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# **Proceedings Paper:**

Huang, Qiyao, Zhang, Yingyue, Zhang, Zhihong et al. (1 more author) (2023) ESSEN: Improving Evolution State Estimation for Temporal Networks using Von Neumann Entropy. In: Thirty-seventh Conference on Neural Information Processing Systems:Proceedings. NeurIPS 2023, 10-16 Dec 2023, USA

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# **ESSEN: Improving Evolution State Estimation for Temporal Networks using Von Neumann Entropy**

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## Abstract

Temporal networks are widely used as abstract graph representations for real-world 1 dynamic systems. Indeed, recognizing the network evolution states is crucial in 2 understanding and analyzing temporal networks. For instance, social networks 3 will generate the clustering and formation of tightly-knit groups or communities 4 over time, relying on the triadic closure theory. However, the existing methods 5 often struggle to account for the time-varying nature of these network structures, 6 hindering their performance when applied to networks with complex evolving 7 states. To mitigate this problem, we propose a novel framework called ESSEN, an 8 Evolution StateS awarE Network, to measure temporal network evolution using 9 von Neumann entropy and thermodynamic temperature difference. The developed 10 framework utilizes the von Neumann entropy aware attention mechanism and 11 network evolution state contrastive learning in the graph encoding. In addition, 12 it employs a unique decoder Mixture of Thermodynamic Experts (MoTE) for 13 decoding. ESSEN extracts local and global network evolution information using 14 thermodynamic features and adaptively recognizes the network evolution states. 15 Moreover, the proposed method is evaluated on link prediction tasks with transduc-16 tive settings and inductive settings, with the corresponding results demonstrating 17 its effectiveness compared to various state-of-the-art baselines <sup>1</sup>. 18

# 19 1 Introduction

20 In recent years, graph representation learning has demonstrated excellent performance in a variety of static graphs [7; 14][28; 18]. Indeed, the success of static graph representation learning has led 21 to a growing interest in continuous-time dynamic graph representation learning. Temporal network 22 representation learning has emerged as an active research area focusing on learning low-dimensional 23 representations that capture their topological and temporal properties. However, in many temporal 24 networks, which are naturally generated in real-world systems, such as social networks[12] and 25 citation networks, learning effective representations is still a difficult task. The evolving nature of 26 these networks poses a significant challenge for network analysis and modeling, as the relationships 27 between nodes and their properties evolve. The existing methods often struggle to account for 28 the time-varying nature of these network structures, hindering their performance when applied to 29 networks with complex evolving states. However, capturing the evolving states of temporal networks 30 suffers from the following challenges: (1) Temporal networks have different types of evolving 31 states, such as periodic, linear, or non-linear changes in their structure over time. Moreover, the 32 evolving patterns can be changed in the network's different evolving stages. As illustrated in Fig.1, 33 the evolution speed varies at different times in both datasets. The MathOverflow network evolves 34 rapidly and has obvious central nodes, which means hot issues will receive long-term attention. 35

<sup>&</sup>lt;sup>1</sup>Code is available at https://github.com/h1o2n3/ESSEN



(a) MathOverflow: 10th Day (b) MathOverflow: 20th Day (c) MathOverflow: 30th Day



(d) BitcoinOTC: 10th Day (e) BitcoinOTC: 20th Day (f) BitcoinOTC: 30th Day

Figure 1: Network snapshots of the MathOverflow website and BitcoinOTC trading platform on the 10th, 20th, and 30th day. The black nodes represent the users who have connections, and the grey nodes represent the users with no edges prior to the snapshot time. The snapshots illustrate that temporal networks have different evolutionary states at different stages.

<sup>36</sup> Instead, in the BitcoinOTC network, early active users may quickly become silent. The phenomenon

requires algorithms that can perform extensive and effective recognition of diverse evolutionary states.
(2) As time passes, temporal networks tend to accumulate more nodes and edges, resulting in an
increasing number of possible connections and a rapidly growing neighborhood for each node. This
growth in the neighborhood can lead to significant computational challenges when analyzing and
modeling evolving patterns. Besides, many connections can quickly make structure recognization
computationally infeasible in large and complex networks, especially the methods based on the

anonymous walk in recent years[24; 6; 20]. The time complexity is tightly related to the length and
 number of paths, so it is challenging to balance time consumption and effectiveness.

45 To overcome these shortcomings, we aim to capture the evolution states using a thermodynamic 46 entropy view. Thermodynamic network entropy is a macroscopic representation of network structures widely used to characterize the salient features of static and dynamic network systems in biology, 47 physics, and social sciences. One of the most sophisticated studies involves the von Neumann entropy, 48 which has been successfully used to describe the structural properties of random, small-world, and 49 scale-free networks [1; 2]. Unfortunately, computing the required network entropies on the temporal 50 network can be computationally burdensome due to spectral decomposition. Hence, we expand 51 the approximate von Neumann entropy into the temporal network. Compared with other graph 52 entropy, approximating von Neumann entropy with low time complexity can better adapt to the 53 constantly evolving complex temporal networks. Moreover, we compute the important approximate 54 thermodynamic quantity temperature for the temporal network. Measuring the thermodynamic 55 56 temperature difference and the von Neumann entropy will provide a better understanding of the network's evolving state at any time. 57

