
Bures-Wasserstein Flow Matching for Graph Generation

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Abstract

1 Graph generation has emerged as a critical task in fields ranging from molecule
2 design to drug discovery. Contemporary approaches, particularly diffusion and
3 flow-based models, have achieved superior generative performance through con-
4 structing an iterative transformation from a simple reference distribution to the data
5 distribution. However, these methods typically use linear interpolations to build
6 the path grounded in Euclidean assumptions, which do not hold for graphs due to
7 their intrinsic non-Euclidean structure. To address this gap, we represent graphs as
8 statistical objects parameterized by Markov random fields (MRF), which permits
9 a closed-form solution for the sampling distribution, transportation distance, and
10 inherent interpolations. Building upon these results, we leverage the corresponding
11 optimal transport displacement interpolation under the MRF assumption and revisit
12 the probability path construction for graph generation. Following the probability
13 path constructed, we then introduce Bures-Wasserstein Flow Matching(BWFlow),
14 which integrates the results into a flow-matching model tailored for graph gen-
15 eration. The novel framework can be adapted to both continuous and discrete
16 flow-matching frameworks depending on the task. Experimental evaluations in
17 plain graph generation and 2D/3D molecule generation validate the effectiveness
18 of BWFlow in preserving key statistical properties while accurately modeling the
19 intricate relationships in graph-structured data.

20 1 Introduction

21 Due to graphs’ capacity to represent complex relationships, graph generation [66, 35] has become an
22 essential task in various fields such as protein design [25], drug discovery [7], and social network
23 analysis [32]. Among various generative models, diffusion models and flow-based models have
24 emerged as two compelling approaches for their ability to achieve state-of-the-art performance in
25 graph generation tasks [42, 57, 16, 48, 24]. In particular, these contemporary generative models rely
26 on constructing a probability path that transforms from the data distribution to an easy-to-sample
27 reference distribution and training a machine learning model to revert the process back [34]. So
28 that one can sample from the reference (a.k.a source) distribution and iteratively transform it to
29 approximate data samples from the target distribution.

30 The flow-based and diffusion models can be unified under the framework of stochastic interpola-
31 tion [1], which consists of four procedures. 1) Drawing samples from the data distribution $p_1(\cdot)$
32 and/or reference distribution $p_0(\cdot)$; 2) Constructing a time-continuous probability path $p_t(\cdot)$, $0 \leq t \leq 1$
33 interpolating between p_0 and p_1 ; 3) Train a model to reconstruct the probability path; and 4) sampling
34 from p_0 and transforming it through the model trained to get samples that approximately follow p_1 .

35 Within such a framework, an important component is constructing the probability path p_t . Existing
36 methods widely consider a linear interpolation between source and target distributions to construct the

probability path, which is derived through the optimal transport (OT) displacement interpolant [56]. This includes continuous generative methods with diffusion [23, 51, 60] and flow [33, 37], as well as the discrete generative models like discrete diffusion [9, 53] and discrete flow [10, 18, 40]. However, such paths have been designed principally under the assumption that the data points lie in the Euclidean space and the cost function for Wasserstein distance is measured by the L^2 norm. Existing models for graph generation, including the diffusion-based models [42, 57, 21, 63, 50] and the flow-based ones [16, 48, 24], widely utilized “straight” probability path in the development of their models. However, graphs are objects lying in a non-euclidean space given their irregular structures and relationships. Such property violates the Euclidean and isotropic assumptions that works as the fundamental building block for linear interpolation. As such, extending diffusion/flow models to graph generation still presents unique challenges.

This observation raises the necessity to re-design the stochastic interpolation methods for graph generative models. To this end, we name two crucial research questions (RQs) when adapting the four-step framework to graph generations, specifically,

1. (RQ1): *How to view graphs as statistical objects, so that one can extend the stochastic interpolation framework between two distributions for graph generations? This includes the definition of distributions, the transportation distances, and the interpolation methods following OT displacement.*
2. (RQ2): *How could we develop the flow-matching model for graph generation based on the derived OT interpolation? This includes the construction of the probability path, the parameterization of the velocity field, the design of training objective and the inference sampling algorithms.*

To solve the first challenge (RQ1), we borrow the idea from statistical relational learning and consider Markov Random Fields (MRF) as a way to model the graph distributions. MRF was initially utilized in statistical physics to model the dynamics of an interconnected multi-body system, such as molecules and proteins [62, 3]. Similarly, any graph can be viewed as a connected network and the joint evolution dynamics of node features and graph structure can be captured by MRF models. Through MRF, the graphs are modeled by a colored Gaussian distribution whose covariance matrix are uniquely determined by the graph structure. Extending from [20], we further derive the Wasserstein distance between two statistical graph objects. The Wasserstein distance is then utilized to construct the Bures-Wasserstein interpolation of two graphs, which works as a replacement of the straight interpolation that does not guarantee the optimal transport displacement in graph generations

To answer RQ2, the results are further used in the development of flow matching for graph generation. Specifically, we utilize the Bures-Wasserstein interpolation to construct the probability path, which thereby models the co-evolution of node features and graph structure and ensures the interpolated points preserve the graphs’ statistical properties by limiting the domain of interpolant. We show that the designed method can be plugged into both continuous and discrete flow frameworks to develop generative models for graph-structured data, which we name Bures-Wasserstein Flow (BWFlow).

