Supplementary Material

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Contents

1	A b	orief literature review of link prediction methods	3
	1.1	Link prediction in static networks	3
		1.1.1 Similarity-based methods	3
		1.1.2 Probabilistic and statistical models	4
		1.1.3 Dimensionality reduction-based methods	5
		1.1.4 Learning-based methods	5
		1.1.5 Summary of static link prediction methods	6
	1.2	Link prediction in dynamic networks	6
		1.2.1 Unsupervised learning methods	6
			8
		1.2.3 Summary of dynamic link prediction	9
2	Tra	ditional heuristic metrics 1	10
	2.1	Common Neighbors (CN)	10
	2.2		1 ()
			10
	2.3		10 10
	2.3 2.4	Resource Allocation Index (RA)	10
		Resource Allocation Index (RA)	10
3	2.4 2.5	Resource Allocation Index (RA)	10 11
3	2.4 2.5	Resource Allocation Index (RA)	10 11 11
3	2.4 2.5 Dat	Resource Allocation Index (RA)	10 11 11 11

4	Supplementary comparison results			
	4.1	Impact of snapshot sampling interval	13	
	4.2	Impact of flight speed	14	

1 A brief literature review of link prediction methods

In the main paper, we provide a concise literature review of related work on link prediction based on methodological differences. Here, we adopt an alternative taxonomy that categorizes the literature into link prediction in static networks and dynamic networks. Interested readers are referred to more comprehensive surveys [1–7] on this topic under different classification schemes.

1.1 Link prediction in static networks

Link prediction for static networks has a long history. Since Liben-Nowell et al. [8] formulated the link prediction problem and proposed a basic framework based on node similarity, the topic has been extensively studied. We discuss the existing methods from three categories: similarity-based methods, probabilistic and statistical models, dimensionality reduction-based methods, and learning-based approaches.

1.1.1 Similarity-based methods

Similarity-based metrics are the simplest class of methods for link prediction. The similarity between node pairs is typically computed using structural properties of the network. Based on the extent of structural information considered, these methods can be grouped into three categories: local, quasi-local, and global.

Local indices are generally calculated using information about common neighbors and node degree. These indices consider immediate neighbors of a node. Examples of such indices contains common neighbor [9], preferential attachment [10], Adamic/Adar [11], Jaccard Coefficient [12], resource allocation [13], etc. Global similarity indices are computed based on the entire topological structure of a network. While these methods often achieve high prediction accuracy by capturing long-range dependencies between nodes, they typically involve higher computational complexity, making them less practical for large-scale networks. Representative global indices include the Katz Index [14], Random Walk with Restart (RWR) [15], Shortest Path [16], Path Entropy [17], and others. Quasi-local indices achieve a balance between local and global approaches by trading off predictive accuracy and

computational cost. These methods generally offer better performance than purely local indices by incorporating a broader range of structural information. However, their performance typically falls short of fully global methods, as they rely on less comprehensive topological information. Representative examples include the Local Path Index [18], Local Random Walk Index [19], and Local Directed Path (LDP) [20].

1.1.2 Probabilistic and statistical models

Probabilistic and statistical models typically assume a known or observable network structure and aim to construct models that fit this structure while estimating parameters using statistical methods. To improve predictive performance, such models often incorporate not only topological information but also node and edge attributes. However, the high computational cost and the requirement for rich attribute data limit the scalability and applicability of probabilistic models in large or dynamic networks.

Wang et al. [21] introduced a local probabilistic model that leverages topological, semantic, and co-occurrence features for link prediction. They proposed the concept of a central neighborhood set and extracted non-derivable frequent itemsets from event logs to serve as input for training a local Markov Random Field (MRF). The model is iteratively optimized using probabilistic inference techniques to estimate the likelihood of potential links. Probabilistic Relational Models (PRMs) [22–24] offer a unified framework for link prediction by incorporating both node and link attributes. They model heterogeneous entities (e.g., persons, articles, institutions) and their relationships by casting link prediction as an attribute inference problem within a relational graph structure. Clauset et al. [25] proposed a hierarchical probabilistic model that learns network structure from data through a tree-based representation. The model estimates link likelihoods based on hierarchical groupings, providing insights into the organization of complex networks. Stochastic Block Models (SBMs) [26, 27] extend the hierarchical structure concept by partitioning nodes into blocks or communities, where the probability of a connection between nodes depends on their respective group memberships. Guimerà et al. [28] utilized SBMs to evaluate the reliability of observed links and to identify potential missing or spurious connections. Exponential Random Graph Models (ERGMs) [29] define a probability distribution over possible network configurations, allowing for the modeling of complex structural dependencies. Several studies [30–32] have applied

ERGMs to discover plausible links by comparing the observed network with random ensembles under predefined structural principles.

