Continuous Graph Flow
for Flexible Density Estimation

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Abstract

In this paper, we propose Continuous Graph Flow, a generative continuous flow based method that aims to model distributions of graph-structured complex data. The model is formulated as an ordinary differential equation system with shared and reusable functions that operate over the graph structure. This leads to a new type of neural graph message passing scheme that performs continuous message passing over time. This class of models offer several advantages: (1) modeling complex graphical distributions without rigid assumptions on the distributions; (2) not limited to modeling data of fixed dimensions and can generalize probability evaluation and data generation over unseen subset of variables; (3) the underlying continuous graph message passing process is reversible and memory-efficient. We demonstrate the effectiveness of our model on two generation tasks, namely, image puzzle generation, and layout generation from scene graphs. Compared to unstructured and structured latent-space VAE models, we show that our proposed model achieves significant performance improvement (up to 400% in negative log-likelihood).

1 Introduction

Accurate modeling of probability densities over sets of random variables is a central part of AI research. Core tasks such as reasoning, planning, and generation benefit from the ability to effectively characterize the probability density over variables pertinent to a domain of interest. As such, the construction of these densities has been a preoccupation of research ranging from seminal work on probabilistic graphical models through to recent efforts utilizing flow-based models.

In this paper, we focus on learning a single representation that can be used to model a density over an arbitrary set of random variables. This task arises in inductive learning scenarios for the aforementioned tasks – learning a model for reasoning over a variable number of related entities, generating layouts of scenes composed of variable numbers of objects. The desiderata of a powerful and expressive model for this task include: (1) flexibility: architectures to enable generalization to new instances with varying numbers of random variables, (2) relations: ability to model dependencies among the random variables to enhance modeling capabilities, (3) high capacity: potential to model complex data distributions, and (4) tractability: exact and efficient computation of the probability density.

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Significant research effort has been devoted in this vein. The classic probabilistic graphical model (PGM) framework [1] allows many algorithms to learn structured representations for complex data. However, PGMs often suffer from rigid assumptions on distributions [2][3]. Furthermore, performing exact inference can be computationally difficult, which led to development of several techniques for approximate inference [4][6]. Alternatively, impressive advances in generative modeling within the variational autoencoder (VAE) [2] formalism offer promise for learning flexible data distributions. In addition, there has been a surge of interest in designing models that focus on bestowing generative models with the ability to learn structured latent space models by unifying PGMs & VAEs [8][11].

Despite the promising success of these modeling efforts, their capacity is still very much limited. This is mainly due to modeling choices enforced by the approximate techniques necessary to alleviate computational difficulty (in case of PGMs) or intractability (in case of VAEs). An immediate consequence of such approximations is restricted distributions or latent space structures, thereby compromising flexibility in the representations obtained from these models.

On that premise, the approach of normalizing flows provides several tools to conduct exact computation of likelihood and perform efficient inference in generative models [12][15]. This line of work uses iterative updates on a composition of invertible transformations at discrete time instances to map points from a simple distribution to complex distributions. However, none of the existing flow-based generative models can be extended to learning flexible representations for variable-sized inputs as the invertible mappings are required to be bijective. This jeopardizes the capability of the modeling approaches to generalize to new unseen tasks relevant to the given data.

Recent extensions of normalizing flows to continuous time versions using ordinary differential equations (ODEs) [16][17] lift all restrictions on the architecture of the flow based generative model. We build on continuous normalizing flow based approaches to accomplish our goal of learning structure-aware flexible models that can generalize across different graph structures while still permitting efficient and exact likelihood computation of variables.

In this paper, we present a new class of models – continuous graph flow, a continuous flow based generative model formulated as a set of related variables having continuous time dynamics. We demonstrate the effectiveness of our model on image puzzle generation and scene graph based layout generation tasks. We illustrate the ability of our model to generalize over variable graph sizes and perform efficient conditional inference. Experimental results clearly show that continuous graph flow achieves significant performance improvement (up to 400% improvement in negative log-likelihood) over state-of-the-art unstructured and structured latent-space VAE models.