To highlight the versatility of our BWFlow method, we test on two tasks: the Discrete Graph Generation and the De-novo Molecule Generation. While existing flow-matching models have already achieved near-saturated performance in the discrete graph generation task, our model inherits the advantage and excess in the task in the general performance. In de-novo molecule generation, our model outperforms the existing ones by a margin. To further illustrate the effectiveness of flowing through the Bures-Wasserstein interpolation, we conduct ablation studies on the types of interpolations within the framework of both continuous and discrete flow matching. We observe that our BWFlow consistently outperforms the competitors - the flow-matching models constructed through arithmetic, geometric, and harmonic interpolations. Finally, we conducted the convergence analysis and found that BWFlow grants better convergence rate and

2 Preliminaries

2.1 Flow Matching and Conditional Flow Matching

Flow Matching (FM). We consider the setting of a pair of data distributions over state space \mathcal{S} with densities $q_0(\mathcal{X})$ and $q_1(\mathcal{X})$ ¹. Generative modeling considers the task of fitting a mapping

¹For clarity, we denote the calligraphic style \mathcal{X} being the random variable, the plain X the relevant realizations and the bold symbol \mathbf{X} the distribution parameters, i.e. $X \sim p(\mathcal{X} | \mathbf{X})$.

from \mathcal{S} to \mathcal{S} that transforms $X_0 \sim q_0$ to $X_1 \sim q_1$. Continuous Normalizing Flow (CNF) [12] parameterizes the transformation through a push-forward equation that interpolates between q_0 and q_1 and constructs a probability path $p_t(\mathcal{X}) = [\psi_t^\dagger q_0](\mathcal{X})$ through a time-dependent function ψ_t (a.k.a flow). A vector field u_t is said to generate p_t between the two distributions if its flow ψ_t satisfies, $\frac{d}{dt}\psi_t(\mathcal{X}) = u_t(\psi_t(\mathcal{X}))$, $\psi_0(\mathcal{X}) = \mathcal{X}$. For simplicity we denote $u_t(\psi_t(\mathcal{X})) := u_t(\mathcal{X})$. The FM objective [33] is designed to match the real velocity field, which yields the training objective:

$$\mathcal{L}_{\text{FM}}(\theta) = \mathbb{E}_{t, p_t(\cdot)} \|v_\theta(X_t) - u_t(X_t)\|^2 \quad (1)$$

where $v_\theta(\cdot) : \mathcal{S} \rightarrow \mathcal{S}$ is the parameterized velocity field, $t \sim \mathcal{U}[0, 1]$ and $X_t \sim p_t(\cdot)$.

Conditional Flow Matching (CFM). Given that the actual vector field and the path are not tractable [56], one can construct the per-sample conditional flow. We condition the probability paths on variable $Z \sim \pi(\cdot)$ (for instance, a pair of source and target points $Z = (X_0, X_1)$) and re-write $p_t(\mathcal{X}) = \mathbb{E}_{\pi(\cdot)} p_t(\mathcal{X} | Z)$ and $u_t(\mathcal{X}) = \mathbb{E}_{\pi(\cdot)} u_t(\mathcal{X} | Z)$ where the conditional probability path and the velocity field are tractable. As an example, linear CFM introduced in [56] set $\pi(\cdot) = q_0(\mathcal{X}) q_1(\mathcal{X})$ to be the independent coupling. Then the conditional flows has a closed form,

$$p_t(\mathcal{X} | Z) = \mathcal{N}(\mathcal{X} | tX_1 + (1-t)X_0, \sigma^2) \text{ and } u_t(\mathcal{X} | X_0, X_1) = X_1 - X_0. \quad (2)$$

The CFM aims at regressing a velocity field $v_\theta(\cdot)$ to $u_t(\mathcal{X} | Z)$, which defines the training objective:

$$\mathcal{L}_{\text{CFM}}(\theta) := \mathbb{E}_{t, Z \sim \pi(\cdot), p_t(\cdot | Z)} \|v_\theta(X_t) - u_t(X_t | Z)\|^2, \quad (3)$$

where it is shown that the CFM optimization has the same optimum as the FM objective [56].

2.2 Optimal Transport and Flow Matching

A natural question is the design of conditional probability path $p_t(\mathcal{X} | Z)$. Existing literature [37, 11] argues that the path should be chosen to recover the optimal transport (OT) displacement interpolant [39]. OT is a classical topic in mathematics that was originally used in economics and operations research [59], and has now become a popular tool in generative models. Specifically, the (Kantorovich) optimal transport problem is to find the transport plan between two probability measures, η_0 and η_1 , with the smallest associated transportation cost, defined as follows.

Definition 1 (Wasserstein Distance). Let (M, d) be a metric space, and let η_0 and η_1 be two probability measures on M . We denote the possible coupling space for η_0 and η_1 as $\Pi(\eta_0, \eta_1)$. A coupling $\pi \in \Pi(\eta_0, \eta_1)$ is a joint probability measure on $M \times M$ whose marginals are η_0 and η_1 respectively. With $c(X, Y)$ being the cost of transporting the mass between X and Y (e.g. the squared difference), the Wasserstein distance is defined as,

$$(W_c(\eta_0, \eta_1))^2 = \inf_{\pi \in \Pi(\eta_0, \eta_1)} \int_{M \times M} c(X, Y) d\pi(X, Y). \quad (4)$$

Specifically, the probability path as shown in Eq. (2) with $\sigma^2 \rightarrow 0$ is a solution to Eq. (4) when q_0 is the standard Gaussian distribution and q_1 can be approximated by a Gaussian distribution. Combined with technologies such as iterative matching [56] and mini batching [47] to approximate the optimal transport cost in Eq. (4), CFM has become the leading method in generative modeling.

