Machine Learning with Graphs (MLG)

# Link Prediction on Time-Evolving Graphs

## A Case of Neural Network-based Link Prediction


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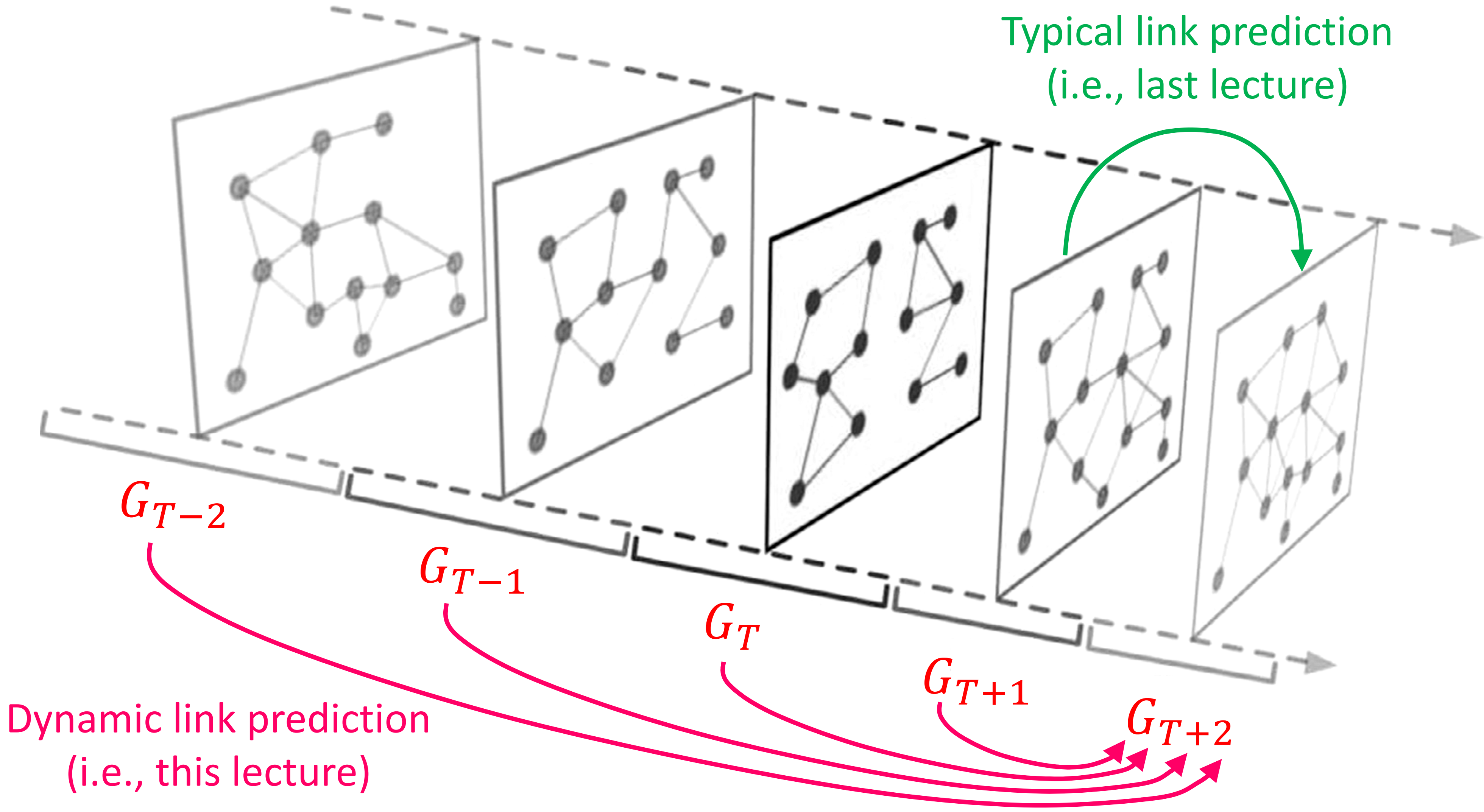
# Time-Evolving Graphs

