

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

B Confusion Matrices

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

Actual	No link	104 40.3%	25 9.7%	80.6% 19.4%
	Link	30 11.6%	99 38.4%	76.7% 23.3%
		77.6% 22.4%	79.8% 20.2%	78.7% 21.3%
		No link	Link	
		Predicted		

(a) ConvE

Actual	No link	105 40.7%	24 9.3%	81.4% 18.6%
	Link	33 12.8%	96 37.2%	74.4% 25.6%
		76.1% 23.9%	80.0% 20.0%	77.9% 22.1%
		No link	Link	
		Predicted		

(b) GAT

Actual	No link	105 40.7%	24 9.3%	81.4% 18.6%
	Link	33 12.8%	96 37.2%	74.4% 25.6%
		76.1% 23.9%	80.0% 20.0%	77.9% 22.1%
		No link	Link	
		Predicted		

(c) GCN

Actual	No link	108 41.9%	21 8.1%	83.7% 16.3%
	Link	32 12.4%	97 37.6%	75.2% 24.8%
		77.1% 22.9%	82.2% 17.8%	79.5% 20.5%
		No link	Link	
		Predicted		

(d) GIN

Actual	No link	109 42.2%	20 7.8%	84.5% 15.5%
	Link	34 13.2%	95 36.8%	73.6% 26.4%
		76.2% 23.8%	82.6% 17.4%	79.1% 20.9%
		No link	Link	
		Predicted		

(e) GraphSAGE

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

Actual	No link	109 42.2%	20 7.8%	84.5% 15.5%
	Link	33 12.8%	96 37.2%	74.4% 25.6%
		76.8% 23.2%	82.8% 17.2%	79.5% 20.5%
		No link	Link	
		Predicted		

(a) ComplEx

Actual	No link	108 41.9%	21 8.1%	83.7% 16.3%
	Link	36 14.0%	93 36.0%	72.1% 27.9%
		75.0% 25.0%	81.6% 18.4%	77.9% 22.1%
		No link	Link	
		Predicted		

(b) CP

Actual	No link	107 41.5%	22 8.5%	82.9% 17.1%
	Link	35 13.6%	94 36.4%	72.9% 27.1%
		75.4% 24.6%	81.0% 19.0%	77.9% 22.1%
		No link	Link	
		Predicted		

(c) DistMult

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

Actual	No link	264 26.6%	233 23.4%	53.1% 46.9%
	Link	57 5.7%	440 44.3%	88.5% 11.5%
		82.2% 17.8%	65.4% 34.6%	70.8% 29.2%
		No link	Link	
		Predicted		

(a) ConvE

Actual	No link	359 36.1%	138 13.9%	72.2% 27.8%
	Link	104 10.5%	393 39.5%	79.1% 20.9%
		77.5% 22.5%	74.0% 26.0%	75.7% 24.3%
		No link	Link	
		Predicted		

(b) GAT

Actual	No link	348 35.0%	149 15.0%	70.0% 30.0%
	Link	95 9.6%	402 40.4%	80.9% 19.1%
		78.6% 21.4%	73.0% 27.0%	75.5% 24.5%
		No link	Link	
		Predicted		

(c) GCN

Actual	No link	394 39.6%	103 10.4%	79.3% 20.7%
	Link	139 14.0%	358 36.0%	72.0% 28.0%
		73.9% 26.1%	77.7% 22.3%	75.7% 24.3%
		No link	Link	
		Predicted		

(d) GIN

Actual	No link	304 30.6%	193 19.4%	61.2% 38.8%
	Link	73 7.3%	424 42.7%	85.3% 14.7%
		80.6% 19.4%	68.7% 31.3%	73.2% 26.8%
		No link	Link	
		Predicted		

(e) GraphSAGE

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

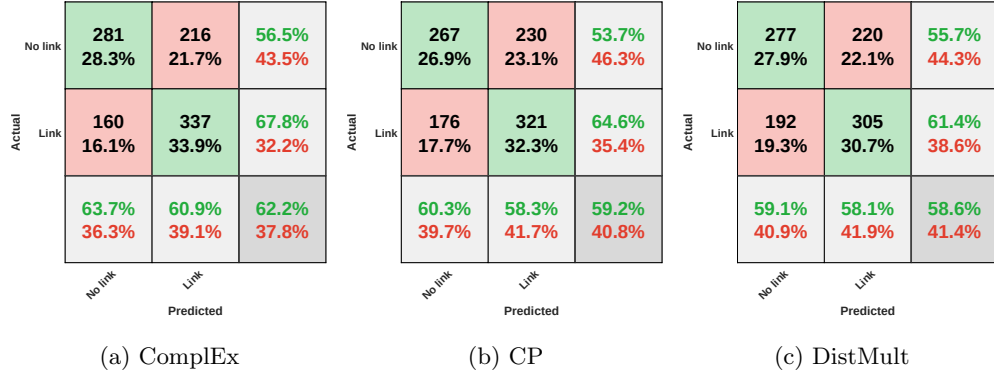


Fig. 5: Confusion Matrices for Drug–Target (Adam Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.