On this basis, we propose a novel framework named ESSEN, an Evolution StateS awarE Network. 58 ESSEN encodes node embeddings with evolution information by utilizing two proposed techniques: 59 von Neumann entropy aware attention mechanism and virtual evolution node representation learning. 60 In addition, ESSEN employs a unique decoder mixture of thermodynamic experts (MoTE) for 61 decoding. Specifically, we project the global network's von Neumann entropy into each edge. The 62 proposed von Neumann entropy aware attention mechanism aggregates the neighborhood in the virtual 63 evolution graph and the original graph based on the von Neumann edge entropy. The virtual evolution 64 graph is defined as supposing the node pair's test connection will truly happen at the specified test time 65 future. The MoTE decoder evaluates the evolutionary state based on the thermodynamic temperature 66 difference and von Neumann entropy in two graph views and provides a comprehensive result from 67

<sup>68</sup> multiple experts. The decoder helps to recognize the network under various evolution states adaptively.

<sup>69</sup> Our framework is evaluated on transductive link prediction, inductive link prediction, and dynamic

<sup>70</sup> node classification tasks. The experimental results demonstrate our method's effectiveness compared

<sup>71</sup> to various state-of-the-art baselines. The overall contributions of our work are summarized as follows:

To our best knowledge, we are the first to utilize the von Neumann entropy in temporal network
 representation learning. We provide a method to expand the approximate von Neumann Entropy
 and approximate thermodynamic temperature difference to temporal networks.

We propose a novel framework, namely ESSEN. The model introduces a new perspective to encode evolution-aware node representations using the von Neumann entropy aware attention mechanism

and virtual evolution node representation learning. Furthermore, the model uses a novel decoder

78 MoTE that adaptively recognizes temporal network evolution states.

<sup>79</sup> • We evaluate our framework on link prediction tasks with transductive and inductive settings.

The results show the effectiveness of our proposed method compared to various state-of-the-art baselines.

# 82 2 Related Work

Temporal Network Representation Learning. Network representation learning is often used to 83 transform large networks into lower-dimensional vectors. For instance, CTDNE [15] learns node 84 embedding from a continuous-time dynamic network instead of a sequence of snapshots. Besides, 85 JODIE [10] uses two recurrent neural networks (RNNs) to learn trajectories of users and items and 86 updates the embedding when interaction occurs. TGAT [25] utilizes a self-attention mechanism and 87 presents an encoding method to learn inductively. CAW [24] and NeuralTWs [6] learn temporal 88 structure using random walk. Specifically, CAW proposes a new anonymization strategy, and 89 NeuralTWs considers structural and tree traversal properties. TDLG[4] aims to model the edges 90 in temporal networks directly instead of calculating from node embedding. However, it remains 91 challenging to model global evolution under acceptable time complexity. 92

Von Neumann Entropy of Static Graph. The von Neumann entropy can be computed in the static
 graph using a quantum analogy[16]. According to this analogy, the Laplacian matrix [17] of a graph
 is interpreted as the density matrix [23] of an equivalent quantum system whose information content
 is given by the von Neumann entropy. The von Neumann entropy can be computed in the static graph
 as follows:

$$S_{VN} = -\sum_{i=1}^{|V|} \frac{\lambda_i}{|V|} \log \frac{\lambda_i}{|V|},\tag{1}$$

where  $\lambda_1, \ldots, \lambda_{|V|}$  are the eigenvalues of Laplacian matrix. This form of von Neumann entropy is 98 effective for network characterization. The thermodynamics entropy could model the structure and 99 100 complexity of a graph, where the von Neumann graph entropy [3; 16; 17] is often used to describe the 101 statistical state of a network system. De Domenico et al. [5] use von Neumann graph entropy for the structural reduction in multiplex networks. Li et al.[11] study convergence through von Neumann 102 entropy for network-ensemble comparison. Liu et al.[13] apply von Neumann graph entropy to study 103 universal patterns of the dynamic genome. Besides, Wang[23] calculates the approximation of von 104 Neumann graph entropy with node degrees to model the network evolution. However, applying von 105 Neumann entropy to represent temporal structure is still scarce. To our best knowledge, there is 106 almost no work using von Neumann entropy to characterize the temporal graph. 107

# **108 3 Preliminaries**

**Definition 1 Temporal Network.** Formally, the temporal network can be denoted as G = (V, E, T), where V represents the set of nodes,  $E \subseteq V \times V$  represents the set of links, and T represents the set of timestamps. Each link (u, v, t) signifies a connection between node u and node v at time t. The temporal network evolves over time, with links appearing at different timestamps. The temporal networks can also include attributes associated with nodes or links, providing further information about the entities or their interactions at specific timestamps.

