Multi-Class and Multi-Task Strategies for Neural Directed Link Prediction

Claudio Moroni(✉)[1,2], Claudio Borile[2], Carolina Mattsson[2], Michele Starnini[2,3], André Panisson[2]

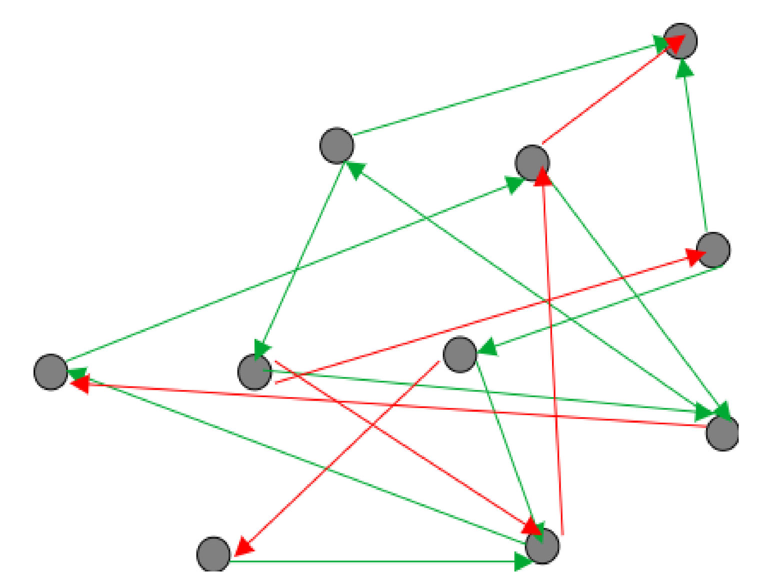
[1]Dedagroup, Torino, Italy, claudio.moroni@dedagroup.it

[2]CENTAI Institute, Torino, Italy, {name.surname}@centai.eu

[3]Department of Engineering, Universitat Pompeu Fabra, Barcelona, 08018, Spain

(NAIVE) DIRECTED LINK PREDICTION

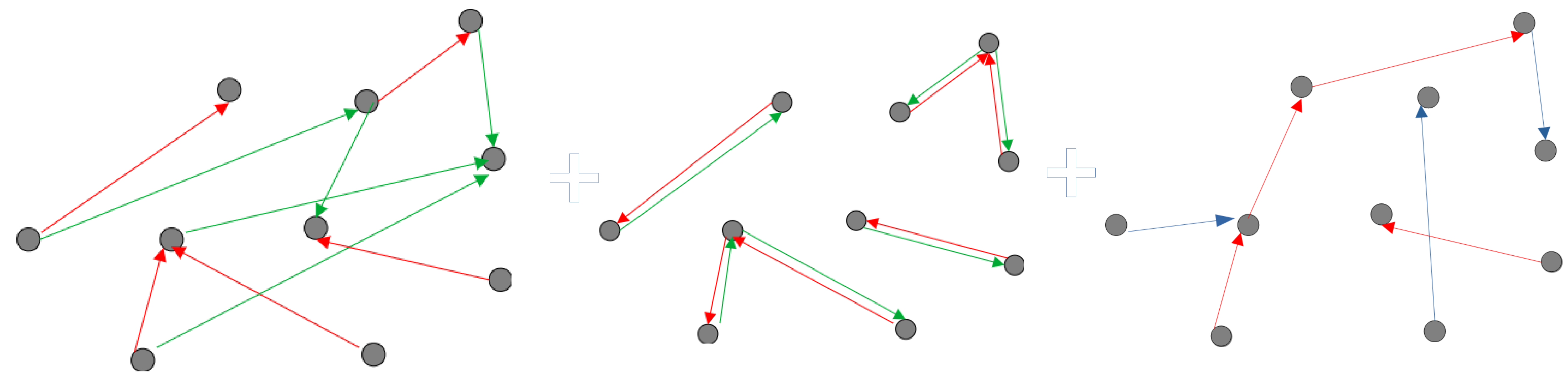
Training



$$\mathcal{L}(\Theta) = \sum_{e \in E_{s+n}} w_p y_e \ln(\hat{p}_\Theta(e)) + (1-y_e)\ln(1-\hat{p}_\Theta(e))$$

