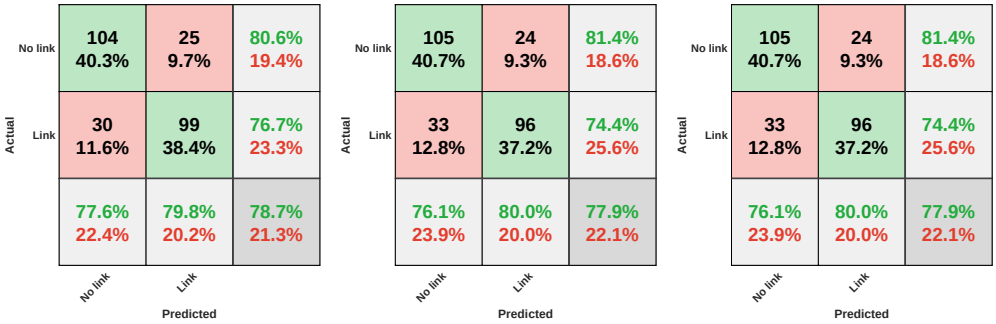
A Hyper-parameter Exploration

Table 1: Hyperparameter list, and values, for all tested Knowledge Graph Embeddings and Graph Neural Network models.

Families	Models	Parameters	Values
KGE	DistMult	*Embedding*	64, 128, 256, 512
		Learning Rate	1.0, 0.5, 0.2, 0.1, 0.05, 0.02, 0.01
		Regularization	1e-7, 1e-5, 1e-3
		Optimizer	AdaGrad
	CP	*Embedding*	64, 128, 256, 512
		Learning Rate	1.0, 0.5, 0.2, 0.1, 0.05, 0.02, 0.01
		Regularization	1e-7, 1e-5, 1e-3
		Optimizer	AdaGrad
	ComplEx	*Embedding*	64, 128, 256, 512
		Learning Rate	1.0, 0.5, 0.2, 0.1, 0.05, 0.02, 0.01
		Regularization	1e-7, 1e-5, 1e-3
		Optimizer	AdaGrad
	ConvE	*Embedding*	64, 128, 256, 512
		Learning Rate	0.001, 0.003
		Regularization	1e-7, 1e-5, 1e-3
		First Shape	16
		Optimizer	Adam
GNN	GCN	*Embedding*	64
		Convolutions	[64, 64], [64, 64, 64]
		Dense	32
		Learning Rate	1e-4, 3e-4, 5e-4, ..., 1e-2, 3e-2, 5e-2
		Regularization	1e-7, 1e-5, 1e-3
		Normalize	True
	GraphSAGE	*Embedding*	64
		Convolutions	64
		Dense	32
		Learning Rate	1e-4, 3e-4, 5e-4, ..., 1e-2, 3e-2, 5e-2
		Regularization	1e-7, 1e-5, 1e-3
		Normalize	True
		Root Weight	True
		Project	True
	GAT	*Embedding*	64
		Convolutions	[64, 64], [64, 64, 64]
		Dense	32
		Learning Rate	1e-4, 3e-4, 5e-4, ..., 1e-2, 3e-2, 5e-2
		Regularization	[1e-7, 1e-5, 1e-3]
		Heads	[4, 8]
	GIN	*Embedding*	64
		Convolutions	[64, 64], [64, 64, 64]
		Dense	[32, 32], [32, 32, 32]
		Learning Rate	1e-4, 3e-4, 5e-4, ..., 1e-2, 3e-2, 5e-2
		Regularization	1e-7, 1e-5, 1e-3
		Epsilon	0.0
		Train Epsilon	True

B Confusion Matrices

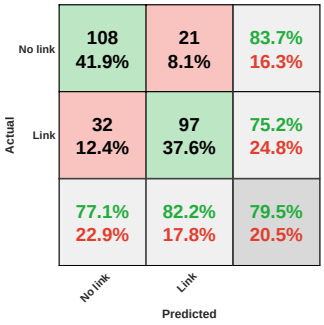
Fig. 1: Confusion Matrices for the Inductive Setting (Adam Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