However, recent research in manifold flow matching [11, 29] suggests that the interpolation trajectories are not appropriate if \mathcal{X} is not designed under the assumption of Euclidean geometry. This calls for the necessity of revisiting the trajectory in generating graphs, a non-euclidean object, as well.

3 Methodology

While the straight flow is proven to be the optimal transport interpolation considering the Euclidean geometry when the data in \mathbb{R}^d , the graph lies in a non-euclidean space thus the linear interpolation of the graph structure and node features does not simply grant optimal transport cost in such a space. In this section, we first consider graphs as a statistical object parameterized by Markov Random Fields in Section 3.2 to solve RQ1. We then develop the relevant OT distance and interpolation methods in Section 3.3. We further develop the flow matching for graphs (BWFlow) in Section 3.4 to solve RQ2. Finally, we extend our method to both continuous and discrete flow matching for more general graph generation tasks in Section 3.5.

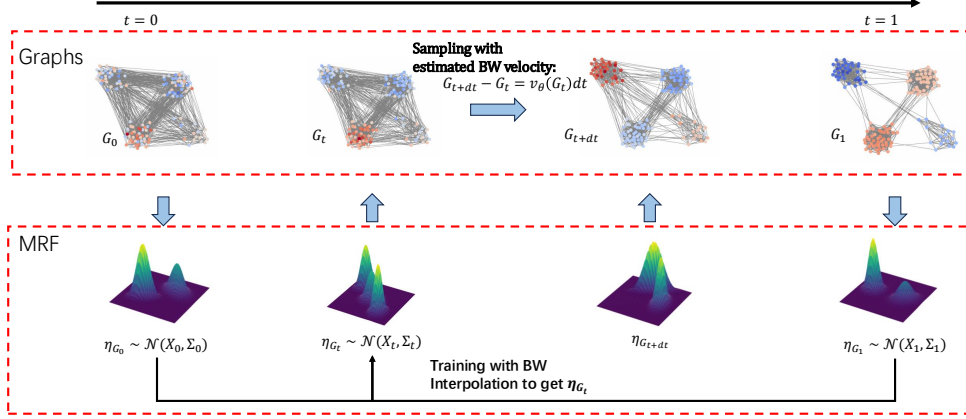


Figure 1: The pipeline for Bures-Wasserstein Flow matching.

3.1 Conditional Flow Matching for Graph Generation

Graphs as statistical objects. CFM is defined over a trajectory between p_1 and p_0 . When considering graph generation, the very first step is to define a data-generating process and model graphs as a statistical object. For notation, we let $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{X}\}$ denote an undirected graph random variable with edges \mathcal{E} , nodes \mathcal{V} , and node features \mathcal{X} . A graph realization is denoted as $G = \{V, E, X\} \sim p(\mathcal{G})$. We consider a group of latent variables that controls the graph distribution, specifically the node feature mean $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{|\mathcal{V}|}]^\top \in \mathbb{R}^{|\mathcal{V}| \times K}$, the weighted adjacency matrices $\mathbf{W} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$, Laplacian matrix as $\mathbf{L} = \mathbf{D} - \mathbf{W} \in \mathbb{R}^{|\mathcal{V}| \times |\mathcal{V}|}$, with $\mathbf{D} = \text{diag}(\mathbf{W}\mathbf{1})$ being the degree matrix. In a nutshell, graphs are statistical objects sampled from $G \sim p(\mathcal{G} | \mathbf{G}) = p(\mathcal{X}, \mathcal{E} | \mathbf{X}, \mathbf{W})$.

A common selection to decompose the probability density assumes the node features and graph structure are independent [24, 48, 16], which gives $p(\mathcal{G}) = p(\mathcal{X}) \cdot p(\mathcal{E})$. Then, the boundary conditions follow Dirac distributions such that $p_i(\mathcal{G}) = \delta(\mathcal{X}_i = \mathbf{X}_i) \cdot \delta(\mathcal{E}_i = \mathbf{W}_i)$, $\forall i = \{0, 1\}$. Such a decomposition causes reverse-starting and exposure biases in graph generation tasks [64]. Unlike them, we aim to mitigate the biases and construct an optimal transport trajectory through modeling the interdependency between node features and graph structures, as we will introduce later.

Graph CFM. We now consider constructing a probability path for graph generation that satisfies $p_t(\mathcal{G}_t) = \mathbb{E}_{(G_0, G_1) \sim \pi(\cdot, \cdot)} p_t(\mathcal{G}_t | G_0, G_1)$. While our method is agnostic of the FM type, we will focus on continuous FM for the sake of concise illustration and postpone the introduction of the discrete counterpart in Section 3.5. Recall that the aim of CFM is to train a parameterized velocity field, $v_t^\theta(\mathcal{G}_t)$ so that the sampling follows $G_{t+dt} = G_t + v_t^\theta(G_t) \cdot dt$, $G_0 \sim p_0(\mathcal{G})$ would generate the path along $p_t(\mathcal{G})$ and terminates at $p_1(\mathcal{G})$. We can parameterize $v_t^\theta(G_t)$ as,

$$v_t^\theta(G_t) = \mathbb{E}_{G_0 \sim p_0(\mathcal{G}), G_1 \sim p_{1|t}^\theta(\cdot, \cdot | G_t)} [v_t(G_t | G_0, G_1)] \quad (5)$$

As such, training the velocity function is replaced by training a denoiser $p_{1|t}^\theta(\cdot, \cdot | G_t)$ to predict the clean datapoint, which is commonly done by maximizing the log-likelihood [48, 10],

$$\mathcal{L}_{\text{CFM}} = \mathbb{E}_{G_1 \sim p_1(\cdot), G_0 \sim p_0(\cdot), t \sim \mathcal{U}_{[0,1]}(\cdot), G_t \sim p_{t|0,1}(\cdot | G_1, G_0)} [\log p_{1|t}^\theta(G_1 | G_t)] \quad (6)$$

where G_1 is sampled from data distribution and G_0 from reference distribution. t is sampled from a uniform distribution $\mathcal{U}_{[0,1]}$ on $[0, 1]$. G_t can be sampled from $p_{t|0,1}$ in a simulation-free manner. This framework avoids the evaluation of the conditional vector field at training time, which both increases the model robustness and training efficiency. However, a closed form of $p_t(\cdot | G_0, G_1)$ is required to construct both the probability path and the velocity field $v_t(G_t | G_0, G_1)$.