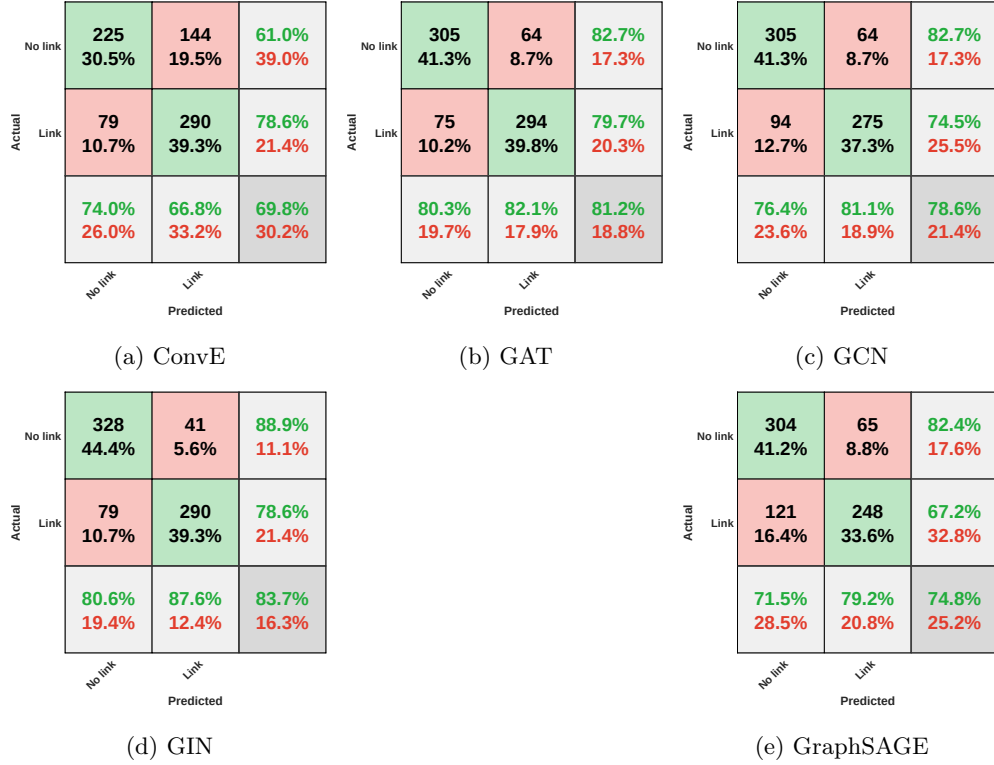


Fig. 6: Confusion Matrices for Drug–Target (AdaGrad Optimizer). Green shades indicate correct classifications, whereas red shades indicate misclassifications.

Actual	No link	180 24.4%	189 25.6%	48.8% 51.2%
	Link	65 8.8%	304 41.2%	82.4% 17.6%
		73.5% 26.5%	61.7% 38.3%	65.6% 34.4%
		No link	Link	Predicted

(a) ComplEx

Actual	No link	187 25.3%	182 24.7%	50.7% 49.3%
	Link	44 6.0%	325 44.0%	88.1% 11.9%
		81.0% 19.0%	64.1% 35.9%	69.4% 30.6%
		No link	Link	Predicted

(b) CP

Actual	No link	188 25.5%	181 24.5%	50.9% 49.1%
	Link	41 5.6%	328 44.4%	88.9% 11.1%
		82.1% 17.9%	64.4% 35.6%	69.9% 30.1%
		No link	Link	Predicted

(c) DistMult

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

Actual	No link	447 40.6%	104 9.4%	81.1% 18.9%
	Link	151 13.7%	400 36.3%	72.6% 27.4%
		74.7% 25.3%	79.4% 20.6%	76.9% 23.1%
		No link	Link	Predicted

(a) ConvE

Actual	No link	422 38.3%	129 11.7%	76.6% 23.4%
	Link	145 13.2%	406 36.8%	73.7% 26.3%
		74.4% 25.6%	75.9% 24.1%	75.1% 24.9%
		No link	Link	Predicted

(b) GAT

Actual	No link	422 38.3%	129 11.7%	76.6% 23.4%
	Link	148 13.4%	403 36.6%	73.1% 26.9%
		74.0% 26.0%	75.8% 24.2%	74.9% 25.1%
		No link	Link	Predicted