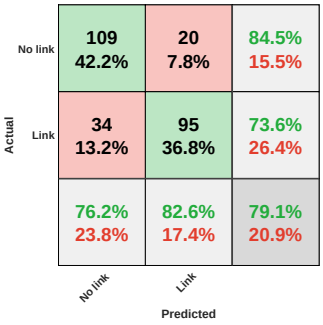
(a) ConvE

(b) GAT

(c) GCN

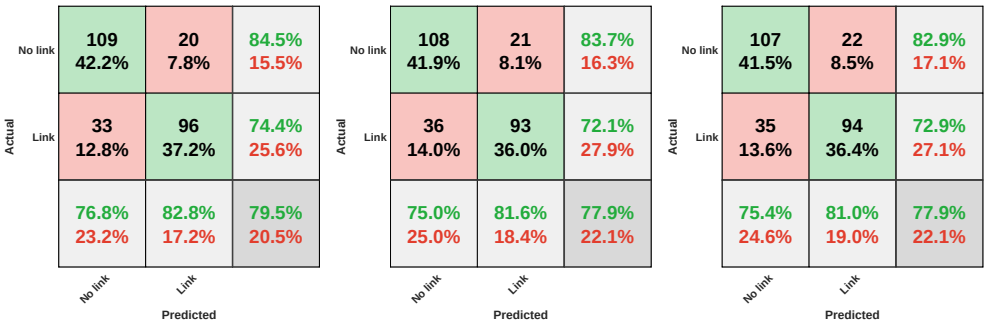


(d) GIN



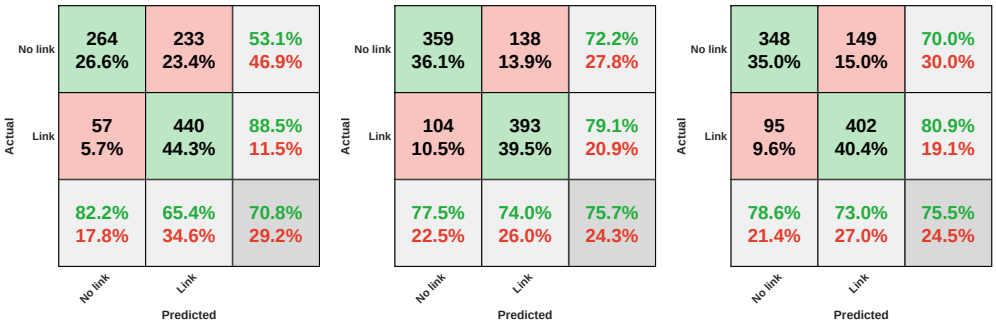
(e) GraphSAGE

Fig. 2: Confusion Matrices for the Inductive Setting (AdaGrad Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



(a) ComplEx (b) CP (c) DistMult

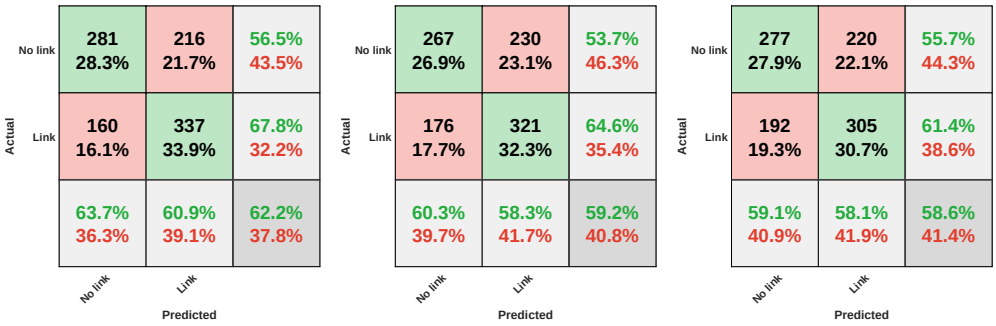
Fig. 3: Confusion Matrices for Drug–Disease (Adam Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



(a) ConvE (b) GAT (c) GCN

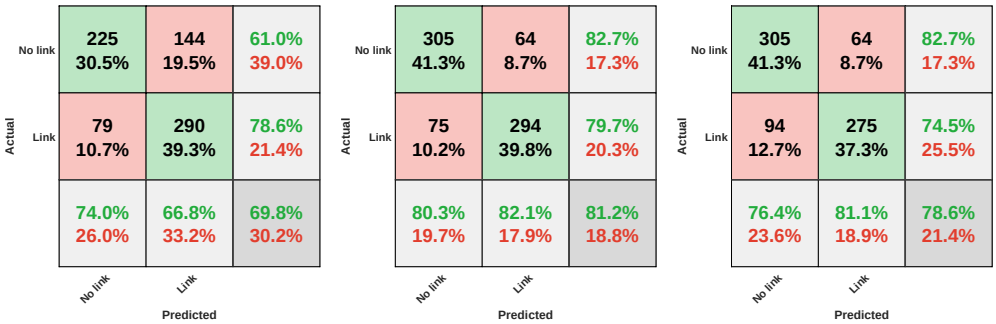
(d) GIN (e) GraphSAGE

Fig. 4: Confusion Matrices for Drug–Disease (AdaGrad Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



(a) ComplEx (b) CP (c) DistMult

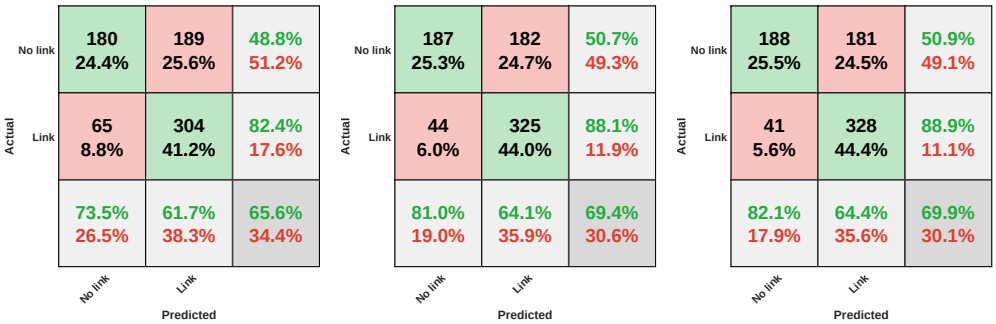
Fig. 5: Confusion Matrices for Drug–Target (Adam Optimizer).Green shades indicate correct classifications, whereas red shades indicate misclassifications.



