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

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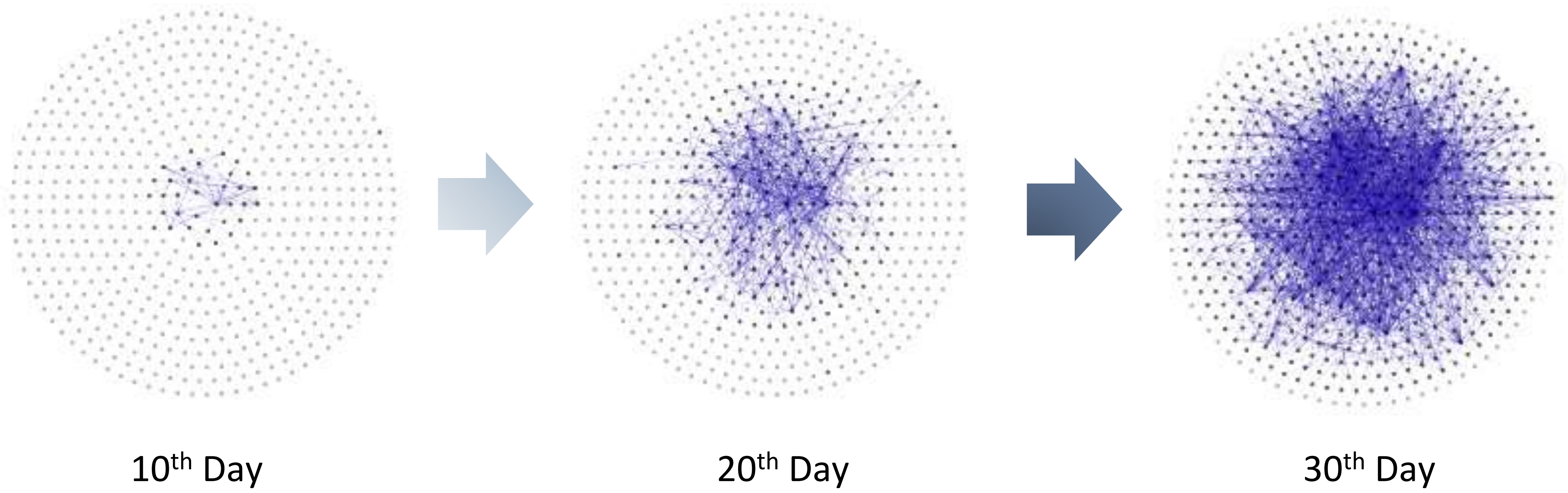
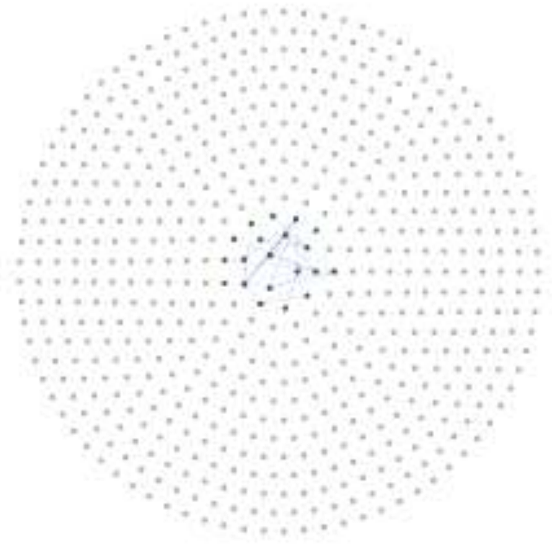
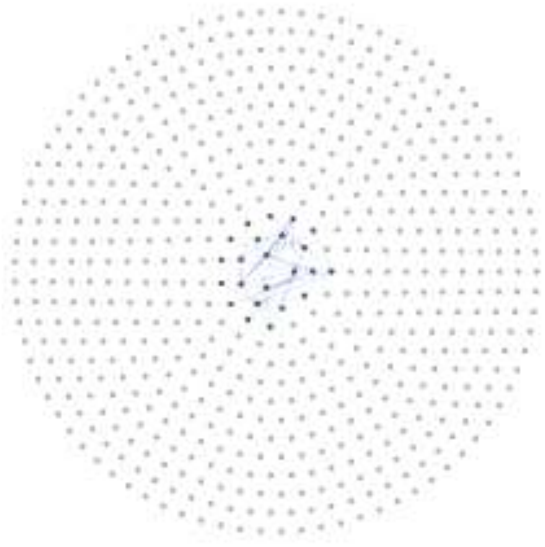
Temporal Network in MathOverflow website