3.2 Markov Random Fields for Graphs

Graph Markov Random Fields Markov random fields (MRF) is a graphical model that is commonly used in modeling interconnected systems in statistical physics, such as molecule dynamics and

multi-body dynamics². We borrow the idea from MRF as a remedy to modeling the complex system organized by graphs, which intrinsically captures the underlying mechanism that jointly generates the nodes and edges. Mathematically, the joint probability density distribution (PDF) of node features and graph structure can be written as $p(\mathcal{G} | \mathbf{G}) = p(\mathcal{X}, \mathcal{E} | \mathbf{X}, \mathbf{W}) = p(\mathcal{X} | \mathbf{X}, \mathbf{W}) \cdot p(\mathcal{E} | \mathbf{W})$. Instead of assuming marginal independence, the node features and graph structure are conditionally independent given latent variables \mathbf{X} and \mathbf{W} . For node features \mathcal{X} , we follow the MRF assumption in Zhu et al. [65] which considers the cliques up to rank 2, i.e., the PDF is decomposed into the node-wise $\varphi_1(v)$ and pair-wise potential $\varphi_2(u, v)$ ³.

$$P(\mathcal{X} | \mathbf{X}, \mathbf{W}) \propto \prod_v \underbrace{\exp\{-(\nu + d_v)\|\mathbf{V}x_v - \boldsymbol{\mu}_v\|^2\}}_{\varphi_1(v)} \prod_{u,v} \underbrace{\exp\{w_{uv}[(\mathbf{V}x_u - \boldsymbol{\mu}_u)^\top (\mathbf{V}x_v - \boldsymbol{\mu}_v)]\}}_{\varphi_2(u,v)}, \quad (7)$$

with $\|\cdot\|$ the L_2 norm. It is shown in Appendix A.2 that Eq. (7) is a colored Gaussian distribution as in Eq. (8). The edges are assumed to be emitted from a Dirac function, i.e. $\mathcal{E} \sim \delta(\mathbf{W})$, yielding our definition for Graph Markov Random Fields (GMRF). The derivation can be found in Appendix A.2

Definition 2 (Graph Markov Random Fields). GMRF statistically describes graphs as follows,

$$p(\mathcal{G}) = p(\mathcal{X}, \mathcal{E}) = p(\mathcal{X} | \mathbf{X}, \mathbf{W}) \cdot p(\mathcal{E} | \mathbf{W}) \text{ where } \mathcal{E} \sim \delta(\mathbf{W}) \text{ and} \quad (8)$$

$$\text{vec}(\mathcal{X}) \sim \mathcal{N}(\mathbf{X}, \Lambda^\dagger), \text{ with } \mathbf{X} = \text{vec}(\mathbf{V}^\dagger \boldsymbol{\mu}), \Lambda = (\nu \mathbf{I} + \mathbf{L}) \otimes \mathbf{V}^\top \mathbf{V}.$$

The \otimes is the Kronecker product, $\text{vec}(\cdot)$ is the vectorization operator and \mathbf{I} is the identity matrix. The linear transformation matrix \mathbf{V} assists in modulating the graph feature emission properties, such as transforming to approximate one-hot encodings. Equipped with a proper prior on \mathbf{X} and \mathbf{W} , the GMRF provides an effective way to organize the graph systems.

Remark. We wish to point out that GMRF is not a universal model for all the graph models and it has constraints. The usage scope of GMRF is discussed in Appendix A.3. Fortunately, the model is capable of capturing the dynamics on most of the graph generation tasks, such as planar, SBM, and molecule graph generation.

3.3 The Optimal Transport Distance between Graph Distributions

The GMRF, simplifying all the way to Eq. (7), provides an elegant and simple framework to consider graphs as statistical objects. We further show that the paired metric spaces are equipped with a well-defined optimal transport distance, which can be used to build CFM models in Section 3.4. For such purpose, we decompose the Wasserstein distance between $\eta_{\mathcal{G}_0}$ and $\eta_{\mathcal{G}_1}$ as the sum of node feature and graph structure distance.

$$(\text{Graph Wasserstein Distance}) \quad \mathcal{W}_c(\eta_{\mathcal{G}_0}, \eta_{\mathcal{G}_1}) = \mathcal{W}_c(\eta_{\mathcal{X}_0}, \eta_{\mathcal{X}_1}) + \mathcal{W}_c(\eta_{\mathcal{E}_0}, \eta_{\mathcal{E}_1}). \quad (9)$$

where $\eta_{\mathcal{X}_j} \sim p(\mathcal{X}_j)$ is measures on node and $\eta_{\mathcal{E}_j} \sim p(\mathcal{E}_j)$ measures on edges with $j \in \{0, 1\}$.