2 Preliminaries

Probabilistic graphical models. A graphical model represents a joint probability distribution over a set of random variables $X = \{x_i\}_{i=1}^n$. A random variable $x_i$ from the set $X$ is represented by a node in the graph. The joint distribution is defined by a set of factor functions $\{f_a\}, a \in A$ where $A$ is a set containing sets of variables over which a factor function instance $f_a$ is defined. Each instance of $\{f_a\}$ corresponds to a type of dependency between a set or subset of graph nodes. We focus on factor function based PGMs for this work that are typically formulated as follows:

$$P(X) = \frac{1}{Z} \prod_a f_a(\{x_a\}; \theta) \quad (1)$$

where $Z$ is the normalization factor and function $f_a$ is defined over a set of variables $\{x_a\}$. Typically, these models allow performing flexible inference when the distributions of variables are simplified such as log-linear, Gaussian distributions.

Graph neural networks. Relational networks such as Graph Neural Networks (GNNs) facilitate learning of non-linear interactions using neural networks. In every layer $\ell \in \mathbb{N}$ of a GNN, the graph node embedding $h_i^{(\ell)}$ accumulates information from its neighbors of the previous layer recursively:

$$h_i^{(\ell)} = g\left(\left\{ f_{ij}(h_i^{(\ell-1)}, x_i^{(\ell-1)}, x_j^{(\ell-1)})|j \in N(i)\right\}\right) \quad (2)$$

where the function $g$ is an aggregator function, $N(i)$ is the set of neighbour nodes of node $i$, and $f_{ij}$ is the message function from node $j$ to node $i$, $x_i$ is the input node features. Our model uses the form
of GNN where embeddings of the graph nodes are kept the same across iterations. This allows using \( x_i \) in the flow-based models (below) while maintaining the same dimensionality across iterations.

**Normalizing flows.** Unlike likelihood based generative models that parameterize distributions with an explicit form, flow-based models allow to construct complex distributions from simple distributions (e.g. Gaussian) through a sequence of invertible mappings \([12]\) by applying a rule for change of variables. The density \( p_K(z_K) \) and the final state \( z_K \) of the variable \( z \) obtained by successively transforming a random variable \( z_0 \) through a chain of \( K \) invertible functions \( f_k \):

\[
z_K = f_K \circ \ldots f_2 \circ f_1(z_0),
\]

\[
\log p_K(z_K) = \log p_0(z_0) - \sum_{k=1}^{K} \log \left| \det \frac{\partial f_k(z_{k-1})}{\partial z_k} \right|
\]

(4)

where \( \frac{\partial f_k(z_{k-1})}{\partial z_k} \) is the Jacobian of \( f \) and \( k \in \{1, 2, ..., K\} \).

Instead of having predetermined number of transformations, continuous normalizing flows (CNFs) \([16,17]\) replace the transformation function with an integral of continuous-time dynamics as follows:

\[
\log p(z(t_1)) = \log p(z(t_0)) - \int_{t_0}^{t_1} \text{Tr} \left( \frac{\partial f(z(t - 1))}{\partial z(t)} \right) dt.
\]

(5)

where the trace computation is computationally less expensive than computation of the Jacobian in Equation (4). Building on CNF based approaches, we present continuous graph flow which effectively models continuous time dynamics of probabilistic graphical models.

## 3 Continuous graph flow

Given a set of random variables \( X \), we represent the joint distribution of \( X \) as \( p(X) \), where \( X = \{ x_i \}_{i=1}^{n} \) and each variable \( x_i \in \mathbb{R}^{m_i} \), associated with each graph node. To model the interactions between graph nodes, we define a set of message functions \( \{ f_a \}, a \in A \) which takes a subset of graph nodes as input and outputs an aggregated message for a target variable. The goal is to learn a joint distribution \( p(X) \).