**Definition 2 Dynamic Link Prediction.** In a temporal network G = (V, E, T), the dynamic link prediction task aims to predict the presence or absence of a link at a future timestamp based on the

observed network evolution history. Given a time window  $T_w \subseteq T$ , which contains the observed link

data, denoted as  $E_{T_w} \subseteq E$ , the goal is to learn a function  $f: (V, E_{T_w}, T_w) \to \{0, 1\}$  that assigns a probability score to the existence of a link (u, v) at the future timestamp t. Mathematically, the

120 function f can be defined as:

$$f(u, v, t) = P(u, v|t, E_{T_w}),$$

$$\tag{2}$$

where  $P((u,v)|t, E_{T_w})$  represents the probability of the link (u,v) being present at the future timestamp t given the observed network and the link data  $E_{T_w}$  within the time window  $T_w$ .

Definition 3 Evolution States. Evolution states denote the specific arrangements of nodes and edges 123 at specific time moments. These states can be characterized by network topology, reflecting the 124 evolving nature of the network over time. For example, social networks at specific evolutionary 125 states will generate the clustering and formation of tightly-knit groups or communities over time 126 by triadic closure theory [29]. The theory is formally defined as  $\exists u, v, w, w' \in V : (u, v), (v, w) \in$ 127  $E_{T_w}, (u, w), (u, w'), (v, w') \notin E_{T_w} \mapsto P(u, w | E_{T_w}) > P(u, w' | E_{T_w})$ . Therefore, analyzing evolu-128 tion states helps in understanding the temporal behavior of the network, identifying recurring patterns, 129 predicting future states, and studying the impact of temporal dynamics on network properties and 130 phenomena. In this paper, we aim to capture evolution states in a thermodynamic entropy view. 131

## **132 4 The Proposed Method**

## 133 4.1 Evolution State Estimation

Von Neumann Entropy in Temporal Network. The von Neumann entropy can be computed in 134 the static graph by Eq. 1. However, the application to temporal networks has two challenges: (1) 135 The dynamic nature of the temporal network. Unlike static networks, where the structure remains 136 constant, temporal networks capture evolving relationships and interactions. This dynamic nature 137 introduces challenges in analyzing and modeling the network's behavior, as the network's topology 138 and connectivity patterns may vary at different time points. (2) The expensive time complexity of 139 140 computing the Laplacian eigenvalues. In Eq. 1, computing the eigenvalues of the Laplacian matrix is a computationally intensive task and the time complexity grows with the size of the network. The 141 time cost is cubic in the number of nodes. In temporal networks, where the network structure changes 142 over time, repeatedly calculating the Laplacian eigenvalues can become prohibitively expensive and 143 time-consuming. 144

To solve these challenges, we must simplify the network and efficiently approximate thermodynamic 145 146 quantities. First, we select a specific time interval from the temporal network and aggregate edge weights or frequencies, where the number of occurrences within the chosen time frame determines 147 the strength of an edge. Following this process, the temporal network can be projected to the 148 time-independent 2-D plane, which provides a simplified representation of the underlying network 149 structure at a specific time. Moreover, inspired by [27], we use the approximate expression for 150 the von Neumann entropy and reduce the computation to quadratic in the number of nodes. The 151 approximate von Neumann entropy is 152

$$S_{VN}(G_t) = 1 - \frac{1}{|V|} - \frac{1}{|V|^2} \sum_{(u,v) \in E} \frac{1}{d_u d_v},$$
(3)

where V is the node set of the temporal network, and  $d_u$ ,  $d_v$  are the degree of node u and v at time t. This approximation allows the von Neumann entropy to be computed without explicitly solving the eigensystem for the normalized Laplacian. The proof of the approximate von Neumann entropy is presented in Appendix A. Thus, the von Neumann entropy can be computed in quadratic time using the node degrees for pairs of nodes connected by edges.

**Thermodynamic Temperature Differences.** In thermodynamics, a thermodynamic state of a system can be fully described by an appropriate set of principal parameters known as thermodynamic variables. Due to the dynamic nature of the temporal network, it is not sufficient to simply evaluate the evolution states for two moments using the von Neumann entropy. Thus, we introduce the thermodynamic temperature difference, defined as the rate of energy change with entropy between two networks, to complement the description of the network dynamics system. The expression which subject to the condition that the volume and number of particles are constant is shown as follows:

$$\mathcal{T}(G_1, G_2) = \frac{de}{dS} = \frac{e(G_1) - e(G_2)}{S(G_1) - S(G_2)},\tag{4}$$

where  $S(G_1)$  is the graph entropy on the graph  $G_1$  and  $e(G_1)$  is the graph average energy. The subject 165 can be applied to temporal networks since the networks do not change significantly in node number 166 during evolution. The thermodynamic temperature difference can bridge the graphs of two moments. 167 More importantly, the thermodynamic temperature difference can also be approximated when we 168 project the temporal network as a weighted graph, like in the computing process of von Neumann 169 entropy. The approximate computation method uses low-order Taylor series that can be computed 170 using the traces of powers of the normalized Laplacian matrix, avoiding explicit computation of the 171 normalized Laplacian spectrum [26]. The detailed derivation process is in Appendix A. In summary, 172 the temperature difference between the two networks can be approximated as 173

$$\mathcal{T}(G_1, G_2) = -\frac{2}{k} + \frac{2}{3k} \cdot \frac{\mathcal{K}(G_1) - \mathcal{K}(G_2)}{\mathcal{J}(G_1) - \mathcal{J}(G_2)},$$
(5)