(a) ConvE (b) GAT (c) GCN

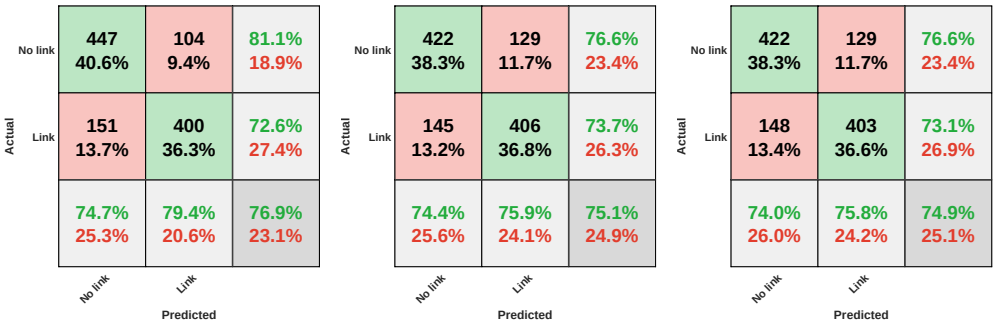
(d) GIN (e) GraphSAGE

Fig. 6: Confusion Matrices for Drug–Target (AdaGrad Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



(a) ComplEx (b) CP (c) DistMult

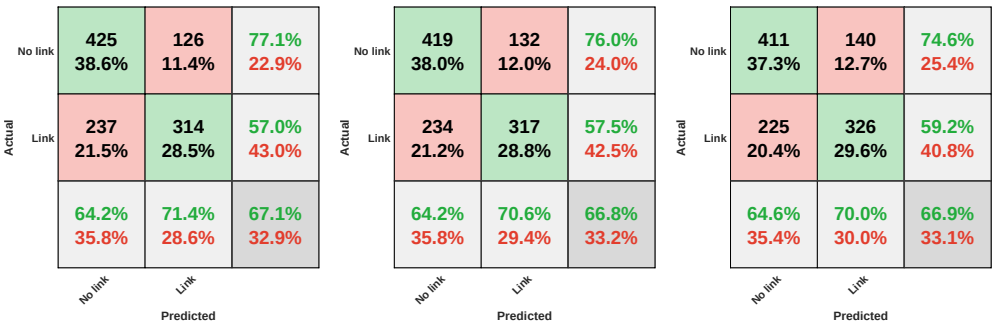
Fig. 7: Confusion Matrices for Patients–Disease (Adam Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



(a) ConvE (b) GAT (c) GCN

(d) GIN (e) GraphSAGE

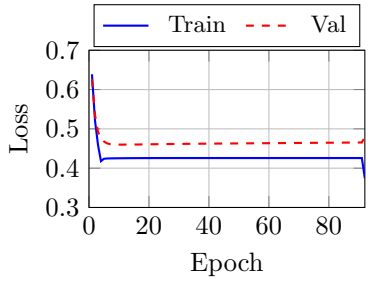
Fig. 8: Confusion Matrices for Patients–Disease (AdaGrad Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.



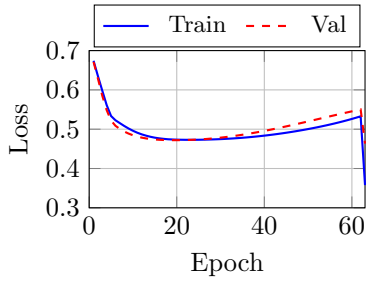
(a) ComplEx (b) CP (c) DistMult

C Additional Material: Training Loss Curves

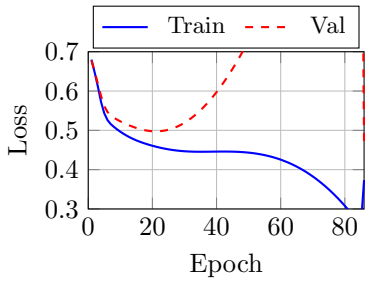
In this appendix, we report the complete training loss trends for all evaluated models across the different experimental settings. These figures complement the quantitative results presented in Section 4, offering insight into convergence stability and generalization behavior.



(a) ComplEx model.

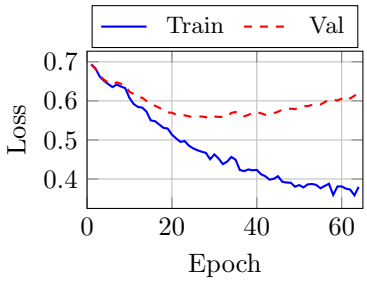


(b) CP model.

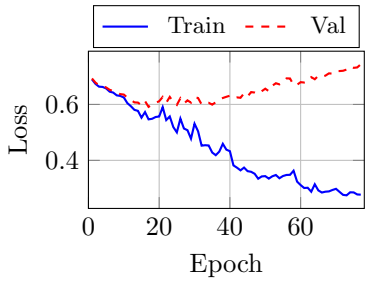


(c) DistMult model.