a.k.a. Dynamic Networks

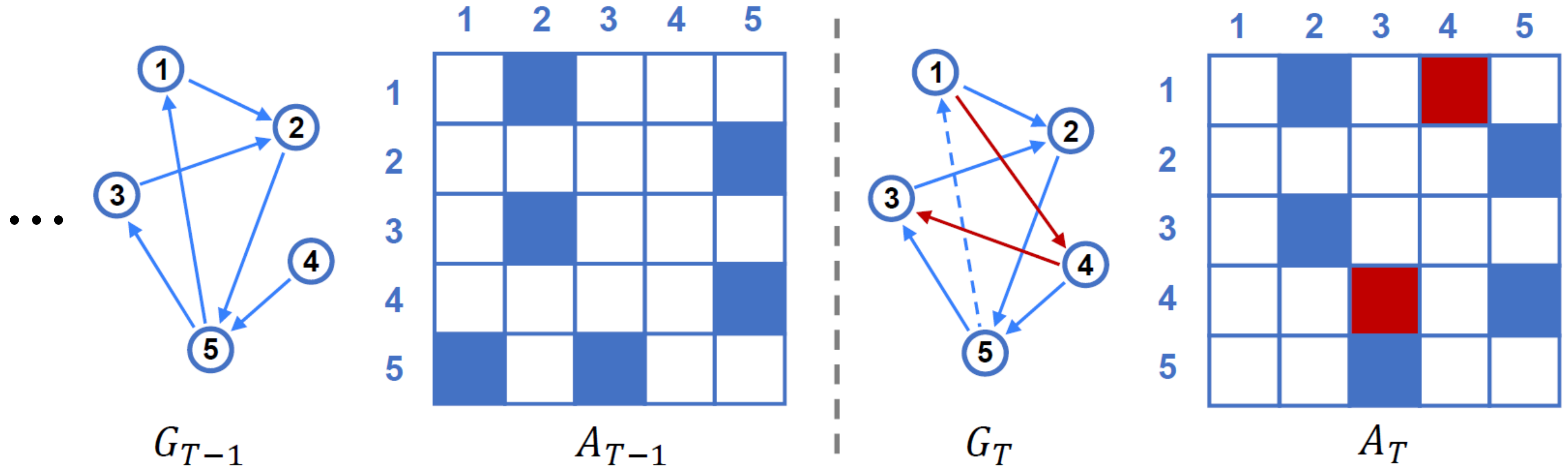


# Applications of Dynamic Link Prediction

- In social networks
  - Predict people's relationship like who will be whose friend in near future
- In information diffusion networks
  - Predict who will adopt the novel info or be infected by coronavirus in the future
- In citation networks
  - Suggest which papers should be cited
- In biological networks
  - Predict protein mutual influence for medicine design

# Dynamic Link Prediction

- Dynamic Network: a sequence of graphs, $S = \{G_1, G_2, \ldots, G_{t-1}\}$, where $G_k = (V, E_k)$ denotes the $k$-th snapshot of a dynamic network
  - $A_k$: the adjacency matrix of $G_k$
- **Dynamic Link Prediction** (DLP)
  - Given $S = \{G_{t-N}, \ldots, G_{t-1}\}$ of length $N$, DLP is to predict $G_t$ by learning a function that maps $S$ to $G_t$



# Deep Learning for DLP

## 1) E-LSTM-D: Encoder-LSTM-Decoder model

- **Encode** each snapshot
- **LSTM** to model the temporal dynamics of structure
- **Decode** embedding to predict next snapshot