(c) GCN

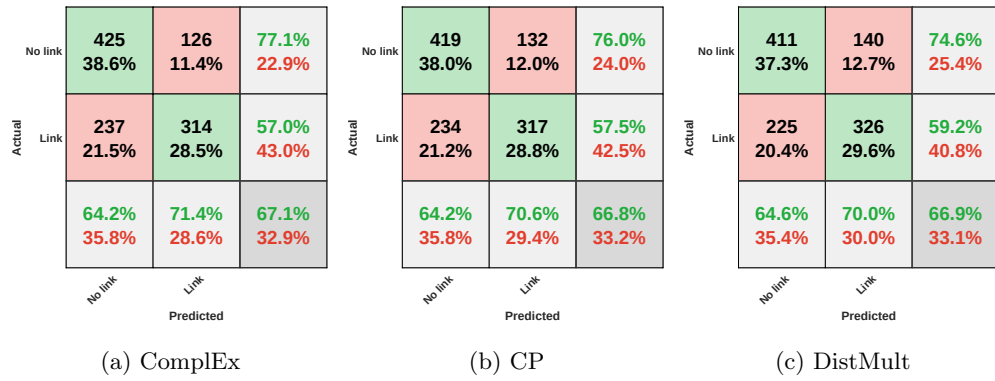
Actual	No link	390 35.4%	161 14.6%	70.8% 29.2%
	Link	119 10.8%	432 39.2%	78.4% 21.6%
		76.6% 23.4%	72.8% 27.2%	74.6% 25.4%
		No link	Link	Predicted

(d) GIN

Actual	No link	448 40.7%	103 9.3%	81.3% 18.7%
	Link	153 13.9%	398 36.1%	72.2% 27.8%
		74.5% 25.5%	79.4% 20.6%	76.8% 23.2%
		No link	Link	Predicted

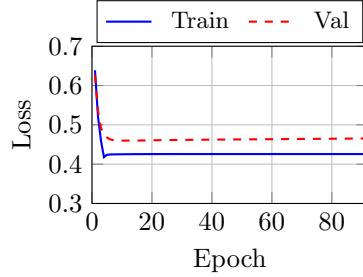
(e) GraphSAGE

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

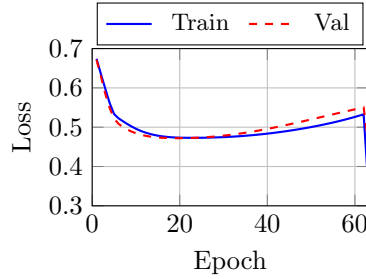


C Additional Material: Training Loss Curves

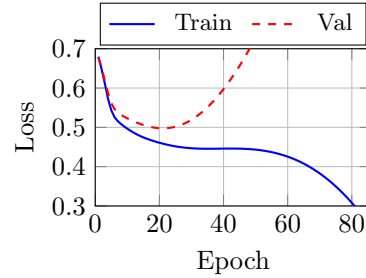
In this appendix, we report the complete training loss trends for all evaluated models across the different experimental settings. These figures complement the quantitative results presented in Section 4, offering insight into convergence stability and generalization behavior.



(a) ComplEx model.

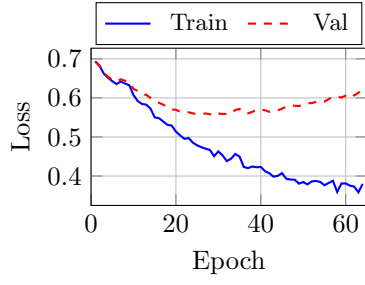


(b) CP model.

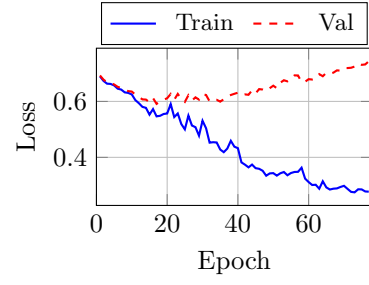


(c) DistMult model.

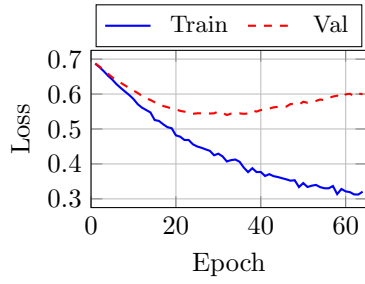
Fig. 9: Training and validation loss curves for inductive KGE models (ComplEx, CP, and DistMult) on the Patients–Diseases dataset using AdaGrad optimizer.



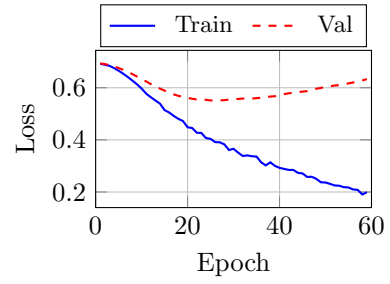
(a) GAT model.



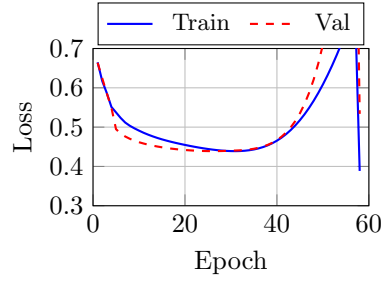
(b) GIN model.



(c) GCN model.