Testing

General | Directional | Bidirectional



model	decoder	GENERAL ROC-AUC	GENERAL AUPRC	DIRECTIONAL ROC-AUC	DIRECTIONAL AUPRC	BIDIRECTIONAL ROC-AUC	BIDIRECTIONAL AUPRC
GAE	$\vec{z}_i \cdot \vec{z}_j$	84.6	88.6	50.0	50.0	62.4	64.0
GR-GAE	$\sigma(\vec{z}_v[0] - \lambda \ln(\|\|\vec{z}_u[1:] - \vec{z}_v[1:]\|\|_2^2))$	89.2	92.4	63.4	61.5	69.1	66.5
MLP-GAE	MLP($\vec{z}_v \|\| \vec{z}_u$)	77.1	78.2	90.7	90.7	69.9	69.7
MAGNET	MLP-like	75.2	77.8	90.4	89.8	71.9	70.4

NEW TRAINING STRATEGIES

Multi Class

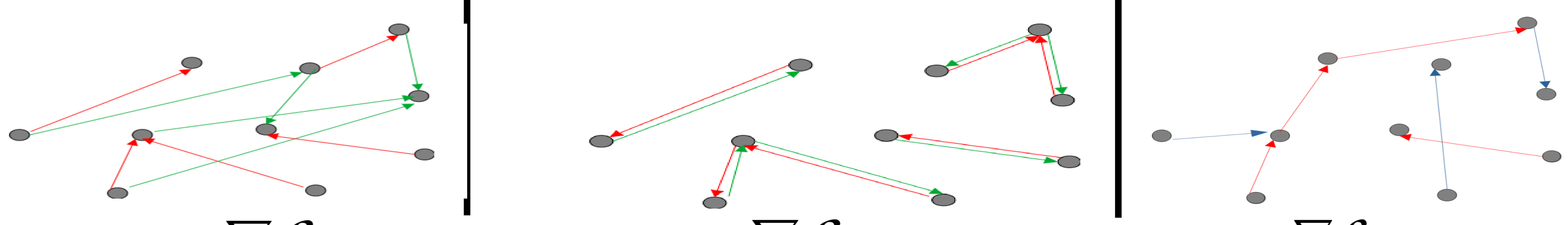
$$[\hat{p}^{nb}_{uv}, \hat{p}^{nu}_{uv}, \hat{p}^{pu}_{uv}, \hat{p}^{pb}_{uv}] = [(1-\hat{p}_{uv})(1-\hat{p}_{vu}),\; (1-\hat{p}_{uv})\hat{p}_{vu},\; \hat{p}_{uv}(1-\hat{p}_{vu}),\; \hat{p}_{uv}\hat{p}_{vu}]$$

$$\mathcal{L}_{MC\text{-}NDLP}(\Theta) = -\sum_{c\in C}\sum_{uv \in T} w_{y_{uv}} \mathbb{I}(y_{uv} = c)\log(\hat{p}^{y_{uv}}_{uv}), w_{y_{uv}} = \frac{n_x}{n_{y_{uv}}}$$

MGDA

Scalarization

General Training Set | Directional Training Set | Bidirectional Training Set



$\nabla\mathcal{L}_G$ | $\nabla\mathcal{L}_D$ | $\nabla\mathcal{L}_B$

$$\vec{g}_{\text{MGDA}} = \min_{||\sum_i \alpha_i \nabla\mathcal{L}_i||_2^2} \sum_i \alpha_i \nabla\mathcal{L}_i \quad \text{s.t} \quad \sum_i \alpha_i = 1$$

