Supplementary materials for "A Systematic Survey on Generative Models for Graph Generation"

1. EVALUATION

A. Statistic-based metrics

Molecule Graph For the evaluation of molecular graphs, both 2D and 3D molecular graphs are considered, where the 2D graph focuses on atom types and their connectivity, while the 3D graph represents the spatial distances between atomic coordinates.

For 2D molecule graphs, mainstream approaches emphasize chemical feasibility through multiple complementary metrics. Atom Stability (AS) measures the proportion of atoms with chemically valid valences:

$$\text{AS} = \frac{1}{N}\sum_{i=1}^{N} 1[valence(a_i) \in V_{valid-valence}(a_i)],$$

where $valence(\cdot)$ computes the chemical valence of a given atom, and $V_{\text{valid-valence}}(\cdot)$ denotes its set of permissible valence states. Molecule Stability (MS) quantifies the fraction of fully stable molecules where all atoms satisfy valence rules:

$$\text{MS} = \frac{|\mathcal{M}_{\text{gen}}[AS = 1]|}{|\mathcal{M}_{\text{gen}}|}.$$

The GuacaMol [1] benchmark proposed a comprehensive evaluation framework for assessing the quality of generated molecular graphs, encompassing multiple metrics that capture different aspects of molecular generation performance. Specifically, Validity captures the overall proportion of molecules adhering to fundamental chemical constraints:

$$\text{Validity} = \frac{|\mathcal{M}_{\text{valid}}|}{|\mathcal{M}_{\text{gen}}|}.$$

Beyond chemical feasibility, the framework incorporates Uniqueness to assess deduplication efficiency:

$$\text{Uniqueness} = \frac{|\mathcal{M}_{\text{unique}}|}{|\mathcal{M}_{\text{gen}}|}.$$

Moreover, they propose Novelty measures exploration beyond the training distribution:

$$\text{Novelty} = \frac{|\mathcal{M}_{\text{gen}} \backslash \mathcal{M}_{\text{train}}|}{|\mathcal{M}_{\text{gen}}|},$$

where $\mathcal{M}_{(\cdot)}$ represents a set of molecules under different metrics. Finally, Diversity [2] evaluates the structural diversity of the generated molecular set, which is quantified using metrics such as the Fréchet ChemNet Distance (FCD) [3]. Specifically, FCD measures the distributional difference between the generated molecules and the reference molecules in the ChemNet [4] embedding space.

$$\text{FCD} = ||m_{\text{ref}} - m_{\text{gen}}||_2^2 + Tr(\Sigma_{\text{ref}} + \Sigma_{\text{gen}} - 2(\Sigma_{\text{ref}}\Sigma_{\text{gen}})^{\frac{1}{2}}),$$

where $m_{\text{ref}}, m_{\text{gen}}, \Sigma_{\text{ref}}, \Sigma_{\text{gen}}$ are the means and covariances of reference and generated molecule sets in ChemNet [4] embedding space, respectively. Together, these metrics provide a comprehensive assessment spanning from atomic-level chemical correctness to collection-level distributional properties, ensuring both the quality and variety of generated molecular structures.

For 3D molecular graphs, namely generated conformers, evaluation relies on geometry-based metrics that compare generated structures against ground truth. Commonly employed MMD-based statistic-based metrics include the distributions of bond lengths, bond angles, and dihedral angles. RMSD-based metrics [5] such as Coverage (Cov), which quantifies conformational diversity by measuring the proportion of reference conformers that have at least one generated conformer within a threshold distance:

$$\text{Cov} = \frac{1}{|\mathcal{C}_{\text{ref}}|}\sum_{C_r \in \mathcal{C}_{\text{ref}}} 1\left[\min_{C_g \in \mathcal{C}_{\text{gen}}} \text{RMSD}(C_r, C_g) < \delta\right].$$

And Average Minimum RMSD (AMR) evaluates overall geometric accuracy by computing the mean of minimum RMSD values from each generated conformer to its closest reference structure:

$$\text{AMR} = \frac{1}{|\mathcal{C}_{\text{gen}}|} \sum_{C_g \in \mathcal{C}_{\text{gen}}} \min_{C_r \in \mathcal{C}_{\text{ref}}} \text{RMSD}(C_g, C_r),$$

where $\mathcal{C}_{\text{ref}}, \mathcal{C}_{\text{gen}}$ denote the reference and generated conformer sets, respectively, and δ is the RMSD threshold (typically 0.5 Å or 1.0 Å). Together, these metrics provide complementary perspectives on conformational generation quality, with higher Cov values indicating better coverage of the conformational space and lower AMR values reflecting more accurate geometric predictions.