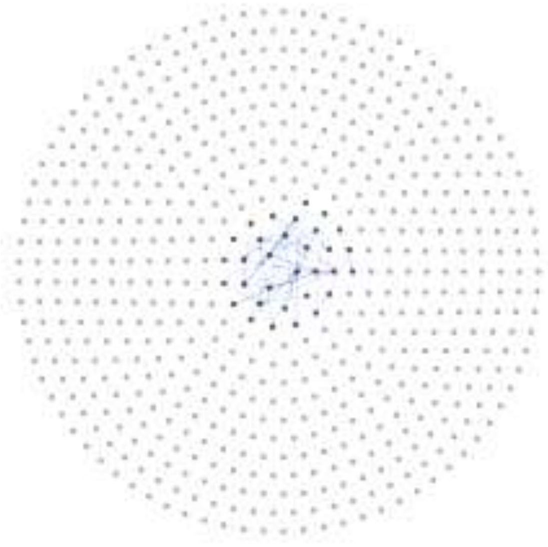
Temporal Network in BitcoinOTC platform



10th Day

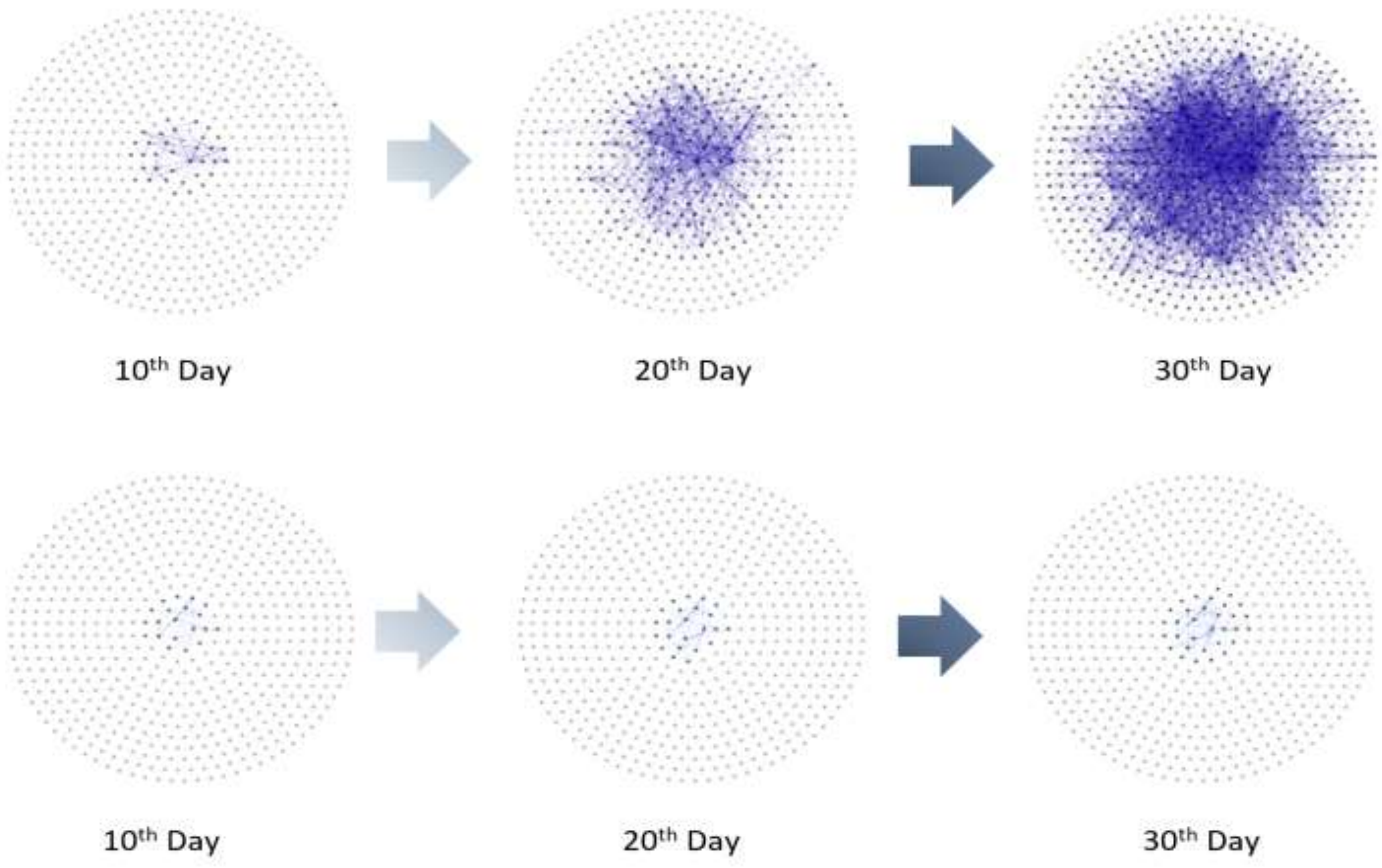


20th Day

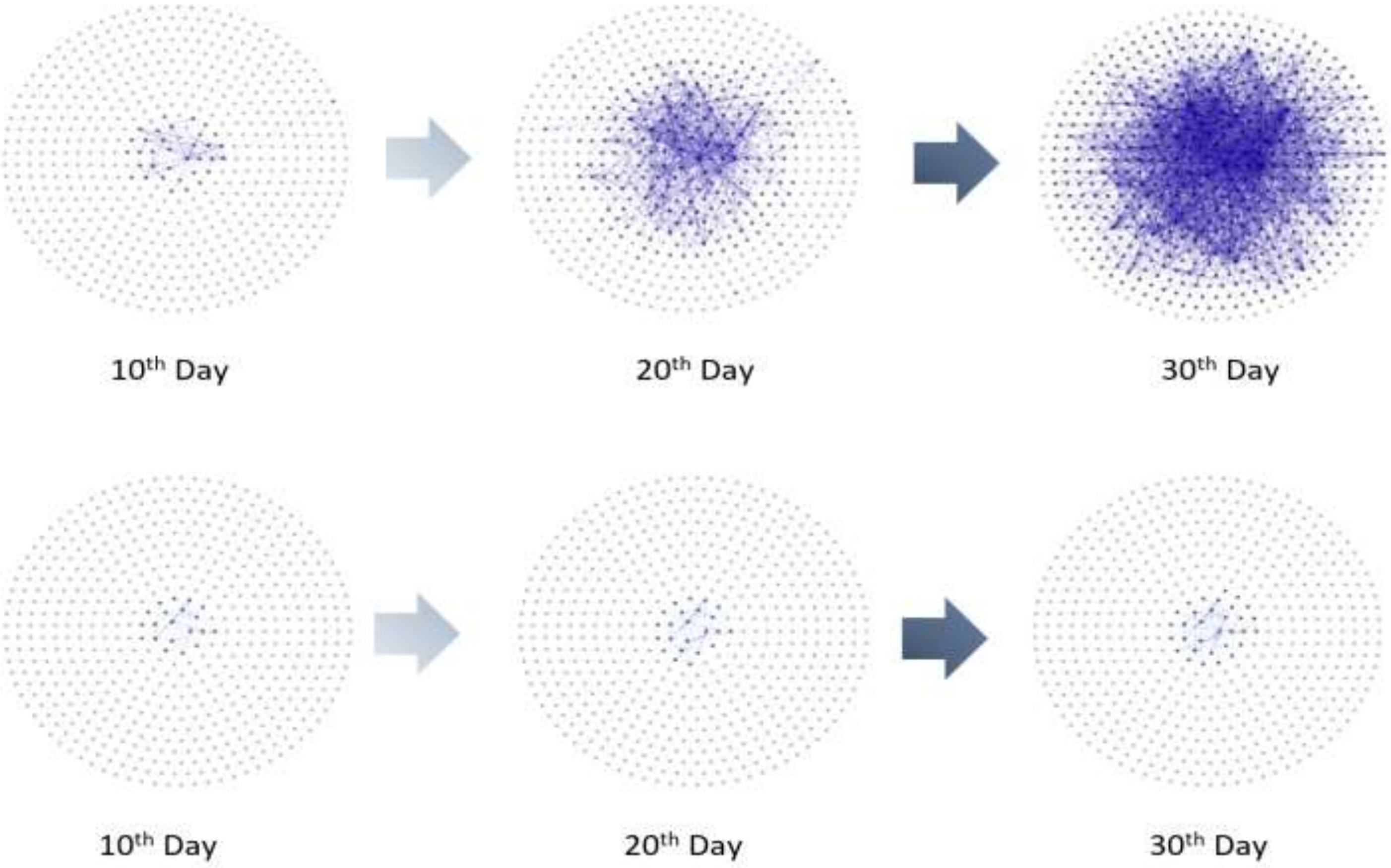


30th Day

Evolution State Estimation

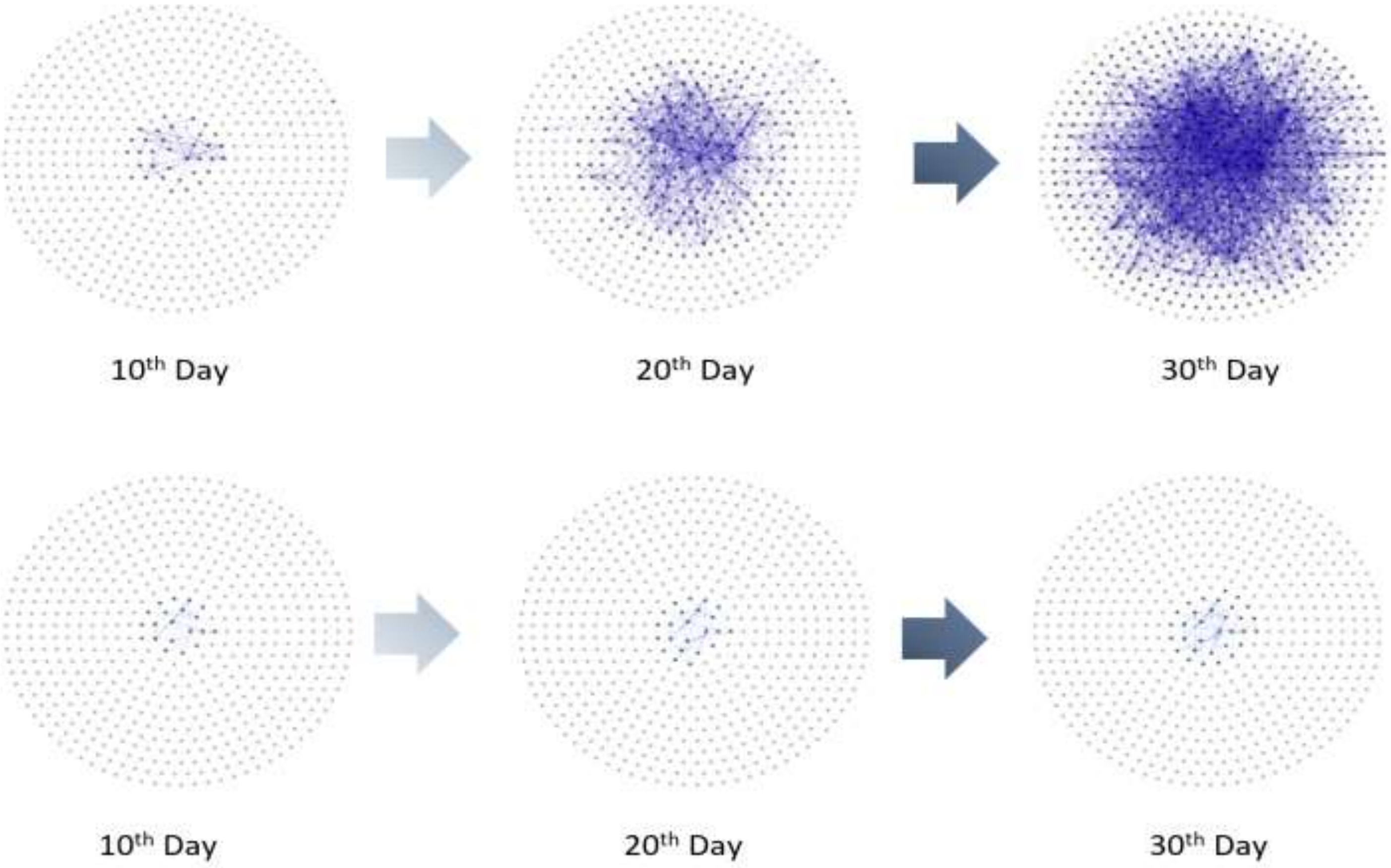


Evolution State Estimation



Generalizability

Evolution State Estimation



Generalizability

Efficiency

Summary of Contribution

- Provides a method to **approximate** the von Neumann entropy for temporal networks.
- Introduces a new perspective to encode evolution aware node representations using the **von Neumann entropy aware attention mechanism** and **virtual evolution node representation learning**.
