolE	100	0	200	200	5	multiclass_nll	0.008342936470924586
	ComplEx	100	0	300	200	5	multiclass_nll	0.00023104489181310494

Table 8. Hyper-parameters for CausalKG-WithBackdoor for causal prediction for different subgraph structures and knowledge graph embedding models