We emphasize that \mathcal{X}_j is a variable controlled by the graph structure, so the BW distance implicitly models interaction between nodes and edges. Given the the question of finding the OT distance boils down to measure the distance between two colored Gaussian distribution, we borrow the results from previous research in probability theory [14, 44, 55] that solves the Wasserstein distance between two Gaussian distributions with an analytical form introduced in Lemma 3. Combining Lemma 3 and Eq. (8) and substituting into Eq. (9), the closed form of the BW distance for graph objects are derived as following (Note that this result is an extension of [20] under the assumption of MRF),

²see Appendix A.1 for a detailed discussion on graph generation, molecule dynamics, and MRF

³The assumption behind, is that the observed $\mathcal{X} = \mathbf{V}^\dagger(\boldsymbol{\mu} + \epsilon)$ so that $\mathbf{V}\mathcal{X} - \boldsymbol{\mu} = \epsilon \sim \mathcal{N}(0, (\nu \mathbf{I} + \mathbf{L})^{-1})$.

Corollary 1 (Bures-Wasserstein Distance). Consider two same-sized graphs $\mathcal{G}_0 \sim P(\mathcal{X}_0, \mathcal{E}_0)$ and $\mathcal{G}_1 \sim P(\mathcal{X}_1, \mathcal{E}_1)$ with \mathbf{V} shared for two graphs, described by the distribution in Definition 2. When the graphs are equipped with signed weighted graph Laplacian matrices \mathbf{L}_0 and \mathbf{L}_1 satisfying 1) is Positive Semi-Definite (PSD) and 2) has only one non-zero eigenvalue. The Bures-Wasserstein distance between these two random graph distributions is given by

$$\mathcal{W}_{BW}(\eta_{\mathcal{G}_0}, \eta_{\mathcal{G}_1}) = \|\mathbf{X}_0 - \mathbf{X}_1\|_F^2 + \beta \text{trace} \left(\mathbf{L}_0^\dagger + \mathbf{L}_1^\dagger - 2 \left(\mathbf{L}_0^{\dagger 1/2} \mathbf{L}_1^\dagger \mathbf{L}_0^{\dagger 1/2} \right)^{1/2} \right), \quad (10)$$

as $\nu \rightarrow 0$ and $\beta = \|\mathbf{V}\|_F^2 + 1$. The proof can be found in Appendix B.2

3.4 Bures-Wasserstein Flow Matching for Graph Generation

With the proper definition of optimal transport distance, we are now capable of introducing the two important components for FM models - the interpolation and the velocity. This provides a closed form for the induced probability path $p(G_t | G_0, G_1)$ that is easy to access without any simulation.

The interpolation. We first derive the OT displacement interpolant for two graphs, which is obtained through the following displacement minimization problem,

$$\mathcal{G}_t = \arg \min_{\tilde{\mathcal{G}}} (1-t)\mathcal{W}(\eta_{\mathcal{G}_0}, \eta_{\tilde{\mathcal{G}}}) + t\mathcal{W}(\eta_{\mathcal{G}_1}, \eta_{\tilde{\mathcal{G}}}). \quad (11)$$

With the Bures-Wasserstein distance defined in Corollary 1, we prove the minimizer of the above problem has the form in Lemma 1. The proof can be found in Appendix B.3.

Lemma 1 (Bures-Wasserstein interpolation). The graph minimizer of Eq. (11) have its node features following a colored Gaussian distribution, $\eta_{\mathcal{X}_t} \sim \mathcal{N}(\mathbf{X}_t, \Lambda_t^\dagger)$ with $\Lambda_t = (\nu \mathbf{I} + \mathbf{L}_t) \otimes \mathbf{V}^\top \mathbf{V}$ and edges following $\mathcal{E}_t \sim \delta(\mathbf{W}_t)$, superficially,

$$\mathbf{L}_t^\dagger = \mathbf{L}_0^{1/2} \left((1-t)\mathbf{L}_0^\dagger + t \left(\mathbf{L}_0^{\dagger 1/2} \mathbf{L}_1^\dagger \mathbf{L}_0^{\dagger 1/2} \right)^{1/2} \right)^2 \mathbf{L}_0^{1/2}, \quad \mathbf{X}_t = (1-t)\mathbf{X}_0 + t\mathbf{X}_1 \quad (12)$$

The velocity. We consider the reparameterization as in Eq. (5) and derive the conditional velocity $v_t(G_t | G_1, G_0)$ as in Lemma 2.

Lemma 2 (Bures-Wasserstein velocity). For the graph \mathcal{G}_t following BW interpolation in Lemma 1 the conditional velocity at time t is given as,

$$v_t(E_t | G_0, G_1) = \dot{\mathbf{W}}_t = \text{diag}(\dot{\mathbf{L}}_t) - \dot{\mathbf{L}}_t, \quad v_t(X_t | G_0, G_1) = \mathbf{X}_1 - \mathbf{X}_0 \quad (13)$$

with $\mathbf{T} = \mathbf{L}_t^{1/2} (\mathbf{L}_t^{\dagger 1/2} \mathbf{L}_1^\dagger \mathbf{L}_t^{\dagger 1/2})^{1/2} \mathbf{L}_t^{1/2}$, $\dot{\mathbf{L}}_t = 2\mathbf{L}_t - \mathbf{T}\mathbf{L}_t + \mathbf{L}_t\mathbf{T}$

where $\mathbf{W}_t = \mathbf{D}_t - \mathbf{L}_t$ and \mathbf{L}_t defined in Eq. (12). Derivation can be found in Appendix C.3.

With Lemma 1 and Lemma 2, we are now able to formally construct the algorithms for Bures-Wasserstein flow matching. Taking continuous flow matching as an example, Algorithms 1 and 2 respectively introduce the training and sampling pipelines for our BWFLOW.