- Proposes a novel **Mixture of Thermodynamic Experts Decoder** which can recognize temporal network evolution states adaptively.

NEURAL INFORMATION PROCESSING SYSTEMS

Von Neumann Entropy

- **VNE** is a representation of structures widely used to characterize the salient features of quantum systems.

- Using quantum analogy, the interpretation of the normalised Laplacian as a density matrix opens up the possibility of computing the von Neumann entropy in networks.

$$S_{VN}(G) = -\operatorname{Tr}(\rho \log \rho) = -\sum_{i=1}^{|\mathcal{V}|} \frac{\lambda_i}{|\mathcal{V}|} \log \frac{\lambda_i}{|\mathcal{V}|}$$

Approximate Von Neumann Entropy for Temporal Networks

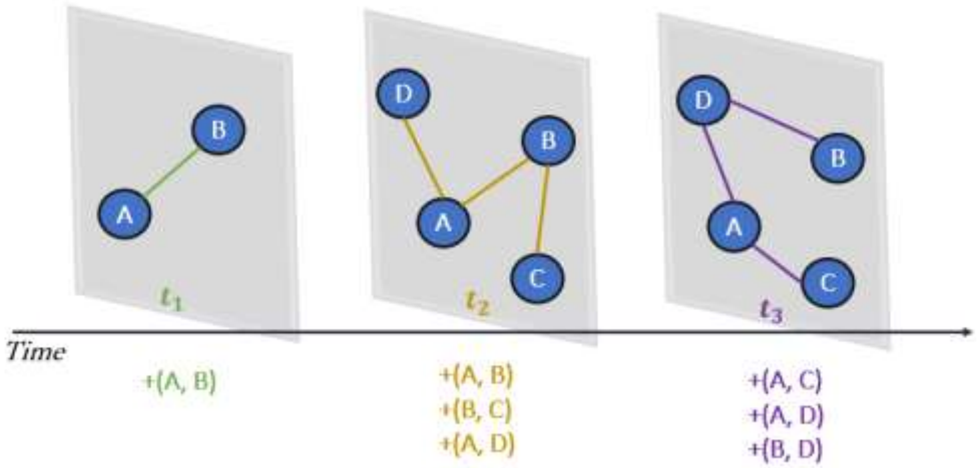
- **The dynamic nature of the temporal network**

Approximate Von Neumann Entropy for Temporal Networks

- **The dynamic nature of the temporal network**

Solution:
(1)Select a specific time interval for the temporal network and aggregate edge weights or frequencies over this interval.

(2)The number of occurrences within the chosen time frame determines the strength of an edge.