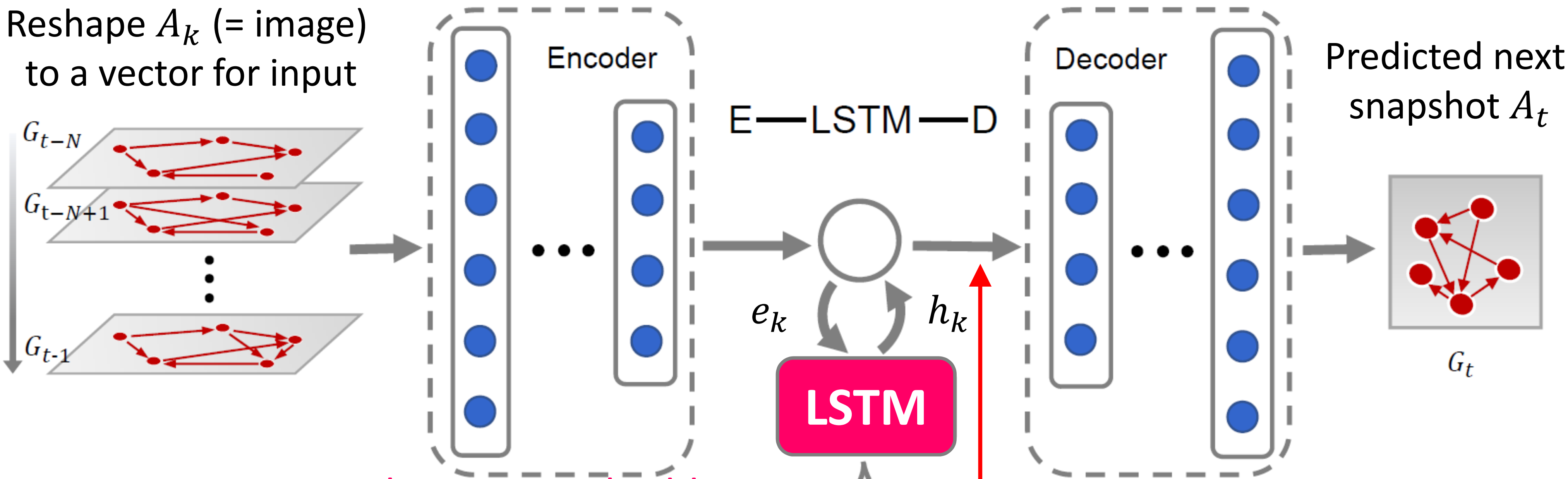
https://arxiv.org/abs/1902.08329 https://github.com/Liang-Liao/e-lstm-d

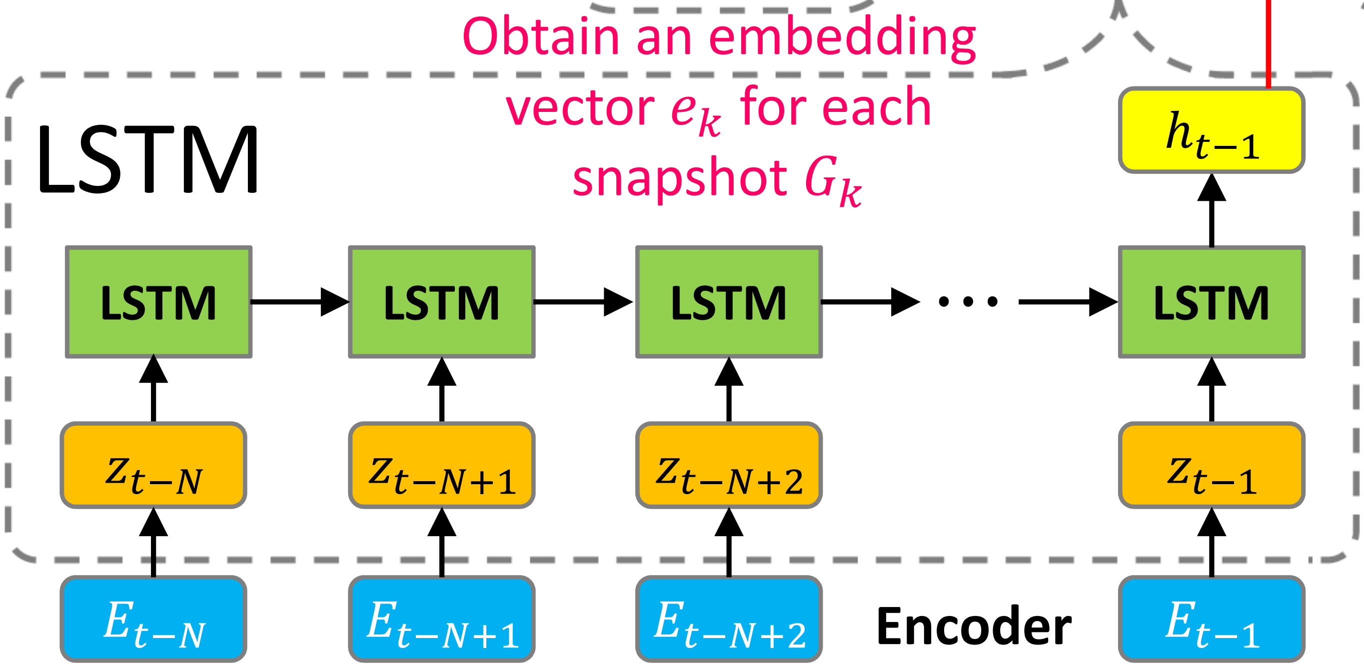
## 2) GRU with Deep Neural Network model

