Optimizing Diffusion Models for Joint Trajectory Prediction and Controllable Generation

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Abstract. Diffusion models are promising for joint trajectory prediction and controllable generation in autonomous driving, but they face challenges of inefficient inference steps and high computational demands. To tackle these challenges, we introduce Optimal Gaussian Diffusion (OGD) and Estimated Clean Manifold (ECM) Guidance. OGD optimizes the prior distribution for a small diffusion time T and starts the reverse diffusion process from it. ECM directly injects guidance gradients to the estimated clean manifold, eliminating extensive gradient backpropagation throughout the network. Our methodology streamlines the generative process, enabling practical applications with reduced computational overhead. Experimental validation on the large-scale Argoverse 2 dataset demonstrates our approach's superior performance, offering a viable solution for computationally efficient, high-quality joint trajectory prediction and controllable generation for autonomous driving. Our project webpage is at https://yixiaowang7.github.io/OptTrajDiff_Page/

Keywords: Diffusion model · Autonomous driving · Trajectory Prediction · Controllable Trajectory Generation

1 Introduction

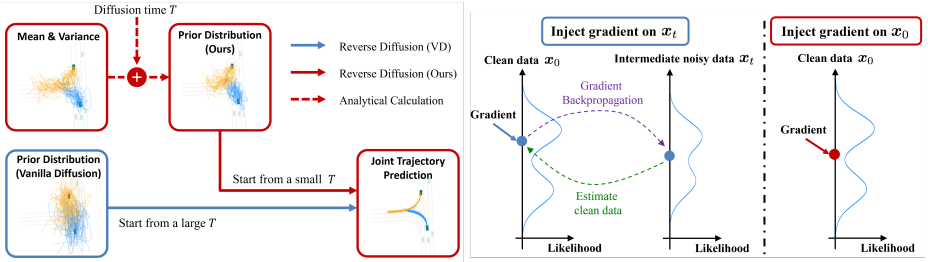
The diffusion model is a class of generative models capable of representing high-dimensional data distributions. In particular, it has demonstrated strong performance in trajectory prediction and generation for autonomous driving [10, 11, 16, 28, 49]. In contrast to traditional trajectory prediction [18, 50] and generative models [41, 45], the unique advantage of diffusion models lies in their ability to deform the generated trajectory distribution to comply with additional requirements at inference stage via gradient-based guided sampling. Notably, it is achieved without extra model training costs. This ability to perform controllable trajectory generation enables various useful applications, such as enforcing additional realism constraints on predicted trajectories, generating directed and user-specified simulation scenarios.

However, computational efficiency is a crucial bottleneck hindering the practical application of diffusion models in autonomous driving. Real-time inference is essential for trajectory prediction, as it provides timely forecasts of surrounding agents' behavior, enabling safe and efficient planning in dynamic traffic scenarios. The high demand for inference speed, coupled with limited onboard computational resources, makes it infeasible to deploy diffusion models for onboard trajectory prediction. While simulations do not occur onboard, lightweight models are still preferred to streamline the closed-loop training and evaluation pipelines. The heavy computational cost is mainly attributed to the following two aspects:

Computationally Expensive Reverse Diffusion. At the inference stage, the diffusion model samples from standard Gaussian distribution and gradually denoises the sample through dynamics described by a Stochastic Differential Equation (SDE) [39], aiming to eventually obtain a sample as if drawn from a target data distribution. The target data distribution can be significantly different from a standard Gaussian distribution, necessitating a large number of denoising steps to yield good performance. Prior works have attempted to reduce the reverse diffusion steps through adaptive noise schedule [17, 32], fast samplers [21,35,43,46], or distillation [31,37]. However, the fixed standard Gaussian prior poses a challenge in accelerating the reverse diffusion process without violating the SDE, which can inevitably compromise the generation quality.

Computationally Expensive Guided Sampling. Controllable generation is typically achieved by guiding the denoising process with the gradient of a guidance cost function. The guidance cost function encodes the desired characteristics of the generated data, which is typically defined on the clean data manifold in trajectory prediction and controllable generation problems. However, guided sampling intends to inject the gradient of the guidance cost function into the series of noisy data at intermediate diffusion steps. It requires a forward pass to estimate the clean data first and then back-propagating throughout the entire network to estimate the gradient with respect to the intermediate noisy data [16, 20, 28], which is very computationally intensive.

Targeted at these challenges, we take a step further to improve the computational efficiency of diffusion models while maintaining their performance for joint trajectory prediction and controllable generation tasks. Specifically, we propose two novel solutions for efficient reverse diffusion and guided sampling respectively. First, we present *Optimal Gaussian Diffusion* (OGD) to accelerate the reverse diffusion process. At the inference stage, instead of a standard Gaussian distribution far away from the desired data distribution, OGD starts from an optimal Gaussian distribution, which minimizes the distance to intermediate data distribution at a specific noise level, cutting down the diffusion steps before that. We show that we can analytically estimate such an optimal Gaussian distribution and also, an optimal perturbation kernel distribution, *at any noise level* from the statistics of the data distribution. It allows flexible tuning of the diffusion steps at the inference stage, without the need to train any additional models [48]. We further derive a practical implementation of OGD for joint trajectory prediction and generation, where the optimal Gaussian prior is computed



(a) Optimal Gaussian Diffusion (OGD) **(b)** Estimated Clean Manifold Guidance (ECM)

Fig. 1: Overview of Optimal Gaussian Diffusion (OGD) and Estimated Clean Manifold Guidance (ECM). **(a)** OGD uses the mean and variance of the data distribution to calculate the optimal prior distribution at a small T. It can largely reduce the diffusion time compared with vanilla diffusion. **(b)** ECM directly injects the gradient of guidance into the clean data manifold to mitigate computational complexity.

using the mean and variance of marginal trajectory distributions estimated with a pre-trained marginal trajectory prediction [18, 24, 50] model.