In addition to unconditional generation of 2D and 3D molecular graphs, conditional molecule generation focuses on designing molecules with specific properties. Evaluations are conducted with respect to the targeted attributes, which can be categorized as 2D or 3D graph-dependent properties depending on whether they rely solely on 2D molecular topology or 3D conformational information.

Among the 2D graph-dependent properties [6], Synthetic Accessibility (SA) assesses the ease of molecular synthesis by integrating fragment-based statistics with structural complexity. Lower SA values indicate higher synthetic feasibility. Penalized $\log P$ (PlogP) measures the lipophilicity of a molecule while penalizing structural complexity, and is defined as

$$\text{PlogP} = \log P - \text{SA},$$

where $\log P$ denotes the octanol–water partition coefficient, and the penalty term (typically using the SA score) accounts for molecular features such as ring count or synthetic difficulty. Quantitative Estimate of Drug-likeness (QED) quantitatively evaluates the overall drug-likeness of a molecule by combining desirability scores of multiple physicochemical properties (e.g., molecular weight, logP, number of hydrogen bond donors/acceptors, and rotatable bonds), computed as

$$\text{QED} = \exp\left(\frac{1}{n}\sum_{i=1}^{n} \ln d_i\right),$$

where d_i represents the desirability value of the i^{th} property and n is the total number of considered properties.

3D graph-dependent properties [7] comprise a broad range of quantum chemical properties characterizing electronic structure and thermodynamic behavior. Dipole Moment (μ) quantifies the separation of positive and negative charges within a molecule, indicating its polarity and response to external electric fields. It is defined as

$$\mu = \sum_i q_i \mathbf{r}_i,$$

where q_i and $\mathbf{r}_i$ denote the charge and position vector of the i^{th} particle, respectively. Polarizability (α) measures the ease with which a molecule's electron cloud can be distorted by an external electric field, reflecting its electronic flexibility and dielectric response. HOMO Energy (ϵ_{HOMO}) represents the energy level of the highest occupied molecular orbital, describing a molecule's electron-donating ability and chemical stability. LUMO Energy (ϵ_{LUMO}) corresponds to the lowest unoccupied molecular orbital and indicates the molecule's electron-accepting tendency and reactivity. Orbital Energy Gap ($\Delta\epsilon$) characterizes molecular chemical stability and excitation potential, defined as

$$\Delta\epsilon = \epsilon_{\text{LUMO}} - \epsilon_{\text{HOMO}}.$$

Heat Capacity (C_v) measures the amount of heat required to increase a system's temperature under constant volume and reflects its ability to store thermal energy. It is given by

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V,$$

where U is the internal energy and T is the temperature. For these 3D-dependent properties, evaluation is usually based on the mean absolute error (MAE) between the properties computed from generated 3D conformers and the corresponding ground truth values.

Protein Graph Protein graph generation quality is typically assessed through complementary metrics that capture both structural fidelity and functional relevance. Specifically, Contact accuracy [8] evaluates the structural realism of generated protein graphs by measuring whether short- and long-range residue-residue distances follow known spatial contact distributions. It is formulated as

$$\text{Contact accuracy} = \frac{|\{(i,j) : \hat{c}_{ij} = 1 \wedge c_{ij} = 1\}|}{|\{(i,j) : c_{ij} = 1\}|},$$

where c_{ij} and $\hat{c}_{ij}$ denote the true and predicted contact states between residues i and j, typically defined by a Cα-C$_\alpha$ distance threshold (e.g., 8 Å).

Perplexity [8] instead focuses on the sequence modeling aspect of the protein graph, assessing how well the model predicts amino acid identities along the sequence. Lower perplexity values indicate higher confidence and accuracy in sequence generation:

$$\text{Perplexity} = \exp\left(-\frac{1}{L}\sum_{i=1}^{L} \ln P(x_i \mid x_1, \cdots, x_{i-1})\right),$$

where L is the sequence length and $P(x_i \mid x_{<i})$ represents the model's predicted probability for residue x_i given preceding residues.

