

# COMPOSITIONAL GENERATIVE INFERENCE USING DIFFUSION-BASED OPTIMIZATION

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## ABSTRACT

Compositional generative tasks, despite being important and having potential applications, have not been thoroughly addressed due to the unclear formulation and the challenges associated with selecting composition strategies. In this paper, we propose a probabilistic graphical approach to tackle the problem of compositional generative tasks and alleviate these challenges. Our approach formulates the problem as a Bayesian inference problem using a representative bipartite Bayesian network. In this network, one set of random variables represents the generation targets, while the other set represents observable variables with explicit or implicit distribution information. To solve this problem, we employ variational inference on the marginal distribution of observable variables. We approximate this distribution using diffusion models. We view the diffusion models as approximate Markov Chain Monte Carlo (MCMC) samplers for the marginals. Based on this perspective, we introduce a novel MCMC-based inference algorithm that incorporates per-step optimization using aggregated objectives from the diffusion models. We demonstrate the generality of our method and conduct experiments to validate its applicability to various compositional generation tasks.

## 1 INTRODUCTION

We understand nature in a highly compositional manner. One good example is our visual memorization Luck & Hollingworth (2008); we decompose the visual scene into small components (e.g., to objects and background) and remember those entities with relation, where we later composite them back when bringing the memory out. The compositional nature of human behavior, while it does affect all aspects of parts of our lives, is especially significant in generative tasks that require creativity. Most of the creative generations involve compositing immanent concepts and ideas.

The need for compositional understanding applies the same to the field of generative AI. Generative AI models have shown remarkable strides in recent advancements for fields requiring creativity, such as text-to-image synthesis Rombach et al. (2022); Kumari et al. (2023); Kawar et al. (2023); Melas-Kyriazi et al. (2023); Nichol et al. (2021), text-to-video synthesis Ho et al. (2022); Blattmann et al. (2023), human motion generation Tevet et al. (2022), and so on. Such advancements are driven by diffusion models: a likelihood-based method that generates plausible samples by iterative denoising any random samples, which have shown astonishing improvements in terms of quality, plausibility, and coherency with given input conditions.

However, there has not been adequate discussion under the perspective of compositionality for generative models, and currently, the models cannot be actively applied to compositional generative tasks as they do not guarantee synergy when composited naively. The lack of compositional ability ultimately results in limitations for alternations in generative tasks, including even the slightest differences. This is because when the compositional ability is not provided, generative models (especially diffusion models) need to be trained on an extensive dataset of conditions and sample pairs for every specific generation task. As there exists a large obstacle to training due to the exhaustive data-collection procedure and costly training procedure, only a few models can be trained under large capital for the limited scope of tasks. This limitation poses a significant obstacle and hinders the exploration of various potential applications.

There do exist prior works that address the compositional generation problem (Refer to Sec. 2). However, these works only suggest a methodology or justification for limited types of data or ways of

054 composition. This is due to challenges within the problem itself: (1) the formulation for the problem  
055 of compositing multiple generative models is ambiguous, unclear, and not mathematically formulated;  
056 (2) for selecting optimal composition strategies, what objectives should aim for are unclear; (3) efforts  
057 must be made to develop generalized formulations that are applicable to a wide range of tasks. In  
058 this paper, we present a probabilistic graphical approach for formulating the problem as a Bayesian  
059 inference problem. We model the situation as a bipartite Bayesian network, consisting of “control  
060 variables” which we can alter directly but do not have distribution information, and “observable  
061 variables” with explicit/implicit distribution information provided but mathematically dependent on  
062 control variables. Under this formulation, we aim to sample the mode of the joint probability, which  
063 is an inference problem.

064 Nonetheless, there exist several obstacles when devising a composition strategy, other than the  
065 challenges of defining the composition problem itself: (1) the inference problem can be notoriously  
066 difficult to solve when the distribution information is not provided for generation targets (i.e., control  
067 variables) or is only provided for partial observations of the targets (i.e., observable variables) as there  
068 are countless ways of compositing information; (2) it is challenging to use the raw explicit/implicit  
069 distribution information directly. To mitigate these challenges, we present an optimization-based  
070 sampling method that resembles Markov Chain Monte Carlo (MCMC) method under the provided  
071 formulation. We suggest a method to utilize diffusion models as approximate MCMC samplers,  
072 which are used to process the information from the raw distribution of observable variables into  
073 feasible score information. We then propose a method to aggregate such information from multiple  
074 diffusion models, to set an optimization objective for control variables. We propose that by adopting  
075 these methods, we can iteratively sample control variables via per-step optimization. This allows us  
076 to sample control variables from the mode effectively.

076 Our method is general and can be applied to arbitrary compositional generative tasks. We validate its  
077 applicability by experiments and empirically show that our method returns trustworthy generation  
078 results.

## 081 2 RELATED WORK

082  
083  
084 **Diffusion Model** Diffusion model Ho et al. (2020); Song et al. (2020a) is a class of methods  
085 generating sample data, generally images, by denoising latent starting from random initial noise. To  
086 guide the diffusion model for image synthesis and editing method work, SDEdit Meng et al. (2021)  
087 introduces a novel method by interpreting the diffusion process as a stochastic differential equation  
088 problem Song et al. (2020b), which is the generalized representation of an ordinary differential  
089 equation. Latent Diffusion Model(LDM) Rombach et al. (2022) improved the quality and efficiency  
090 by performing diffusion in reduced latent space and larger dataset Schuhmann et al. (2021). Classifier-  
091 Free Guidance(CFG) Ho & Salimans (2022) is an approach that combines score estimation Hyvärinen  
092 & Dayan (2005) of condition and unconditional diffusion models to obtain a similar quality of  
093 classifier guidance Dhariwal & Nichol (2021) result.