174 where

$$\mathcal{J}(G) = \sum_{u,v \in V} \frac{A_{uv}}{d_u d_v},\tag{6}$$

175

$$\mathcal{K}(G) = \sum_{u,v,w \in V} \frac{A_{uv}A_{vw}A_{wu}}{d_u d_v d_w},\tag{7}$$

<sup>176</sup> k is the Boltzmann constant, and A is the adjacency matrix of the network. Especially we denote <sup>177</sup>  $G'_{uv}$  as the graph G adds a new connection between u and v, the computation of  $\mathcal{T}(G, G'_{uv})$  can <sup>178</sup> be reduced as quadratic in the number of nodes. Because the expressions  $\mathcal{J}(G'_{uv}) - \mathcal{J}(G)$  and <sup>179</sup>  $\mathcal{K}(G'_{uv}) - \mathcal{K}(G)$  can be rewritten as

$$\mathcal{J}(G'_{uv}) - \mathcal{J}(G) = \sum_{i \in V} \frac{A_{iv}}{d_i d_v (d_v + 1)} + \frac{A_{iu}}{d_i d_u (d_u + 1)},$$
  
$$\mathcal{K}(G'_{uv}) - \mathcal{K}(G) = \sum_{i,j \in V} \frac{A_{iv} A_{jv} A_{ij}}{d_i d_j d_v (d_v + 1)} + \frac{A_{iu} A_{ju} A_{ij}}{d_i d_j d_u (d_u + 1)} + \sum_{i \in V} \frac{A_{iv} A_{iu} A_{uv}}{d_i d_u d_v (d_u + 1) (d_v + 1)}.$$
(8)

In summary, by simplifying the network representation and using efficient approximations, the von Neumann entropy and thermodynamic temperature difference can be computed effectively in temporal networks. These measures provide insights into the evolving nature of the network and enable the estimation of its evolution state.

#### 184 4.2 Evolution States Aware Graph Encoder

**Von Neumann Entropy Aware Attention Mechanism.** In graph encoding, we utilize the von Neumann entropy to explore a more diverse and balanced distribution of attention weights with the attention mechanism in the input neighborhood. This strategy helps the model learn network evolution states adaptively. According to Eq. 3, the global network entropy is a sum of contributions from individual edges. Thus, we decompose the global network entropy into components residing on the individual edges, so the von Neumann entropy of the edge connecting nodes u and v is

$$S_{VN}^{uv}(G_t) = \frac{1}{|E|} - \frac{1}{|V||E|} - \frac{1}{|E||V|^2} \frac{1}{d_u d_v},\tag{9}$$

To better encode entropy features into attention layers, we incorporate the edge expression of von Neumann entropy via a bias term to the attention module[22]. Moreover, we use a time position encoding module[25] to supplement the continuous time information of edges simplified in the von Neumann entropy. Concretely, given a target node u at time t, the attention weight  $\alpha_v^{(l)}$  from the neighbor node v on the  $l^{th}$  layer as

$$\alpha_{v}^{(l)} = \frac{Q_{u}^{(l)} \left(K_{v}^{(l)}\right)^{T}}{\sqrt{d}} + S_{VN}^{uv}(G_{t}),$$
(10)

196 197

$$Q_u^{(l)} = (h_u^{(l-1)} \| e_0 \| \phi(0)) W_Q, \tag{11}$$

$$K_v^{(l)} = M_{v,t}^{(l)} W_K, (12)$$

198

$$M_{v,t}^{(l)} = \left(h_v^{(l-1)} \|e_{uv,t}\|\phi(t_q - t)\right) W_M,$$
(13)

where *d* is the dimension of the node representation and "||" is the concatenation operation.  $W_K \in \mathbb{R}^{(d+d_t+d_e)\times d}$  and  $W_Q \in \mathbb{R}^{(d+d_t+d_e)\times d}$  are the projection matrices to obtain the query matrices and key matrices.  $e_0$  is an all-zero vector to keep the same dimension as *K* and *V*, and  $\phi$  (\*) is the generic time position encoding module from [25], which encodes the difference between the edge's timestamp and query timestamp.  $M_{v,t}^{(l)}$  is the message representation at time *t* from node *v* to *u*, where  $h_v^{(l-1)}$  is node *v*'s hidden representation on the  $(l-1)^{th}$  layer,  $e_{uv,t} \in \mathbb{R}^{d_e}$  is the edge feature, and  $t_q$  is the query time.

Next, the model combines values with the attention weight aware of generating hidden representation  $z_u^{(l)}(t)$  for node u. Finally, an MLP is used to combine the node representation of the previous layer with the neighborhood information:

$$h_u^{(l)} = MLP(h_u^{(l-1)} \| z_u^{(l)}(t)),$$
(14)

$$z_u^{(l)}(t) = \sum_{v \in \mathcal{N}_v} \operatorname{softmax}_v(\alpha_v(t)) V_v(t),$$
(15)

210

209

$$V_v^{(l)} = M_{uut}^{(l)} W_V, \tag{16}$$

where  $V_v^{(l)}$  is the value vector of neighbor node v, and  $\mathcal{N}_u$  is a neighbor node set that connects with node u before time t.