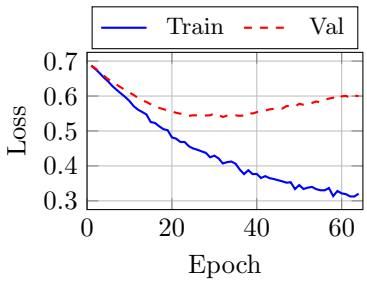
Fig. 9: Training and validation loss curves for inductive KGE models (ComplEx, CP, and DistMult) on the Patients–Diseases dataset using AdaGrad optimizer.



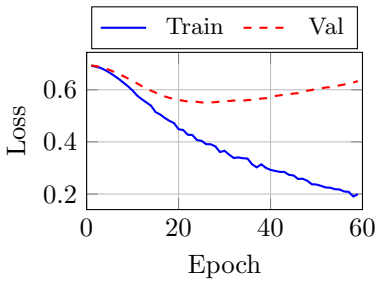
(a) GAT model.



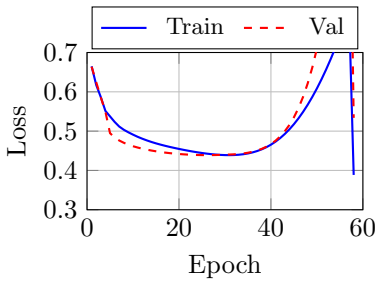
(b) GIN model.



(c) GCN model.

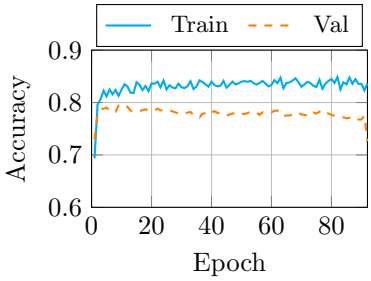


(d) SAGE model.

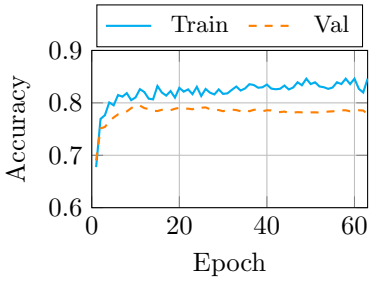


(e) ConvE model.

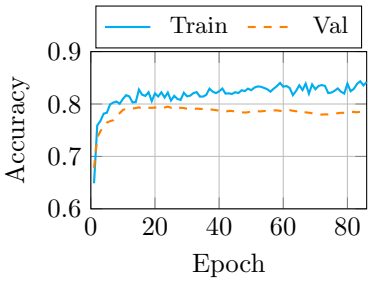
Fig. 10: Training and validation loss curves for inductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Disease dataset using Adam optimizer.



(a) ComplEx model.

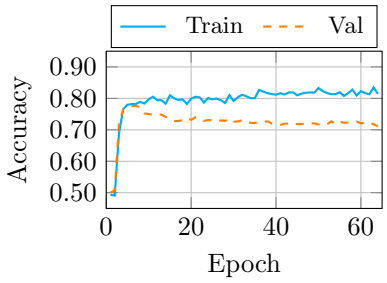


(b) CP model.

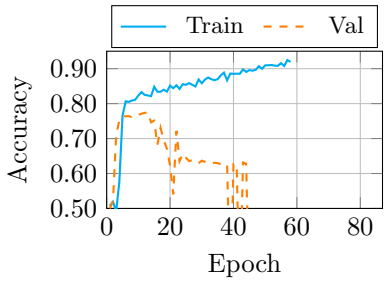


(c) DistMult model.

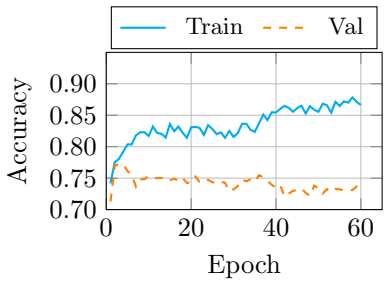
Fig. 11: Training and validation accuracy curves for inductive KGE models (ComplEx, CP, and DistMult) on the Patients–Diseases dataset using AdaGrad optimizer.



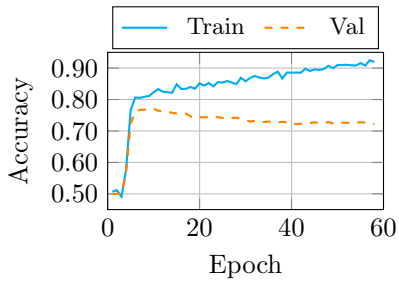
(a) GAT model.



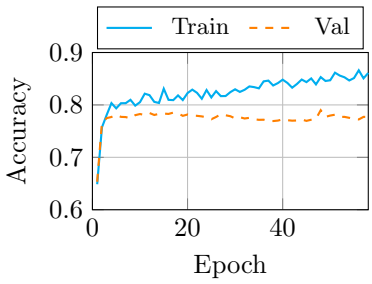
(b) GIN model.



(c) GCN model.

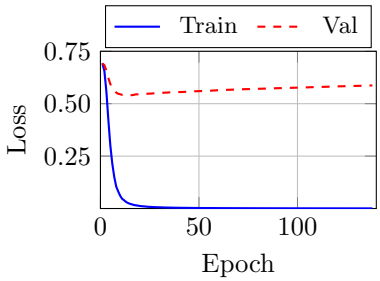


(d) SAGE model.