094 **Text-guided Diffusion Models** Most of the recent diffusion-based work is strongly correlated to  
095 text-guided image synthesis Rombach et al. (2022); Kumari et al. (2023); Kavar et al. (2023); Melas-  
096 Kyriazi et al. (2023); Nichol et al. (2021); Blattmann et al. (2022) with the help of text embedding  
097 networks Radford et al. (2021b;a) for latent spaces. For text and image guiding for Diffusion models,  
098 Instruct-Pix2Pix-based recent works Brooks et al. (2023); Kamata et al. (2023); Haque et al. (2023)  
099 suggests the fine-tuned Stable Diffusion Rombach et al. (2022) in a supervised manner with custom  
100 datasets automatically leveraging Prompt-to-Prompt and GPT-3 Hertz et al. (2022); Brown et al.  
101 (2020). Also, ControlNet Zhang & Agrawala (2023) suggests guidance using various methods, such  
102 as Canny Edge Canny (1986), OpenPose Cao et al. (2019), user scribe, or text prompt.

102 **Compositional GAN** GIRAFFE Niemeyer & Geiger (2021) is a compositional GAN model gener-  
103 ating scenes together with objects, i.e., a street with cars. To enable us to arrange objects freely, it  
104 models a scene in 3D and asks us to locate 3D objects in the scene, where each of them is represented  
105 implicitly. GIRAFFE generates composited images by rendering all entities together using NeRF  
106 pipeline Mildenhall et al. (2021), and it’s trained with GAN loss Goodfellow et al. (2014); Mescheder  
107 et al. (2018). Though GIRAFFE can generate controllable high-quality 3D scenes, it has limitations  
on image resolution and scene scale.

**Large Image Synthesis with Diffusion** Though most diffusion models have translational equivariance, which allows us to generate an arbitrary-sized image, they are failed to produce plausible large images without additional fine-tuning Rombach et al. (2022); Avrahami et al. (2022).

**Compositional Generation Using Composable Diffusion** MultiDiffusion and DiffCollage Bar-Tal et al. (2023); Zhang et al. (2023) are the works to address the composition strategy for multiple diffusion. Two works have the purpose of compositing multiple text-to-image diffusion models to generate holistic images for images of local regions.

### 3 PRELIMINARIES

#### 3.1 DIFFUSION MODELS

In this paper, we follow the formulation of Denoising Diffusion Implicit Models (DDIM) Song et al. (2020a) to derive the training process and inference process. In a nutshell, diffusion models sample start from the initial random sample  $\mathbf{y}^T$  from the prior distribution  $\mathcal{N}(0, \mathbf{I})$  and generate samples iteratively  $(\mathbf{y}^{T-1}, \dots, \mathbf{y}^0)$  by removing the noise from the sample, which can be viewed as MCMC sampling process for  $\mathbf{y}^0$ 's.

**Training** To train diffusion models, we first sample a data  $\mathbf{y}^0$  from the dataset and sample the noisy latents  $\mathbf{y}^t$  ( $t = 1, \dots, T$ ) from  $\mathbf{y}^0$  via non-Markovian forward kernel:

$$q(\mathbf{y}^{1:T} | \mathbf{y}^0) = q(\mathbf{y}^T | \mathbf{y}^0) \prod_{t=2}^T q(\mathbf{y}^{t-1} | \mathbf{y}^t, \mathbf{y}^0) \quad (1)$$

where the forward kernel for each step is provided as:

$$q(\mathbf{y}^{t-1} | \mathbf{y}^t, \mathbf{y}^0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{y}^0 + \sqrt{1 - \bar{\alpha}_{t-1} - \sigma_t^2} \cdot \frac{\mathbf{y}^t - \sqrt{\bar{\alpha}_t} \mathbf{y}^0}{\sqrt{1 - \bar{\alpha}_t}}, \sigma_t^2 \mathbf{I}) \quad (2)$$

$$q(\mathbf{y}^T | \mathbf{y}^0) = \mathcal{N}(\sqrt{\bar{\alpha}_T} \mathbf{y}^0, (1 - \bar{\alpha}_T) \mathbf{I}) \quad (3)$$

Note that  $\bar{\alpha}_t, \sigma_t$  are hyperparameter constants where  $\bar{\alpha}_T \approx 0$ , and  $\sigma_t$  is the scale for Langevin noise term Song et al. (2020a). We then approximate the distribution of latents  $q(\mathbf{y}^{0:T} | \mathbf{y}^0)$  with the reverse process of diffusion model:  $p_\theta(\mathbf{y}^{0:T})$  where the design choice of approximate distribution  $p_\theta$  is set as Markovian:

$$p_\theta(\mathbf{y}^{t-1} | \mathbf{y}^t) = \begin{cases} \mathcal{N}(f_\theta^{(1)}(\mathbf{y}^1), \sigma_1^2 \mathbf{I}) & \text{if } t = 1 \\ q(\mathbf{y}^{t-1} | \mathbf{y}^t, f_\theta^{(t)}(\mathbf{y}^t)) & \text{otherwise} \end{cases} \quad (4)$$

$$f_\theta^{(t)}(\mathbf{y}^t) = (\mathbf{y}^t - \sqrt{1 - \bar{\alpha}_t} \cdot \epsilon_\theta^{(t)}(\mathbf{y}^t)) / \sqrt{\bar{\alpha}_t} \quad (5)$$

here  $\epsilon_\theta^{(t)}$  is known as ‘‘score predictor’’ Song & Ermon (2019); Song et al. (2020a), where the ‘‘score’’ is the gradient of log-probability distribution. We can obtain optimal  $\theta$  by minimizing the following variational inference objective:

$$J(\theta) = \mathbb{E}_{\mathbf{y}^{0:T} \sim q(\mathbf{y}^{0:T})} [\log q(\mathbf{y}^{0:T} | \mathbf{y}^0) - \log p_\theta(\mathbf{y}^{0:T})] \quad (6)$$

According to Song et al. Song et al. (2020a), minimizing this objective is equivalent to minimizing a surrogate objective:

$$J_{\text{surr}}(\theta) = \sum_{t=1}^T \mathbb{E}_{\mathbf{y}^0 \sim q(\mathbf{y}^0), \epsilon_t \sim \mathcal{N}(0, \mathbf{I})} [\|\epsilon_\theta^{(t)}(\sqrt{\bar{\alpha}_t} \mathbf{y}^0 + \sqrt{1 - \bar{\alpha}_t} \epsilon_t) - \epsilon_t\|^2] \quad (7)$$

This process can be viewed as variational inference for the distribution of  $\mathbf{y}^{0:T}$ , and the approximated reverse process  $p_\theta$  can be viewed as an MCMC sampler. Also, the surrogate objective in Eq. 7 is equivalent to the surrogate objective for Denoising Diffusion Probabilistic Models (DDPM) Ho et al. (2020), which enables us to use the pretrained DDPM model for DDIM inference.