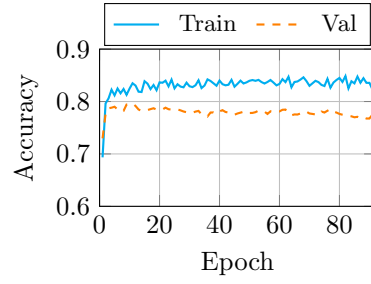


(d) SAGE model.

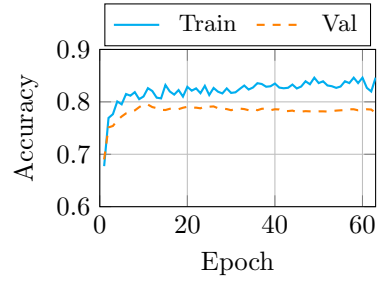


(e) ConvE model.

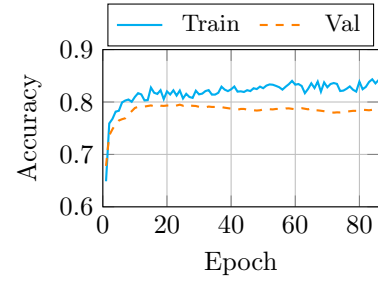
Fig. 10: Training and validation loss curves for inductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Disease dataset using Adam optimizer.



(a) ComplEx model.

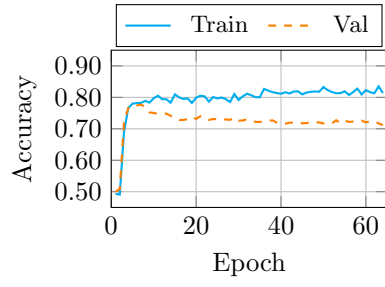


(b) CP model.

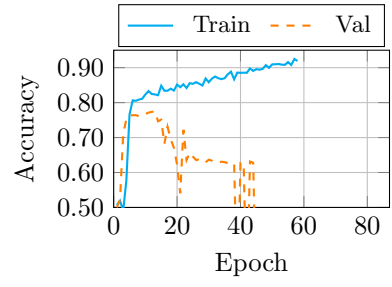


(c) DistMult model.

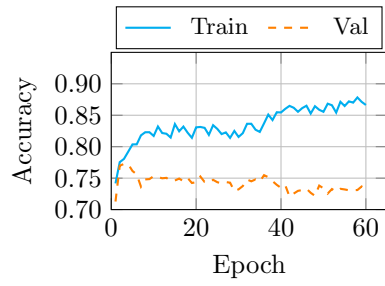
Fig. 11: Training and validation accuracy curves for inductive KGE models (ComplEx, CP, and DistMult) on the Patients-Diseases dataset using AdaGrad optimizer.



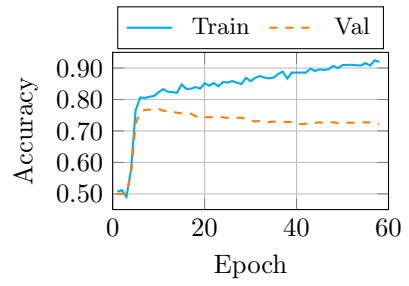
(a) GAT model.



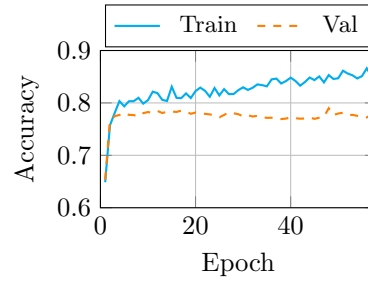
(b) GIN model.



(c) GCN model.

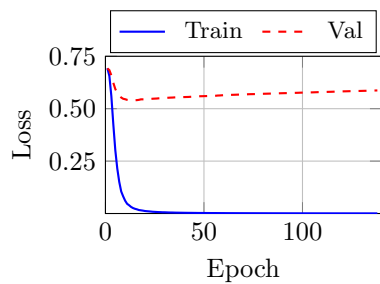


(d) SAGE model.

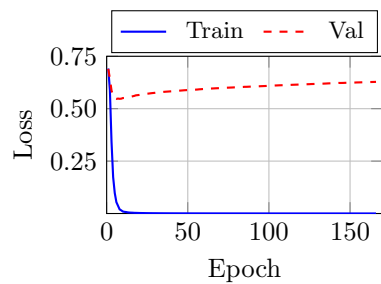


(e) ConvE model.

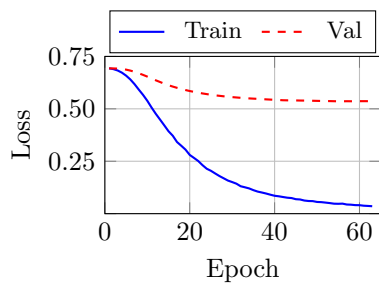
Fig. 12: Training and validation accuracy curves for inductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Patient.Disease dataset using Adam optimizer.



(a) ComplEx model.

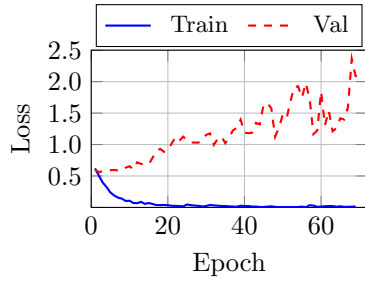


(b) CP model.