Second, we propose *Estimated Clean Manifold Guidance* (ECM) to accelerate guided sampling for controllable generation. To save the computational cost due to estimating the guided gradient on the noisy data, we aim to directly inject the gradient into the clean data manifold without lengthy backpropagation. ECM is motivated by the insight that guided sampling can be regarded as a multi-objective optimization problem on the clean data manifold: The first objective is to maximize the likelihood of the samples on the estimated real data distribution; the second objective is to achieve low guidance cost. ECM hierarchically solves this multi-objective problem without backpropagation throughout the entire diffusion model. We show that it leads to faster inference time and much better performance than existing approaches. Also, to tackle the challenges imposed by the multi-modal nature of vehicle interactions, we propose to warm-start the multi-objective optimization problem with reference joint trajectory points estimated using a marginal trajectory predictor. We refer to the complete algorithm as *Estimated Clean Manifold with Reference Joint Trajectory* (ECMR).

To evaluate the proposed OGD and ECM methods on real-world tasks, we implement the OGD model leveraging a pre-trained marginal prediction model, QCNet [50], and conduct extensive experiments on the Argoverse 2 dataset. We show that OGD can achieve better joint trajectory prediction performance than vanilla diffusion with significantly fewer diffusion steps—it only takes $1/12$ of the diffusion steps used by the vanilla diffusion model. OGD also achieves outstanding prediction accuracy compared to non-diffusion joint prediction models. In addition, ECMR, coupled with OGD, can generate samples with significantly lower guidance costs with the same level of realism scores compared to conducting controllable generation on the vanilla diffusion model using existing guided sampling approaches used in autonomous driving [16, 28], but using around $1/5$ of their inference step.

2 Related Work

Diffusion models. Diffusion models have demonstrated their ability to produce high-quality, diverse samples in a variety of applications, such as image, video, and 3D generation [13, 22, 29]. Recently, diffusion models have been applied to trajectory prediction in autonomous driving. It shows great performance on representing future trajectory distribution [10, 16]. However, diffusion models need to run lengthy reverse diffusion processes to generate high-quality samples [5, 10]. This makes it hard to apply diffusion models to trajectory prediction in autonomous driving since it requires in-time prediction for the downstream planning module to promptly respond to dynamically changing traffic scenarios. Previous works [17, 21, 31, 32, 35, 37, 43, 46] mostly focused on mitigating this issue by investigating how to solve reverse SDE in a faster manner. In addition, similar to ours, some works sought alternative initialization of the reverse diffusion process to achieve faster inference. For example, [3] initialized the reverse diffusion process with samples generated by another generative backbone network. However, the backbone network is not deliberately trained for the reverse diffusion process. [48] proposed to learn the initial diffusion with a generative adversarial network (GAN) [8]. However, it requires training a large additional model with a complex training procedure. Also, it requires specifying the reverse diffusion time as a hyperparameter prior to GAN training, which is hard to tune.

Guided sampling. Diffusion models have been successfully used to tackle controllable tasks through guided sampling, such as image inpainting [36] and motion planning [15]. A notable feature of diffusion models with guided sampling is their ability to condition the generation process on the user's preference, which was not available during the training phase. In the driving domain, recent works used guided sampling to generate controllable traffic [16, 49], and controllable pedestrian animation [28]. Our work belongs to the prior category, where user-specified guidance cost is used to guide generation in the trajectory space. In this case, the guidance cost function encodes certain desired properties of the generated trajectories. Thus, it is normally defined on the realistic trajectory samples, which are on the so-called clean manifold, instead of the noisy manifold containing the intermediate noisy data. Some works attempted to learn the guidance cost function on the noisy manifold [15]. Otherwise, it will lead to numerical instability when evaluating guidance cost at intermediate noisy data [28, 49]. To avoid the additional computational costs introduced by a learned guidance cost function, [16, 28] proposed to project the intermediate noisy data into the clean manifold through the diffusion model, and evaluate the guidance cost on the projected point. This approach requires back-propagating throughout the entire diffusion model, which is also computationally intensive.

Trajectory prediction. In autonomous driving [26, 27], it is vital to precisely forecast how other participants in traffic will move in the future so that ego vehicle can plan a safe and efficient trajectory to execute in the future. Marginal trajectory prediction is used to predict the trajectory distribution for single vehicle and recent works involve kinematic constraints of the vehicles, restrictions of complex topology of roads, and interaction from the surrounding

vehicles [18, 24, 50]. Recently, joint trajectory prediction has attracted attention from several researchers. It consists in predicting the joint future trajectories for all agents so that these trajectories are consistent with one another [25], an aspect which marginal trajectory prediction does not consider. Scene-Transformer [25] uses a fixed set of learnable scene embeddings to generate corresponding joint trajectories for all the vehicles in the given scene. Models like M2I [40], and FJMP [30] adopt a conditional approach, predicting the motions of other agents based on the movements of controlled agents. Diffusion model [16] has also been used to predict the joint trajectory. However, joint trajectory prediction is still a challenging problem since the complexity increases exponentially with the number of vehicles in the scene. The efficiency problem becomes more serious when using diffusion model to predict the joint trajectory distribution [16], and largely limits the application of diffusion models in autonomous driving.

3 Preliminaries

3.1 Diffusion Models

The diffusion process continuously perturbs the unknown data distribution p_{data} with a perturbation kernel and generates intermediate data with a given diffusion time T. Denote the distribution of the time-dependent intermediate nosiy data $\boldsymbol{x}_t$ as $p_t(\boldsymbol{x}_t)$, $t \in [0, T]$, where $p_0(\boldsymbol{x}_0) = p_{data}$ is the clean data distribution and $\boldsymbol{x}_0$ is the clean data. The series of intermediate data $\boldsymbol{x}_t$ are generated through the Stochastic Differential Equation (SDE) [39]:

$$\mathrm{d}\boldsymbol{x}_t = f(\boldsymbol{x}_t, t)\mathrm{d}t + g(t)\mathrm{d}\boldsymbol{w}, \boldsymbol{x}_0 \sim p_{data} = p_0(\boldsymbol{x}_0), \tag{1}$$

where $f(\cdot, t)$ is the drift coefficient, $g(t)$ is the diffusion coefficient, and $\boldsymbol{w}$ is the Wiener process. We can recover p_{data} from reverse-time SDE

$$\mathrm{d}\boldsymbol{x}_t = [f(\boldsymbol{x}_t, t) - g(t)^2 \nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)]\mathrm{d}t + g(t)\mathrm{d}\bar{\boldsymbol{w}}, \boldsymbol{x}_T \sim p_T(\boldsymbol{x}_T), \tag{2}$$

where $\bar{\boldsymbol{w}}$ is another Wiener process, $\mathrm{d}t$ is negative timestep.