**Inference** After training, we can sample plausible  $\mathbf{y}^0$  by sampling initial latent  $\mathbf{y}^T \sim \mathcal{N}(0, \mathbf{I})$  and sequentially sampling the previous timestep latent given the current timestep latent:  $p_\theta(\mathbf{y}^{t-1} | \mathbf{y}^t)$ . Hence, the inference procedure for the diffusion model can be viewed as an approximate MCMC sampling for distribution  $q(\mathbf{y}^0)$ .

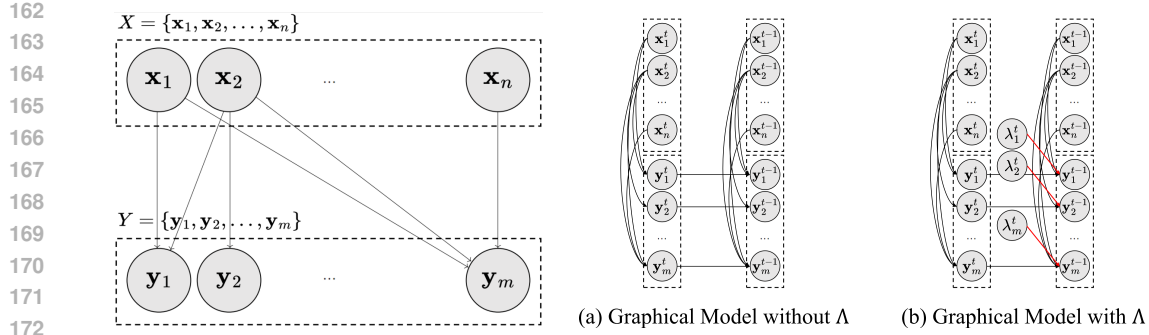


Figure 1: (left) Bipartite Bayesian network introduced in Formulation. (right) Graphical model for MCMC Sampling at timestep  $t$ .

### 3.2 LATENT DIFFUSION MODELS

In Sec. 5.2, we use publicly available Latent Diffusion Models Rombach et al. (2022) for approximating the distribution of observable variables via variational inference. Latent Diffusion Model (LDM) is a diffusion model that operates on the latent space of an image, where the images are encoded into latents and decoded back to the image via pretrained VAE Rombach et al. (2022); Kingma & Welling (2013); Van Den Oord et al. (2017). Specifically, when given pretrained VAE encoder  $\mathcal{E}$  and decoder  $\mathcal{D}$ , the relation between the latent and image satisfies:

$$z = \mathcal{E}(x), x \approx \mathcal{D}(z) \quad (8)$$

LDMs generate the latents  $z$  from initial random noise latent, which can be transformed to an image using the decoder as in Eq. 8. On account of this, we represent the image and image latent with the same notation (a  $y$ -notation, i.e.,  $\mathbf{y}^t$  or  $\mathbf{y}_i^t$ ) for brevity. It is noteworthy that LDMs are trained following the DDPM training procedure Ho et al. (2020). Since the training procedure of DDPM and DDIM are equivalent, as we have mentioned earlier in Sec. 3.1, it is fine to use DDIM’s inference procedure for approximate MCMC sampling, as we have done in our research.

## 4 FORMULATION

In this section, we will provide a general mathematical formulation for the compositional generation problem. Consider the following Bayesian inference problem. Given the bipartite Bayesian graphical model  $G_B(V, E)$ , where vertices can be decomposed into two mutually exclusive sets  $V = \{X, Y\}$ . We denote  $X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$  as a set of “control variables” and  $Y = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_m\}$  as a set of “observable variables”. Refer to Fig. 1-(left) for the visualization of the graphical model. Control variables are the target variables we aim to generate or possibly alter to have a higher probability. Observable variables are the variables we can “observe”, which means that we can obtain the distribution information  $p(Y)$ :

$$p(Y) = \prod_{i=1}^m p(\mathbf{y}_i) \quad (9)$$

which suffices for each observable variable, obtaining distribution information  $p(\mathbf{y}_i)$  either explicitly or implicitly. We may consider variables “containing explicit distribution information” if the exact marginal probability value  $p(\mathbf{y}_i)$  can be evaluated and variables “containing implicit distribution information” (1) if the information is obtained from the generative models for the marginal distribution  $p(\mathbf{y}_i)$ ; (2) if we can sample from the distribution; or so on.

This formulation represents the composition problem well, as we need to composite the information from observable variables in order to achieve meaningful updates for the compositions (which are represented as control variables). Under the intuition that the compositions we try to generate will likely have a mathematical relationship with each separate component in the direction starting from composition to the component (i.e., the component is dependent on composition), we formulate the

dependency between control variables and observable variables as a conditional distribution:

$$p(Y | X) = \prod_{i=1}^m p(\mathbf{y}_i | \text{PA}(\mathbf{y}_i)) \quad (10)$$

where  $\text{PA}(\cdot)$  denotes the parents of a given random variable. Note that such composition is assured since the graphical model is bipartite and the parents of  $\mathbf{y}_i$  is a subset of  $X$ . Given the distribution information for observable variables  $Y$  and stochastic dependency between  $X$  and  $Y$ , the problem’s goal is to find all realizations of control variables  $X$  that maximize the marginal probability of  $X$ :

$$X^* = \arg \max_X p(X) \quad (11)$$

This is a general formulation encompassing a wide range of compositional generation tasks, where the definition of tasks varies by the type of information provided for the marginal distribution of observable variables (i.e.,  $p(Y)$ ) or type of stochastic dependency between control variables and observable variables (i.e.,  $p(Y | X)$ ).