Remark 1: Even though the GMRF in Definition 2 does rely on an implicit linear emission matrices \mathbf{V} , the BW interpolation Theorem 1 can be obtained without explicitly accessing to the \mathbf{V} matrices. The property was attractive as in practice we can construct the probability path without explicitly fitting a \mathbf{V} beforehand.

Remark 2: The BW interpolation and velocity both deviate from the linear flow matching framework and require extra computational cost. However, there exist multiple ways to analytically calculate or numerically approximate the velocity for training and inference. The choice of these methods depends on the trade-off between training stability, sampling efficiency, etc. In Appendix E, we provide a detailed discussion about the design space of BW interpolation and velocity, and compare

3.5 Discrete Bures Wasserstein Flow Matching for Graph Generation

Up to now we are working on the scenario when $p(\mathcal{X} | \mathbf{X}_i, \mathbf{W}_i)$ is a Gaussian and $p(\mathcal{E} | \mathbf{W}_i)$ is a Dirac distribution. However, previous studies have observed a significant improvement of the discrete

Algorithm 1: BWFlow Training

Input: Ref. dist p_0 and dataset $\mathcal{D} \sim p_1$.**Output:** Trained model $f_\theta(G_t, t)$.

```

1 Initialize model  $f_\theta(G_t, t)$ ;
2 while  $f_\theta$  not converged do
  /* Sample Boundary Graphs */
3   Sample batched  $\{G_0\} \sim p_0, \{G_1\} \sim \mathcal{D}$ ;
  /* Prob.path Construction */
4   Sample  $t \sim \mathcal{U}(0, 1)$ ;
5   Calculate the BW interpolation
      $p(G_t | G_0, G_1)$  via Eq. (12);
  /* Denoising - x-prediction */
6    $p_{1|t}^\theta(\cdot | G_t) \leftarrow f_\theta(G_t, t)$ ;
7   Loss calculation via Eq. (6);
8   optimizer.step();

```

Algorithm 2: BWFlow Sampling

Input: Reference distribution p_0 , TrainedModel $f_\theta(G_t, t)$, Small time step dt ,**Output:** Generated Graphs $\{\hat{G}_1\}$.

```

1 Initialize samples  $\{\hat{G}_0\} \sim p_0$ ;
2 Initialize the model  $p_{1|t}^\theta(\cdot | G_t) \leftarrow f_\theta(G_t, t)$ 
  for  $t \leftarrow 0$  to  $1 - dt$  by  $dt$  do
  /* Denoising - x-prediction */
3   Predict  $\hat{G}_1 \leftarrow p_{1|t}^\theta(\cdot | G_t)$ ;
  /* Velocity calculation */
4   Calculate  $v_\theta(\hat{G}_t | \hat{G}_0, \hat{G}_1)$  via Eq. (13);
  /* Numerical Sampling */
5   Sample  $\hat{G}_{t+dt} \sim \hat{G}_t + v_\theta(\hat{G}_t)dt$ 

```

204 counterpart of the continuous graph generation models [57, 63, 48]. To benefit our model from such
 205 a nature, we derive the discrete Bures-Wasserstein Flow Matching for graph generation.

206 As such, we design the probability path as,

$$p_t(\mathcal{X}) = \text{Cat}(\mathbf{X}_t), p_t(\mathcal{E}) = \text{Bernoulli}(\mathbf{W}_t) \text{ s.t. } p(\mathcal{G}_0) = \delta(G_0), p(\mathcal{G}_1) = \delta(G_1) \quad (14)$$

207 where $\mathbf{W}_t = \mathbf{D}_t - \mathbf{L}_t$ with \mathbf{X}_t and \mathbf{L}_t defined the same in Eq. (12). We consider the fact that the
 208 Dirac distribution is a special case when the Categorical/Bernoulli distribution has probability 1 or
 209 0, so the boundary condition $p_0(\mathcal{G}) = \delta_{G_0}(\mathcal{G}), p_1(\mathcal{G}) = \delta_{G_1}(\mathcal{G})$ holds. Even though now we are not
 210 sampling from Gaussian distributions anymore, it is possible to approximate the Wasserstein distance
 211 between two multivariate Bernoulli distributions with the Gaussian counterpart so the conclusions,
 212 such as optimal transport displacements, still hold. We left the discussion in Appendix D.1.

213 The distribution of \mathcal{X}_t can be re-written as $p_t(\mathcal{X}) = (1 - t)\delta(\cdot, \mathbf{X}_0) + t\delta(\cdot, \mathbf{X}_1)$ so the conditional
 214 velocity $v_t(X_t | G_0, G_1) = \delta(\cdot, \mathbf{X}_1) - \delta(\cdot, \mathbf{X}_0)$. However, the velocity of \mathcal{E}_t cannot be written as a
 215 mixture of two boundary conditions. Instead, we derive in Appendix C.3 that the discrete velocity as,

$$v_t(E_t | G_1, G_0) = (1 - 2E_t) \frac{\dot{\mathbf{W}}_t}{\mathbf{W}_t \circ (1 - \mathbf{W}_t)}, \quad (15)$$

216 where $\mathbf{W}_t = \mathbf{D}_t - \mathbf{L}_t$, $\dot{\mathbf{W}}_t = \text{diag}(\dot{\mathbf{L}}_t) - \dot{\mathbf{L}}_t$ with $\mathbf{L}_t, \dot{\mathbf{L}}_t$ defined in Eqs. (12) and (13) respectively.
 217 With the interpolation and velocity defined, the discrete flow matching is built in Algorithms 3 and 4

218 4 Experiments

219 We evaluate the BWFlow algorithm through both the plain graph generation and real-world molecule
 220 generation tasks. We first outline the experimental setup in Section 4.1 followed by a general
 221 comparison on both tasks in Section 4.2. Next, we conduct ablation studies to analyze the impact
 222 of interpolation methods and the corresponding velocity construction on graph generation perfor-
 223 mance in Section 4.3 and demonstrate the effectiveness and benefit of flow along Bures-Wasserstein
 224 interpolation.