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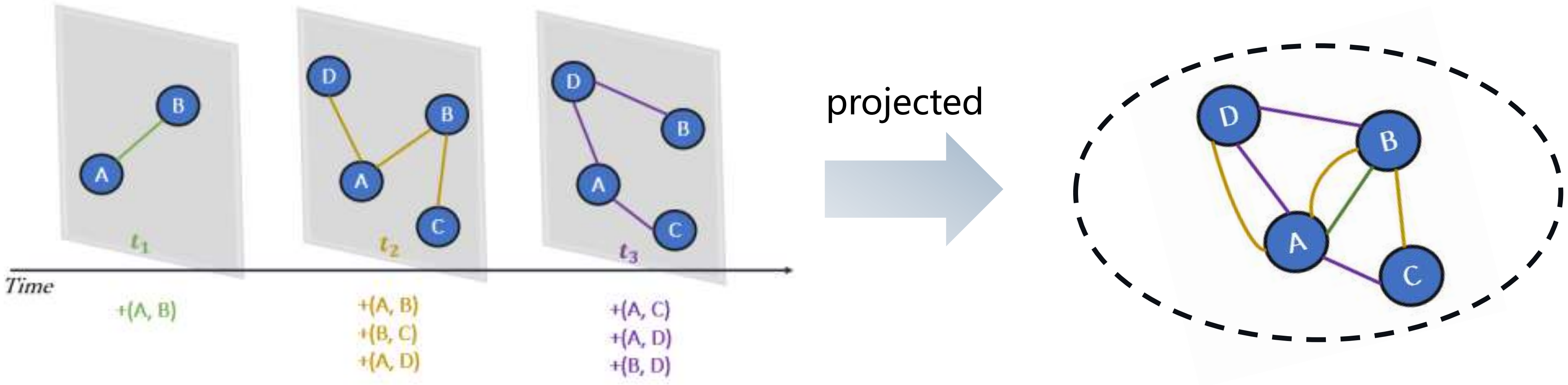


Approximate Von Neumann Entropy for Temporal Networks

- **The computationally expensive time complexity of obtaining the Laplacian eigenvalues.**

Approximate Von Neumann Entropy for Temporal Networks

- **The computationally expensive time complexity of obtaining the Laplacian eigenvalues.**

Solution:
(1) Taylor expansion for $\ln \frac{\hat{\lambda}_j}{|V|}$ and keep the first item

(2) Using the nature of normalized Laplacian matrix

$$S_{VN}(G) = -\sum_j \frac{\hat{\lambda}_j}{|V|} \ln \frac{\hat{\lambda}_j}{|V|} \simeq \sum_j \frac{\hat{\lambda}_j}{|V|} \left(1 - \frac{\hat{\lambda}_j}{|V|}\right)$$
$$= \frac{1}{|V|} \sum_j \lambda_j - \frac{1}{|V|^2} \sum_j \lambda_j^2$$
$$= \frac{\mathrm{Tr}[\hat{L}]}{|V|} - \frac{\mathrm{Tr}\left[\hat{L}^2\right]}{|V|^2}$$
$$= \frac{|V|}{|V|} - \frac{|V|}{|V|^2} - \sum_{(u,v)\in e} \frac{1}{|V|^2 d_u d_v}$$
$$= 1 - \frac{1}{|V|} - \frac{1}{|V|^2} \sum_{(u,v)\in e} \frac{1}{d_u d_v}$$