In this work, we focus on the case where we can sample from the marginal distribution of observable variable  $p(\mathbf{y}_i)$  and no other distribution information is provided. We formulate the stochastic dependency  $p(Y | X)$ , as a deterministic observation with “observation noise”  $\Psi_i$  (for  $i = 1, \dots, m$ ):

$$p(Y | X) = \prod_{i=1}^m \mathcal{N}(\mathbf{y}_i | f_i(\text{PA}(\mathbf{y}_i)), \Psi_i) \quad (12)$$

where observation functions  $f_i$  and observation noise  $\Psi_i$ , vary by the characteristics specific to the task. For brevity, we will denote  $f_i(\text{PA}(\mathbf{y}_i))$  as  $f_i(X)$ , considering the function to be constant for inputs other than  $\text{PA}(\mathbf{y}_i)$ . In this work, we formulate  $\Psi_i$  to be scaled identity, i.e.,  $\Psi_i = \psi_i^2 \mathbf{I}$ .

## 5 METHOD

### 5.1 OVERVIEW

We now discuss our method under the provided formulation. Our method mitigates the aforementioned challenges by introducing various strategies. The method starts by training diffusion models on the marginal distribution of observable variables  $p(\mathbf{y}_i)$  for  $\forall i = 1, \dots, m$ , where the dataset is sampled from  $p(\mathbf{y}_i)$ ’s. This procedure can be viewed as variational inference, and the trained diffusion model can be viewed as an approximate MCMC sampler, in which the resulting distribution information (for our method, score function value) is easier to use than just direct sampling. We then aggregate the score function values for  $\mathbf{y}_i$ ’s to create an optimization objective with respect to control variables  $X$ , which resembles the objectives in Expectation-Maximization (EM) algorithm Moon (1996). We optimize  $X$  according to the objective, which can be viewed as sampling from an adaptive proposal. The method repeats the aforementioned process, finally giving optimal  $X$ .

### 5.2 DIFFUSION AS APPROXIMATE MCMC

The method trains diffusion models, with different parameters  $\theta_i$  for each observable variable  $\mathbf{y}_i$  to approximate the marginal distribution  $p(\mathbf{y}_i)$ . The training procedure starts by sampling  $\mathbf{y}_i^0$ ’s from each marginal distribution  $p(\mathbf{y}_i)$ . Then, following the provided forward kernel represented in Eq. 1, we sample the sequence of noisy latents  $\mathbf{y}_i^{0:T}$  from each sample  $\mathbf{y}_i^0$ . Using the collected dataset, we minimize the surrogate objective  $J_{\text{surr}}(\theta_i)$  from Eq. 7 for each  $i$ , resulting  $m$  different diffusion models:

$$\theta_i^* = \arg \min_{\theta_i} J_{\text{surr}}(\theta_i) \text{ for } \forall i = 1, \dots, m \quad (13)$$

As mentioned in Sec. 3.1, this process can be viewed as variational inference. After training, the method utilizes trained diffusion models as approximate MCMC sampler, in which the adaptive proposal can be derived from Eq. 2~5 as:

$$\mathbf{y}_i^{t-1} = \sqrt{\bar{\alpha}_{t-1}} \left( \frac{\mathbf{y}_i^t - \sqrt{1 - \bar{\alpha}_t} \epsilon_{\theta_i}^{(t)}(\mathbf{y}_i^t)}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1 - \bar{\alpha}_{t-1} - \sigma_t^2} \cdot \epsilon_{\theta_i^*}^{(t)}(\mathbf{y}_i^t) + \sigma_t \mathbf{z}_t, \mathbf{z}_t \sim \mathcal{N}(0, \mathbf{I}) \quad (14)$$

270 In this work, we use the deterministic sampling process with zero Langevin noise, i.e.,  $\sigma_t = 0$  (Note  
271 that  $\sigma_t$  is a hyperparameter):

$$272 \mathbf{y}_i^{t-1} = \sqrt{\bar{\alpha}_{t-1}} \left( \frac{\mathbf{y}_i^t - \sqrt{1 - \bar{\alpha}_t} \epsilon_{\theta_i}^{(t)}(\mathbf{y}_i^t)}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1 - \bar{\alpha}_{t-1}} \cdot \epsilon_{\theta_i}^{(t)}(\mathbf{y}_i^t) \quad (15)$$

### 276 5.3 OPTIMIZATION-BASED ADAPTIVE PROPOSAL

277 Now that we have a diffusion-based approximate MCMC sampler for the marginal distribution  
278  $p(\mathbf{y}_i)$ 's, we aim to sample  $X$  concurrent to the MCMC sampling process of  $\mathbf{y}_i$ 's. Specifically, when  
279 given control variables at timestep  $t$  ( $X^t = \{\mathbf{x}_i^t\}_{i=1}^n$ ), we aim to sample the updated control variables  
280  $X^{t-1}$  to eventually reach  $X^0$ , which is what we aim to generate. This process resembles sampling  
281 from an adaptive proposal, which is optimization-based. Such a sub-problem can be formulated  
282 again as an inference problem for the graphical model consisting of  $X^t, Y^t, X^{t-1}, Y^{t-1}$ . Refer to  
283 Fig. 1-(right)-(a) for visualization of the graphical model at timestep  $t$ .