In order to solve Eq. (2), we first need to approximate $p_T(\boldsymbol{x}_T)$. In previous works, $p_T(\boldsymbol{x}_T)$ is typically approximated by some prior distributions p_{prior} which contain no information of p_{data}. In this paper, we adopt the setting of Variance Preserving (VP) SDE [12, 39]. In VP-SDE, $p_T(\boldsymbol{x}_T) \approx p_{prior}$ when $T \to \infty$. The perturbation kernels are in the form of $p_t(\boldsymbol{x}_t|\boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1 - \bar{\alpha}_t)\boldsymbol{\Sigma}_p)$ where scalar $\bar{\alpha}_t$ is diffusion schedule parameter, $|\boldsymbol{\Sigma}_p| = 1$. A common choice for $\boldsymbol{\Sigma}_p$ is the identity matrix $\mathbf{I}$ [12, 39]. Second, we need to approximate $\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)$ for all $t \in (0, T]$. Some works solve score-matching problem [14, 38] and learn a score function $\boldsymbol{s}_\theta(\boldsymbol{s}_t, t)$ to approximate $\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)$. In this paper, we follow the practice in DDPM [12] to learn the noise $\boldsymbol{\epsilon}$ using a network $\boldsymbol{\epsilon}_\theta(\boldsymbol{x}_t, t)$:

$$\arg\min_\theta \mathbb{E}_{\boldsymbol{x}_0 \sim p_{data}, \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_p)} ||\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\boldsymbol{x}_t, t)||_2^2 \tag{3}$$

where $\boldsymbol{x}_t = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}_\theta(\boldsymbol{x}_t, t) = -\sqrt{1 - \bar{\alpha}_t}\boldsymbol{s}_\theta(\boldsymbol{x}_t, t)$. With these two approximation, we can learn $q_\theta(\boldsymbol{x}_0)$ to estimate unknown data distribution $p_0(\boldsymbol{x}_0)$ solving Eq. (2) from $t = T$ to $t = 0$.

3.2 Guided Sampling

In prior diffusion-based controllable generation frameworks [15,16,20,28,49], controllable generation is achieved via biasing of the score function for sampling:

$$\nabla_{\boldsymbol{x}_t} \log \left[p_t(\boldsymbol{x}_t) \exp(-\mathcal{C}(\boldsymbol{x}_t))\right] = \nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t) - \nabla_{\boldsymbol{x}_t} \mathcal{C}(\boldsymbol{x}_t) \tag{4}$$

where $\mathcal{C}(\cdot)$ is the guidance function. It requires estimating the guidance gradient with respect to the noisy data $\boldsymbol{x}_t$. Some approaches introduce an additional neural network to approximate $\mathcal{C}(\cdot)$ at different noisy levels [4,15,49]. The additional neural network imposes additional training costs and heavier computational burden at the inference stage. To this end, some works define an analytical guidance function $\mathcal{J}(\cdot)$ on the clean data $\boldsymbol{x}_0$. They first estimate $\hat{\boldsymbol{x}}_0 = f_\theta(\boldsymbol{x}_t)$ based on $\boldsymbol{x}_t$ with the diffusion model, then calculate $\mathcal{C}(\boldsymbol{x}_t)$ as $\mathcal{J}(\hat{\boldsymbol{x}}_0)$. However, when taking the gradient of $\mathcal{J}(\hat{\boldsymbol{x}}_0)$ with respect to $\boldsymbol{x}_t$, we get

$$\nabla_{\boldsymbol{x}_t} \mathcal{J}(\hat{\boldsymbol{x}}_0) = \nabla_{\hat{\boldsymbol{x}}_0} \mathcal{J}(\hat{\boldsymbol{x}}_0) \cdot \nabla_{\boldsymbol{x}_t} f_\theta(\boldsymbol{x}_t). \tag{5}$$

Estimating $\nabla_{\boldsymbol{x}_t} f_\theta(\boldsymbol{x}_t)$ requires backpropagating throughout the entire diffusion model, i.e., $f_\theta(\boldsymbol{x}_t)$. It requires heavy computing resources and GPU memory.

3.3 Trajectory Prediction and Controllable Generation

Joint trajectory prediction aims to predict the future joint trajectories $\boldsymbol{x}_0$ for all the vehicles in the scene, conditioned on context information $\boldsymbol{c}$. It can be regarded as a conditional generation task where the goal is to train a generative model to approximate the distribution $p_0(\boldsymbol{x}_0|\boldsymbol{c})$. For simplicity, we omit $\boldsymbol{c}$ and represent $p_0(\boldsymbol{x}_0|\boldsymbol{c})$ as $p_0(\boldsymbol{x}_0)$. We denote n as the number of vehicles in the same scene and $\boldsymbol{x}_{0,i}$ as the future trajectory for vehicle i, $i \in \{1, 2, ..., n\}$, so $\boldsymbol{x}_0 = [\boldsymbol{x}_{0,1}, \boldsymbol{x}_{0,2}, ..., \boldsymbol{x}_{0,n}]$. Joint trajectory prediction can be very challenging. The complex interactions among vehicles, especially in highly interactive and dense traffic, result in a complicated high-dimensional $p_0(\boldsymbol{x}_0)$, which is difficult to accurately model with lightweight and computationally efficient models. A simplified solution is to approximately decompose the joint trajectory distribution into marginal ones, i.e., $p_0(\boldsymbol{x}_0) \approx \prod_i^n p_0(\boldsymbol{x}_{0,i})$. It leads to the marginal trajectory prediction task, which has been extensively studied with mature solutions [18,24,50]. One drawback is that it omits the interactions among vehicles in the predicted horizon, which leads to large errors in highly interactive scenes.