To define the transformations for the probability density we formulate a multi-variate ordinary differential equation system. The form of this system follows the below template:

\[
\begin{bmatrix}
\dot{x}_0(t) \\
\dot{x}_1(t) \\
\vdots \\
\dot{x}_n(t)
\end{bmatrix} =
\begin{bmatrix}
f^0(\{x(t)\}) \\
f^1(\{x(t)\}) \\
\vdots \\
f^n(\{x(t)\})
\end{bmatrix}
\]

(6)

\[
x_i(t_1) = x_i(t_0) + \int_{t_0}^{t_1} f^i(\{x(t)\}) dt
\]

(7)
where $\dot{x}_i = dx_i/dt$ and $\{x(t)\}$ is the set of variables at time $t$. The random variable $x_i$ at time $t_0$ follows a simple prior distribution, i.e., $x_i(t_0) \sim q(x_i(t_0))$. In the above transformation, function $f^t$ implicitly defines the interaction and density transformation over the variables. It transforms the value of the variable $x_i$ at time $t_0$ to the value of the variable at time $t_1$ which follows the data distribution to be learned. The prior distributions $q(x_i(t_0))$ can have simple forms such as Gaussian distributions.

### 3.1 Continuous message passing over graphs

The above form in Eq. (7) represents a generic multi-variate update. However, it does not take into account the structure between nodes and the form of update functions $f(\cdot)$ does not naturally permit generalization to new random variables.

To alleviate these shortcomings, we define a message passing process that operates over graphs, by making the update functions reusable and defined over variables according to the graph structure. The above form in Eq. (7) represents a generic multi-variate update. However, it does not take into account the structure between nodes and the form of update functions $f(\cdot)$ does not naturally permit generalization to new random variables.

The updates are defined as discrete steps of updating the set of node variables $X = \{x_i\}_{i=1}^n$. The process begins from timestep $t_0$ where variables $\{x_i(t_0)\}_{i=1}^n$ only contain local information, and these variables update node variables based on information gathered from other relevant graph nodes in the graphical model after a fixed number of message passing steps. Instead of treating the message passing process as a discrete process, we formulate it as a continuous process which eliminates the requirement of having a predetermined number of steps of message passing. By further pushing the message passing process to update at smaller steps and continuing the updates for an arbitrarily large number of steps, each variable update can be represented as a continuous differential equation (ODE) system with shared and reusable functions:

$$
\begin{bmatrix}
\dot{x}_0(t) \\
\dot{x}_1(t) \\
\vdots \\
\dot{x}_n(t)
\end{bmatrix} =
\begin{bmatrix}
g(\{\hat{f}_{a(0,j)}(x_0(t), x_j(t))|j \in N(0)\}) \\
g(\{\hat{f}_{a(1,j)}(x_1(t), x_j(t))|j \in N(1)\}) \\
\vdots \\
g(\{\hat{f}_{a(n,j)}(x_n(t), x_j(t))|j \in N(n)\})
\end{bmatrix}
$$

(8)

where $\dot{x}_i = dx_i/dt$, $\hat{f}_{a(i,j)}(\cdot)$ is a reusable message function, $N(i)$ is the set of neighbours of node $i$, and $g(\cdot) \cdot$ is a function that aggregates the information passed to a variable. The above formulation describes the case of pairwise message functions, though this can be generalized to higher-order interactions. The function $\hat{f}_{a(i,j)}$ to use in passing information between nodes $i$ and $j$ depends on the nodes; we implement this as a fixed library of functions, the selection from which $a(\cdot, \cdot)$ depends on the type of node to allow for generalization to new graph structures. Performing message passing to derive final states is equivalent to solving an initial value problem for an ODE system. Following the ODE formulation, the final states of variables can be computed as:

$$
x_i(t_1) = x_i(t_0) + \int_{t_0}^{t_1} g \left( \{\hat{f}_{a(i,j)}(x_i(t), x_j(t))|j \in N(i)\} \right), \quad i \in \{1, 2, \ldots, n\}
$$

(9)

This formulation can be solved with an ODE solver.