284 We sample  $X^{t-1(*)}$  when  $X^t$  is given via optimization:

$$285 X^{t-1(*)} = \arg \max_{X^{t-1}} \mathcal{Q}(X^{t-1} | X^t) \quad (16)$$

286 where  $\mathcal{Q}$  is an optimization objective which resembles the EM algorithm Moon (1996):

$$287 \mathcal{Q}(X^{t-1} | X^t) := \mathbb{E}_{Y^t, Y^{t-1}} [\log p(X^{t-1}, Y^{t-1}, Y^t | X^t)] \quad (17)$$

288 From the graphical model provided in Fig. 1-(right)-(a), we can derive that pairs  $(\mathbf{y}_i^t, \mathbf{y}_i^{t-1})$ 's for all  
289  $i$ 's are mutually independent when given  $X$ . Hence, we can decompose the log-probability term as  
290 below:

$$291 \log p(X^{t-1}, Y^{t-1}, Y^t | X^t) = \sum_{i=1}^m \log p(X^{t-1}, \mathbf{y}_i^{t-1}, \mathbf{y}_i^t | X^t) \quad (18)$$

292 We can further factorize the log-probability term as:

$$293 \log p(X^{t-1}, Y^{t-1}, Y^t | X^t) = \sum_{i=1}^m [\log p(\mathbf{y}_i^{t-1}, X^{t-1} | \mathbf{y}_i^t) + \log p(\mathbf{y}_i^t | X^t)] \quad (19)$$

294 Using Eq. 19, we can also decompose the optimization objective as below:

$$295 \mathcal{Q}(X^{t-1} | X^t) = \sum_{i=1}^m \mathbb{E}_{\mathbf{y}_i^t, \mathbf{y}_i^{t-1}} [\log p(\mathbf{y}_i^{t-1}, X^{t-1} | \mathbf{y}_i^t) + \log p(\mathbf{y}_i^t | X^t)] \quad (20)$$

296 Inspired by the Hard EM algorithm Ruggieri et al. (2020), we approximate the expectation term w.r.t.  
297  $\mathbf{y}_i^t$  into a maximization term to approximate the optimization objective:

$$298 \mathcal{Q}(X^{t-1} | X^t) \approx \sum_{i=1}^m \mathbb{E}_{\mathbf{y}_i^{t-1}} [\log p(\mathbf{y}_i^{t-1}, X^{t-1} | \tilde{\mathbf{y}}_i^t) + \log p(\tilde{\mathbf{y}}_i^t | X^t)] \quad (21)$$

299 where  $\tilde{\mathbf{y}}_i^t = \arg \max_{\mathbf{y}_i^t} p(\mathbf{y}_i^t | X^t)$ . Recall from Eq. 12 that  $\tilde{\mathbf{y}}_i^{t-1} \sim \mathcal{N}(f_i(X^{t-1}), \psi_i^2 \mathbf{I})$ . From this, we  
300 can easily derive that  $\tilde{\mathbf{y}}_i^t = f_i(X^t)$ . We now argue that:

$$301 \log p(\mathbf{y}_i^{t-1}, X^{t-1} | \tilde{\mathbf{y}}_i^t) = \begin{cases} \log p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}, \tilde{\mathbf{y}}_i^t) & \text{if } \mathbf{y}_i^{t-1} = \tilde{\mathbf{y}}_i^{t-1} \\ 0 & \text{otherwise} \end{cases} \quad (22)$$

302 where  $\tilde{\mathbf{y}}_i^{t-1}$  is obtained via deterministic sampling described in Eq. 15 using  $\tilde{\mathbf{y}}_i^t$ , since for any  
303  $\mathbf{y}_i^{t-1} \neq \tilde{\mathbf{y}}_i^{t-1}$ :

$$304 \int p(\mathbf{y}_i^{t-1}, X^{t-1} | \tilde{\mathbf{y}}_i^t) dX^{t-1} = p(\mathbf{y}_i^{t-1} | \tilde{\mathbf{y}}_i^t) = 0 \quad (23)$$

305 hence for  $\forall X^{t-1}$ :

$$306 p(\mathbf{y}_i^{t-1}, X^{t-1} | \tilde{\mathbf{y}}_i^t) = 0 \quad (24)$$

and for the case of  $\mathbf{y}_i^{t-1} = \tilde{\mathbf{y}}_i^{t-1}$ :

$$p(\tilde{\mathbf{y}}_i^{t-1}, X^{t-1} | \tilde{\mathbf{y}}_i^t) = p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}, \tilde{\mathbf{y}}_i^t) p(\tilde{\mathbf{y}}_i^{t-1} | \tilde{\mathbf{y}}_i^t) = p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}, \tilde{\mathbf{y}}_i^t) \quad (25)$$

since sampling for  $\tilde{\mathbf{y}}_i^{t-1}$  is a deterministic procedure. Using Eq. 22, the optimization objectives can be reduced to:

$$\mathcal{Q}(X^{t-1} | X^t) \approx \sum_{i=1}^m [\log p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}, \tilde{\mathbf{y}}_i^t) + \log p(\tilde{\mathbf{y}}_i^t | X^t)] \quad (26)$$

Applying Bayes' rule, we get:

$$\mathcal{Q}(X^{t-1} | X^t) \approx \sum_{i=1}^m [\log \frac{p(\tilde{\mathbf{y}}_i^{t-1} | X^{t-1}) p(X^{t-1})}{p(\tilde{\mathbf{y}}_i^{t-1}, \tilde{\mathbf{y}}_i^t)} + \log p(\tilde{\mathbf{y}}_i^t | X^t)] \quad (27)$$