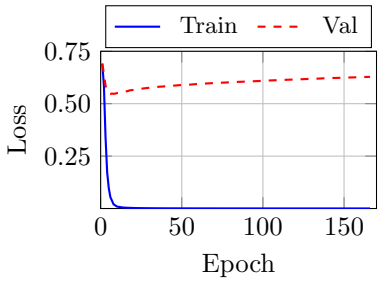


(e) ConvE model.

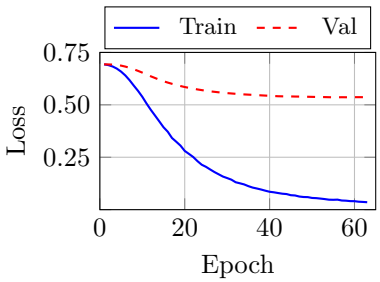
Fig. 12: Training and validation accuracy curves for inductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Patient_Disease dataset using Adam optimizer.



(a) ComplEx model.

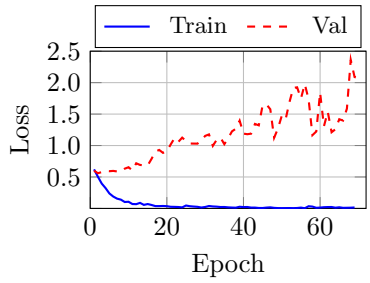


(b) CP model.

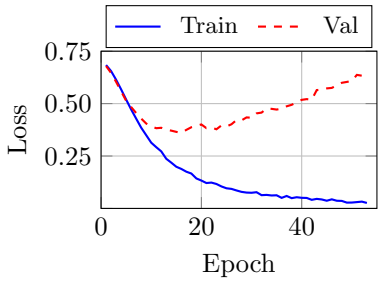


(c) DistMult model.

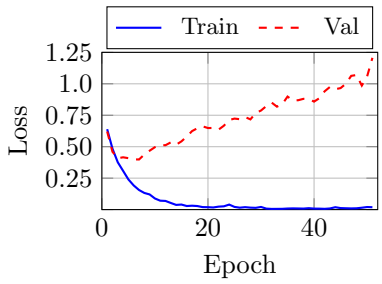
Fig. 13: Training and validation loss curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Target dataset using Adagrad optimizer.



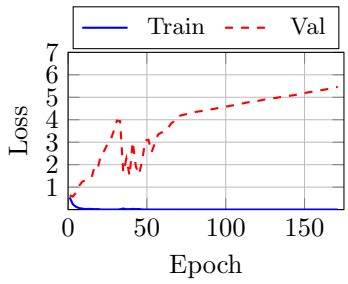
(a) GAT model.



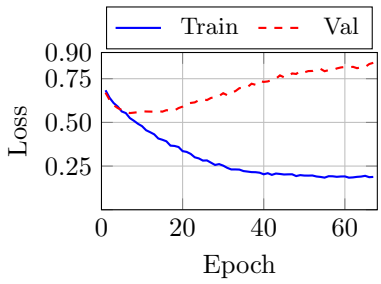
(b) GIN model.



(c) GCN model.

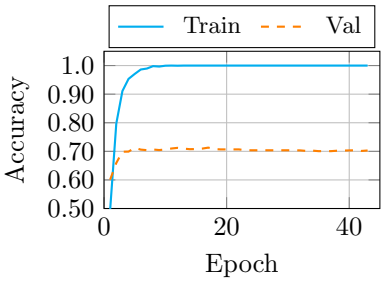


(d) SAGE model.

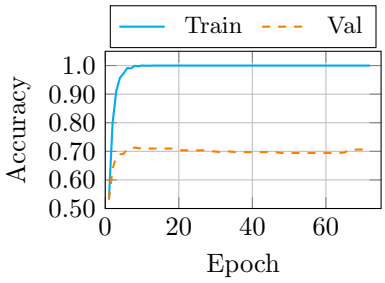


(e) ConvE model.

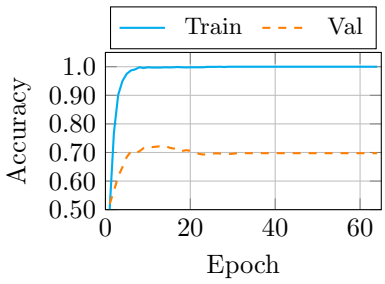
Fig. 14: Training and validation loss curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Target dataset using Adam optimizer.



(a) ComplEx model.

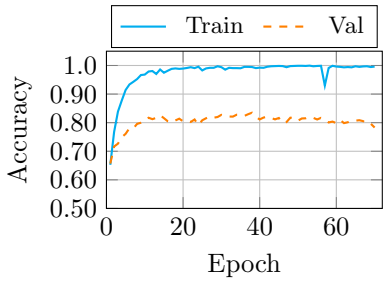


(b) CP model.

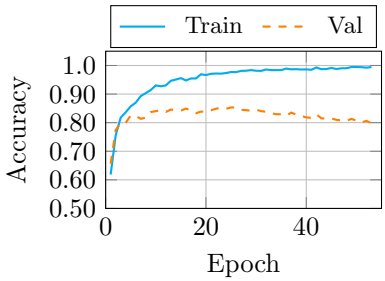


(c) DistMult model.