Finally, Fitness [8] evaluates the functional aspect of generated proteins, quantifying how well the generated sequences preserve or enhance biological activity. It is often estimated from predicted or experimentally measured mutation effect scores.

Together, these metrics provide a holistic evaluation of protein graph generation—Contact accuracy ensuring structural plausibility, Perplexity verifying sequence coherence, and Fitness reflecting biological functionality.

Spatial Graph Spatial graphs, or specifically geo-spatial graphs, are spatiotemporal networks modeling the dynamic interactions between nodes (locations) and edges (flows) over time. The Origin-Destination (OD) matrix quantifies flow volumes between geographic locations, serving as the adjacency matrix in transportation graphs to encode connection strength [9].

Consequently, in spatial graph generation, OD matrix prediction is a critical evaluation metric as it directly reflects the accuracy of travel pattern predictions and the effectiveness of transportation models. Three evaluation metrics are typically adopted [10]: (1) Numerical error metrics, which measure the numerical discrepancy between the generated OD matrix and the ground truth. Root Mean Square Error (RMSE) captures the overall magnitude of traffic flow prediction errors, and Normalized Root Mean Square Error (NRMSE) normalizes RMSE to facilitate comparison across datasets of different scales. (2) Common Part of Commuting (CPC), which quantifies the overlapping portion between the generated and real OD matrix; higher CPC values correspond to closer similarity. (3) Distributional consistency, where Jensen-Shannon Divergence (JSD) is used to measure the similarity between the generated and real distributions of inflow, outflow, and OD flows.

Human Motion Graph A human motion graph refers to complex graphs representing human motion, scaffolded by realistic human motion sequences [11]. For motion graph evaluation, most works [12, 13] employ the distance metrics (e.g., mean squared error (MSE)) to measure the difference between synthesized motion and ground truth motion. DanceFormer [14] utilizes Normalized Power Spectrum Similarity (NPSS) for evaluating long-term motion synthesis capabilities. NPSS operates in the frequency domain and is less sensitive to frame misalignment compared to MSE. Additionally, Normalized Directional Motion Similarity (NDMS) [15] is introduced to measure the similarity of motion directions. Similar to the CPC metric used in geo-spatial graphs, some works [16] compute the Percentage of Correct 3D Keypoints (PCK), which measures the accuracy of predicted 3D keypoints. Additionally, like image generation metrics, some studies [17–19] employ Fréchet Inception Distance (FID) and Inception Score (IS) to evaluate the quality of generated human motion sequences. FID measures the distance between the distributions of generated and real motion features, while IS assesses the diversity and quality of generated motions by feeding them into a pre-trained classifier [20].

Social Graph In evaluating social graph generation, several key metrics are used to assess the unique characteristics of scale-free graphs. One important metric is power-law fitness, measured by the Power-law Exponent Gap between the reference and generated social graphs [21]. Other metrics focus on local connectivity patterns, such as wedge count and claw count. The wedge count measures nodes connected to two others, forming a wedge structure, while the claw count measures nodes connected to three others, forming a claw structure [22]. Recently, TIS [23] used LLM-based simulations to identify key opinion leaders (KOLs) in social graphs. By comparing the distributions of KOLs, they assess the quality of the generated graphs.

User-Item Bipartite Graph In the generation of user-item bipartite graphs, LLM-based simulation methods are primarily used to model user-item interaction graphs in recommendation systems. Therefore, the evaluation metrics largely adopt those commonly used in recommendation system evaluations, such as Mean Reciprocal Rank (MRR), Hit Rate, and Recall@k, to assess the ranking quality of the model's candidate edges [24].

Synthetic Graph The evaluation of synthetic graphs is based on the distributions of several key properties [25], primarily including degree (DEG), clustering coefficients (CC), eigenvalues of the normalized Laplacian matrix (Spec), and orbit counts (Orb), which represent the distribution of all substructures of size 4. These metrics provide a comprehensive and generalizable assessment of the graph's structural characteristics across different synthetic graphs.