From  $\tilde{\mathbf{y}}_i^{t-1} \sim \mathcal{N}(f_i(X^{t-1}), \psi_i^2 \mathbf{I})$ , if the magnitude of observation noise  $\psi_i$  is small, we can assume that marginal distribution  $p(X^{t-1})$  is ‘‘locally constant’’ compared to  $p(\tilde{\mathbf{y}}_i^{t-1} | X^{t-1})$  within the region around optimal  $X^{t-1}$ . The underlying idea behind this assumption is that the conditional distribution  $p(\tilde{\mathbf{y}}_i^{t-1} | X^{t-1})$  will undergo significant changes when  $X^{t-1}$  deviates from the optimal point, particularly when the magnitude of  $\Psi_i$  is small. In contrast, the marginal distribution  $p(X^{t-1})$ , which represents the true probability value as an expectation considering numerous possible values of  $\mathbf{y}_i^{t-1}$ , will exhibit smoother behavior compared to the prior distribution. Using this assumption, the optimization problem suffices to:

$$X^{t-1(*)} \approx \arg \max_{X^{t-1}} \sum_{i=1}^m \log p(\tilde{\mathbf{y}}_i^{t-1} | X^{t-1}) \quad (28)$$

where we have also neglected all constant terms w.r.t.  $X^{t-1}$ . Using  $\tilde{\mathbf{y}}_i^{t-1} \sim \mathcal{N}(f_i(X^{t-1}), \psi_i^2 \mathbf{I})$ , the problem becomes:

$$X^{t-1(*)} \approx \arg \min_{X^{t-1}} \sum_{i=1}^m \frac{1}{2\psi_i^2} \|\tilde{\mathbf{y}}_i^{t-1} - f_i(X^{t-1})\|^2 \quad (29)$$

We apply a gradient descent approach for optimizing  $X^{t-1}$ .

#### 5.4 AUXILIARY VARIABLE $\Lambda$ FOR ADDITIONAL FLEXIBILITY

During experiments, we noticed some failure cases. We conjectured that the failure can be attributed to the excessive restriction imposed by the deterministic procedure described in Equation 15, which severely limits the flexibility in sampling. To mitigate this issue, we introduce auxiliary random variables  $\Lambda^t = \{\lambda_i^t\}_{i=1}^m$  to the graphical model, as shown in Fig. 1-(right)-(b).  $\lambda_i^t$  replaces the deterministic procedure from Eq. 15 to:

$$\mathbf{y}_i^{t-1}(\lambda_i^t) = \sqrt{\bar{\alpha}_{t-1}} \left( \frac{\mathbf{y}_i^t - \sqrt{1 - \bar{\alpha}_t} \cdot \lambda_i^t \cdot \epsilon_{\theta_i^*}^{(t)}(\mathbf{y}_i^t)}{\sqrt{\bar{\alpha}_t}} \right) + \sqrt{1 - \bar{\alpha}_{t-1}} \cdot \lambda_i^t \cdot \epsilon_{\theta_i^*}^{(t)}(\mathbf{y}_i^t) \quad (30)$$

This is based on the intuition that predicted  $\epsilon_{\theta_i^*}^{(t)}(\mathbf{y}_i^t)$  value is equivalent to a score Song & Ermon (2019); Ho et al. (2020); Song et al. (2020a); the gradient of log-probability distribution  $p_{\theta_i^*}(\mathbf{y}_i)$ . Hence, the procedure above can be viewed as pushing  $\mathbf{y}_i^t$  towards the direction of  $\epsilon_{\theta_i^*}^{(t)}(\mathbf{y}_i^t)$  with step-size  $\lambda_i^t$ , which increases the marginal probability of  $\mathbf{y}_i$ . Then, we can re-define the optimization problem as below:

$$X^{t-1(*)}, \Lambda^{t(*)} = \arg \max_{X^{t-1}, \Lambda^t} \mathcal{Q}'(X^{t-1}, \Lambda^t | X^t) \quad (31)$$

where the optimization objective is defined as:

$$\mathcal{Q}'(X^{t-1}, \Lambda^t | X^t) := \mathbb{E}_{\mathbf{y}_i^t, Y^{t-1}} [\log p(X^{t-1}, Y^{t-1}, Y^t, \Lambda^t | X^t)] \quad (32)$$

Following the similar way of Eq. 18~21, the optimization objective is approximated as:

$$\mathcal{Q}'(X^{t-1}, \Lambda^t | X^t) \approx \sum_{i=1}^m \mathbb{E}_{\mathbf{y}_i^{t-1}} [\log p(\mathbf{y}_i^{t-1}, X^{t-1} | \lambda_i^t, \tilde{\mathbf{y}}_i^t) + \log p(\lambda_i^t) + \log p(\tilde{\mathbf{y}}_i^t | X^t)] \quad (33)$$

where  $\tilde{\mathbf{y}}_i^t = \arg \max_{\mathbf{y}_i^t} p(\mathbf{y}_i^t | X^t) = f_i(X^{t-1})$ . We now argue that:

$$\log p(\mathbf{y}_i^{t-1}, X^{t-1} | \lambda_i^t, \tilde{\mathbf{y}}_i^t) = \begin{cases} \log p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t), \tilde{\mathbf{y}}_i^t) & \text{if } \mathbf{y}_i^{t-1} = \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) \\ 0 & \text{otherwise} \end{cases} \quad (34)$$

where  $\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t)$  is obtained via Eq. 30 using  $\tilde{\mathbf{y}}_i^t$  and  $\lambda_i^t$ , since for any  $\mathbf{y}_i^{t-1} \neq \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t)$ :

$$\int p(\mathbf{y}_i^{t-1}, X^{t-1} | \lambda_i^t, \tilde{\mathbf{y}}_i^t) dX^{t-1} = p(\mathbf{y}_i^{t-1} | \lambda_i^t, \tilde{\mathbf{y}}_i^t) = 0 \quad (35)$$

hence for  $\forall X^{t-1}$ :

$$p(\mathbf{y}_i^{t-1}, X^{t-1} | \lambda_i^t, \tilde{\mathbf{y}}_i^t) = 0 \quad (36)$$

and for the case of  $\mathbf{y}_i^{t-1} = \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t)$ :

$$p(\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t), X^{t-1} | \lambda_i^t, \tilde{\mathbf{y}}_i^t) = p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t), \lambda_i^t, \tilde{\mathbf{y}}_i^t) p(\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) | \lambda_i^t, \tilde{\mathbf{y}}_i^t) = p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t), \tilde{\mathbf{y}}_i^t) \quad (37)$$

since sampling for  $\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t)$  when  $\lambda_i^t, \tilde{\mathbf{y}}_i^t$  given is a deterministic procedure. Using Eq. 34, the optimization objectives can be reduced to:

$$\mathcal{Q}'(X^{t-1}, \Lambda^t | X^t) \approx \sum_{i=1}^m [\log p(X^{t-1} | \tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t), \tilde{\mathbf{y}}_i^t) + \log p(\lambda_i^t) + \log p(\tilde{\mathbf{y}}_i^t | X^t)] \quad (38)$$