225 4.1 Experiment Settings

226 **Dataset.** For planar graph generation, we evaluate the quality of generated graphs on three benchmark
 227 datasets following previous works [38, 57, 6], specifically, **planar** graphs, **tree** graphs, and stochastic
 228 blocking models (**SBM**). Two datasets, namely MOSES [46] and GUACAMOL [8], are benchmarked
 229 to test the model performance on 2D molecule generation. For 3D molecule generation with
 230 coordinate data, we test the model on QM9 [49] and GEOM-DRUGS [2].

231 **Metrics.** In plain graph generation, the evaluation metrics include the percentage of Valid, Unique,
 232 and Novel (**V.U.N.**) graphs, and the average maximum mean discrepancy ratio (**A.Ratio**) of graph

statistics between the set of generated graphs and the test set are reported (details in Appendix L.1). For molecule generation, since our model ignores the edge types but only consider the graph structure when generating the graphs, we develop a new relaxed metric when measuring the stability and validity of atoms and molecules. Specifically, the atom-wise stability is relaxed as:

$$\text{Stability of Atom } i : s_i = \mathbb{I}[\exists (b_{ij})_{j \in \mathcal{N}_i} \in \prod_{j \in \mathcal{N}_i} B_{ij} : \sum_{j \in \mathcal{N}_i} b_{ij} = E_i] \quad (16)$$

which means atom i is “relaxed-stable” if there is at least one way to pick allowed bond types (B_{ij}) to its neighbors \mathcal{N}_i so that their total exactly matches the expected valences (E_i). Such a relaxed stability of atoms (**Atom.Stab.**) inherently defines molecule stability (**Mol.Stab.**) and the **V.U.N.** of a molecule, which are the shared metrics for both 2D/3D molecule generation. In addition to these metrics, distribution metrics are also used for 2D molecules (FCD, Scaf, etc.), and 3D generations (charge distributions, atom total variation, angels, etc.). Details in Appendix L.1

Setup. To isolate the impact from model architecture, we follow [48] to fix the backbone model as the same graph transformers in their paper. Furthermore, it is shown in [48] that sample distortion, training distortion and target guidance have a significant impact on the performance of graph generation tasks. In our paper, in addition to the best model performance, we also show the results when these technologies are disabled, i.e., identity time distortion and unconditional generation without any graph-level labeling.

4.2 Main Results for Graph Generation

Plain Graph Generation. We first validate the ability of BWFlow to generate plain graphs without node attributes. In Table 1, we report V.U.N. and A.Ratio. We only keep the main diffusion/flow model for comparison, while other models are included in the full version at Table 6. As the model performance is near-saturated in these datasets, we not only report the best performance achieved by the models but also gives the results when all the models are without training distortion and sampling distortion as in Qin et al. [48]. One exception is tree graph datasets, where our model performance is not satisfying. This is due to the fact that tree graphs lie in a hyperbolic space which do not strictly follow our MRF assumptions.

Table 1: Graph generation performance on the synthetic datasets: Planar, Tree, and SBM. Given that the synthetic datasets are usually unstable in evaluation, we applied an exponential moving average to stabilize the results and sample 5 times (each run generates 40 graphs) to calculate the mean and standard deviation.

Model	Class	Planar		Tree		SBM	
		V.U.N. \uparrow	A.Ratio \downarrow	V.U.N. \uparrow	A.Ratio \downarrow	V.U.N. \uparrow	A.Ratio \downarrow
Train set	—	100	1.0	100	1.0	85.9	1.0
DiGress [57]	Diffusion	77.5	5.1	90.0	1.6	60.0	1.7
EDGE [13]	Diffusion	0.0	431.4	0.0	850.7	0.0	51.4
HSpectre [6]	Diffusion	95.0	2.1	100.0	4.0	75.0	10.5
GruM [27]	Diffusion	90.0	1.8	—	—	85.0	1.1
CatFlow [16]	Flow	80.0	—	—	—	85.0	—
Cometh [50]	Diffusion	99.5 \pm 0.9	—	—	—	75.0 \pm 3.7	—
DeFoG [48]	Flow	99.5 \pm 1.0	1.6 \pm 0.4	96.5 \pm 2.6	1.6 \pm 0.4	90.0 \pm 5.1	4.9 \pm 1.3
BWFlow	Flow	97.5 \pm 2.5	1.37 \pm 0.4	75.5 \pm 2.4	3.6 \pm 1.2	83.5 \pm 6.0	3.8 \pm 0.9
DeFoG (S.ed)	Flow	77.5 \pm 1.0	3.5 \pm 0.4	75.3 \pm 2.6	1.32 \pm 0.4	90.0 \pm 5.1	4.9 \pm 1.3
BWFlow (S.ed)	Flow	84.8 \pm 1.0	2.7 \pm 0.4	75.5 \pm 2.4	3.6 \pm 1.2	90.5 \pm 4.0	3.8 \pm 0.9

257

2D Molecule Graph Generation The model performance compared to SOTA diffusion/flow models is illustrated in Table 2. In GUACAMOL, almost all the modern generative models, including our BWflow, can achieve V.U.N close to 100%. Given that MOSES and GUACAMOL benchmarks are approaching saturation, the fact that BWFlow achieves results on par with the SOTA models serves as strong evidence of its effectiveness.