Virtual Evolution Node Representation Learning. Temporal net-213 works follow evolution laws in the progress of time. The emergence 214 of nodes and edges is often predictive, i.e., future network states 215 can be predicted by past states and evolutionary laws. The network 216 evolution state representation learning utilizes historical evolution 217 information and the future virtual evolution graph to generate node 218 representations. Specifically, the dynamic link prediction task aims 219 to predict the probability of the link between two nodes appearing 220 at a future moment. We suppose the link has been generated at the 221 query moment and further construct the virtual evolution graph be-222 longing to the query node pair on this suppose. For example, given a 223 node pair (u, v) and the query time t, there is a virtual bridge at time 224



Figure 2: Virtual evolution graph of u, v at time t.

t that connects the node u and v in the virtual evolution graph  $G'_{uv}$ . The approach makes the two node's neighborhoods interconnected. We denote  $h'_u$  and  $h'_v$  as the virtual future node embedding of u and v. Our framework will further measure the evolution differences through the decoding process.

#### 228 4.3 Mixture of Thermodynamic Experts Decoder

Expert Assessment Features. We use the von Neuman entropy of the original graph, the von Neuman 229 230 entropy of the virtual evolution graph, and the thermodynamic temperature difference between both networks to combine a unique vector as expert assessment features. The vector represents the 231 232 network's evolution states in the 3-D thermodynamic space, which is made up of current time and future time's von Neumann entropy and the thermodynamic temperature. We use Eq. 5 to approximate 233 the thermodynamic temperature difference and Eq. 3 to compute the von Neumann graph entropy for 234 the original and virtual evolution graphs. Furthermore, to control evolution-aware ranges, which is 235 important for large temporal networks, we compute these approximate thermodynamic quantities in 236 the node's neighborhood and set the sampled neighborhood size N. 237

Decoding Process. The mixture of thermodynamic experts decoder dynamically selects the appropriate thermodynamic expert model based on the input expert assessment feature vectors. For each expert, we use a two-layers MLP model to represent. Then the MoTE decoder combines the output embedding of each expert model using respective expert weights to produce the final target score as follows:

$$score(u, v, t) = \sum_{i=1}^{M} \sigma(W_i(h_u, h_v, h'_v - h_v, h'_u - h_u))\pi_i,$$
(17)

Task	Methods	MathOverflow	BitcoinAlpha	BitcoinOTC	Wikipedia
Transductive	JODIE	86.07 ±0.48	91.14 ±0.18	92.29 ±0.11	94.62 ±0.50
	DyRep	$80.77 \pm 0.65$	79.39 ±3.17	79.21 ±4.10	94.59 ±0.20
	TGN	$80.47 \pm 3.24$	86.71 ±1.00	86.78 ±2.29	98.46 ±0.10
	TGAT	$71.80 \pm 0.91$	78.99 ±0.50	79.53 ±0.67	95.34 ±0.10
	CAW	$53.82 \pm 0.28$	64.70 ±0.93	73.95 ±1.22	98.96 ±0.10
	TDLG	84.02 ±0.16	92.83 ±0.22	93.48 ±0.22	88.93 ±0.09
	P-INT	$54.09 \pm 3.24$	88.11 ±0.60	91.26 ±0.69	98.78 ±0.10
	NeurTWs	<u>92.56 ±0.51</u>	<u>93.95 ±0.41</u>	<u>95.75 ±0.01</u>	94.54 ±0.87
	ESSEN	98.60 ±0.40	99.10 ±0.16	98.88 ±0.42	99.03 ±0.33
Inductive	JODIE	67.06 ±0.42	74.47 ±0.16	76.21 ±0.47	93.11 ±0.40
	DyRep	$63.50 \pm 0.66$	66.27 ±0.73	65.09 ±0.86	$92.05 \pm 0.30$
	TGN	$64.50 \pm 1.17$	69.36 ±0.94	76.52 ±1.25	97.81 ±0.10
	TGAT	$60.02 \pm 0.75$	66.42 ±1.17	66.62 ±1.99	93.99 ±0.30
	CAW	57.67 ±0.33	64.38 ±1.01	72.99 ±0.46	<u>98.75 ±0.14</u>
	TDLG	74.31 ±1.58	83.85 ±1.65	85.22 ±3.89	45.77 ±3.06
	P-INT	$50.16 \pm 1.46$	77.88 ±0.93	83.76 ±0.98	$98.38 \pm 0.40$
	NeurTWs	<u>91.83 ±0.13</u>	<u>94.20 ±0.26</u>	<u>96.08 ±0.38</u>	94.63 ±0.47
	ESSEN	98.33 ±0.28	98.07 ±0.64	98.67 ±0.31	98.80 ±0.10

Table 1: Performance of AUC(%) for link prediction. The best results in each column are highlighted in bold font and the second-best results are underlined. We report the AP results in Appendix B.