Applying Bayes' rule, we get:

$$\mathcal{Q}'(X^{t-1}, \Lambda^t | X^t) \approx \sum_{i=1}^m [\log \frac{p(\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) | X^{t-1}) p(X^{t-1})}{p(\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t), \tilde{\mathbf{y}}_i^t)} + \log p(\lambda_i^t) + \log p(\tilde{\mathbf{y}}_i^t | X^t)] \quad (39)$$

Again, from  $\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) \sim \mathcal{N}(f_i(X^{t-1}), \psi_i^2 \mathbf{I})$ , if the magnitude of observation noise  $\psi_i$  is small, we can assume that marginal distribution  $p(X^{t-1})$  is ‘‘locally constant’’ compared to  $p(\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) | X^{t-1})$  within the region around optimal  $X^{t-1}$ , which reduces the optimization problem to:

$$X^{t-1(*)}, \Lambda^{t(*)} \approx \arg \max_{X^{t-1}, \Lambda^t} \sum_{i=1}^m [\log p(\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) | X^{t-1}) + \log p(\lambda_i^t)] \quad (40)$$

where we have also neglected all constant terms w.r.t.  $X^{t-1}$  and  $\Lambda^t$ . Using  $\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) \sim \mathcal{N}(f_i(X^{t-1}), \psi_i^2 \mathbf{I})$ , the problem becomes:

$$X^{t-1(*)}, \Lambda^{t(*)} \approx \arg \min_{X^{t-1}, \Lambda^t} \sum_{i=1}^m [\frac{1}{2\psi_i^2} \|\tilde{\mathbf{y}}_i^{t-1}(\lambda_i^t) - f_i(X^{t-1})\|^2 - \log p(\lambda_i^t)] \quad (41)$$

Intuitively, the above problem can be viewed as optimizing  $X^{t-1}$  with flexibility on the step size for an update in observable variables, and the negative-log-prior term (i.e.,  $-\log p(\lambda_i^t)$ ) can be seen as a regularization term for  $\lambda_i^t$ . In this work, we use L1-regularization for  $\lambda_i^t - 1$ ; hence, Eq. 41 resembles the LASSO regression Ranstam & Cook (2018). We apply a gradient descent approach, same as in Sec. 5.3, for optimizing  $X^{t-1}$  and  $\Lambda^t$ .

## 6 EXPERIMENTS

Our approach is a general solution for compositional generative tasks, providing broad applicability to diverse scenarios. In this section, we present a series of experiments that we conducted to evaluate the performance and effectiveness of our method. We provide detailed descriptions of these experiments along with their corresponding results.

### 6.1 EXTENSIVE IMAGE GENERATION

Our method is capable of generating large images by generating local patches. such as panorama images. We demonstrate our method in the task of generating a panorama image composed of three consecutive local patches. In this case, the panorama image can be viewed as a control variable (i.e.,



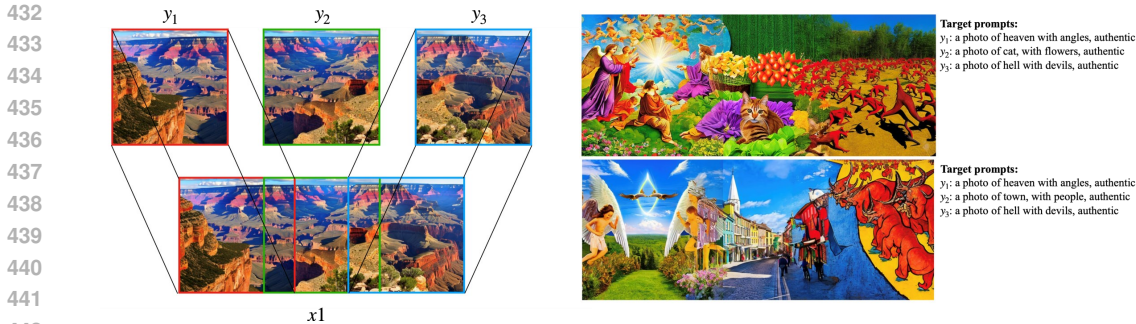


Figure 2: (left) Generated Panorama images using prompts with a shared prompt, "a photo of the grand canyon". (right) Generated Panorama images using different prompts for each patch

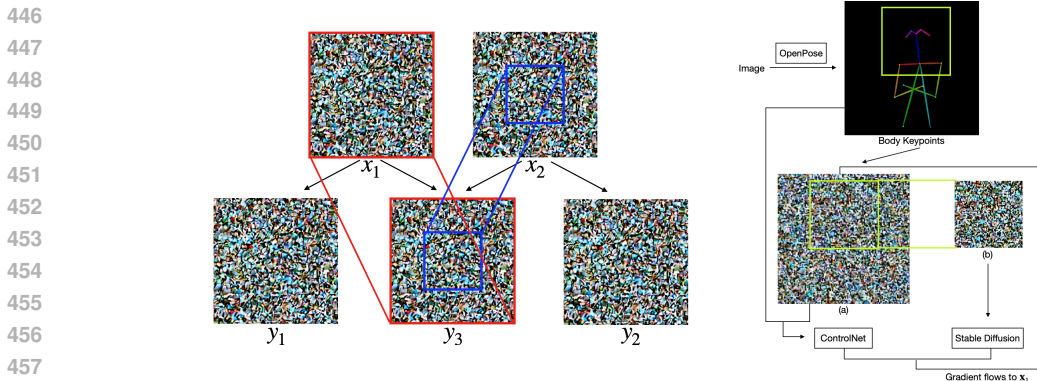


Figure 3: (left) Pipeline for producing  $y$  latent values using  $x$  values. (right) Pipeline for producing aligned face and body for Sec. 6.3.