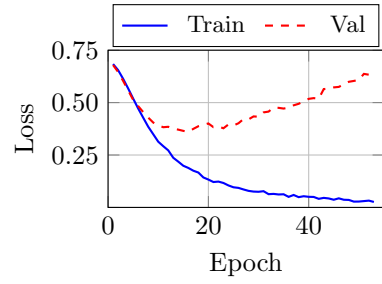


(c) DistMult model.

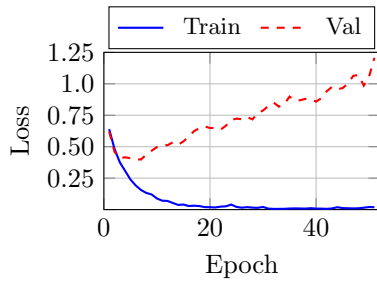
Fig. 13: Training and validation loss curves for transductive models (ComplEx, CP, and DistMult) on the Drug-Target dataset using Adagrad optimizer.



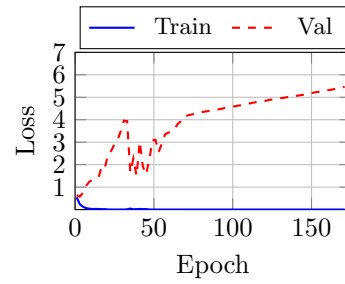
(a) GAT model.



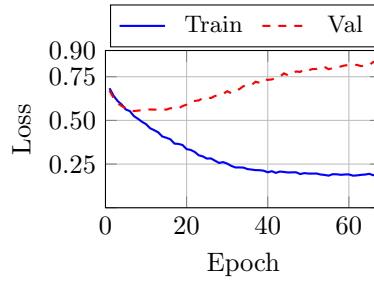
(b) GIN model.



(c) GCN model.

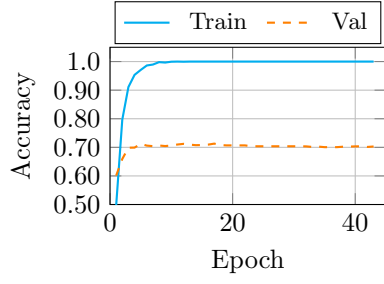


(d) SAGE model.

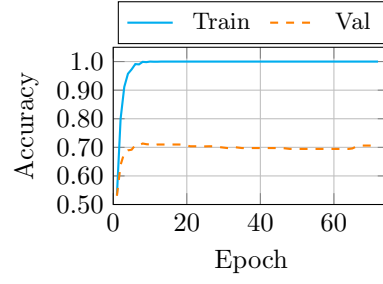


(e) ConvE model.

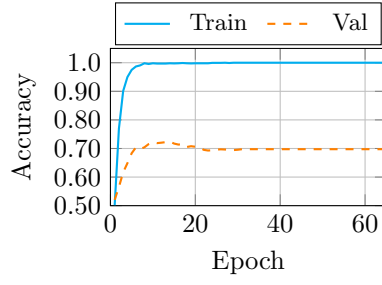
Fig. 14: Training and validation loss curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug-Target dataset using Adam optimizer.



(a) ComplEx model.

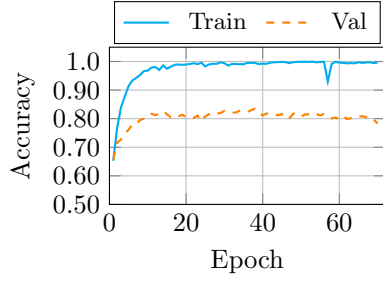


(b) CP model.

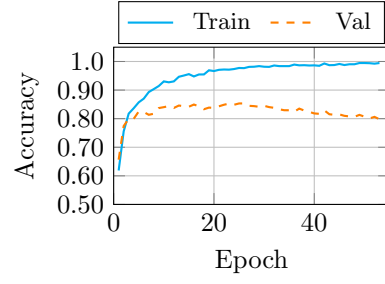


(c) DistMult model.

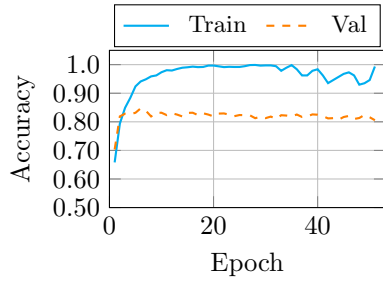
Fig. 15: Training and validation accuracy curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Target dataset using Adagrad optimizer.



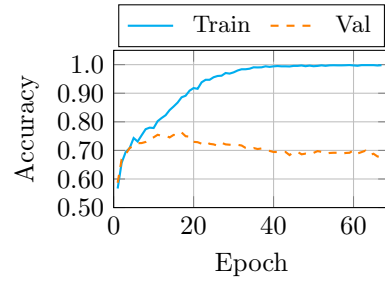
(a) GAT model.