Controllable trajectory generation is closely related to trajectory prediction. In addition to generating realistic trajectory samples resembling the ground-truth $p_0(\boldsymbol{x}_0)$, controllable generation imposes an additional objective—the generated trajectories should comply with specified guidance cost function $\mathcal{J}(\cdot)$. We term the former objective as *realism* and the latter as *guidance effectiveness*. The guidance cost function $\mathcal{J}(\cdot)$ can be some goal points of the vehicles, kinematic constraints, etc, which are mostly defined on the clean manifold rather than on the noisy data when it comes to diffusion-based controllable generation.

4 Methodology

4.1 Optimal Gaussian Diffusion

As discussed in Sec. 3.1, diffusion models typically select a non-informative prior distribution p_{prior}, such as a standard Gaussian, as the initial data distribution for the reverse diffusion process. Such a non-informative p_{prior} is reasonable since $p_T(\boldsymbol{x}_T)$ converges to it when $T \to \infty$. However, it also means that a large T is required at inference time to yield good performance, which undermines computational efficiency and limits its wide real-time applications in autonomous driving. In this section, we aim to investigate a practical solution to tackle this challenge for joint trajectory prediction. Given the inherent limitation imposed by a non-informative prior, the key question we look into is: *can we instead adopt an informative prior so that we can obtain the same level of performance with much smaller reverse diffusion steps?*

First, we still consider a Gaussian prior, but with learnable parameters, i.e., we parameterize p_{prior} as $q_\phi(T) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are learnable. We aim to optimize $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ to enhance the generation performance for small T. We got inspiration from [5], where an upper bound of the Kullback–Leibler divergence of the clean data distribution $p_0(\boldsymbol{x}_0)$ and learned distribution $q_\theta(\boldsymbol{x}_0)$ was derived as a function of the diffusion time T:

$$\mathrm{KL}[p_0(\boldsymbol{x}_0)||q_\theta(\boldsymbol{x}_0)] \leq \mathcal{G}(\boldsymbol{x}_\theta, T) + \mathrm{KL}[p_T(\boldsymbol{x}_T)||p_{prior}] \tag{6}$$

where $\mathcal{G}(\boldsymbol{x}_\theta, T)$ is the positive accumulated error between $\nabla_{\boldsymbol{x}} \log p_t(\boldsymbol{x}_t)$ and $\boldsymbol{s}_\theta(\boldsymbol{x}_t, t)$ from 0 to T [5]. Note that $\mathcal{G}(\boldsymbol{x}_\theta, T)$ is an accumulated error so $\mathcal{G}(\boldsymbol{x}_\theta, T_1) \leq \mathcal{G}(\boldsymbol{x}_\theta, T_2)$, $T_1 \leq T_2$. If we can achieve lower $\mathrm{KL}[p_{T_1}(\boldsymbol{x}_{T_1})||q_\phi(T_1)]$, then a tighter upper bound can be obtained. This opens up the possibility to achieve better performance with less diffusion time. Thus, we propose to optimize the prior distribution by minimizing $\mathrm{KL}[p_T(\boldsymbol{x}_T)||q_\phi(T)]$. As shown in Proposition 1 (See proof in Appendix A), it turns out that the optimal μ and Σ can be expressed analytically as functions of the ground-truth data statistics. In addition, we find that we can further minimize the target KL divergence if we set a learnable $\boldsymbol{\Sigma}_p$ in the perturbation kernel $p_t(\boldsymbol{x}_t|\boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\boldsymbol{\Sigma}_p)$, whose optimal value can also be expressed as a function of the data statistics.

Proposition 1. *Denote $\boldsymbol{\mu}_d$ and $\boldsymbol{\Sigma}_d$ as the mean and variance of p_{data}. Denote $\boldsymbol{\Sigma}^*(i,j)$ and $\boldsymbol{\Sigma}_p^*(i,j)$ as the element at ith row and jth column of matrix $\boldsymbol{\Sigma}^*$ and $\boldsymbol{\Sigma}_p^*$. The optimal solution to* $\min KL[p_T(\boldsymbol{x}_T)||q_\phi(\boldsymbol{x}_T, T)]$ *is*

$$\begin{cases} \boldsymbol{\mu}^* \approx \sqrt{\bar{\alpha}_T}\boldsymbol{\mu}_d \\ \boldsymbol{\Sigma}_p^*(i,j) \approx \frac{1}{|\boldsymbol{\Sigma}_d|}\boldsymbol{\Sigma}_d(i,j) \\ \boldsymbol{\Sigma}^*(i,j) \approx \bar{\alpha}_T\boldsymbol{\Sigma}_d + (1-\bar{\alpha}_T)^2\boldsymbol{\Sigma}_p^* = (\bar{\alpha}_T^2 + \frac{(1-\bar{\alpha}_T)^2}{|\boldsymbol{\Sigma}_d|})\boldsymbol{\Sigma}_d(i,j) \end{cases} \tag{7}$$

Thus, if we are able to estimate the mean and variance of the ground-truth data distribution, we can then analytically determine the optimal prior distribution $\mathcal{N}(\boldsymbol{\mu}^*, \boldsymbol{\Sigma}^*)$ and the optimal perturbation kernel variance $\boldsymbol{\Sigma}_p^*$ at *any noise*

level $T \in [0, \infty)$. It leads to a crucial advantage against prior efforts on prior learning [48], where a target noise level has to be determined at training time in order to train an additional neural network to represent the prior distribution at the pre-selected noise level. In contrast, our method enables flexible tuning of the number of diffusion steps at inference time, without additional training costs. Since the learnable $q_\phi(T)$ and perturbation kernel are both Gaussian, we refer to our proposed diffusion framework as Optimal Gaussian Diffusion (OGD).