### 3.2 Continuous message passing as density transformation

Continuous graph flow leverages the continuous message passing mechanism (described in Sec. 3.1) and formulates the message passing as implicit density transformations of the variables in the graphical model (illustrated in Figure 1). Given a set of variables $X = \{x_i\}_{i=1}^n$ with dependencies between variables (as in graphical model), the goal is to obtain the true distribution over $X$ by fitting a model based on data sampled from the true distribution. Assume that at initial time $t_0$, the joint distribution $p(X(t_0))$ has a simple form such as independent Gaussian distribution for different variables $x_i$ where the mean and variance of Gaussian are learnable. The continuous message passing process allows the transformation of the variables from $X(t_0) = \{x_i(t_0)\}_{i=1}^n$ to $X(t_1) = \{x_i(t_1)\}_{i=1}^n$. Moreover, this process also converts the distributions over variables from simple distributions (e.g., Gaussian distributions) to complex data distributions. Building on the single-variable continuous dynamics proposed by [10] where each variable in the system has a single coherent meaning, we define the following dynamics over joint distributions corresponding to multiple-variables that subsequently can be solved using initial value problem of ODE as follows:

$$
\frac{\partial \log p(X(t))}{\partial t} = -Tr \left( \frac{\partial F}{\partial X(t)} \right) \cdot \log p(X(t_1)) = \log p(X(t_0)) - \int_{t_0}^{t_1} Tr \left( \frac{\partial F}{\partial X(t)} \right)
$$

(10)
where the set of variables $X$ is a concatenation of all variables $x_i$ in the graph (varies depending on the size of the input graph) and $F$ represents the set of factor functions $\{g(f_a(\{x_a\}))\}$. The changes in log probability along with the sequential changes of variables can be reduced to the trace computation of Jacobian matrix $\partial F/\partial X(t)$ [16].

In this work, we use two forms of density transformations for message passing: (1) *generic message transformations* – transformations with generic update functions whose trace (refer Eq. [10]) can be approximated instead of computed by brute force, and (2) *multi-scale message transformations* – transformations with generic update functions at multiple scales of information.

**Generic message transformations.** We represent a message passing block as neural network. The trace estimation of Jacobian matrix by a generic neural network function can be estimated using the trace estimator proposed in [17]:

$$\log p(X(t_1)) = \log p(X(t_0)) - \mathbb{E}_{\epsilon} \int_{t_0}^{t_1} [\epsilon^T \frac{\partial F}{\partial X(t)} \epsilon] dt$$

(11)

where $F$ denotes a generic neural network based message passing block, and $\epsilon$ is a noise vector and usually can be sampled from standard Gaussian or Rademacher distributions.

**Multi-scale message transformations.** As a generalization of generic message transformations, we design a model with multi-scale message passing to encode different levels of information in the variables. As in [15], we construct our overall multiscale flow model by stacking several blocks wherein each block contains message passing blocks based on generic message transformations. After passing the input through a block, we factor out a portion of the output and feed it as input to the subsequent block.

$$\log p(X(t_b)) = \log p(X(t_{b-1})) - \mathbb{E}_{\epsilon} \int_{t_{b-1}}^{t_b} [\epsilon^T \frac{\partial F}{\partial X(t_{b-1})} \epsilon] dt$$

(12)

where $b = 1, 2, \ldots, (B - 1)$ with $B$ as the total number of blocks in the design of the multi-scale architecture. Assume at time instance $t_0 < t_b < t_1$, the variable $X(t_b)$ is factored out into two to obtain $\tilde{X}(t_b)$ and $\hat{X}(t_b)$, we input one of these as the input to the $(b + 1)^{th}$ block. Let $\tilde{X}(t_b)$ be the input to the next block, the density transformation is formulated as:

$$\log p(\tilde{X}(t_{b+1})) = \log p(\tilde{X}(t_b)) - \mathbb{E}_{\epsilon} \int_{t_b}^{t_{b+1}} [\epsilon^T \frac{\partial F}{\partial \tilde{X}(t_b)} \epsilon] dt$$

(13)

4 Experiments

To show the effectiveness and generalizability of our Continuous Graph Flow (CGF) on graphical distributions, we evaluate our model on two tasks: (1) image puzzle generation; and (2) layout generation from scene graphs. These two tasks have high complexity in variable distributions and offer a challenging evaluation setup for our model.