B. Downstream Tasks

Beyond distributional similarity to reference graphs, a complementary line of work evaluates generated graphs by their utility on downstream tasks. Rather than directly matching structures, these protocols assess the practical usefulness of generated graphs in standard graph learning scenarios. Under this evaluation framework, the generated graphs are primarily assessed across five types of downstream tasks.

(1) Machine Learning Tasks. This line asks whether generated graphs can substitute for reference graphs when training discriminative models. A representative framework [26, 27] trains link prediction and node classification models separately on the reference and generated graphs, then evaluates both models on the same test split of the reference graph. When the performance ratio of the two models approaches 1, the synthetic graph's topology and attributes are deemed sufficient to support comparable learning.

(2) Data Augmentation Tasks. Several studies evaluate the effectiveness of GGMs by addressing the data sparsity issue in long-tail categories. Early work focused on enhancing the textual features of nodes or edges in graphs using LLMs. LLM4NG [28] introduced a lightweight, plug-and-play paradigm that uses LLMs to generate semantically consistent node texts. This process effectively incorporates labeled synthetic nodes and edges without modifying the reference graph structure, significantly improving performance in few-shot node classification tasks. Building on this, SAVE-TAG [29] proposed a semantic proximity risk minimization framework for text-based graphs under long-tail distributions. The method uses LLMs to perform semantic interpolation in the text space, generating semantically coherent and diverse node/edge text content.

(3) Robust Graph Generation Tasks. Enhancing the robustness of generated graphs against noise is another key evaluation task. For instance, in relation extraction tasks, unstructured text is aligned with a knowledge base to automatically label training data, but this process often introduces noisy labels. To address this, LLM-CG [30] proposed a constraint-based graph enhancement framework using LLMs to improve the robustness and semantic accuracy of distant supervision relation extraction (DSRE). LLM4RGNN [31] introduced a graph structure reasoning framework based on LLMs to identify and repair anomalous structures using the cognitive capabilities of large models. The framework integrates a local LLM module to detect potential malicious or false edges (e.g., edges introduced by adversarial attacks), alongside a language model-based edge predictor to infer potentially missing critical connections. LLM4RGNN can reconstruct a more robust and semantically consistent graph structure, thereby enhancing the stability of downstream tasks such as node classification and link prediction in adversarial environments.

(4) Generative Pretraining Tasks. Here, graph generation (or reconstruction) is viewed as self-supervised pretraining to boost downstream performance in target domain. Two transfer settings are common: temporal transfer (pretrain on earlier time windows, then fine-tune and test on later ones) and domain transfer (pretrain and finetune/test on different domains) [25, 32]. Early work VGAE[33] established unsupervised graph representation learning via generative reconstruction for link prediction. With the rise of LLMs and text-attributed graphs, GPT-GNN [32] pretrains a GNN on large graph corpora, initializes downstream models with pretrained weights, and finetunes with task-specific decoders for node classification and link prediction. GraphMaster [34] adopts a similar pretrain-finetune paradigm, demonstrating gains from generative learning. LGGM [25] further explores joint evaluation of generation quality and downstream performance on the test graph.

(5) Conditional Graph Generation Tasks. Conditional generation focuses on synthesizing graphs that meet user-defined conditions or properties, ensuring specific functional or structural requirements. This approach is crucial in areas like drug discovery and materials design. In molecular graph generation, it typically involves generating molecules based on property conditions, such as hydrophilicity, toxicity, synthetic accessibility, or conformational energy [35, 36]. Representative methods such as ChemFlow [6],

GGFlow [37], and Next-Mol [38] explicitly incorporate target property values as conditional variables into the generation process, often by integrating this information into the latent space of graph neural networks or variational autoencoders, to steer the directional generation of molecular structures and enable exploration and optimization within targeted property ranges. The other, more challenging mode involves target-based molecular generation, which requires generating molecules capable of effectively binding to specific protein targets (e.g., kinases, GPCRs). Methods like UniMoMo [39], TargetDiff [40], and Pocket2Mol [41] utilize the 3D structure of the target protein or key interaction fingerprints as semantic conditions, encoded via geometric deep learning or protein language models, to guide the generation of molecular structures highly complementary to the binding pocket in terms of spatial fit and interaction patterns. This mode emphasizes not only the structural validity of the molecule itself but also its functional compatibility with biomacromolecules, significantly advancing de novo drug design for specific targets.