For joint trajectory prediction and generation, we need to estimate the mean and variance of the joint trajectory distribution $p_0(\boldsymbol{x}_0)$. It is not straightforward as only a limited number of trajectory samples exist in the dataset under the same context. Considering there exists mature and accurate marginal trajectory prediction models [18, 24, 50], we can conveniently extract statistics of the marginal trajectory distributions, i.e., $p_0(\boldsymbol{x}_{0,i}), i \in \{1, 2, ..., n\}$ from a pre-trained marginal trajectory predictor. Since Proposition 1 provides element-wise optimal value, we can easily get:

Corollary 1. *Denote* $\boldsymbol{\mu}_d(\boldsymbol{x}_{0,i})$ *and* $\boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,i})$ *as the mean and variance of marginal distribution for vehicle* i *and set both* $\boldsymbol{\Sigma}$ *and* $\boldsymbol{\Sigma}_p$ *are block-diagonal matrices where each block represents the marginal characteristics of one single vehicle. The optimal solution to* $\min KL[p_T(\boldsymbol{x}_T)||q_\phi(\boldsymbol{x}_T, T)]$ *is*

$$\begin{cases} \boldsymbol{\mu}^* = [\sqrt{\bar{\alpha}_T}\boldsymbol{\mu}_d(\boldsymbol{x}_{0,1}), ..., \sqrt{\bar{\alpha}_T}\boldsymbol{\mu}_d(\boldsymbol{x}_{0,n})]^T \\ \boldsymbol{\Sigma}_p^* = \frac{1}{\sum_{i=1}^n |\boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,i})|} diag[\boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,1}), ..., \boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,n})] \\ \boldsymbol{\Sigma}^* = \bar{\alpha}_T diag[\boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,1}), ..., \boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,n})] + (1 - \bar{\alpha}_T)^2 \boldsymbol{\Sigma}_p^* \end{cases} \tag{8}$$

Corollary 1 implies that, if we further confine $\boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}_p$ to be block-diagonal without covariance between the states of different vehicles, then we can determine their optimal values purely from the estimated marginal statistics $\boldsymbol{\mu}_d(\boldsymbol{x}_{0,i})$ and $\boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,i})$, $i \in \{1, 2, ..., n\}$, which enables a practical implementation of the proposed OGD model for joint trajectory prediction and generation tasks. Specifically, for vehicle i, we leverage a pre-trained marginal trajectory predictor [18, 24, 50], predict diverse marginal trajectory sample set $\mathcal{R}_i = \{\boldsymbol{r}_i^l\}_{l=1}^L$ and corresponding likelihood set $\{p(\boldsymbol{r}_i^l)\}_{l=1}^L$, and estimate $\boldsymbol{\mu}_d(\boldsymbol{x}_{0,i})$ and $\boldsymbol{\Sigma}_d(\boldsymbol{x}_{0,i})$. For example, $\boldsymbol{\mu}_d(\boldsymbol{x}_{0,i})$ can be estimated as $\frac{1}{L}\sum_{l=L} p(\boldsymbol{r}_i^l)\boldsymbol{r}_i^l$.

4.2 Estimated Clean Manifold Guidance with Reference

As discussed in Sec. 3.2, the intensive computation required for guided sampling comes from the calculation of $\nabla_{\boldsymbol{x}_t} f_\theta(\boldsymbol{x}_t)$. Previous guided sampling approaches bias the score function defined on the intermediate noisy data $\boldsymbol{x}_t$. In this section, we aim to investigate whether we can inject the gradient directly into $\boldsymbol{x}_0$ to avoid the gradient propagation process. We first reformulate the controllable generation as a multi-objective optimization problem directly over $\boldsymbol{x}_0$ and propose an iterative algorithm to solve the formulated problem. In addition, we use reference trajectory points to create the region of interest, which helps solve the local optimal problem caused by multi-modal joint trajectory distribution and accelerate the guided sampling process.

Estimated Clean Manifold Guidance. The objective of controllable generation of sample $\boldsymbol{x}_0$ includes two different objectives. The most important is the negative likelihood, ensuring the sample lies in the clean manifold. The second important is the guidance cost representing the user preference on the generated sample $\boldsymbol{x}_0$. This multi-objective optimization problem can be represented as

$$\min_{\boldsymbol{x}_0} \quad [-\log q_\theta(\boldsymbol{x}_0), \mathcal{J}(\boldsymbol{x}_0)]^T \tag{9}$$

Inspired by lexicographic optimization [33], we solve this multi-objective optimization problem hierarchically. The main idea is to optimize each objective in the order of importance regardless of the degradation of the other less significant objectives. We first optimize the most important objective, $-\log q_\theta(\boldsymbol{x}_0)$, to generate realistic and high-likelihood samples. The diffusion model achieves this goal effectively by reversing the diffusion process from noisy samples at specific noise level. However, exact noise level of current sample $\boldsymbol{x}_0$ is unknown. To address this, we inject noise at level t into $\boldsymbol{x}_0$, and then denoise it from t with learned diffusion model. This approach, similar to *noise injection and denoising* [1,23,37], improves the desired sample quality. We iteratively repeat this process K times, injecting guidance at each iteration to strengthen user preference.

Specifically, denote $\boldsymbol{x}_0(k)$ as the sample at iteration k. We first regenerate high-likelihood sample $\hat{\boldsymbol{x}}_0(k)$ by diffusion model:

$$\hat{\boldsymbol{x}}_0(k) \leftarrow \mathbb{E}[q_\theta(\boldsymbol{x}_0(k)|\boldsymbol{x}_{t_k}(k))] = \frac{1}{\sqrt{\bar{\alpha}_{t_k}}}(\boldsymbol{x}_{t_k} - \sqrt{1-\bar{\alpha}_{t_k}}\boldsymbol{\epsilon}_\theta(\boldsymbol{x}_{t_k}(k), t_k)), \tag{10}$$

where $\boldsymbol{x}_{t_k}(k) = \sqrt{\bar{\alpha}_{t_k}}\boldsymbol{x}_0(k) + \sqrt{1-\bar{\alpha}_{t_k}}\boldsymbol{\epsilon}$, $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_p)$. $t_k \in [0, T]$ is a tunable parameter. Then we minimize the guidance cost function with a small degradation of the most important objective $-\log q_\theta(\boldsymbol{x}_0)$,

$$\boldsymbol{x}_0(k-1) \leftarrow \hat{\boldsymbol{x}}_0(k) - \zeta \nabla_{\hat{\boldsymbol{x}}_0(k)} \mathcal{J}(\hat{\boldsymbol{x}}_0(k)) \tag{11}$$

where ζ is the step size. Small degradation of $-\log q_\theta(\boldsymbol{x}_0)$ is realized by one-step gradient update and proper step size ζ. See the derivation of the optimization process and the parameter tuning in Appendix B.