4.1 Graphical distribution – density estimation

4.1.1 Image puzzle generation

**Task description.** We design image puzzles for image datasets. Given an image of size $N \times N$, we design a puzzle by dividing the original image into non-overlapping unique patches (each forming a puzzle patch). A puzzle patch is of size $W \times W$ and each image is divided into $p = N/W$ puzzle patches both horizontally and vertically. Each of the $p^2$ patches forms a node in the graph. To evaluate the performance of our model on dynamic graph sizes, instead of training the model with all $p^2$ nodes, we sample $p'$ adjacent patches where $p'$ is uniformly sampled from $\{1, \ldots, p^2\}$ as input to the model during training and test using the same setup. In our experiments, we use patch size $W = 16$, the number of puzzle patches $(p^2)$ where $p \in \{2, 3, 4\}$ and edge function for each direction (left, right, up, down) within a neighbourhood of a node. Additional details are provided in Appendix.

**Datasets and baselines.** We design the image puzzle generation task (described above) for each of three image datasets: MNIST [13], CIFAR10 [19], and CelebA [20]. We perform training and testing

CelebA dataset does not have a validation set, thus, we split the original dataset into a training set of 27,000 images and test set of 3,000 images.
Table 1: **Quantitative results on image puzzle generation.** Comparison of our CGF model with standard VAE and state-of-the-art VAE based models in bits/dimension (lower is better). These results are for unconditional generation using multi-scale version of continuous graph flow.

| Method          | MNIST     | CIFAR-10  | CelebA-HQ |
|-----------------|-----------|-----------|-----------|
| BiLSTM + VAE    | 4.97 4.77 | 6.02 5.20 | 5.72 5.66 |
| GraphVAE [9]    | 4.89 4.65 | 6.03 5.02 | 5.66 5.43 |
| Graphite [10]   | 4.90 4.64 | 6.06 5.09 | 5.71 5.50 |
| VMP-SIN [8]     | 5.13 4.92 | 6.00 4.96 | 5.70 5.43 |
| GAE [22]        | 4.91 4.89 | 5.83 4.95 | 5.71 5.63 |
| NRI [23]        | 4.58 4.35 | 5.44 4.82 | 5.36 5.43 |
| **Ours**        | 1.24 1.21 | 2.42 2.31 | 3.44 3.17 |

Figure 2: **Qualitative results on MNIST for image puzzle generation.** Samples generated using our model for 2x2 MNIST puzzles in (a) unconditional generation and (b) conditional generation settings. For setting (b), generated patches (highlighted in green bounding boxes) are conditioned on the remaining patches (obtained from ground truth). Best viewed in color.

Figure 3: **Qualitative results on CelebA-HQ for image puzzle generation.** Samples generated using our model for 3x3 CelebA-HQ puzzles in (a) unconditional generation and (b) conditional generation settings. For setting (b), generated patches (highlighted in green bounding boxes) are conditioned on the remaining patches (obtained from ground truth). Best viewed in color.

Table 2: **Quantitative performance measurement of generalizability of our CGF model** in three different evaluation settings for image puzzle sizes 3x3 for three image datasets in bits/dimension. These results are for unconditional generation using multiscale version of continuous graph flow.

| Settings       | MNIST     | CIFAR-10  | CelebA-HQ |
|----------------|-----------|-----------|-----------|
| Odd to even    | 1.33      | 2.81      | 3.31      |
| Less to more   | 1.37      | 2.91      | 3.66      |
| More to less   | 1.34      | 2.83      | 3.44      |

using the training and validation set provided in the original dataset respectively. We compare our model with four state-of-the-art VAE based models which focus on learning structured representations: (1) GraphVAE [9], (2) Graphite [10], (3) Variational message passing using structured inference networks (VMP-SIN) [8], (4) BiLSTM + VAE: a bidirectional LSTM used to model the interaction between node latent variables (obtained after serializing the graph) in an autoregressive manner similar to [21], (5) Variational graph autoencoder (GAE) [22], and (6) Neural relational inference [23]: we adapt this to model data for single time instance and model interactions between the nodes.