2. FUTURE OPPORTUNITY

We explore several promising future opportunities, including improving scalability of deep learning models, enhancing controllability with target properties, advancing multimodal graph generation using diverse data sources, and establishing more robust and generalizable evaluation metrics.

A. Scalability

Deep learning-based generative models have gained prominence as a research hotspot by automatically capturing intricate graph statistics through reconstruction tasks, leveraging neural architectures to encode/decode graph structures without manual feature engineering. However, these models exhibit super-linear time complexity relative to node count, restricting applications to small graphs (dozens to thousands of nodes). Only a handful of approaches achieve linear time complexity (O(M)) [42, 43], while most existing works focus on small graphs with node counts ranging from dozens to thousands. This limitation is especially problematic for real-world networks, such as the Internet, biological neural systems, and social graphs, which often span millions to billions of nodes [44]. On the other hand, most simulation-based generators focus on producing large-scale graphs. Yet, their reliance on simplified statistical rules lead to synthetic graphs with unrealistic topologies, since real-world networks often deviate from idealized statistical rules. This dichotomy highlights a pivotal trade-off: while simulation-based methods dominate large-scale graph generation due to computational efficiency, deep learning approaches excel in modeling complex, high-order dependencies but remain restricted to niche applications. Simulation-based models dominate large-scale graph generation due to their efficiency, while deep learning-based models excel in capturing complex, real-world graph statistics. Future work may focus on hybrid frameworks that combine the scalability of simulation-based methods with the expressive power of deep learning-based methods.

B. Controllability

Controllability in content generation is a crucial aspect for real-world applications and has been a popular topic in GGMs [45, 46]. In molecular generation, controllability primarily refers to generating molecules that satisfy specific properties, such as drug activity, toxicity, synthetic accessibility [47, 48], and binding affinity with specific pockets [49]. In protein design, it is about generating protein structures with specific functions or stabilities, like enzyme activity or binding affinity [50]. In social network analysis, controllability involves generating network structures that align with particular social behaviors or propagation patterns, such as community structure and information diffusion [23]. With the advancement of LLM-based agent simulations for graph generation, some research has started focusing on the impact of macro-level communication patterns (e.g., chain, tree or star) within MAS systems on task performance [51]. However, most existing work still concentrates on generating graphs with specific statistical features at the graph level [52], lacking control over higher-level semantics or functional requirements. Future research could explore more effective control mechanisms to enhance the controllability of GGMs by incorporating prior knowledge.

C. Multimodality

Real-world graphs inherently encode complex multimodal information beyond pure topology. Capturing attributed graphs, like textual descriptions, OD flows, and molecule types, is essential for generating results that are both structurally sound and semantically meaningful [53]. Recent research has progressively advanced the attribute modalities of generated graphs, evolving from non-attributed structures to categorical/numeric attributes, and ultimately to textual or multimodal representations. For instance, molecular graphs may include textual annotations, 3D spatial structures, and physicochemical properties [54], whereas social graphs often involve user profiles, interaction content, and temporal dynamics [55]. Future models are expected to accommodate even richer modalities. Current limitations include: (1) insufficient integration of domain knowledge (e.g., chemical knowledge graphs); (2) complex cross-modal alignment mechanisms with high computational costs; and (3) limited self-supervised learning approaches for extracting and synthesizing knowledge across modalities, since existing methods often treat each modality independently rather than learning their inherent correlations and complementary information for graph generation.

D. Evaluation

The evaluation of graph generative models faces several key challenges that need to be addressed: (1) Non-uniqueness: Unlike discriminative tasks, graph generation lacks unique ground truth labels for direct comparison, making quality assessment inherently subjective. (2) Computational complexity: Complex evaluation metrics can better capture structural patterns but scale poorly to large graphs. Simple metrics are more efficient but may miss important properties [56]. (3) Domain specialization: Many applications require expensive domain-specific validation (e.g., wet-lab experiments for molecules) or custom metrics aligned with downstream tasks [57]. Future research should focus on developing more robust, efficient, and standardized evaluation frameworks that can effectively assess both the statistical quality and practical utility of generated graphs.