- **GRU** for model the structural dynamics of every node
- Make linked nodes have similar embeddings
- **DNN** for predict next snapshot

https://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=8365780

# Encoder-LSTM-Decoder for DLP




**Loss function**

$$\mathcal{L} = \sum_{i=1}^{n}\sum_{j=1}^{n}(a_{t;i,j} - \hat{a}_{t;i,j}) * p_{i,j}$$

$$= \| (A_t - \hat{A}_t) \odot P \|_F^2,$$

Element-wise product

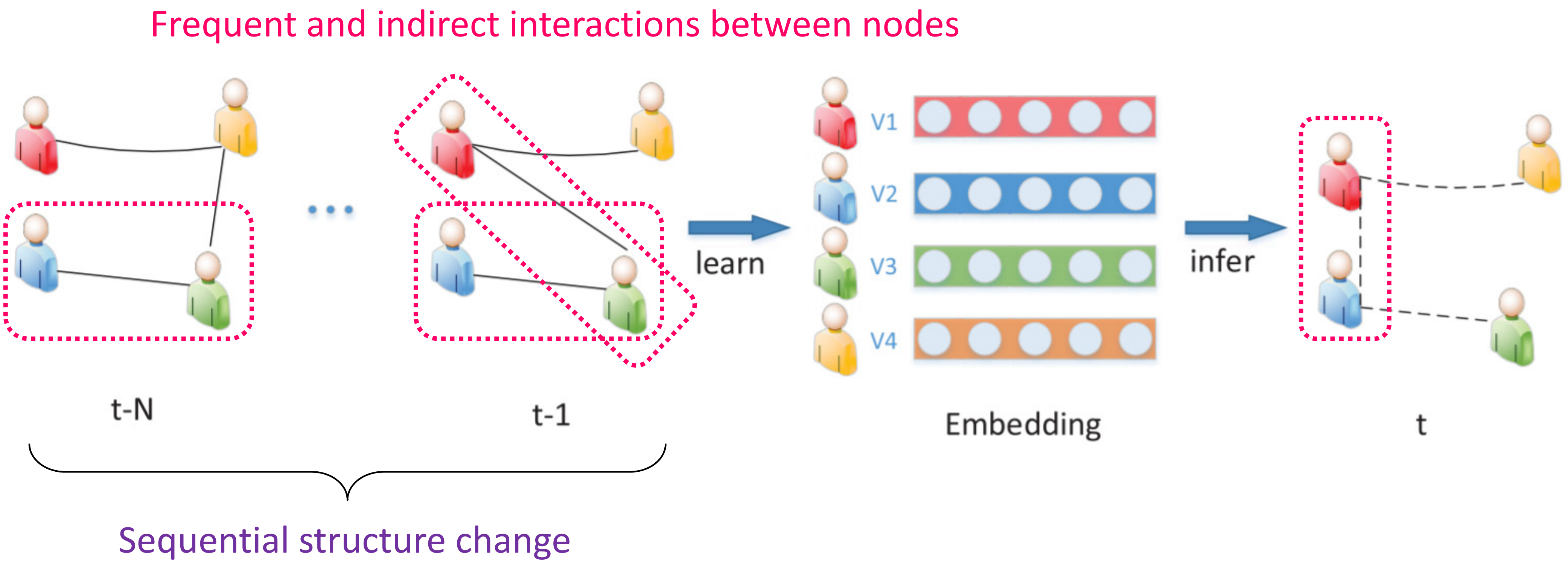
$$p_{i,j} = 1 \text{ if } a_{t;i,j} = 0$$