$$\theta' = \theta - \eta\vec{g}_{\text{MGDA}}$$

$$\vec{g}_{\text{S}} = \sum_i \alpha_i \nabla\mathcal{L}_i$$

$$\theta' = \theta - \eta\vec{g}_{\text{S}}$$

model	strategy	GENERAL ROC-AUC	GENERAL AUPRC	DIRECTIONAL ROC-AUC	DIRECTIONAL AUPRC	BIDIRECTIONAL ROC-AUC	BIDIRECTIONAL AUPRC
GR-GAE	BASELINE	**89.2 ± 0.4**	**92.4 ± 0.2**	63.4 ± 2.5	61.5 ± 2.7	69.1 ± 3.1	66.5 ± 3.3
	MO-NDLP	84.5 ± 1.1	86.3 ± 1.1	80.6 ± 0.7	80.2 ± 0.9	79.6 ± 4.3	84.6 ± 3.5
	MC-NDLP	88.6 ± 0.4	90.0 ± 0.4	82.1 ± 0.5	**81.8 ± 0.7**	77.3 ± 2.2	76.3 ± 1.7
	S-NDLP	87.8 ± 0.6	89.5 ± 0.5	**82.3 ± 0.5**	81.6 ± 0.4	**89.6 ± 1.6**	**92.4 ± 1.1**
DiGAE	BASELINE	**80.4 ± 1.1**	**85.3 ± 0.8**	57.5 ± 1.3	63.0 ± 1.4	70.4 ± 2.2	68.6 ± 1.2
	MO-NDLP	70.2 ± 3.8	72.6 ± 3.6	73.6 ± 5.4	76.0 ± 4.2	67.3 ± 4.6	69.6 ± 4.1
	MC-NDLP	75.4 ± 0.9	77.4 ± 1.0	**84.3 ± 0.6**	**85.4 ± 0.8**	68.9 ± 1.5	69.3 ± 1.1
	S-NDLP	72.5 ± 4.0	77.4 ± 4.4	61.6 ± 1.3	69.2 ± 1.4	**72.1 ± 5.6**	**74.4 ± 5.7**
MLP-GAE	BASELINE	**77.1 ± 0.9**	**78.2 ± 0.6**	90.7 ± 0.6	90.7 ± 0.6	69.9 ± 3.2	69.7 ± 3.7
	MO-NDLP	76.0 ± 0.8	76.4 ± 0.7	93.4 ± 0.6	93.5 ± 0.6	**80.7 ± 1.6**	**79.2 ± 2.4**
	MC-NDLP	74.5 ± 0.7	75.6 ± 0.7	**94.3 ± 0.6**	**94.4 ± 0.5**	71.7 ± 2.4	65.7 ± 1.8
	S-NDLP	74.7 ± 1.0	74.9 ± 0.9	90.5 ± 0.7	90.0 ± 0.9	72.0 ± 2.6	70.5 ± 2.9
MAGNET	BASELINE	**75.2 ± 1.4**	**77.8 ± 1.0**	90.4 ± 0.9	89.8 ± 0.8	**71.9 ± 2.3**	**70.4 ± 2.8**
	MO-NDLP	74.4 ± 1.4	77.4 ± 1.1	91.3 ± 1.0	90.9 ± 1.0	70.6 ± 2.7	68.6 ± 2.7
	MC-NDLP	74.4 ± 1.0	77.4 ± 1.0	**92.1 ± 0.7**	**91.6 ± 0.7**	71.8 ± 2.6	70.0 ± 2.6
	S-NDLP	74.6 ± 1.3	77.5 ± 1.1	91.0 ± 1.0	90.4 ± 1.0	71.8 ± 2.8	70.2 ± 2.9

- Salha, G., Limnios, S., Hennequin, R., Tran, V.A., Vazirgiannis, M.: Gravityinspired graph autoencoders for directed link prediction. In: Proceedings of the 28th ACM International Conference on Information and Knowledge Management. pp. 589–598 (2019)
- Zhang, X., He, Y., Brugnone, N., Perlmutter, M., Hirn, M.: Magnet: A neural network for directed graphs. In: Advances in Neural Information Processing Systems (2021)
- Kollias, G., Kalantzis, V., Id'e, T., Lozano, A.C., Abe, N.: Directed graph autoencoders. In: AAAI Conference on Artificial Intelligence (2022)
- Désidéri, J.A.: Multiple-gradient descent algorithm (mgda) for multiobjective optimization. Comptes Rendus Mathematique 350(5), 313–318 (2012)