$x_1$ ), and the local patches as observable variables (i.e.,  $y_1 \sim y_3$ ). Instead of training a diffusion model as in Sec. 5.2, we leverage a publicly available pretrained latent diffusion model Rombach et al. (2022) conditioned with the prompt we provide. We crop the control variable  $x_1$  to generate observable variables  $y_1 \sim y_3$  along the wide panorama axis and force the patches to have consecutive, overlapped latent values. Each stable diffusion model computes the score functions value for each  $y_i$ 's and optimizes control variable  $x_1$  to maximize our aggregated objective functions mentioned in Eq. 32.

We refer the readers to Fig. 2 for results. We observe that our method creates continuous and seamless panorama images. The generated local patches align with the provided prompt. We also provide additional results using different prompts for each local patch in Fig. 2. The results show a smooth transition between scenes, which demonstrates our method's compositional ability.

## 6.2 COMPOSITIONAL SCENE GENERATION

In this section, we focus on the task of generating a background image and object simultaneously. To be specific, the control variables  $x_1, x_2$  each denote the background without/with an object. The observable variables  $y_1, y_2$  each are identical to  $x_1, x_2$ . Observable variable  $y_3$  is an image composited of "background region" of  $x_1$  and "object region" of  $x_2$ . We manually set the background region of  $x_1$  and object region of  $x_2$  as partitions, where the object region is defined as an arbitrary bounding box. Refer to Fig 3-(left) for more details.

Our aim is to generate realistic and plausible composition  $y_3$ , maintaining the background from  $y_1$  and object from  $y_2$ . We set the conditioning prompt for  $y_1, y_2, y_3$  each to represent the background without an object, an object, and an overall scene with  $y_1$ 's background and object from  $y_2$ . For  $y_3$ 's conditioning prompt, we do not provide a detailed description of the object as we represent the overall scene.

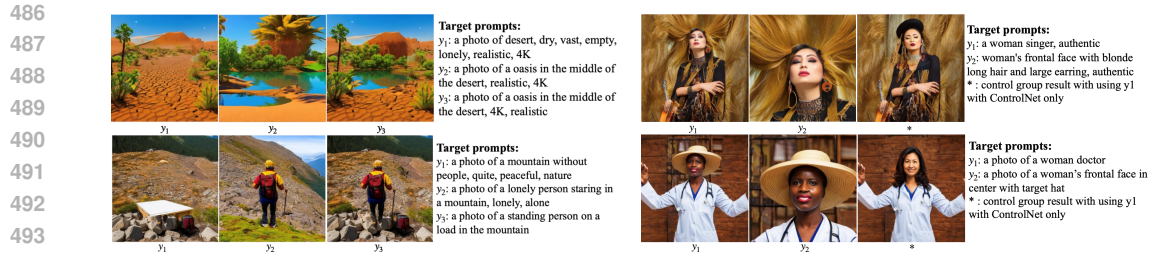


Figure 4: (left) A result of the compositional scene generation in Sec. 6.2 with used target prompts. (right) Generated body image with different prompt conditioning.

Results are shown in Fig. 4-(left). The first row of generated images aligns with the conditioning prompt as well, and we observe that  $y_3$  blends naturally. From the second row, we observe that we can generate an overall scene with the detailed object in  $y_3$  without directly inserting the detailed explanation to  $y_3$ .

### 6.3 COMPOSABLE BODY SYNTHESIS

Our method can be applied to generate a full body with detailed local parts by compositing multiple diffusion models with diverse conditions. Compared to compositional scene generation in Sec. 6.2, it requires accurate alignment between body and parts as plausible locations of parts are strongly conditioned on body pose. Here we show a few examples of merging the full body and face as local parts. In this task, we define single control variable  $x_1$  corresponding to  $96 \times 96$  dimension latent, which encodes  $768 \times 768$  body image. Then set two observation variables corresponding to full body  $y_1$  identical to  $x_1$  and  $y_2$  for closed-up face area, which is a crop of  $x_1$  with latent size  $48 \times 48$ . Different from Sec. 6.2, instead of randomly placing cropping bounding box for  $y_2$ , we place the bounding box on a fixed point where the head locates. To adjust the head positioning of the generated image, we used ControlNet Zhang & Agrawala (2023) to estimate the score for full body  $y_1$  with OpenPose Cao et al. (2019) body keypoint conditioning as shown in Fig. 3-(right).

To check the composition of the head and body is successful, we gave a detailed prompt only on the diffusion model for face  $y_2$ . As shown in Fig. 4-(right), our method succeed in generating images consistent with both of the prompts, even though the composed result is rare in the real world. When comparing the generated results to a control group, where the influence of  $y_2$  has been eliminated, we can observe that the desired property of the prompt is effectively injected into the outcome in a compositional manner.

## 7 CONCLUSION

We have presented a novel approach to address the compositional generation problem by formulating it as a Bayesian inference problem. Our formulation is versatile and applicable to a wide range of tasks in different scenarios. Under the provided formulation, we propose an optimization-based sampling method inspired by Markov Chain Monte Carlo (MCMC) techniques. The method leverages variational inference with diffusion models and aggregates information from these models to devise optimization-based adaptive proposals used for iterative sampling. Our method has demonstrated high performance across various tasks, as evidenced by our qualitative results.

However, it is important to acknowledge the limitations of our method. Specifically, our approach is currently only justified for scenarios with zero Langevin noise. It would be valuable for future work to explore and address the case with non-zero Langevin noise, as this may potentially enhance the performance of our method.

Furthermore, our provided formulation for the compositional generation problem offers flexibility in terms of the choice of stochastic dependency (i.e.,  $p(Y | X)$ ) and the information types for observables (i.e.,  $p(Y)$ ). This implies that there are numerous design choices available, which we leave as avenues for future research.

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