$$p_{i,j} = \beta > 1 \text{ otherwise}$$

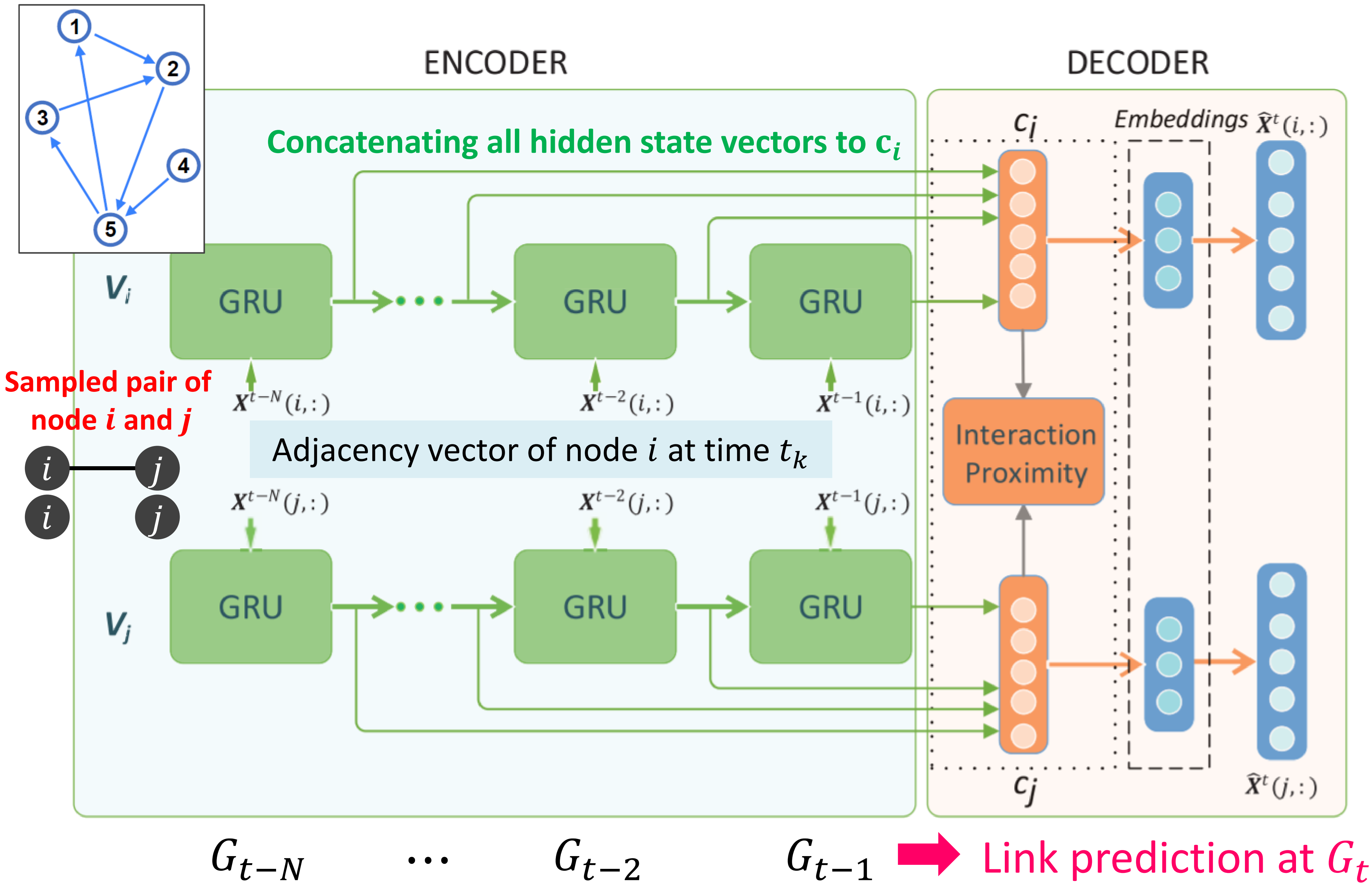
Penalty exerts more on non-zero elements to avoid overfitting

# Two Issues in DLP

- Incorporating dynamic structure info over time
- Node interactions (i.e., matrix form ignores node correlation)



# Deep Dynamic Network Embedding for DLP



# Loss Function Design

- Cross-entropy loss for link prediction
  - The loss of non-zero elements can be highlighted and the linkage information will be preserved

$$\mathcal{L}_s = -\sum_{i=1}^{n}\sum_{j=1}^{n} Z(i,j)\underbrace{X^t(i,j)}_{\text{Ground truth}} \log \underbrace{\hat{X}^t(i,j)}_{\text{Predicted links}}$$

$Z(i,j) = 1, if\ X(i,j) = 0$
$Z(i,j) = \alpha > 1, if\ X(i,j) = 0$

- Similarity by L2 norm for interaction proximity
  - Two nodes with frequent connections are more likely to have similar latent representations

$$\mathcal{L}_c = \sum_{u,v=1}^{n} N_{ij}\|\mathbf{c}_i - \mathbf{c}_j\|_2$$

$N_{ij}$: connection frequency of nodes $i$ and $j$ in the historical networks

- Final loss function $\mathcal{L}_{all} = \mathcal{L}_s + \beta\mathcal{L}_c + \gamma\mathcal{L}_{reg}$