**Quantitative results.** We report the negative log likelihood (NLL) in bits/dimension for each of the three datasets (lower is better). We observe that our model outperforms the VAE-based baselines with a significant margin as shown in Table 1.
Qualitative evaluation. In addition to the quantitative results, we perform two types of sampling based evaluation: (1) Unconditional Generation, i.e., samples from a base distribution (e.g. Gaussian) are transformed into learnt data distribution using the flow, and (2) Conditional Generation: we map $x_a \in X_a$ where $X_a \subset X$ to the points in base distribution to obtain $z_a$ and subsequently concatenate the samples from Gaussian distribution to $z_a$ to obtain $z'$ that match the dimensions of desired graph and generate samples by transforming from $z'$ to $x \in X$ using the trained graph flow.

For our experiments, we perform two sets of generation experiments using CGF: (1) Unconditional Generation: Given a puzzle size $p$, $p^2$ puzzle patches are generated using a vector $z$ sampled from Gaussian distribution (refer Fig. 2(3(a))); and (2) Conditional Generation: Given $p_1$ patches from an image puzzle having $p^2$ patches, we generate the remaining $(p^2 - p_1)$ patches of the puzzle using our model (see Fig. 2(3(b))). We believe the task of conditional generation is easier than unconditional generation one as there is more relevant information in the input while performing flow based transformations.

4.1.2 Layout generation from scene graphs

Task description. Layout generation from scene graphs bridges the gap between the symbolic graph-based scene description and the object layouts in the scene [24]. Scene graphs represent scenes as directed graphs, where nodes are objects and edges give relationships between objects. Object layouts are described by the set of corresponding bounding box annotations [24, 25]. Continuous graph flow is computed on the graph that resembles the scene graph (nodes correspond to objects and relations to directed edges). One edge function is defined for each relationship type. The output contains a set of object bounding boxes described by $\{[x_i, y_i, h_i, w_i]^{n_i=1}\}$, where $x_i, y_i$ represents the top-left coordinates, and $w_i, h_i$ represents the bounding box width and height respectively. In general, this task is challenging because a single instance of a scene graph can potentially correspond to multiple instances of scene layouts. Additional details are provided in Appendix.

Datasets and baselines. We evaluate our proposed model on Visual Genome [26] and COCO-Stuff [27] datasets. The preprocessing is the same as [24]. Visual Genome contains 175 object and 45 relation types. The training, validation and test set contain 62565, 5506 and 5088 images respectively. The average number of objects and relations is 10 and 5 for each image. COCO-Stuff contains 80 things and 91 stuff categories. Object relations are defined by their geometric positions and are categorized into 6 relations: left of, right of, above, below, inside, and surrounding. The final dataset contains 24972 train, 1024 validation, and 2048 test scene graphs. We use the same baselines as the image puzzle generation tasks in Sec. 4.1.1.

Results and analysis. We show the main results in Table 3. We use negative log likelihood for evaluating models on scene layout generation. The negative log likelihood is calculated per node (lower is better). The results indicate that our CGF model significantly outperforms the VAE-based baselines illustrating the benefits of exact likelihood computation and flexible architectures. Moreover,
the results also indicate that our model is able to reason over varied numbers of relation type (or edge types) described by the scene graphs. Fig. 4 shows some qualitative results.