243

$$\pi_i = softmax_i((\mathcal{T}(G, G'_{uv}) \| S_{VN}(G)) \| S_{VN}(G'_{uv})) W_{\pi}), \tag{18}$$

where *M* is the total number of experts,  $\pi_i$  is the mixing coefficient of expert *i*.  $W_i \in \mathbb{R}^{4d \times 1}$  is the weight matrices for expert *i*. And  $W_{\pi} \in \mathbb{R}^{3 \times M}$  is the weight matrix of the gate unit.  $h_v$  and  $h'_v$  are the embeddings of node *v* in the original graph and virtual evolution graph generated by the encoder.

## 247 4.4 Optimization

During training, we evaluated the convergence behavior of our model by monitoring the training and
validation loss, ensuring that the model was not underfitting or overfitting. The loss function is shown
as follows:

$$\ell = \sum_{(v_i, v_j, t_{ij}) \in \mathcal{E}} -\log P(v_i, v_j \mid t_{ij}) - \mathcal{Q} \cdot \mathbf{E}_{\tilde{v} \sim P(\tilde{v})} \log P(v_i, \tilde{v} \mid t_{ij}),$$
(19)

where  $(v_i, v_j, t_{ij})$  is the observed edge on the temporal network, Q denotes the number of negative samples, and  $P(\tilde{v})$  is the negative sampling distribution over the node space **E**.

## 253 4.5 Computational Complexity Analysis

This section aims to highlight the efficiency of our approach in calculating approximate thermo-254 dynamic quantities of temporal networks. Based on Eq.3, Eq. 5, and Eq. 8, the time complexity 255 of computing approximate von Neumann entropy and the approximate temperature difference is 256  $O(|V|^2)$ , where |V| is the number of nodes in the network. Moreover, we compute the approximate 257 thermodynamic quantities in the neighborhood for the large networks and set the sampled neighbor-258 hood size N. In this setting, the computational complexity can be reduced to  $O(N^2)$ , where N is 259 the settable number. Therefore, the time complexity demonstrates scalability and feasibility for our 260 method to operate in moderate or large networks. The controllable time complexity ensures efficient 261 computation. 262

# **263 5 Experiments**

#### 264 5.1 Experimental Setup

265	Datasets. The temporal network datasets of our	
266	experiment are divided into three types: (a) QA:	-
267	The "answers to questions" dataset of MathOver-	-
268	flow. (b) Bitcoin trading data: BitcoinAlpha	
269	Dataset and BitcoinOTC Dataset [9; 8]. (c) So-	
270	cial networks: Wikipedia Dataset[10]. Table 2	
271	reports more details about these datasets.	-

Table 2: Statistics of the datasets.						
Dataset	Nodes	Edges	Timespan			
MathOverflow	21,688	107,581	2350 days			
BitcoinOTC	5,881	35,592	1903 days			
BitcoinAlpha	3,783	24,186	1901 days			
Wikipedia	9,227	157,474	30 days			

Baselines. In addition to reporting our ESSEN method's performance, we report results for several popular dynamic methods: a) JODIE [10]; b) DyRep [21]; c) TGAT [25]; d) TGN [19]; e) CAW [24];
f) TDLG[4]; g) P-INT[20]; and h) NeurTWs[6]. We report more details about baselines in Appendix C.

Link Prediction Task Settings. We evaluate our model on the link prediction task with two significant
 settings:

• **Transductive Setting.** The model under the transductive setting is trained on available nodes and their connections to predict links between these nodes in the future. The setting assumes the network will not add unseen nodes in the future test time. It mainly evaluates the model's transductive ability.

Inductive Setting. The inductive setting predicts missing links for existing nodes and potential
 new nodes that may be added in the future. It generalizes link prediction beyond known nodes,
 considering the possibility of new nodes. It learns network patterns and characteristics to make
 predictions applicable to both known and unknown nodes.

**Implementation Training Details.** For each dataset, we used the training time points  $T_{tr} = 70\%$ 286 to split the dataset results in approximately 70%-15%-15% of the total edges [25]. The principal 287 288 hyperparameters are set as follows: a) the number of attention heads  $\mathcal{U} = \{2, 3\}$ , b) the number of 289 the GNN layers  $\mathcal{L} = 2$ , c) the maximum number of aggregated neighbors  $n \in \{60, 80, 100\}$ , d) the total number of experts in MoTE  $M = \{4, 6, 8, 10\}$ , and e) the dimension of the node embedding 290 D = 172. We use the ADAM optimization algorithm for model training with a learning rate 1e-3 291 and batch size of 128. All the models are implemented in PyTorch and evaluated on a single Tesla 292 A100 GPU. 293