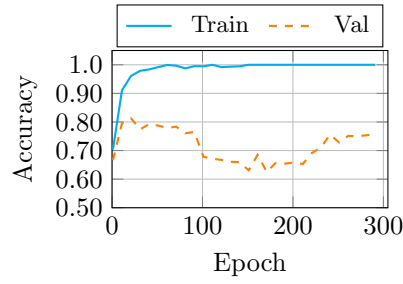
(b) GIN model.



(c) GCN model.

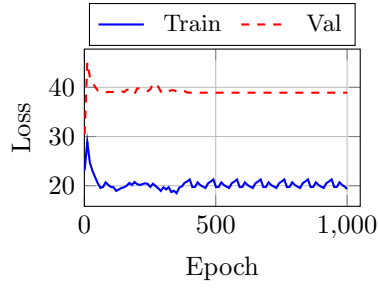


(d) ConvE model.

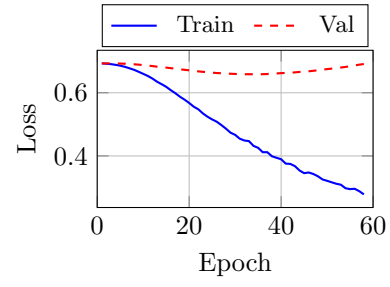


(e) SAGE model.

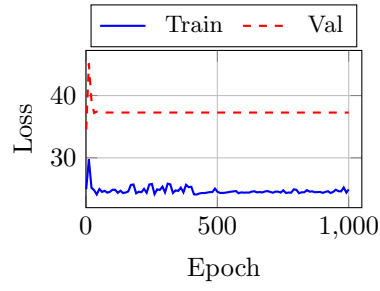
Fig. 16: Training and validation accuracy curves for transductive GNN models (GAT, GIN, GCN, ConvE, and SAGE) on the Drug-Target dataset using Adam optimizer. All data extracted from real files.



(a) ComplEx model.

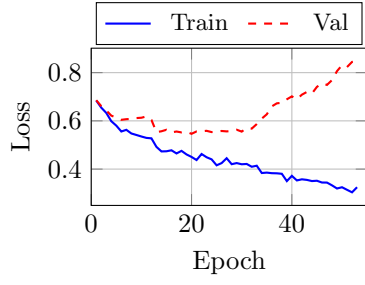


(b) CP model.

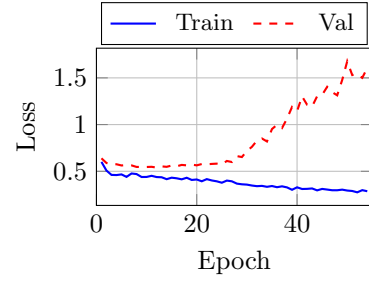


(c) DistMult model.

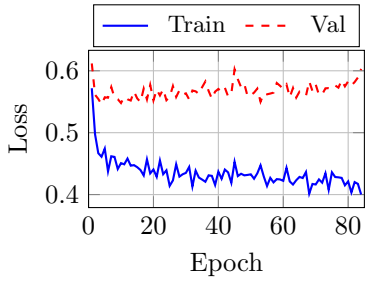
Fig. 17: Training and validation loss curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Disease dataset using Adagrad optimizer.



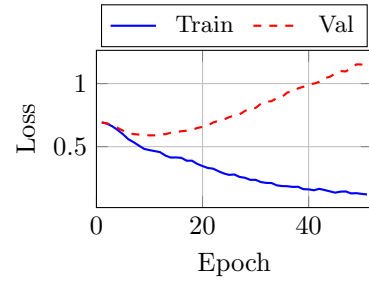
(a) GAT model.



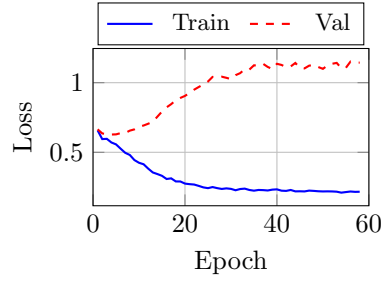
(b) GIN model.



(c) GCN model.

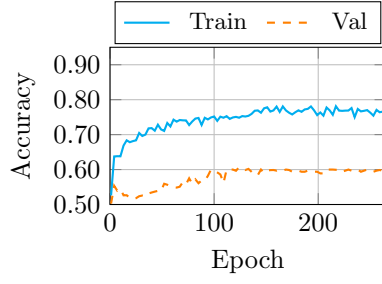


(d) SAGE model.

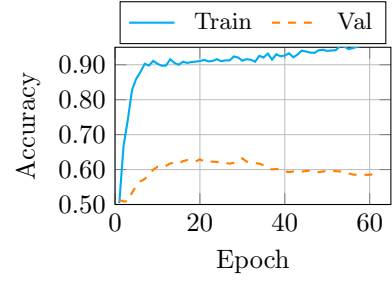


(e) ConvE model.