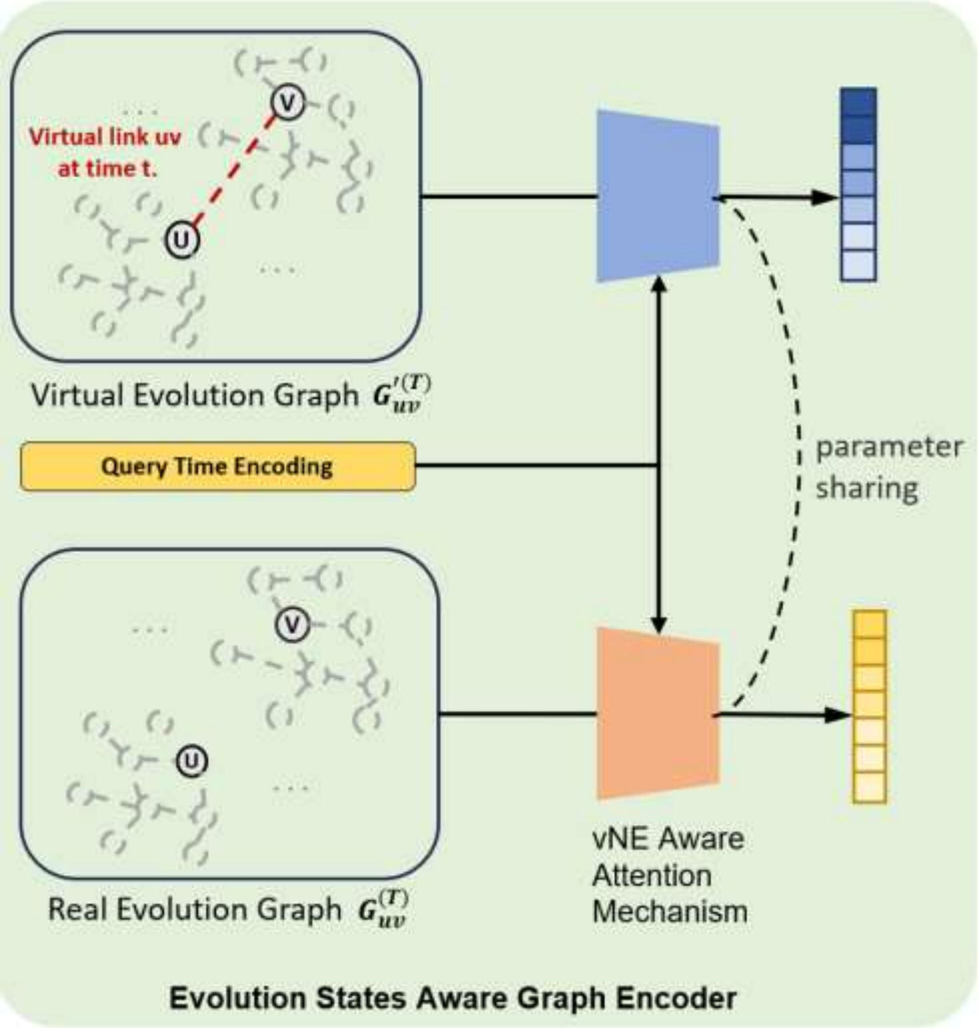
Evolution States Aware Graph Encoder

1) Von Neumann Entropy Aware Attention Mechanism

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

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

$$\alpha_v^{(l)} = \frac{Q_u^{(l)} \left(K_v^{(l)}\right)^T}{\sqrt{d_n}} + S_{VN}^{uv}(G_t)$$

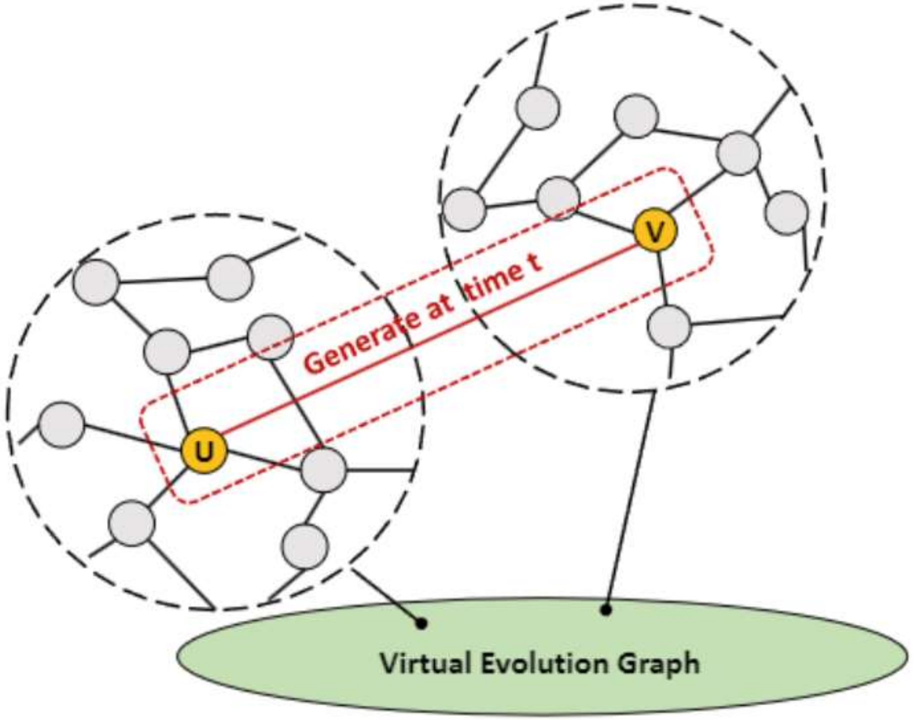


Evolution States Aware Graph Encoder

2) Virtual Evolution Node Representation Learning

+ query edge (u,v,t)

$G \rightarrow G'_{uv}$



The change of virtual evolution is instantaneous. View the evolution process as an **isochoric process** in the network.

The **thermodynamic temperature** of the virtual evolution path can be computed.