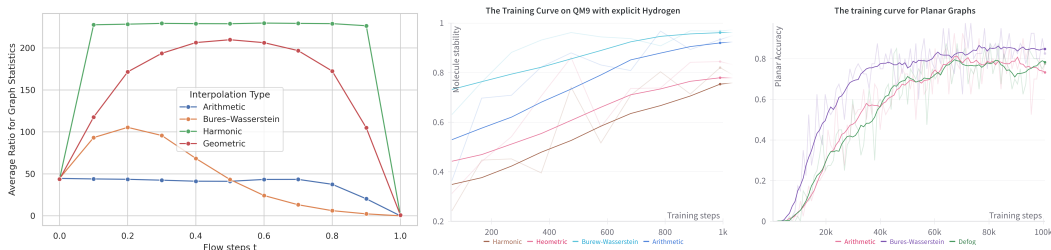
3D Molecule Generation. Table 3 gives the results on the 3D molecule generation task with explicit hydrogen, where we ignore the bond type but just view the adjacency matrix as a binary one for fair comparison. Interestingly, the empirical results show that even without edge type, the de novo graph generation model already can capture the molecule data distribution. And our BWFlow significantly outperforms the SOTA models, including MiDi [58] and FlowMol [15]. We believe a promising

Table 2: Large molecule generation results. Only iterative denoising-based methods are reported.

Model	Guacamol					MOSES						
	Val. \uparrow	V.U. \uparrow	V.U.N. \uparrow	KL div \uparrow	FCD \uparrow	Val. \uparrow	Unique. \uparrow	Novelty \uparrow	Filters \uparrow	FCD \downarrow	SNN \uparrow	Scaf \uparrow
Training set	100.0	100.0	0.0	99.9	92.8	100.0	100.0	0.0	100.0	0.01	0.64	99.1
DiGress [57]	85.2	85.2	85.1	92.9	68.0	85.7	100.0	95.0	97.1	1.19	0.52	14.8
DisCo [63]	86.6	86.6	86.5	92.6	59.7	88.3	100.0	97.7	95.6	1.44	0.50	15.1
Cometh [50]	98.9	98.9	97.6	96.7	72.7	90.5	99.9	92.6	99.1	<u>1.27</u>	0.54	16.0
DeFoG [48]	99.0	99.0	97.9	97.7	73.8	92.8	<u>99.9</u>	92.1	<u>98.9</u>	1.95	0.55	14.4
BWFlow (Ours)	98.8	98.9	97.4			91.7	91.7	91.2	92.3	57.9		

Dataset	Interpolation	Metrics							
		μ	V.U.N.(%)	Mol.Stab.	Atom.Stab.	Connected(%)	Charge(10^{-2})	Atom(10^{-2})	Angles($^{\circ}$)
QM9 (with h)	MiDi	1.01	93.13	93.98	99.60	99.21	0.2	3.7	2.21
	FlowMol	1.01	87.53	88.45	99.13	99.09	0.4	4.2	2.72
	BWFlow	1.01	96.45	97.84	99.84	99.24	0.1	2.3	1.96
GEOM (with h)	Midi	1.34	78.23	32.42	89.61	79.15	0.6	11.2	9.6
	FlowMol		35.7		/				
	BWFlow	1.20	87.75	46.80	95.08	73.53	0.1	6.5	3.96

Table 3: Quantitative experimental results on De Novo Molecule Generation with explicit hydrogen.



(a) The evolution of graph statistics ratio. (b) Training Curves for QM9. (c) Training Curves for Planar.

Figure 2: Training curves on QM9 and planar datasets with explicit hydrogen.

future direction is to incorporate the processing of multiple bond types into our framework, which would further raise the performance by a margin.

4.3 Ablation Studies.

Superiority of BWFlow in constructing paths. We compute the A.Ratio on SBM between generated graph interpolants and test data for $t \in [0, 1]$, as shown in Fig. 2a. Under arithmetic interpolation, the A.Ratio hovers around a high value until $t \approx 0.8$. By contrast, BW interpolation initially exposes the model to more out-of-distribution samples with increased A.Ratio. After this early exploration, the A.Ratio rapidly converges, yielding more accurate velocity estimates toward the true data distribution. This behavior—early exposure to diverse samples followed by steady denoising—enhances both the model robustness and velocity estimation. In comparison, harmonic and geometric interpolations step outside the valid graph domain, making the learning problem ill-posed.

Interpolation metrics

Following our analysis of probability paths constructed by different interpolation methods, we evaluate the impact of these methods on the overall model performance. Fig. 2b illustrated the a bar plot that compares interpolation methods on the ability of capturing data distributions. Fig. 2c illustrated an example of the convergence curve at the training stage. Full results can be found in Table 8. The results suggest that BW flow matching can bring a significant performance boost compared to FM methods constructed with arithmetic and other interpolation methods.

5 Discussion and Future Work

Limitations: *Extension to multiple relation types.* As our framework is built upon the interpolation parameterized by the Laplacian Matrices, it is not generalizable to the probability path with multiple edge types. *Increased Computational Complexity.* While constructing the probability path and the

290 velocity, our BW interpolation suffers from an $O(N^3)$ extra cost due to its request to compute the
291 pseudo-inverse of the Laplacian matrix. Compared to linear interpolation, empirically this brings 2x
292 training time and inference time.

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