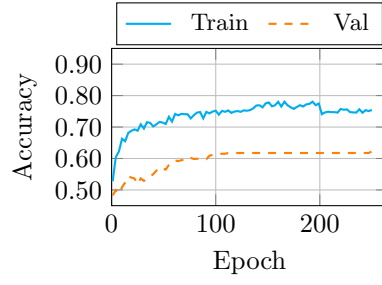
Fig. 18: Training and validation loss curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Disease dataset using Adam optimizer.



(a) ComplEx model.

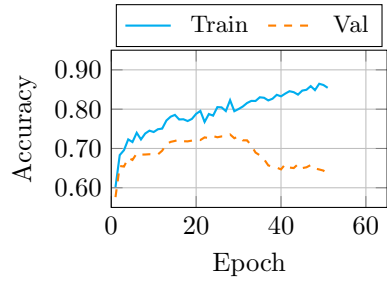


(b) CP model.

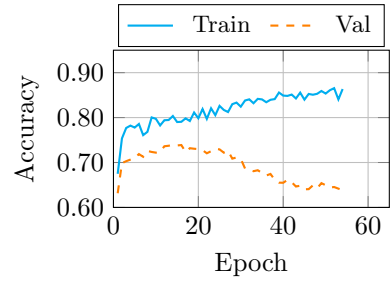


(c) DistMult model.

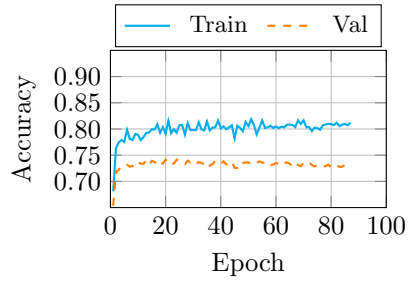
Fig. 19: Training and validation accuracy curves for transductive models (ComplEx, CP, and DistMult) on the Drug_Disease dataset using Adagrad optimizer.



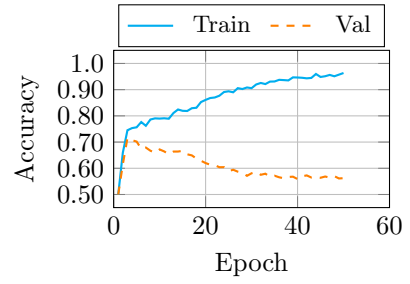
(a) GAT model.



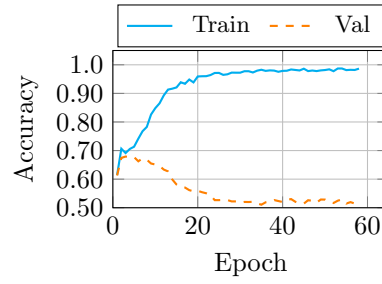
(b) GIN model.



(c) GCN model.

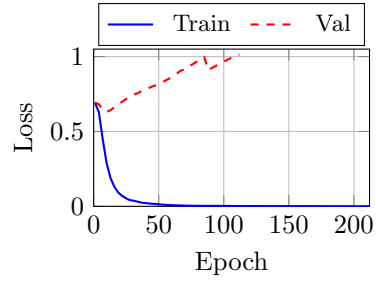


(d) SAGE model.

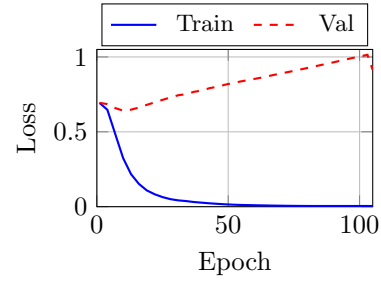


(e) ConvE model.

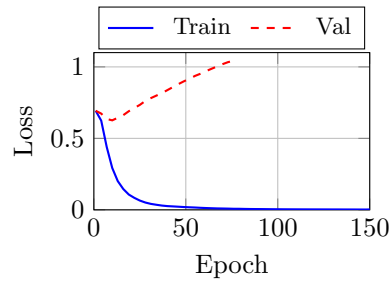
Fig. 20: Training and validation accuracy curves for transductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Drug_Disease dataset using Adam optimizer.



(a) ComplEx model.

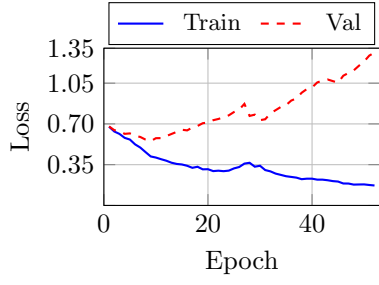


(b) CP model.

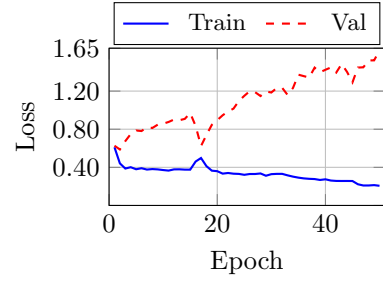


(c) DistMult model.