Table 1. Geometric Graph Generative Models

Model	Year	Journal	Probabilistic Modeling	Attribute	Application
motion-framework [58]	2016	TOG	VAE	Non-Attribute	Human Motion Prediction
ORGAN [59]	2017	arXiv	GAN	Categorical/Numerical Attribute	Molecule Generation
GraphVAE [60]	2018	ICANN	VAE	Categorical/Numerical Attribute	Molecule Generation
CharVAE [61]	2018	ACS Central Science	VAE	Categorical/Numerical Attribute	Molecule Generation
JT-VAE [62]	2018	ICML	VAE	Categorical/Numerical Attribute	Molecule Generation
MolGAN [63]	2018	ICML	GAN	Categorical/Numerical Attribute	Molecule Generation
GCPN [64]	2018	NIPS	GAN	Categorical/Numerical Attribute	Molecule Generation
CGVAE [65]	2018	NIPS	VAE	Categorical/Numerical Attribute	Molecule Generation
CVAE [66]	2018	cheminformatics	VAE	Categorical/Numerical Attribute	Molecule Generation
NeVAE [67]	2019	AAAI	VAE	Categorical/Numerical Attribute	Molecule Generation
MolecularRNN [68]	2019	arXiv	AR	Categorical/Numerical Attribute	Molecule Generation
GraphMCTS [69]	2019	chemical science	AR	Categorical/Numerical Attribute	Molecule Generation
G-SchNet [70]	2019	NIPS	VAE	Categorical/Numerical Attribute	Molecule Generation
VJTNN [71]	2019	ICLR	VAE	Categorical/Numerical Attribute	Molecule Generation
Graphnvp [72]	2019	arXiv	Flow	Categorical/Numerical Attribute	Molecule Generation
MoFlow [73]	2020	KDD	Flow	Categorical/Numerical Attribute	Molecule Generation
BIMODAL [74]	2020	JCIM	AR	Categorical/Numerical Attribute	Molecule Generation
ALMGIG [75]	2020	ECML PKDD	GAN	Categorical/Numerical Attribute	Molecule Generation
MoGlow [18]	2020	TOG	Flow	Categorical/Numerical Attribute	Human Motion Prediction
GraphAF [76]	2020	ICLR	AR	Categorical/Numerical Attribute	Molecule Generation
GraphDF [77]	2021	ICML	Flow	Categorical/Numerical Attribute	Molecule Generation
MGRNN [78]	2021	molecular informatics	AR	Categorical/Numerical Attribute	Molecule Generation
MG2N2 [79]	2021	Neurocomputing	AR	Categorical/Numerical Attribute	Molecule Generation
MGM [80]	2021	Nature Communications	AR	Categorical/Numerical Attribute	Molecule Generation
ENF [81]	2021	NIPS	Flow	Categorical/Numerical Attribute	Molecule Generation
GraphCNF [82]	2021	ICLR	Flow	Categorical/Numerical Attribute	Molecule Generation
CGCF [83]	2021	ICLR	Flow	Categorical/Numerical Attribute	Molecule Generation
MolGrow [84]	2021	AAAI	Flow	Categorical/Numerical Attribute	Molecule Generation
GraphEBM [85]	2021	ICLR	Diffusion	Categorical/Numerical Attribute	Molecule Generation
FastFlows [86]	2022	ELLIS workshop	Flow	Categorical/Numerical Attribute	Molecule Generation
STGEN [87]	2022	ecml PKDD	GAN	Categorical/Numerical Attribute	Transportation Network Modeling
EDM [88]	2022	ICML	Diffusion	Categorical/Numerical Attribute	Molecule Generation
G-SphereNet [89]	2022	ICLR	Flow	Categorical/Numerical Attribute	Molecule Generation
DeMo [90]	2022	CIKM	Flow	Categorical/Numerical Attribute	Molecule Generation
MiCaM [91]	2023	ICLR	VAE	Categorical/Numerical Attribute	Molecule Generation
DeepRank-GNN [92]	2023	Bioinformatics	Diffusion	Categorical/Numerical Attribute	Molecule Generation
GraphGPT(1) [93]	2023	IJMS	AR	Categorical/Numerical Attribute	Molecule Generation
EquiFM [94]	2023	NIPS	Flow	Categorical/Numerical Attribute	Molecule Generation
MOLDR [95]	2023	ACS Omega	GAN	Categorical/Numerical Attribute	Molecule Generation
CDGS [35]	2023	AAAI	Diffusion	Categorical/Numerical Attribute	Molecule Generation
EEGSDE [96]	2023	ICLR	Diffusion	Categorical/Numerical Attribute	Molecule Generation
DiffODGen [97]	2023	arXiv	Diffusion	Categorical/Numerical Attribute	Transportation Network Modeling
MoVAE [98]	2023	SIAM	VAE	Categorical/Numerical Attribute	Molecule Generation
GeoLDM [99]	2023	ICML	Diffusion	Categorical/Numerical Attribute	Molecule Generation
GGFlow [37]	2024	NIPS	Flow	Categorical/Numerical Attribute	Molecule Generation
LLM4GraphGen [52]	2024	SIGKDD Explorations	AR	Categorical/Numerical Attribute	General Graph Modeling
OLR [100]	2024	TMLR	AR	Categorical/Numerical Attribute	Molecule Generation
GeoMol [5]	2024	Computers and Chemical Engineering	AR	Categorical/Numerical Attribute	Molecule Generation
TransFlower [101]	2024	arXiv	AR	Categorical/Numerical Attribute	Transportation Network Modeling
Lingo3DMol [102]	2024	Nature Machine Intelligence	AR	Categorical/Numerical Attribute	Molecule Generation
ChemFlow [6]	2024	NIPS	Flow	Categorical/Numerical Attribute	Molecule Generation
GeoBFN [103]	2024	ICLR	Flow	Categorical/Numerical Attribute	Molecule Generation
FlowMol [104]	2024	arXiv	Flow	Categorical/Numerical Attribute	Molecule Generation
CatFlow [105]	2024	NIPS	Flow	Categorical/Numerical Attribute	Molecule Generation
ETFlow [106]	2024	NIPS	Flow	Categorical/Numerical Attribute	Molecule Generation
FragGen [107]	2024	Chemical Science	GAN	Categorical/Numerical Attribute	Molecule Generation
MotionDiffuse [19]	2024	TPAMI	Diffusion	Categorical/Numerical Attribute	Human Motion Prediction
TACS [36]	2024	NIPS	Diffusion	Categorical/Numerical Attribute	Molecule Generation
Uni-3DAR [108]	2025	arXiv	AR	Categorical/Numerical Attribute	Molecule Generation
BindGPT [109]	2025	AAAI	AR	Categorical/Numerical Attribute	Molecule Generation
SemlaFlow [110]	2025	AISTATS	Flow	Categorical/Numerical Attribute	Molecule Generation
GOAT [111]	2025	ICLR	Flow	Categorical/Numerical Attribute	Molecule Generation
Mol-AIR [112]	2025	JCIM	GAN	Categorical/Numerical Attribute	Molecule Generation
Next-Mol [38]	2025	ICLR	Diffusion	Textual Attribute	Molecule Generation
A-GFN [113]	2025	arXiv	Flow	Categorical/Numerical Attribute	Molecule Generation