Table 3: Quantitative results for layout generation for scene graph in negative log-likelihood. These results are for unconditional generation using CGF with generic message transformations.

| Method           | Visual Genome | COCO-Stuff |
|------------------|---------------|------------|
| BiLSTM + VAE     | -1.20         | -1.60      |
| GraphVAE [9]     | -1.05         | -1.36      |
| Graphite [10]    | -1.17         | -0.93      |
| VMP-SIN [11]     | -0.61         | -0.85      |
| GAE [22]         | -1.85         | -1.92      |
| NRI [23]         | -0.76         | -0.91      |
| Ours             | **-4.24**     | **-6.21**  |

4.2 Graphical distribution – generalization test

Can CGF generalize to unseen subset of variables? To test the generalizability of our model to variable graph sizes (variable number of nodes), we design three different evaluation settings and test it on image puzzle task: (1) odd to even: training with graphs having odd graph sizes and testing on graphs with even numbers of nodes, (2) less to more: training on graphs with smaller sizes and testing on graphs with larger sizes, and (3) more to less: training on graphs with larger sizes and testing on graphs with smaller. In the less to more setting, we test the model’s ability to use the factors learned from small graphs on more complicated ones, whereas the more to less setting evaluates the model’s ability to learn disentangled functions without explicitly seeing them during training. In our experiments, for the less to more setting, we use sizes less than \(G/2\) for training and more than \(G/2\) for testing where \(G\) is the size of the full graph. Similarly, for the less to more setting, we use sizes less than \(G/2\) for training and more than \(G/2\) for testing. Tab. 2 reports the NLL for these settings. The NLL of these models are close to the performance on the original experiments when trained with variable graph sizes indicating that our model is able to generalize to unseen graph sizes.

5 Related work

Probabilistic graphical models. Probabilistic graphical models (PGMs) serve as a statistical framework for modeling dependencies among random variables and building multivariate statistical models [3]. Traditional modeling algorithms include belief propagation networks [28–30], Markov Random Fields [31–33], Conditional Random Fields (CRFs) [34–36] and Restricted Boltzmann Machines (RBMs) [37, 38]. Neural networks have also been explored for inference in PGMs to model the inference steps as feedforward or recurrent networks [39, 40]. Based on the similarities in the message passing mechanism of graph neural networks (GNNs) and iterative updates for dependencies between variables in PGMs [41], we use GNN based architectures to represent graphical models in our work.

Generative modeling. Recent generative modeling techniques such as autoregressive methods [42, 43], variational autoencoders (VAEs) [7–10][22, 23] and generative adversarial networks (GANs) [44] have demonstrated considerable success in modeling complex data distributions. These models focus on learning a joint probability distribution over variables in the data. However, none of these models allow exact computation of likelihood of the data. More recently, flow-based generative models [12–15] have been designed allowing the computation of exact likelihood of the data. Continuous time of normalizing flows [16, 17] allow flow-based models to have completely unrestricted architectures, but have been shown to be effective for modeling dynamics for a single variable(with coherent meaning). In this work, we use continuous normalizing flows to model the multivariate dynamics to procure data distributions that incorporate statistical dependencies in complex graphical models.

Learning structured representations. Recently, there has been a surge of interest in modeling efforts that focus on improving generative models with the ability to learn structured latent space by unifying PGMs and VAEs [8][9][11][45]. However, these models still have limited capacity mainly because they are based on approximate computation of likelihood of data.

Learning graph representations. Random walk approaches [46, 47], factorization-based approaches [48][49] and GNN based approaches [50, 52] are three main approaches for representation
learning on graphs. Our work is closely related with GNNs, in which nodes repeatedly accumulate information from their neighbors in a recursive manner. However, as opposed to the conventional discrete time updates, our model employs continuous normalizing flow based techniques to build flexible graph representations.

6 Conclusion
In this paper, we presented a new class of models – continuous graph flow, a continuous flow-based generative model that aims to model distributions of graph-structured complex data. In particular, we proposed a novel message passing scheme that performs continuous-time message passing formulated as an ordinary differential equation system with shared and reusable functions that operate over the graph structure. Our model effectively learns flexible representations for generalization to new tasks, models dependencies in complex data distributions, and performs exact computation of the likelihood of the variables in the data. We conducted empirical evaluation for two generation tasks, namely, image puzzle generation and layout generation for scene graph. Experimental results showed that continuous graph flow achieves significant performance improvement (up to 400% in negative log-likelihood) over state-of-the-art unstructured and structured latent-space VAE models.
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Appendix for Continuous Graph Flow for Flexible Density Estimation

We provide supplementary materials to support the contents of the main paper. In this part, we describe implementation details of our model. We also provide additional qualitative results for both the generation tasks, namely, image puzzle generation and layout generation from scene graphs.