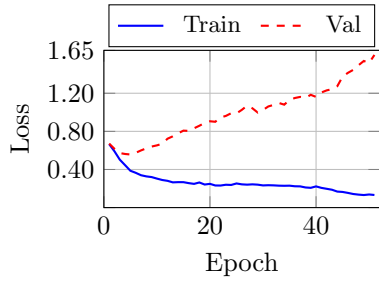
Fig. 21: Updated training and validation loss curves for Patients–Diseases using the new best checkpoints (sampled every 3 epochs).



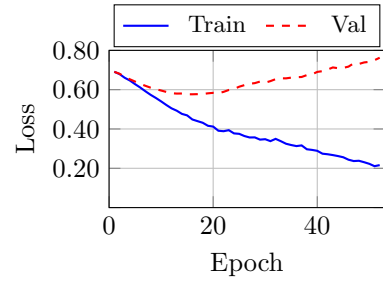
(a) GAT model.



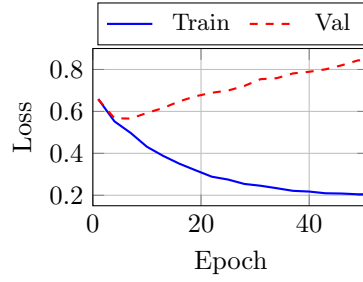
(b) GIN model.



(c) GCN model.

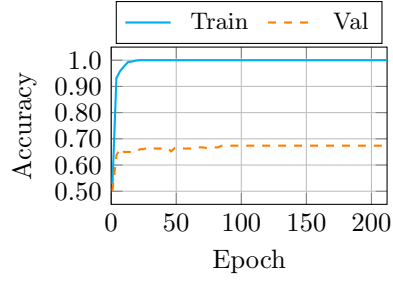


(d) SAGE model.

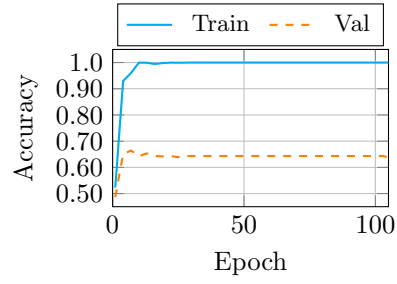


(e) ConvE model.

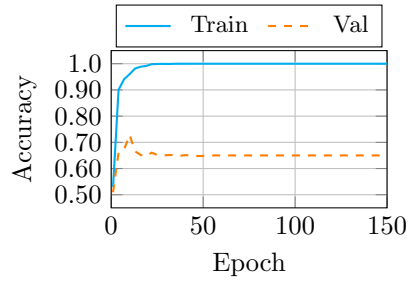
Fig. 22: Training and validation loss curves for inductive GNN models (GAT, GIN, GCN, SAGE, and ConvE) on the Patient_Disease dataset using Adam optimizer.



(a) ComplEx model.

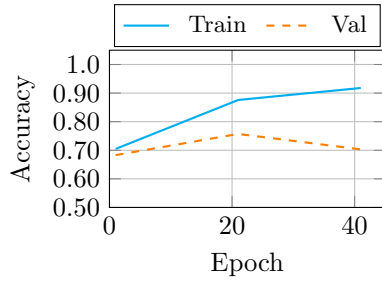


(b) CP model.

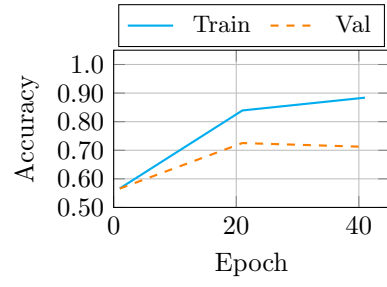


(c) DistMult model.

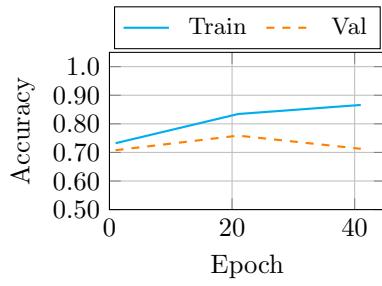
Fig. 23: Updated accuracy curves (Train/Val) from the new checkpoints.



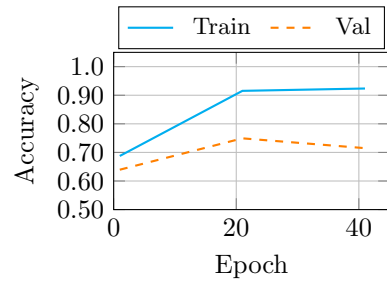
(a) GAT model.



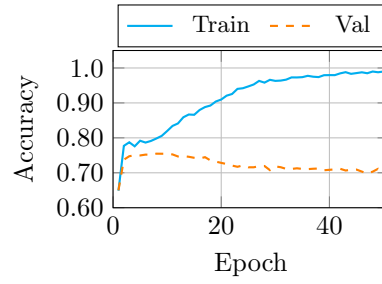
(b) SAGE model.



(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.