Table 2. General Graph Generative Models

Model	Year	Journal	Probabilistic Modeling	Attribute	Application
GraphRNN [114]	2018	ICML	AR	Categorical/Numerical Attribute	General Graph Modeling
GraphGAN [115]	2018	AAAI	GAN	Non-Attribute	General Graph Modeling
NetGAN [116]	2018	ICML	GAN	Non-Attribute	General Graph Modeling
GRAN [117]	2019	NIPS	AR	Non-Attribute	General Graph Modeling
Graphite [118]	2019	ICML	VAE	Non-Attribute	General Graph Modeling
CONDGEN [119]	2019	NIPS	GAN	Categorical/Numerical Attribute	General Graph Modeling
BiGG [43]	2020	ICML	AR	Non-Attribute	General Graph Modeling
GraphGen [120]	2020	WWW	AR	Categorical/Numerical Attribute	General Graph Modeling
GPT-GNN [32]	2020	KDD	VAE	Categorical/Numerical Attribute	General Graph Modeling
EDP-GNN [121]	2020	AISTATS	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
AGE [122]	2020	PAKDD	VAE	Categorical/Numerical Attribute	General Graph Modeling
GraphGen-Redux [123]	2021	IJCNN	AR	Categorical/Numerical Attribute	General Graph Modeling
D2G2 [124]	2021	SIAM	AR	Categorical/Numerical Attribute	General Graph Modeling
GDSS [125]	2022	ICML	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
GraphMAE [126]	2022	KDD	VAE	Categorical/Numerical Attribute	General Graph Modeling
EDGE [42]	2023	ICML	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
Digress [127]	2023	ICLR	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
BwR [128]	2023	ICML	Depend On Backbone(AR/VAE/Difussion)	Categorical/Numerical Attribute	General Graph Modeling
GraphGPT(2) [129]	2024	arXiv	AR	Categorical/Numerical Attribute	General Graph Modeling
GEEL [130]	2024	ICLR	AR	Categorical/Numerical Attribute	General Graph Modeling
LGGM [25]	2025	ICLR	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
THePUff [131]	2025	ICLR	Diffusion	Categorical/Numerical Attribute	General Graph Modeling