A.1 Implementation Details

The ODE formulation for continuous graph flow (CGF) model was solved using ODE solver provided by NeuralODE [16]. In this section, we provide specific details of the configuration of our CGF model used in our experiments on two different generation tasks used for evaluation in the paper.

**Image puzzle generation.** Each graph for this task comprise nodes corresponding to the puzzle pieces. The pieces that share an edge in the puzzle grid are considered to be connected and an edge function is defined over those connections. In our experiments, each node is transformed to an embedding of size 64 using convolutional layer. The graph message passing is performed over these node embeddings. The image puzzle generation model is designed using a multi-scale continuous graph flow architecture. We use two levels of downscaling in our model each of which factors out the channel dimension of the random variable by 2. We have two blocks of continuous graph flow before each downscaling with four convolutional message passing blocks in each of them. Each message passing block has a unary message passing function and binary passing functions based on the edge types – all containing hidden dimensions of 64.

**Layout generation for scene graphs.** For scene graph layout generation, a graph comprises node corresponding to object bounding boxes described by \{[x_i, y_i, h_i, w_i]\}_{i=1}^n, where \(x_i, y_i\) represents the top-left coordinates, and \(w_i, h_i\) represents the bounding box width and height respectively and edge functions are defined based on the relation types. In our experiments, the layout generation model uses two blocks of continuous graph flow units, with four linear graph message passing blocks in each of them. The message passing function uses 64 hidden dimensions, and takes the embedding of node label and edge label in unary message passing function and binary message passing function respectively. The embedding dimension is also set to 64 dimensions. For binary message passing function, we pass the messages both through the direction of edge and the reverse direction of edge to increase the model capacity.

A.2 Image Puzzle Generation: Additional Qualitative Results for CelebA-HQ

Fig 5 and Fig 6 presents the image puzzles generated using unconditional generation and conditional generation respectively.

![Image Puzzle Generation](image)

Figure 5: Qualitative results on CelebA-HQ for image puzzle generation. Samples generated using our model for 3x3 CelebA-HQ puzzles in unconditional generation setting. Best viewed in color.

A.3 Layout Generation from Scene Graph: Qualitative Results

Fig 7 and Fig 8 show qualitative result on unconditional and conditional layout generation from scene graphs for COCO-stuff dataset respectively. Fig 9 and Fig 10 show qualitative result on unconditional and conditional layout generation from scene graphs for Visual Genome dataset respectively. The generated results have diverse layouts corresponding to a single scene graph.
Figure 6: **Qualitative results on CelebA-HQ for image puzzle generation.** Samples generated using our model for 3x3 CelebA-HQ puzzles in conditional generation setting. Generated patches are highlighted in green. Best viewed in color.

Figure 7: **Examples of Unconditional generation of layouts from scene graphs for COCO-Stuff dataset.** We sample 4 layouts. The generated results have different layouts, but sharing the same scene graph. Best viewed in color. Please zoom in to see the category of each object.
Figure 8: **Conditional generation of layouts from scene graphs for COCO-stuff dataset.** We sample 4 layouts. The generated results have different layouts except the conditional layout objects in (b), but sharing the same scene graph. Best viewed in color. Please zoom in to see the category of each object.

Figure 9: **Unconditional generation of layouts from scene graphs for Visual Genome dataset.** We sample 4 layouts for each scene graph. The generated results have different layouts, but sharing the same scene graph. Best viewed in color. Please zoom in to see the category of each object.
Figure 10: *Conditional generation of layouts from scene graphs for Visual Genome dataset*. We sample 4 layouts for each scene graph. The generated results have different layouts except the conditional layout objects in (b), but sharing the same scene graph. Best viewed in color. Please zoom in to see the category of each object.