1.1.3 Dimensionality reduction-based methods

The curse of dimensionality poses significant challenges in link prediction. To address this, dimensionality reduction techniques such as network embedding and matrix factorization have gained increasing attention.

Network embedding methods learn low-dimensional vector representations of nodes that preserve network proximity. Classical techniques include Laplacian Eigenmaps [33], Locally Linear Embedding (LLE) [34], and Isomap [35]. However, these methods often face scalability issues. Recent advances exploit the sparsity of real-world networks to improve scalability. For example, DeepWalk [36] treats truncated random walks as sentences in a language model to capture higher-order proximities, while Node2vec [37] introduces biased random walks that balance breadth-first and depth-first search strategies, demonstrating improved performance over DeepWalk. Complex embeddings, as introduced by Trouillon et al., leverage matrix and tensor factorization with complex-valued vectors to model diverse binary relations, including symmetric and antisymmetric ones. Menon et al. [38] proposed a supervised matrix factorization framework that addresses class imbalance by optimizing ranking loss and integrating explicit node and link features for improved link prediction. Similar approaches by Chen et al. [39] combined topological and attribute matrices via non-negative matrix factorization.

1.1.4 Learning-based methods

In learning-based methods, link prediction is often formulated as a binary classification problem, where each data point corresponds to a node pair and the label indicates the presence or absence of a link. Various classifiers [40,41] (e.g., SVM, decision trees, naive Bayes) can be employed; however, a key challenge lies in selecting effective features. Most existing works [42] rely on topological features, which are domain-independent and computationally efficient.

In recent years, deep learning techniques have shown great promise in link prediction by learning high-level representations from structural and attribute data. Schlichtkrul et al. developed the Relational Graph Convolutional Network (R-GCN) [43], which models knowledge graphs as di-

rected multigraphs with labeled nodes and edges, enabling link prediction via autoencoding. Kipf et al. proposed the Variational Graph Autoencoder (VGAE) [44], which learns latent node representations from the adjacency and feature matrices of graphs. The input is normalized and self-loops are added to improve stability during training. More recent models, such as the Weisfeiler–Lehman Neural Machine (WLNM) [45], capture higher-order local structures through subgraph extraction and use neural networks to learn link patterns. The SEAL framework [46] further integrates local subgraphs, embeddings, and attributes within a unified GCN-based model, demonstrating superior performance over heuristic and latent feature-based methods.

1.1.5 Summary of static link prediction methods

For Static link prediction, similarity-based methods offer intuitive and computationally efficient solutions by leveraging local to global network structures. Probabilistic models predict links via statistical inference, often integrating topological information along with node or edge attributes to improve accuracy. Dimensionality reduction methods, including network embedding and matrix factorization, effectively address high-dimensionality issues by learning compact node representations. Learning-based approaches, especially those leveraging deep learning, have recently advanced the field by capturing complex patterns and high-order structures, leading to improved prediction accuracy. Together, these diverse methodologies provide a solid foundation for tackling various static link prediction problems.

1.2 Link prediction in dynamic networks

Dynamic link prediction is a fundamental problem in the analysis of evolving networks, with applications in social networks, communication systems, and biological networks. As networks change over time, accurately predicting future links requires capturing both structural and temporal dependencies. To this end, a wide range of learning-based methods have been proposed, which can be broadly categorized into unsupervised and supervised approaches.

1.2.1 Unsupervised learning methods

Unsupervised methods have been widely explored for dynamic link prediction, as they can effectively capture network structure and evolution without

requiring labeled data. In this section, we categorize these methods into two main types: random walk-based approaches and matrix analysis-based approaches.

Random walk-based methods. Random walk-based methods aim to learn low-dimensional representations of nodes and are widely applicable to dynamic networks. Zhang et al. [47] proposed a time-constrained random walk approach that avoids manually defined snapshot intervals and preserves temporal continuity. Nguyen et al. [48] introduced a general framework that incorporates temporal dependencies into random-walk-based models, effectively capturing time-ordered interactions while minimizing information loss. Causal Anonymous Walks (CAWs) [49] further enhance temporal modeling by using time-based random walks to extract temporal features, replacing node identities with node hitting counts, and establishing temporal correlations. These methods effectively capture temporal dynamics, though integrating rich node attribute information remains a significant challenge.