#### 294 5.2 Results and Discussion

Table 1 reports the transductive and inductive link prediction task results on four datasets, demonstrat-295 ing our method's state-of-the-art performance on link prediction tasks. Indeed, our model significantly 296 outperforms all baselines on all datasets. In particular, in the MathOverflow dataset, compared with 297 NeurTWs, the second strongest baseline, ESSEN improved the AUC(%) by 5.04% and 6.50% on 298 average on the transductive and inductive setting. The results demonstrate that our method has a 299 300 clear advantage for temporal networks. Specifically, our method performs well on both long and short evolution time networks, while the effectiveness of baseline models varies significantly. CAW 301 and TGAT have enormous performance gaps between MathOverflow and Wikipedia in all tasks. 302 It indicates that our framework represents the network with ever-changing evolution states better. 303 The superiority can be attributed to our von Neumann entropy aware mechanism, virtual evolution 304 node representation learning, and MoTE decoder. In addition, our method is effective under both 305 transductive and inductive settings. On the contrary, the baseline method JODIE cannot predict 306 interactions well between unseen nodes because it pays more attention to node identities rather than 307 the evolution states of temporal networks. 308

#### 309 5.3 Ablation Study and Time Comparison

Ablation Study. To validate the effectiveness of the elements comprising ESSEN, we conduct a series of ablation studies and report the AUC results. We investigated the proposed modules with three ablated models on the Bitcoin-alpha dataset: a)ESSEN-*E*, the model removes the von Neumann edge entropy bias in the attention mechanism of ESSEN. b)ESSEN-*V*, the model removes virtual evolution node representation and



Figure 3: Ablation Study



Figure 5: Study on important settings. We report the results of the inductive link prediction.

only uses the node embeddings of the original graph for decoding. c)ESSEN-*D*, the model replaces
the MoTE decoder with a simple MLP decoder. In Fig. 3, we can see the performance degradation
without considering the von Neumann entropy information of edges, demonstrating the effectiveness
of the proposed von Neumann entropy aware attention mechanism. Disabling the virtual evolution
node representation also hurts performance. Furthermore, when the MoTE decoder is removed,
BitcoinOTC and BitcoinAlpha exhibit more severe performance drops, demonstrating that the MoTE
decoder excels on temporal networks with a long time span and more evolution states.

Time Comparison. Fig.4 compares the training times of ESSEN 324 against the second-strongest baseline NTW. For fairness, we use the 325 same batch size for both models and experiment in the same environ-326 ment. Note that the running time of ESSEN is down quickly because 327 the approximate thermodynamic quantities have been computed at 328 the first epoch and use cache after that. If we pre-computed thermo-329 dynamic quantities for the model, ESSEN would run considerably 330 faster than NTW. 331



Figure 4: Time Comparison.

#### 332 5.4 Parametric Sensitivity

we investigate the sensitivity of our ESSEN to various parameters and evaluate their impact on 333 the model's performance. In Fig. 5, We report the results and have the following observations: a) 334 Through the exploration of different training time points, our model keeps excellent performance, 335 even if the number of samples in the training set is reduced since the training time shift. Especially, 336 lowering the training time point means increasing the testing of more samples in the future. It clearly 337 shows the robustness of ESSEN for complex evolutionary states. b) Regarding the number of experts 338 M, there are sweet spots in both datasets. This finding indicates that different datasets exhibit a 339 preference for specific numbers of experts in the MoTE decoder, which can be attributed to the 340 varying complexity of evolutionary states in the temporal network. c) We observe a strong correlation 341 between the evolution-aware size N and the node number of the temporal network. For instance, 342 the MathOverflow with more number nodes has better performance with the large evolution-aware 343 neighborhood. On the contrary, it negatively impacts the performance of BitcoinAlpha when N is 344 higher than 100. 345

# 346 6 Conclusion

In this paper, we propose ESSEN, an Evolution StateS awarE Network for recognizing and analyzing 347 the evolution states on temporal networks. We addressed the limitations of existing methods in 348 capturing the time-varying nature of network structures, especially in complex evolving states. Our 349 framework incorporates a von Neumann entropy aware attention mechanism and network evolution 350 state contrastive learning in the graph encoding. The decoding stage utilizes a unique decoder called 351 Mixture of Thermodynamic Experts (MoTE). We evaluated ESSEN on link prediction tasks in 352 transductive and inductive settings and compared it to state-of-the-art baselines. The experimental 353 354 results demonstrate the effectiveness of our proposed method in capturing temporal dynamics and outperforming existing approaches. Our work contributes to advancing the field of temporal network 355 analysis and opens up possibilities for future research in other domains and additional network 356 dynamics. In the future, we will focus on improving ESSEN's efficiency and scalability, allowing it 357 to handle larger datasets and real-time analysis. 358