Mixture of Thermodynamic Experts Decoder

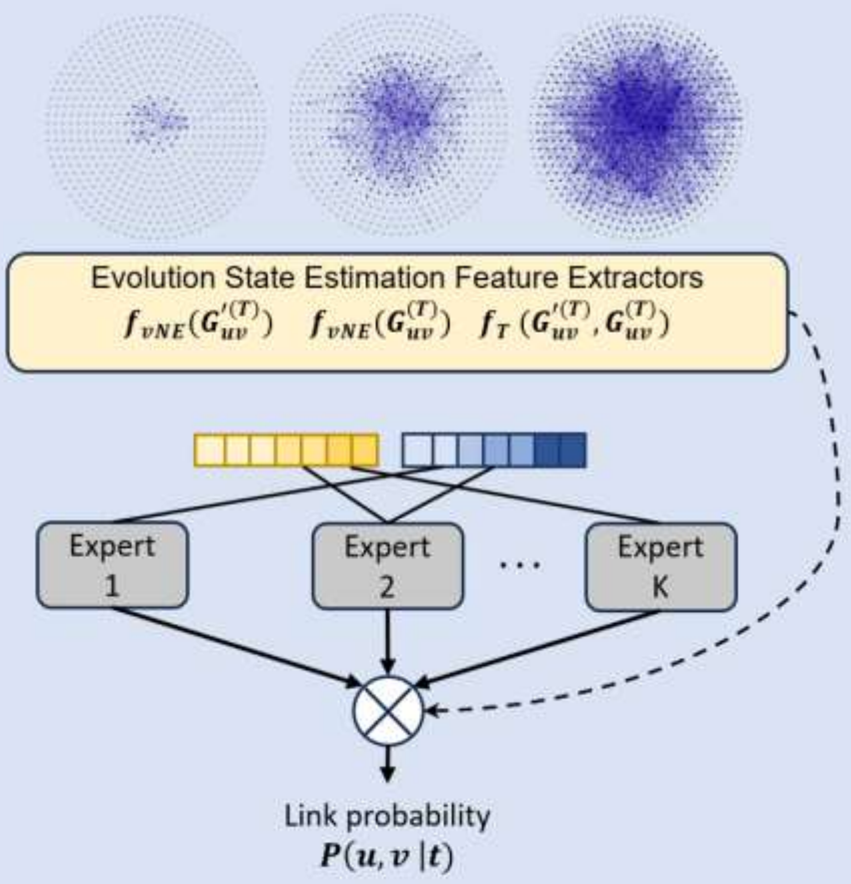
Evolution State Feature Extractor:

Computing thermodynamic vector that includes **vNE** of original and virtual evolution graphs and **thermodynamic temperature** of the virtual evolution path.

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

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

Time Complexity: $O(|V|^2)$, where V can be replaced with the neighborhood size under the sampling setting.



Mixture of Thermodynamic Experts Decoder

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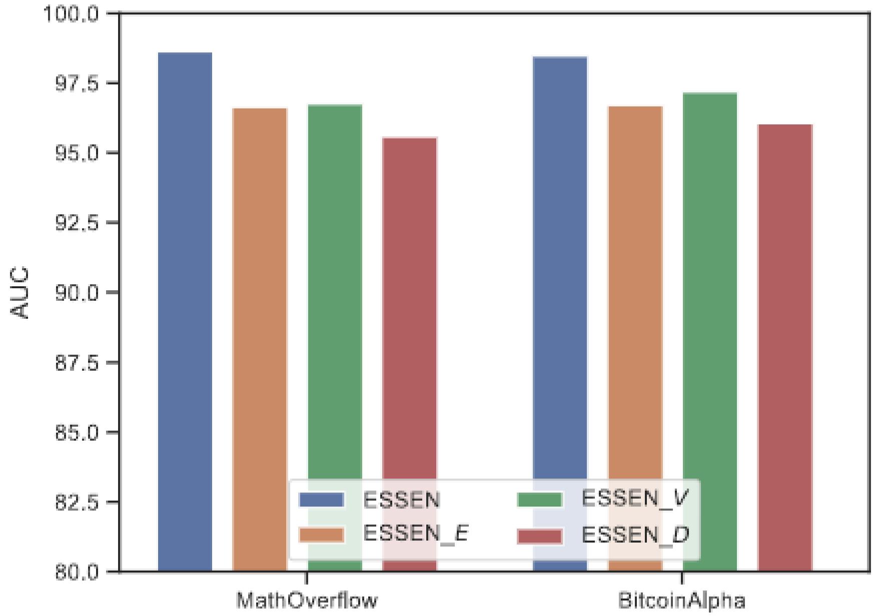
Performance