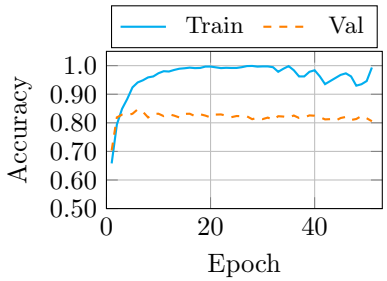
Fig. 15: Training and validation accuracy curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Target dataset using Adagrad optimizer.



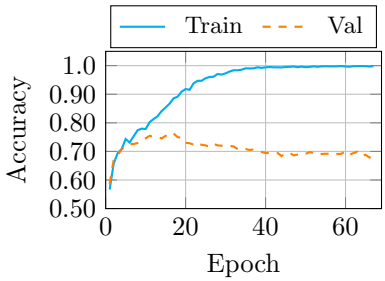
(a) GAT model.



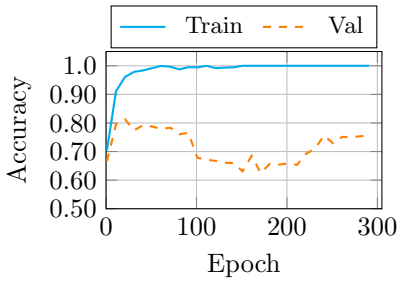
(b) GIN model.



(c) GCN model.

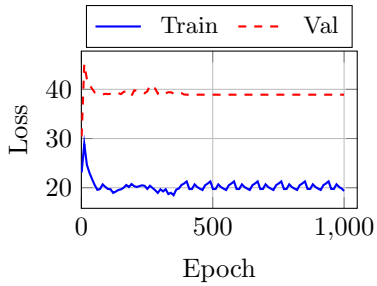


(d) ConvE model.

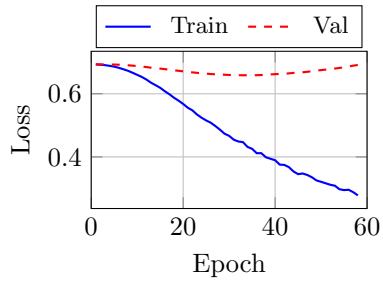


(e) SAGE model.

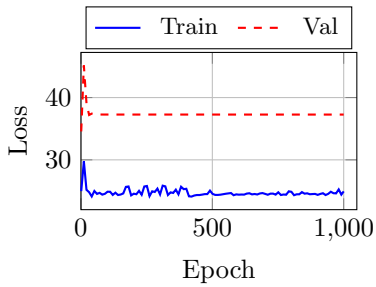
Fig. 16: Training and validation accuracy curves for transductive GNN models (GAT, GIN, GCN, ConvE, and SAGE) on the Drug_Target dataset using Adam optimizer. All data extracted from real files.



(a) ComplEx model.

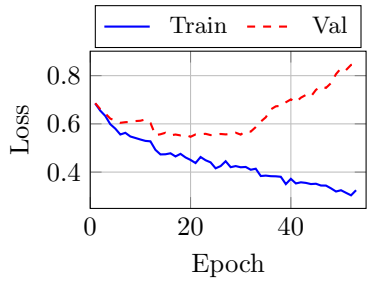


(b) CP model.

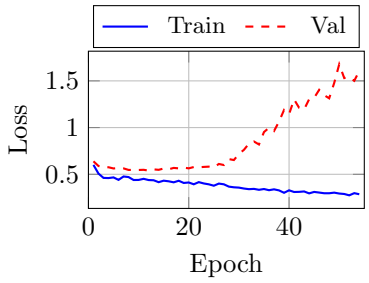


(c) DistMult model.

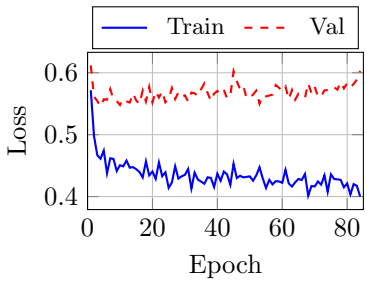
Fig. 17: Training and validation loss curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Disease dataset using Adagrad optimizer.



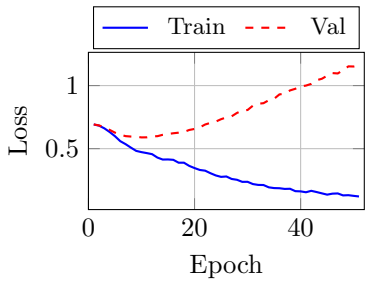
(a) GAT model.



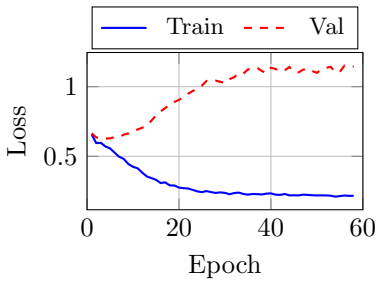
(b) GIN model.



(c) GCN model.

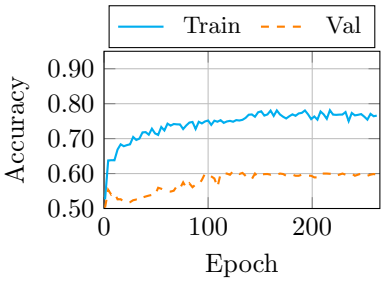


(d) SAGE model.