During the iterations, $\boldsymbol{x}_0(k)$, $\forall k \in \{0, 1, ..., K-1\}$ are not exactly on the clean manifold. We minimize its negative log-likelihood through diffusion model, resulting in it lying on an estimated clean manifold. Thus, we call our method Estimated Clean Manifold (ECM) Guidance.

Reference Joint Trajectories. To generate trajectories with low guidance cost, we are essentially searching low-cost trajectories within the high-likelihood region. At the same time, joint trajectory distribution is a multi-modal distribution resulting from road topologies and different decision variables, meaning the likelihood has multiple peaks. This leads to the optimal solution of Problem 9 having multiple local optimals, and each optimal is far away from the other. Guided sampling methods [15,16,28,49], including our method ECM, suffer from

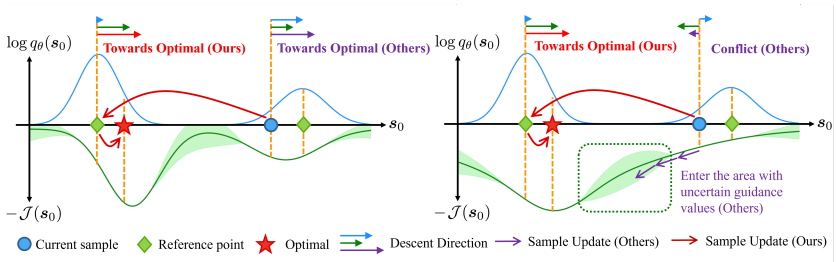


Fig. 2: Two challenges with multi-peak function optimization: 1) Gradients may lead to suboptimal local optima (left); 2) There exist regions with low likelihood but high guidance cost uncertainty, leading to instability (right). Our approach can bypass the lengthy paths between peaks, search for better optima, and avoid uncertain areas.

two challenges (See Fig. 2): 1) it can be trapped at the local optimal around the initial position; 2) it takes massive efforts to drag the sample from one peak to another and transferring from one modal to another will need to pass through the region of low-likelihood (off clean-manifold), leading to numerical instability.

To overcome this, we generate high-likelihood reference joint trajectories, choose the best one as the initialization. Note that combinations of samples with high marginal likelihood tend to exhibit high joint likelihood. Therefore, we can utilize the marginal sample set $\mathcal{R} = \{\mathcal{R}_i\}_{i=1}^{n}$ obtained from pre-trained marginal models to generate the references. Specifically, for iteration k, we construct candidate joint trajectory set $\mathcal{R} \bigotimes \hat{\boldsymbol{x}}_0(k) = \{[\boldsymbol{w}_1, \boldsymbol{w}_2, ..., \boldsymbol{w}_n] | \boldsymbol{w}_i \in \mathcal{R}_i \cup \{\hat{\boldsymbol{x}}_{0,i}\}, i = 1, 2, ..., n\}$. We calculate the guidance cost of all possible combinations, $\mathcal{J}(w), w \in \mathcal{R} \bigotimes \hat{\boldsymbol{x}}_0(k)$, and choose the minimal-cost one as the reference. The guided sampling algorithm, ECM with reference joint trajectories (ECMR), is introduced in Algorithm 1.

Algorithm 1: ECMR

Input: $\mathcal{J}(\cdot)$, $\{\bar{\alpha}_t, \beta_t\}_{t=0}^{T-1}$, $\{t_k\}_{k=0}^{K-1}$
$\boldsymbol{x}_0(K) \sim \mathcal{N}(0, \boldsymbol{\Sigma}_p)$
for $k = K-1, ..., 1$ **do**
  $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{\Sigma}_p)$
  $\boldsymbol{x}_{t_k}(k) = \sqrt{\bar{\alpha}_{t_k}}\boldsymbol{x}_0(k) + \sqrt{1-\bar{\alpha}_{t_k}}\boldsymbol{\epsilon}$
  $\hat{\boldsymbol{x}}_0(k) = \frac{1}{\sqrt{\bar{\alpha}_{t_k}}}(\boldsymbol{x}_{t_k}(k) - \sqrt{1-\bar{\alpha}_{t_k}}\boldsymbol{\epsilon}_\theta(\boldsymbol{x}_{t_k}(k), t))$
  $\hat{\boldsymbol{x}}_0(k) = \arg\min \mathcal{J}(w), w \in \mathcal{R} \bigotimes \hat{\boldsymbol{x}}_0(k)$
  $\boldsymbol{x}_0(k-1) \leftarrow \hat{\boldsymbol{x}}_0(k) - \zeta \nabla_{\hat{\boldsymbol{x}}_0(k)} \mathcal{J}(\hat{\boldsymbol{x}}_0(k))$
end for
Output: $\boldsymbol{x}_0(0)$

5 Experiments

5.1 Experimental setup

Dataset. We use Argoverse 2 [44], a widely used and large-scale trajectory prediction dataset, to test the effectiveness of our approaches for joint trajectory prediction and controllable generation. It has a large observation window of 5s and a long prediction horizon of 6s.