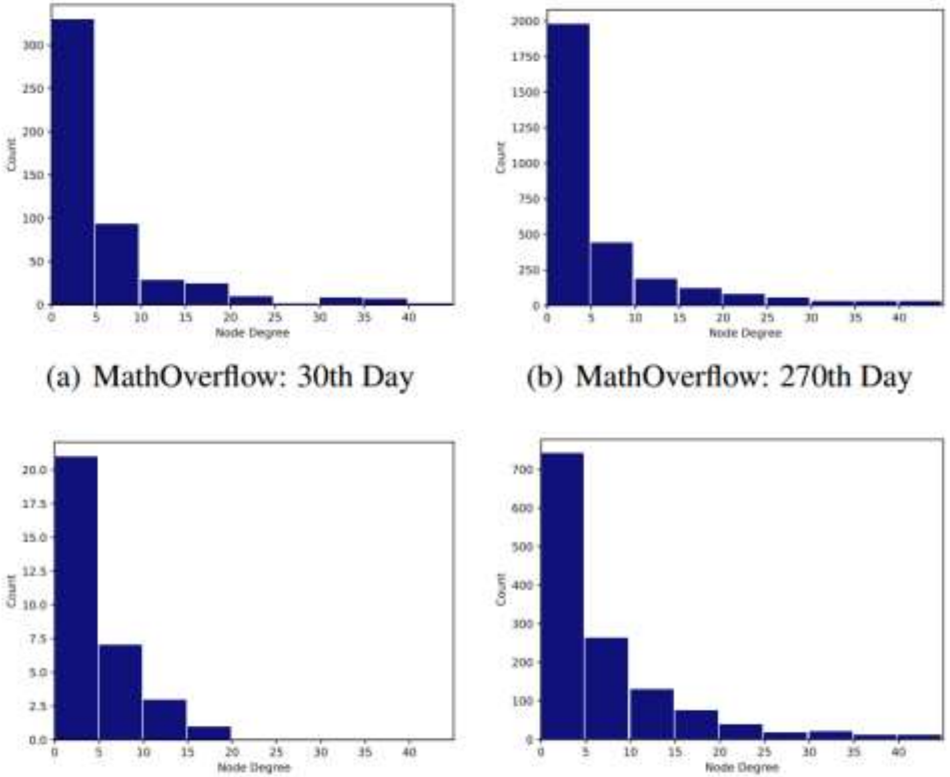
Task	Methods	MathOverflow	BitcoinAlpha	BitcoinOTC	Wikipedia
Transductive	JODIE	86.07 ±0.48	91.14 ±0.18	92.29 ±0.11	93.58 ±2.00
	DyRep	80.77 ±0.65	79.39 ±3.17	79.21 ±4.10	94.22 ±0.27
	TGN	80.47 ±3.24	86.71 ±1.00	86.78 ±2.29	98.46 ±0.10
	TGAT	71.80 ±0.91	78.99 ±0.50	79.53 ±0.67	95.34 ±0.10
	CAW	53.82 ±0.28	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
	NeurTWs	92.56 ±0.51	93.95 ±0.41	95.75 ±0.01	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	91.44 ±1.99
	DyRep	63.50 ±0.66	66.27 ±0.73	65.09 ±0.86	91.03 ±0.34
	TGN	64.50 ±1.17	69.36 ±0.94	76.52 ±1.25	97.70 ±0.18
	TGAT	60.02 ±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	98.75 ±0.14
	TDLG	74.31 ±1.58	83.85 ±1.65	85.22 ±3.89	45.77 ±3.06
	NeurTWs	91.83 ±0.13	94.20 ±0.26	96.08 ±0.38	94.63 ±0.47
	ESSEN	**98.33 ±0.28**	**98.07 ±0.64**	**98.67 ±0.31**	**98.80 ±0.10**

Link Prediction



Ablation Study

Qualitative Analysis



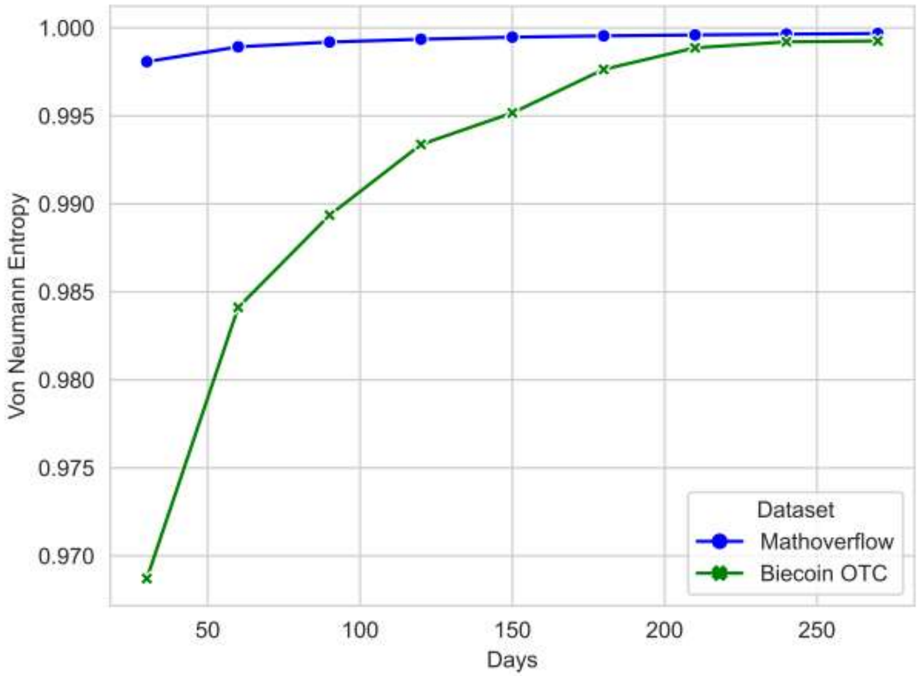
(a) MathOverflow: 30th Day

(b) MathOverflow: 270th Day

(c) BitcoinOTC: 30th Day

(d) BitcoinOTC: 270th Day

Degree distribution



Approximate von Neumann entropy can help model to understand network evolution structure.

NEURAL INFORMATION PROCESSING SYSTEMS

XIAMEN UNIVERSITY

UNIVERSITY of York

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Thank You for Listening!