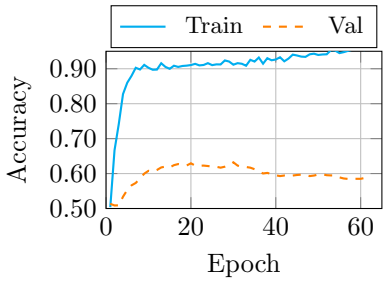


(e) ConvE model.

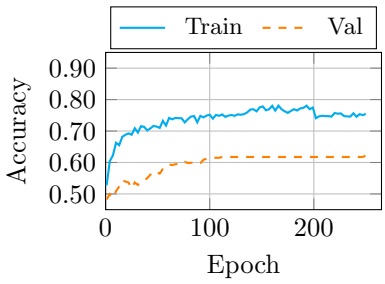
Fig. 18: Training and validation loss curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Disease dataset using Adam optimizer.



(a) ComplEx model.

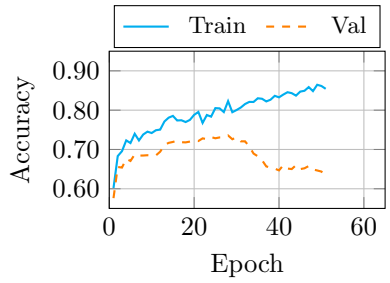


(b) CP model.

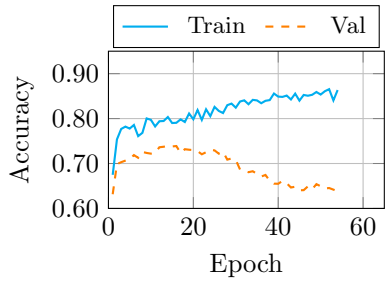


(c) DistMult model.

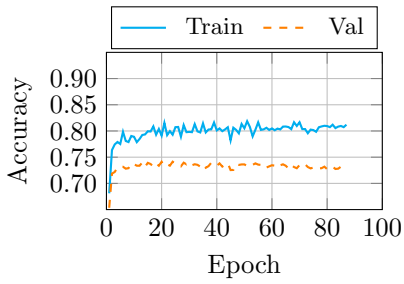
Fig. 19: Training and validation accuracy curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Disease dataset using Adagrad optimizer.



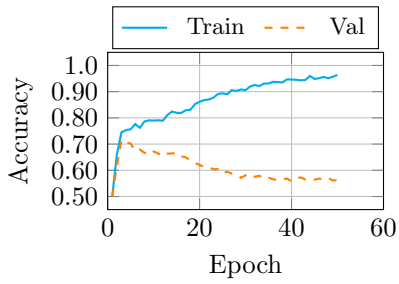
(a) GAT model.



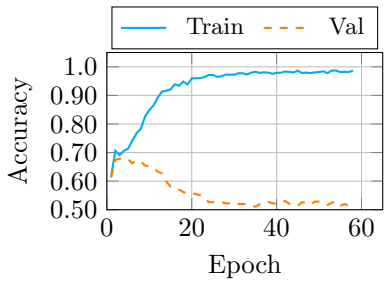
(b) GIN model.



(c) GCN model.

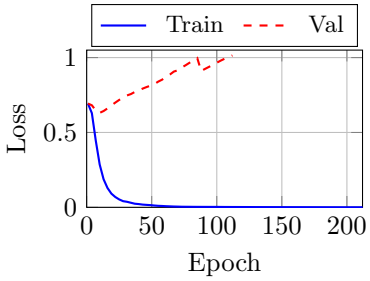


(d) SAGE model.

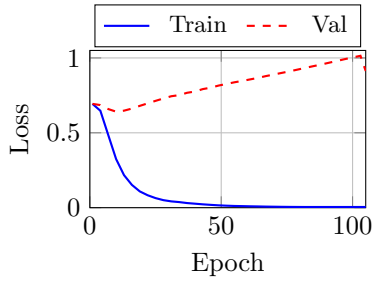


(e) ConvE model.

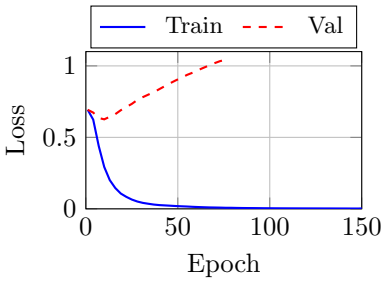
Fig. 20: Training and validation accuracy curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Disease dataset using Adam optimizer.



(a) ComplEx model.

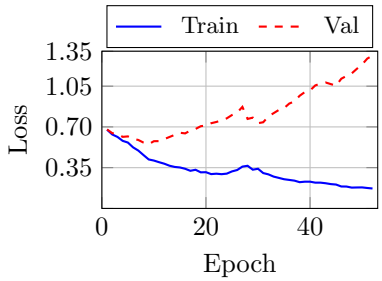


(b) CP model.

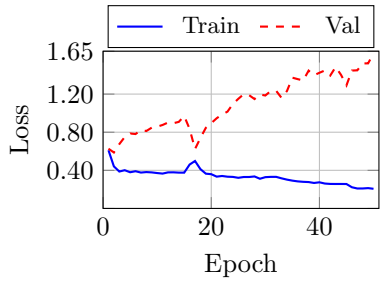


(c) DistMult model.