Implementation Details. We use the fixed scene context encoder of pre-trained QCNet [50] to extract compact and representative context features from context information $\boldsymbol{c}$. Then, we utilize a cross-attention layer to update the intermediate noisy data $\boldsymbol{x}_t$ with multiple contexts, including the history encodings of the target agent, the map encodings, the neighboring agents' encodings. Inspired by [7], we also add a cross-attention layer to update $\boldsymbol{x}_t$ with the diverse marginal trajectory samples $\boldsymbol{r}_i^l$ and its corresponding likelihood. In addition, we use self-attention to allow the interaction between $\boldsymbol{x}_{t,i}$ and $\boldsymbol{x}_{t,j}$. Then the model predicts the noise $\boldsymbol{\epsilon}_\theta(\boldsymbol{x}_t, t)$. According to [16], compact trajectory representation helps the diffusion model to generate high-quality trajectories efficiently. Inspired by this, we also learn a linear mapping between the 10-dimensional latent and 120-dimensional trajectories. Similar to [16], we design a rapid sample clustering algorithm so that we can generate a representative joint trajectory set. To increase the efficiency of sampling, we use DDIM [35] to accelerate the inference, and the DDIM step stride is 10. See Appendix C for details and analysis.

5.2 Joint trajectory prediction

We now evaluate OGD for joint trajectory prediction. Given K joint trajectories, the evaluation metrics are 1) $\textbf{avgMinFDE}_K$/$\textbf{avgMinADE}_K$: the average of lowest final/average displacement error (FDE/ADE) of joint trajectory samples; 2) $\textbf{actorMR}_K$: the rate of trajectory predictions that are considered to be "missed" (>2m FDE) in the lowest minFDE joint trajectory samples; 3) $\textbf{actorCR}_K$: the rate of collisions across "best" (lowest avgMinFDE) joint trajectory samples; 4) $\textbf{avgBrierMinFDE}_K$: calculated similarly to avgMinFDE_K but scaled by the probability score of joint trajectory samples. We denote metrics with superscript "*" as those after sample clustering (see Appendix C.3).

As a baseline, we train a vanilla diffusion (VD) baseline that shares the same neural network architecture as OGD. Specifically, we train an Optimal Gaussian Diffusion model with diffusion time $T_{train} = 100$ (OGD), vanilla diffusion with two different diffusion times $T_{train} = 100, 500$ (VD_{100}, VD_{500}). Note that T is denoted as the diffusion time from which the reverse diffusion process starts. First, during the inference, we change T and evaluate OGD and VD_{100} who have the same $T_{train} = 100$. Figure 3 shows that, with the decrease of the reverse steps, avgMinFDE_{128} of OGD keeps lower than VD_{100} and it is more stable with the change of T. It is also interesting to note that the performance of OGD even becomes better in the early stage. We hypothesize that it is because that $\text{KL}[p_T(\boldsymbol{x}_T)||p_{prior}]$ of OGD is small and the accumulated error of $\mathcal{G}(\boldsymbol{x}_\theta, T)$ is sufficiently reduced by a small T. It also shows an advantage of OGD, which is that it is easy for OGD to tune a suitable T for reverse diffusion without training an additional model for every T [48]. Table 1 shows that OGD outperforms VD_{500} with only 40 diffusion steps.

We also compare our OGD with the other state-of-the-art methods on the Argoverse multi-world leaderboard; our approach OGD ranks 4^{th} on the leaderboard ranked by avgBrierMinFDE_K, which demonstrates the effectiveness of our

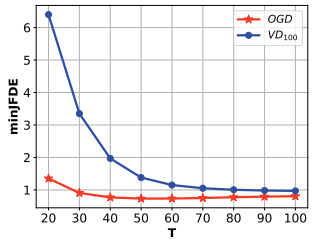


Fig. 3: Evaluation of Optimal Gaussian Diffusion and vanilla diffusion over reverse steps T.

Table 1: Evaluation on joint trajectory prediction task. For each metric, the best result is in **bold** and the second best result is underlined. $T = 70$ is the best T from Fig. 3. $T = 40$ is the minimal diffusion time when OGD outperforms VD_{500} on all metrics.

Model	T	avgMinFDE$^*_6$	avgMinADE$^*_6$	avgMinFDE$_{128}$	avgMinADE$_{128}$
VD_{100}	100	0.62	1.38	0.49	0.97
VD_{500}	500	0.61	1.36	0.48	0.91
OGD	100	0.60	1.32	0.43	0.81
OGD	70	**0.59**	**1.31**	**0.42**	**0.75**
OGD	40	0.61	1.34	0.47	0.77

OGD framework. Note that we only list the entries with publications or technical reports in Tab. 2. Please refer to the official website for the full leaderboard.

5.3 Controllable Generation

Tasks. Future behaviors of vehicles can be effectively can be effectively represented by a set of goal points [9, 47] such as acceleration, braking, and right or left turn. Generating such diverse modes of joint trajectories is a typical motivation for using controllable generation. Thus, we study the controllable generation task where the goal is to reach diverse goal points at a specific time to fully test our guided sampling method. Considering that goal points should lie in realistic routes, and the trajectories to reach such goal points should also lie in such routes, we generate such target goal points in some realistic routes $\text{Route}(\tau_g)$. The guidance cost function can be expressed as

$$\mathcal{J}(\boldsymbol{x}_0) = \frac{1}{n}||\text{Position}(\boldsymbol{x}_0, \tau_d) - \text{Route}(\tau_g)||_2^2, \tag{12}$$

where $\text{Position}(\boldsymbol{x}_0, \tau_d)$ is the positions of $\boldsymbol{x}_0$ at time τ_d. We choose ground-truth trajectories and a random combination set of diverse marginal samples, i.e., $\mathcal{U} = \{[\boldsymbol{u}_1, \boldsymbol{u}_2, ..., \boldsymbol{u}_n] | \boldsymbol{u}_i \in \mathcal{R}_i, i = 1, 2, ..., n\}$ as the realistic routes. We denote

Table 2: Quantitative results on the Argoverse 2 Multi-world Forecasting leaderboard. For each metric, the best result is in **bold** and the second best result is underlined.