Matrix analysis-based methods. Matrix analysis-based methods predict links via matrix decomposition or completion. Non-negative Matrix Factorization (NMF) is widely used for learning latent structural features. Ahmed et al. [50] proposed an NMF-based method that employs novel iterative rules to construct matrix factors capturing key network features, thereby effectively representing the network dynamics. Ma et al. [51] established the equivalence between feature decomposition and NMF algorithms, providing a theoretical foundation for designing dynamic link prediction methods based on NMF. Building on this, they proposed a novel algorithm that factorizes each network snapshot, utilizes graph communicability to extract features, and then folds the resulting feature matrix to predict links. Lei et al. [52] proposed a novel method called Adaptive Multiple Non-negative Matrix Factorization (AM-NMF), which embeds dynamic networks into a low-dimensional space while preserving features across different snapshots. The method introduces an adaptive parameter that automatically adjusts the contribution of various terms and effectively fuses hidden information from multiple time slices. Ma et al. [53] proposed the Graph Regularized Nonnegative Matrix Factorization (GrNMF) algorithm, which decomposes the adjacency matrix of each time slice while simultaneously leveraging information from other slices as structural regularization to preserve both intra-slice structural features and inter-slice temporal continuity.

1.2.2 Supervised learning methods

Supervised methods learn from labeled data to predict the existence of links through classification or regression. Compared to unsupervised approaches, they often achieve higher predictive accuracy. These methods include both traditional machine learning models and deep learning frameworks.

Traditional machine learning methods. Methods like logistic regression, SVMs, and random forests treat link prediction as a binary classification task. They rely on manually extracted features such as node attributes and temporal patterns. Liu et al. [54] established time series features of dynamic networks based on network topology features and link generation time and combined statistical models with supervised learning methods to predict links on a weighted dynamic network. Singh et al. [55] proposed a PILHNB method for dynamic social network link prediction based on Latent Dirichlet Allocation (LDA) and Hidden Naive Bayes (HNB). It considers behavioral control elements such as relationship network structure, node attributes, node location information, and node popularity, and learns the changing patterns of these factors of the network. Currently, traditional machine learning methods are relatively mature, providing many options for constructing complete prediction models. However, they are sensitive to quality and quantity of training data.

Deep learning models. Deep learning methods, particularly Graph Neural Networks (GNNs), have achieved remarkable success in dynamic link prediction. GNNs are generally categorized into four types: Recurrent Graph Neural Networks (RecGNNs), Convolutional Graph Neural Networks (ConvGNNs), Graph Autoencoders (GAEs), and Spatio-Temporal Graph Neural Networks (STGNNs). In practice, a complete dynamic link prediction model often integrates multiple types of GNNs.

Jiao et al. [56] proposed a dynamic network embedding approach that learns low-dimensional node representations while preserving non-linear temporal patterns, using attention-enhanced RecGNNs to update embeddings with temporal dependencies. Pham et al. [57] introduced ComGCN, a hybrid model combining RecGNNs and ConvGNNs for dynamic link prediction. Kumar et al. [58] developed GNS, a simulator that models system dynamics

through an encoder-processor-decoder architecture, demonstrating strong generalization capabilities. Zheng et al. [59] proposed a transition structure that adaptively personalizes node modeling and captures node dynamics by performing multi-step transition propagation and leveraging dual GNNs to extract informative neighborhood features. Chen et al. [60] proposed a deep learning model called Encoder-LSTM-Decoder (E-LSTM-D) for predicting dynamic links. This model can automatically learn structural and temporal features within a unified framework. Min et al. [61] proposed the Spatio-Temporal Graph Social Network (STGSN), which extracts structural features of dynamic social networks using ConvGNNs and captures temporal patterns through a temporal attention mechanism. Yu et al. [62] introduced DyGFormer, a Transformer-based method that models first-order historical interactions by encoding neighbor co-occurrence and segmenting node interaction sequences, enabling effective learning from long-term dependencies. Wen et al. [63] designed a framework called TREND, which integrates temporal events and dynamic nodes to jointly capture local and global features, and further incorporates the Hawkes process to model the interplay between temporal events.