## 359 **References**

- [1] Alstott, J., Pajevic, S., Bullmore, E., Plenz, D.: Opening bottlenecks on weighted networks by local
   adaptation to cascade failures. Journal of Complex Networks 3(4), 552–565 (2015)
- [2] Anand, K., Krioukov, D., Bianconi, G.: Entropy distribution and condensation in random networks with a
   given degree distribution. Physical Review E 89(6), 062807 (2014)
- [3] Braunstein, S.L., Ghosh, S., Severini, S.: The laplacian of a graph as a density matrix: a basic combinatorial
   approach to separability of mixed states. Annals of Combinatorics 10(3), 291–317 (2006)
- [4] Chanpuriya, S., Rossi, R.A., Kim, S., Yu, T., Hoffswell, J., Lipka, N., Guo, S., Musco, C.: Direct
   embedding of temporal network edges via time-decayed line graphs. In: ICLR (2022)
- [5] De Domenico, M., Nicosia, V., Arenas, A., Latora, V.: Structural reducibility of multilayer networks.
   Nature communications 6(1), 1–9 (2015)
- [6] Jin, M., Li, Y.F., Pan, S.: Neural temporal walks: Motif-aware representation learning on continuous-time
   dynamic graphs. In: NeurIPS (2022)
- [7] Kipf, T.N., Welling, M.: Semi-supervised classification with graph convolutional networks. In: ICLR
   (2016)
- [8] Kumar, S., Hooi, B., Makhija, D., Kumar, M., Faloutsos, C., Subrahmanian, V.: Rev2: Fraudulent user
   prediction in rating platforms. In: WSDM. pp. 333–341. ACM (2018)
- [9] Kumar, S., Spezzano, F., Subrahmanian, V., Faloutsos, C.: Edge weight prediction in weighted signed networks. In: ICDM. pp. 221–230. IEEE (2016)
- [10] Kumar, S., Zhang, X., Leskovec, J.: Predicting dynamic embedding trajectory in temporal interaction
   networks. In: SIGKDD. ACM (2019)
- [11] Li, Z., Mucha, P.J., Taylor, D.: Network-ensemble comparisons with stochastic rewiring and von neumann
   entropy. SIAM journal on applied mathematics 78(2), 897–920 (2018)
- [12] Liben-Nowell, D., Kleinberg, J.: The link-prediction problem for social networks. Journal of the American
   society for information science and technology 58(7), 1019–1031 (2007)
- [13] Liu, S., Chen, P.Y., Hero, A., Rajapakse, I.: Dynamic network analysis of the 4d nucleome. bioRxiv p.
   268318 (2018)
- [14] Monti, F., Boscaini, D., Masci, J., Rodola, E., Svoboda, J., Bronstein, M.M.: Geometric deep learning on
   graphs and manifolds using mixture model cnns. In: CVPR. pp. 5115–5124 (2017)
- [15] Nguyen, G.H., Lee, J.B., Rossi, R.A., Ahmed, N.K., Koh, E., Kim, S.: Continuous-time dynamic network
   embeddings. In: WWW. pp. 969–976 (2018)
- [16] Passerini, F., Severini, S.: The von neumann entropy of networks. Available at SSRN 1382662 (2008)
- [17] Passerini, F., Severini, S.: Quantifying complexity in networks: the von neumann entropy. International
   Journal of Agent Technologies and Systems (IJATS) 1(4), 58–67 (2009)
- [18] Ren, H., Leskovec, J.: Beta embeddings for multi-hop logical reasoning in knowledge graphs. In: NeurIPS.
   vol. 33, pp. 19716–19726 (2020)
- [19] Rossi, E., Chamberlain, B., Frasca, F., Eynard, D., Monti, F., Bronstein, M.: Temporal graph networks for
   deep learning on dynamic graphs. In: ICLR (2020)
- Souza, A., Mesquita, D., Kaski, S., Garg, V.: Provably expressive temporal graph networks. Advances in
   Neural Information Processing Systems 35, 32257–32269 (2022)
- [21] Trivedi, R., Farajtabar, M., Biswal, P., Zha, H.: Dyrep: Learning representations over dynamic graphs. In:
   ICLR (2019)
- [22] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, Ł., Polosukhin, I.:
   Attention is all you need. Advances in neural information processing systems **30** (2017)
- [23] Wang, J.: Statistical Mechanics for Network Structure and Evolution. Ph.D. thesis, University of York
   (2018)

- [24] Wang, Y., Chang, Y.Y., Liu, Y., Leskovec, J., Li, P.: Inductive representation learning in temporal networks
   via causal anonymous walks. In: ICLR (2021)
- [25] Xu, D., Ruan, C., Korpeoglu, E., Kumar, S., Achan, K.: Inductive representation learning on temporal
   graphs. In: ICLR (2020)
- Ye, C., Comin, C.H., Peron, T.K.D., Silva, F.N., Rodrigues, F.A., Costa, L.d.F., Torsello, A., Hancock,
   E.R.: Thermodynamic characterization of networks using graph polynomials. Physical Review E 92(3),
   032810 (2015)
- 412 [27] Ye, C., Wilson, R.C., Comin, C.H., Costa, L.d.F., Hancock, E.R.: Approximate von neumann entropy for
   413 directed graphs. Physical Review E 89(5), 052804 (2014)
- [28] Zhang, M., Chen, Y.: Link prediction based on graph neural networks. Advances in neural information
   processing systems **31** (2018)
- [29] Zhou, L., Yang, Y., Ren, X., Wu, F., Zhuang, Y.: Dynamic network embedding by modeling triadic closure process. In: Proceedings of the AAAI conference on artificial intelligence. vol. 32 (2018)