Model	avgMinFDE$^*_6$	avgMinFDE$^*_1$	actorMR$^*_6$	avgMinADE$^*_6$	avgMinADE$^*_1$	avgBrierMinFDE$^*_6$	actorCR$^*_6$
QCXet [51]	**1.02**	**2.29**	**0.13**	**0.50**	**0.94**	**1.65**	**0.01**
Gnet [6]	1.46	3.05	0.19	0.69	1.23	2.12	0.01
Forecast-MAE [2]	1.55	3.33	0.19	0.69	1.30	2.24	0.01
FJMP [30]	1.89	4.00	0.23	0.81	1.52	2.59	0.01
OGD (Ours)	1.31	2.71	0.17	0.60	1.08	1.95	0.01

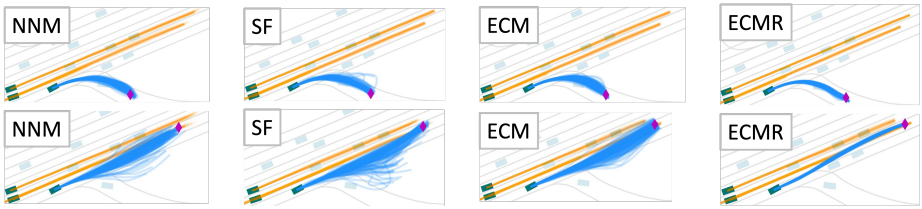


Fig. 4: Evaluation on controllable generation: route set **U** and **Deceleration**. Magenta diamonds represent goal points. In the first (second) row, goal points are set at the fork lane (right lane). NNM [49] and SF [16, 28] struggle to drag samples from one modal to another. Our methods can achieve better guidance effectiveness and realism.

the former as **GT** set and the latter as **U** set. The underlying assumption is that diverse samples from a good marginal trajectory predictor are realistic. We design different velocity settings to cover the diverse controllable generation tasks in autonomous driving: first is **Normal Speed** (**N**), $\tau_d = \tau_g = 6s$; second is **Acceleration** (**A**), $\tau_d = 5s < \tau_g = 6s$; third is **Deceleration** (**D**), $\tau_d = 6s < \tau_g = 5s$.

Metrics. We use the following metrics to evaluate controllable generation performance: Joint Route Deviation Error (JRDE), which measures the displacements to the routes to evaluate the realism, and Joint Final Displacement Error (JFDE), which evaluates the guidance effectiveness. We also evaluate from the "min" and "mean" perspectives: The "min" metric considers the best sample's performance, while the "mean" metric assesses the ratio of valid samples.

Baselines. Guided sampling in controllable generation is mainly divided into two approaches: the first is to directly calculate $\nabla_{\boldsymbol{x}_t}\mathcal{J}(\boldsymbol{x}_t)$ [49]; the second is to calculate $\nabla_{\boldsymbol{x}_t}\mathcal{J}(\hat{\boldsymbol{x}}_0)$ [16, 28]. We denote the former as Next Noisy Mean Guidance (NNM) and the latter as Score Function Guidance (SF). For a fair comparison, we use one guidance step followed by one DDIM step. We also tune the gradient step size for different guided sampling with Optimal Gaussian Diffusion and vanilla diffusion and report the results with the optimal step size. See Appendix D for the details of baseline derivation and step size tuning. We evaluate the following experiments with 128 joint trajectory samples.

Evaluation. First, we evaluate the performance and efficiency with our diffusion model (OGD) and guided sampling method (ECM and ECMR) in Tab. 3, which demonstrates our methods can generate more realistic and effective samples with 5 times less DDIM steps. In addition, with reference joint trajectories, ECM significantly improves 'mean' metrics, indicating it addresses the issues discussed in Sec. 4.2 to a certain extent. Second, we compare solely on different guided sampling methods using the same OGD model shown in Fig. 5. Our ECM achieves better performance both in guidance effectiveness and realism. In Fig. 4, our ECM can generate trajectories that reach goal points more closely than NNM and SF. And with reference joint trajectory, ECMR can easily move samples from one modal to another . Third, we evaluate the average inference time and average GPU memory usage in Tab. 4. Our methods can generate

Table 3: Evaluation on controllable generation: route set **U** and **Deceleration**. For each metric, the best result is in **bold** and the second best result is underlined.

Model	Sampling	DDIM Steps	Guidance Effectiveness		Realism	
			minJFDE	meanJFDE	minJRDE	meanJRDE
VD_{500}	No Guid	50	1.961	5.229	0.165	0.492
VD_{500}	NNM [49]	50	0.778	2.913	0.130	0.309
VD_{500}	SF [16, 28]	50	0.538	2.339	0.158	0.500
OGD	No Guid	10	1.772	5.172	0.138	0.469
OGD	ECM (Ours)	10	0.072	0.237	0.128	0.236
OGD	ECMR (Ours)	10	**0.053**	**0.146**	**0.110**	**0.154**

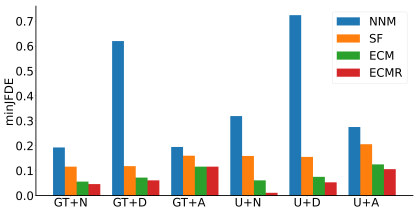


Fig. 5: Evaluation of different guided sampling methods on various tasks. See Appendix E for other metrics.

Table 4: We evaluate the average inference time per step and GPU incremental memory on **U** + **Deceleration**. We test on single RTX A6000, batch size is 16 and number of samples is 128.

Sampling	minJFDE	minJRDE	time(ms)	memory (GB)
NNM [49]	0.724	0.119	113	3.21
SF [16, 28]	0.155	0.126	247	7.96
ECM(Ours)	0.075	0.116	111	3.21
ECMR(Ours)	0.053	0.110	116	3.22

realistic trajectories satisfying guidance quite well with low inference time and GPU memory usage. More results on controllable generation can be found in Appendix E.

6 Conclusion

In this work, we introduce Optimal Gaussian Diffusion (OGD) and Estimated Clean Manifold (ECM) Guidance to significantly improve the computational efficiency and performance of diffusion models in autonomous driving. These methodologies enable a substantial reduction in inference steps and computational demands while ensuring enhanced joint trajectory prediction and controllable generation capabilities. Our approaches and experimental results underscore the potential of diffusion models for real-time applications in dynamic environments, marking a pivotal advancement in the deployment of diffusion models for autonomous driving. One limitation of the current implementation is that the performance is affected by the accuracy of marginal trajectory predictors. Enhancements could be achieved with superior marginal models or by directly learning joint predictions' mean and variance, areas for future work.

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