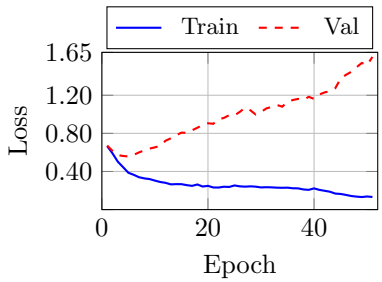
Fig. 21: Updated training and validation loss curves for Patients–Diseases using the new best checkpoints (sampled every 3 epochs).



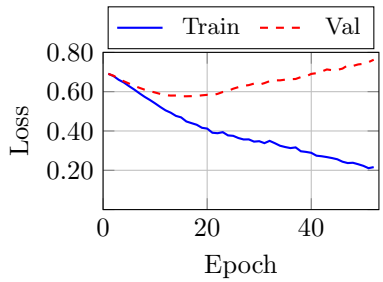
(a) GAT model.



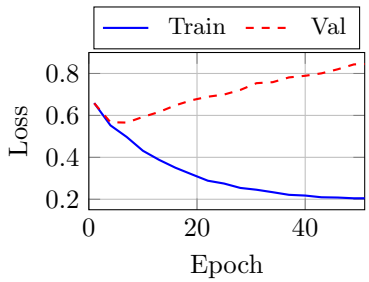
(b) GIN model.



(c) GCN model.

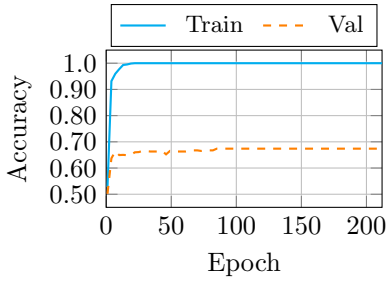


(d) SAGE model.

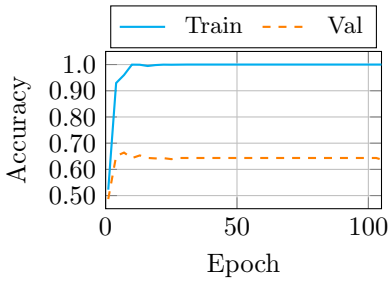


(e) ConvE model.

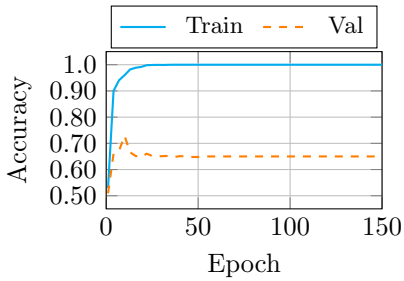
Fig. 22: Training and validation loss curves for inductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Patient_Disease dataset using Adam optimizer.



(a) ComplEx model.

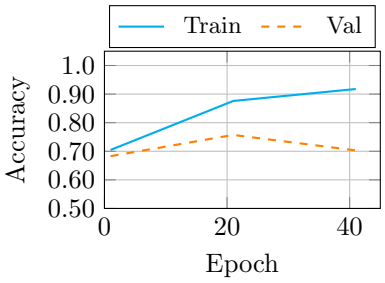


(b) CP model.

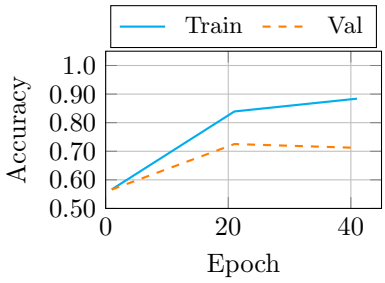


(c) DistMult model.

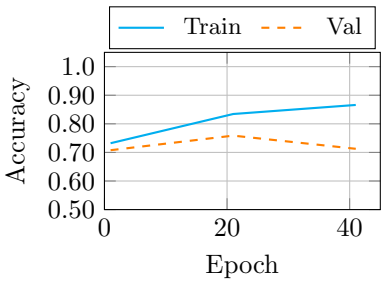
Fig. 23: Updated accuracy curves (Train/Val) from the new checkpoints.



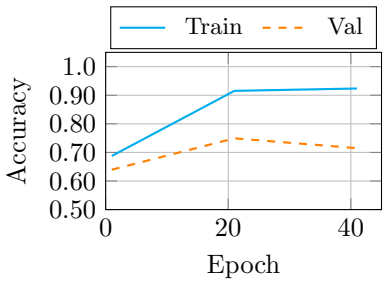
(a) GAT model.



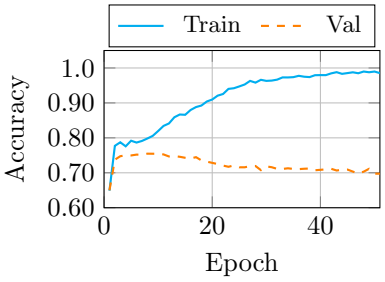
(b) SAGE model.



(c) GIN model.



(d) GCN model.



(e) ConvE model.

Fig. 24: Training and validation accuracy curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Patient Disease dataset using Adam optimizer.