Table 3. Scale-Free Graph Generative Models

Model	Year	Journal	Probabilistic Modeling	Attribute	Application
Erdös-Rényi [132]	1960	Publicationes Mathematicae	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
Barabási-Albert [133]	1999	Science	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
ERGM [134]	2007	Social Networks	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
Affiliation Network [135]	2009	STOC	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
FastKronecker [136]	2010	JMLR	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
AND [137]	2012	Scientific Reports	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
ROLL-Tree [138]	2016	SIGMOD	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
VGAE [33]	2016	NIPS	VAE	Non-Attribute	Dynamic Graph Modeling
TrillionG [139]	2017	SIGMOD	Statistical-Based Simulation	Non-Attribute	Social Network Analysis
TG-GAN [140]	2020	WWW	GAN	Categorical/Numerical Attribute	Dynamic Graph Modeling
TagGen [22]	2020	KDD	GAN	Categorical/Numerical Attribute	Dynamic Graph Modeling
FastSGG [141]	2021	ICDE	Statistical-Based Simulation	Categorical/Numerical Attribute	Social Network Analysis
DYMOND [142]	2021	WWW	Statistical-Based Simulation	Categorical/Numerical Attribute	Social Network Analysis
TIGGER [143]	2022	AAAI	AR	Categorical/Numerical Attribute	Dynamic Graph Modeling
GenCAT [144]	2023	Information Systems	Statistical-Based Simulation	Categorical/Numerical Attribute	Social Network Analysis
S3 [145]	2023	arXiv	LLM-Based Simulation	Textual Attribute	Social Network Analysis
FairWire [146]	2024	NIPS	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
GraphMaker [27]	2024	TMLR	Diffusion	Categorical/Numerical Attribute	General Graph Modeling
SUBER [147]	2024	ECAI	LLM-Based Simulation	Textual Attribute	Recommender Systems
AgentCF [148]	2024	WWW	LLM-Based Simulation	Textual Attribute	Recommender Systems
BASES [149]	2024	EMNLP	LLM-Based Simulation	Textual Attribute	Recommender Systems
SRAP-Agent [150]	2024	EMNLP	LLM-Based Simulation	Textual Attribute	Social Network Analysis
FUSE [151]	2024	arXiv	LLM-Based Simulation	Textual Attribute	Social Network Analysis
TIS [23]	2024	arXiv	LLM-Based Simulation	Textual Attribute	Social Network Analysis
OASIS [152]	2024	arXiv	LLM-Based Simulation	Textual Attribute	Social Network Analysis
Y Social [153]	2024	arXiv	LLM-Based Simulation	Textual Attribute	Social Network Analysis
VRDAG [154]	2024	ICDE	VAE	Categorical/Numerical Attribute	Dynamic Graph Modeling
DGGEN [155]	2025	AAAI	AR	Categorical/Numerical Attribute	Dynamic Graph Modeling
RecUserSim [156]	2025	WWW	LLM-Based Simulation	Textual Attribute	Recommender Systems
Social Simulacra [157]	2025	UIST	LLM-Based Simulation	Textual Attribute	Social Network Analysis
RecAgent [24]	2025	TOIS	LLM-Based Simulation	Textual Attribute	Recommender Systems
GAG [55]	2025	ACL	LLM-Based Simulation	Textual Attribute	Social Network Analysis

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