Many methods have been developed to handle more complex scenarios, such as dynamic weighted and heterogeneous networks. Qin et al. [64] proposed IDEA, which combines error and scale difference minimization objectives to generate weighted snapshots, using a generator–discriminator structure within an encoder–decoder framework. Wei et al. [65] introduced NeiDy-HNE for dynamic heterogeneous attributed networks, leveraging hierarchical structural and convolutional temporal attention modules to capture node semantics, neighborhood structures, and network evolution over time.

1.2.3 Summary of dynamic link prediction

Dynamic link prediction has seen substantial progress through both unsupervised and supervised learning paradigms. Unsupervised approaches, including random walk and matrix factorization methods, offer scalability and flexibility in learning from unlabeled data, while supervised techniques, ranging from classical machine learning to advanced deep learning models, demonstrate superior capability in capturing complex spatio-temporal dependencies. Recent research trends also address more sophisticated settings such as weighted, heterogeneous, and attributed dynamic networks. These developments suggest that the integration of multiple strategies, particularly hybrid

models, is a growing trend in dynamic link prediction.

2 Traditional heuristic metrics

In this supplementary material, we present five representative heuristic methods for link prediction, which are used in the comparative experiments reported in the main paper. The methods considered are Common Neighbors [9], Adamic-Adar Index [11], Resource Allocation Index [13], Local Path Index [18], and Katz Index [14]. While these methods were originally designed for static link prediction, we adapt them to the dynamic link prediction setting. Specifically, we aggregate the first l-1 graph snapshots of each sample into a single static graph, and then apply the heuristic methods to this aggregated graph to compute the likelihood scores for potential links in the l-th snapshot. The details of these methods are as follows:

2.1 Common Neighbors (CN)

This index counts the number of common neighbors between two nodes u and v. The underlying assumption is that two nodes with more shared neighbors are more likely to be connected.

$$CN(u, v) = |\Gamma(u) \cap \Gamma(v)|,$$

where $\Gamma(u)$ denotes the set of neighbors of node u.

2.2 Adamic-Adar Index (AA)

This metric refines the CN index by assigning lower weights to high-degree common neighbors, assuming that rare shared neighbors are more informative.

$$AA(u,v) = \sum_{w \in \Gamma(u) \cap \Gamma(v)} \frac{1}{\log |\Gamma(w)|}.$$

2.3 Resource Allocation Index (RA)

The RA index models a resource allocation process, where node u sends a unit resource to v through common neighbors. Common neighbors with

higher degrees distribute their resource more thinly among their neighbors, resulting in less resource allocated to v.

$$RA(u, v) = \sum_{w \in \Gamma(u) \cap \Gamma(v)} \frac{1}{|\Gamma(w)|}.$$

2.4 Local Path Index (LP)

The LP index extends the CN metric by incorporating paths of length 3, enhancing predictive power while maintaining computational efficiency.

$$LP(u, v) = (A^2)_{uv} + \beta (A^3)_{uv},$$

where A is the adjacency matrix and β is a damping factor (typically $\beta = 0.01$).

2.5 Katz Index

The Katz index considers all paths between two nodes, giving exponentially smaller weights to longer paths.

$$Katz(u, v) = \sum_{l=1}^{\infty} \beta^{l} \cdot (A^{l})_{uv},$$

where β is a decay parameter and A^l denotes the number of paths of length l between u and v. To ensure convergence, β must be smaller than the reciprocal of the largest eigenvalue of A.

3 Dataset specification

In this section, we provide a detailed specification of the datasets used in the main paper, including the simulation tool, data generation process, and data partitioning.

3.1 Simulation tool

Due to the lack of real UANET datasets, we employ the freely available mobility scenario generation and analysis tool BonnMotion [66] to produce UAV

mobility traces. BonnMotion is widely used in the simulation of MANETs, VANETs, and UANETs, and supports various classic mobility models, including the RW (Random Waypoint), MG (Manhattan Grid), RPG (Random Point Group), and GM (Gauss–Markov) models used in our work. The tool's command-line interface enables precise reproduction of experimental configurations, such as the number of nodes, flight speed, and simulation duration.

3.2 Dataset generation

The data generation process is as follows. First, based on the selected mobility model and input parameters, BonnMotion generates trajectory data for each node, capturing the temporal variations of node position, velocity, and direction. Next, it outputs a sequence of UAV location records in the format (node ID, timestamp, x-coordinate, y-coordinate). Using the coordinate information of all nodes, we generate the UAV network topology. For each timestamp, if the distance between two nodes is less than the communication radius, a link is established between them, and the link weight is calculated according to Eq. (1) in the main paper. This generates a snapshot sequence for the UANET, which relies solely on the UAV location information produced by BonnMotion.

3.3 Dataset partitioning

A sliding window of size 11 with a step size of 1 is applied over the snapshot sequence of length 80, yielding 70 samples. Among these, the first 50 samples are used as the training set, and the remaining 20 samples as the test set. For each sample, the first 10 snapshots serve as the historical graph data input to the model, and the last snapshot is used as the target graph for prediction. The generated datasets have been publicly released at https://github.com/turtlo6/MUST.

4 Supplementary comparison results

In the main paper, we compare the performance of MUST with state-ofthe-art learning-based methods across varying sampling intervals and flight speeds, showing that MUST consistently outperforms them in terms of AUC

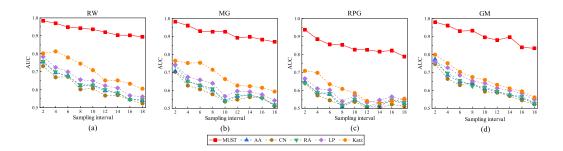


Figure 1: AUC vs. Sampling interval for MUST and traditional heuristic methods across the four mobility models.

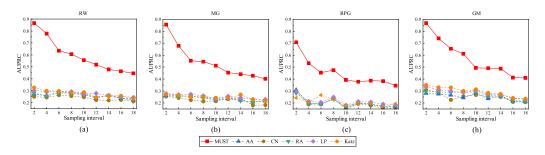


Figure 2: AUPRC vs. Sampling interval for MUST and traditional heuristic methods across the four mobility models.

and AUPRC. In this supplementary material, we further provide a comparison between MUST and representative heuristic methods, including CN, AA, RA, LP, and Katz, under varying sampling intervals and flight speeds, as a complement to the main paper. The experimental setup is identical to that described in the main paper.

4.1 Impact of snapshot sampling interval

Figs. 1 and 2 illustrate the AUC and AUPRC results under different sampling intervals, respectively. We observe that both MUST and the heuristic methods exhibit a decline in performance as the sampling interval increases. This is because larger sampling intervals reduce the temporal correlation between consecutive snapshots, thereby increasing the difficulty of link prediction. Among the heuristic methods, Katz achieves the best overall performance, while CN performs the worst. The superior performance of Katz

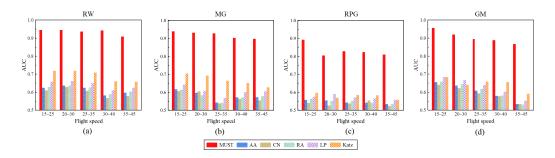


Figure 3: AUC vs. Flight speed for MUST and traditional heuristic methods across the four mobility models.

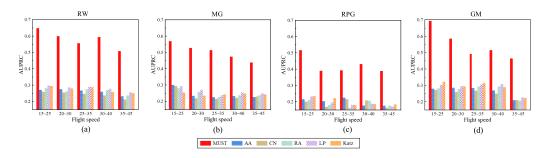


Figure 4: AUPRC vs. Flight speed for MUST and traditional heuristic methods across the four mobility models.

can be attributed to its ability to aggregate contributions from paths of all lengths, providing a more comprehensive characterization of node associations, whereas CN relies solely on direct connections among local neighbors and ignores information from longer paths between node pairs. Our method, MUST, significantly outperforms all heuristic methods across all sampling intervals, as heuristics are inherently based on handcrafted static topological rules and thus fail to effectively capture the evolving patterns of UANET topology.

4.2 Impact of flight speed

Figs. 3 and 4 present the performance of MUST and the heuristic methods under different flight speeds. As the flight speed increases, both MUST and the heuristic methods exhibit a decline with fluctuations in AUC and AUPRC. This is because higher flight speeds induce more rapid topologi-

cal changes, thereby making link prediction more challenging. Among the heuristic methods, Katz once again achieves the best overall performance, whereas CN performs the worst. In contrast, MUST consistently outperforms all heuristic methods across different flight speeds.

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