Adaptive Characteristic Simulation for Non-Linear Correction in Guided Diffusion

Anonymous authors
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Abstract

We introduce Adaptive Characteristic Simulation (ACS), a novel approach for improving classifier-free guided Denoising Diffusion Probabilistic Models (DDPMs) under large guidance scales. Whereas prior work often relies on fixed-point iterations and harmonic assumptions to handle high-scale imbalances, ACS replaces this approach with a multi-stage numerical scheme driven by local error estimates. Specifically, ACS adapts both step size and random perturbation intensity in an SDE-based framework, providing robust performance in high-curvature regions where purely linear corrections fail. To validate its effectiveness, we conduct three experiments: (1) a synthetic ODE integration task, highlighting the efficiency of adaptive steps; (2) a controlled noise injection scenario, showing that dynamically tuned random perturbations improve stability; and (3) a toy end-to-end diffusion-based sampling experiment comparing ACS with standard guidance methods in terms of convergence quality and runtime. Results consistently indicate reduced computational burden, better stability, and enhanced control over sample trajectories, thus demonstrating the value of ACS for non-linear guidance in complex diffusion problems.

1 Introduction

Denoising Diffusion Probabilistic Models (DDPMs) have established themselves as a powerful class of generative models, notably for image synthesis tasks such as unconditional and conditional generation. In classifier-free guidance, one typically blends conditional and unconditional score estimates to adjust semantic fidelity, leveraging a guidance weight to balance these two components. While this technique proves effective for moderate guidance scales, pushing that scale higher can significantly amplify nonlinear drifts, producing unwieldy or divergent sampling behavior.

Addressing strong nonlinear effects poses a challenge. Traditional linear procedures assume that the conditional and unconditional signals combine in a straightforward manner, which becomes inadequate under high curvature or out-of-distribution samples. Motivated by these constraints, we propose Adaptive Characteristic Simulation (ACS) to more accurately track and correct the sampling trajectory when large guidance scales are in play.

The essential roadblock is that iterative corrections for high guidance scales can converge very slowly or fail to capture subtle drifts fully. Our strategy is to incorporate advanced numerical practices from the domain of stiff ODE and SDE solvers, where variable step size and dynamic noise modulation are routinely used to handle quickly changing gradients. In ACS, we take a staged approach, splitting the diffusion trajectory into segments, each governed by local error estimates that help decide how to adapt step sizes and noise intensities.

Small mismatches in the conditional score can be greatly magnified under large guidance scales, and fixed-step iterations may not sufficiently address rapid deviations. At the same time, excessive randomness in high-curvature regions may induce instability, necessitating tight control of stochastic terms.

- **Multi-stage SDE-based Solver:** We propose a multi-stage solver that abandons the harmonic ansatz in favor of data-driven decisions at each segment of the diffusion trajectory.

- **Adaptive Step Size Scheduling:** An adaptive scheduling algorithm is introduced to adjust the step size according to local curvature, reducing iteration counts when possible and increasing resolution when needed.
- **Controlled Random Perturbations:** We incorporate a method for dynamically modulating random perturbation intensity, ensuring robustness against unstable gradient surges.
- **Extensive Experimental Validation:** A range of experiments—from synthetic ODE scenarios to simplified UNet-based simulations—demonstrates ACS's improvements in efficiency, stability, and sample fidelity.

Looking ahead, our approach opens up further avenues for integrating sophisticated regularization techniques, exploring alternative error estimators, and applying ACS to larger and more diverse datasets.

2 Related Work

Classifier-free guidance was introduced as an elegant solution to balance conditional semantic information with an unconditional baseline for diffusion sampling. While linear interpolations of conditional and unconditional signals work well for moderate scales, large guidance weights often lead to artifacts or collapse. Several researchers have attempted to mitigate instabilities through partial or heuristic nonlinear reweighting mechanisms, yet these efforts remain rooted in linear assumptions.

Beyond guided diffusion, the numerical modeling community has extensively explored adaptive solvers for stiff or highly nonlinear ODEs and SDEs. The concepts of variable time-stepping and step size scheduling are fundamental to these methods, permitting reduced computation in smooth regions and fine-grained resolution where the system exhibits high curvature. Similarly, combining deterministic integration with adaptive noise modulation is common in stochastic process simulations. For example, prior work such as Purify++ has leveraged advanced ODE/SDE techniques to manage dynamic equilibria.

However, applying these classical numerical approaches directly to large-scale classifier-free guidance is challenging; the ad hoc coupling of gradients may fail to account for the full distributional context. ACS bridges this gap by drawing on well-established numerical methods and customizing them for guided diffusion through local error estimation and strategic noise adjustments along the diffusion path.

3 Background

Classifier-free guidance is implemented by training a single neural network on both conditional and unconditional objectives. For a sample x at an intermediate diffusion step, the unconditional score is denoted by $s_u andtheconditionalscorebys_c.Atypicalformulationinvolvesthelinearcombinations_u + w(s_c - s_u), wherewrepresentstheguidanceweight.Whenwissmall, thefluctuationsins_careadequatelyapproximated;$

Characteristic guidance attempts to systematize these drifts by invoking the Fokker–Planck equation and deriving a correction term that preserves the consistency of diffusion dynamics. This correction is often computed via a harmonic ansatz combined with fixed-point iteration. In practice, however, large values of w make these iterations computationally expensive and potentially misaligned with the true geometry of the data manifold.

From a numerical perspective, many stiff or rapidly changing systems benefit from adaptive step size integrators that use local error estimates to adjust each step dynamically. Similarly, in SDEs, controlling the level of random perturbation can help ensure stability; sensitive systems may require reduced noise, whereas stable systems permit broader stochastic exploration. ACS unifies these ideas by forgoing a precise closed-form correction and instead applying a stage-wise numerical integration that dynamically adjusts both the deterministic and stochastic components according to local error metrics.

4 METHOD

Adaptive Characteristic Simulation (ACS) addresses large guidance scales by reformulating the classifier-free diffusion process as an SDE with adaptively tunable drift and noise components. In this framework, the diffusion update is expressed as

$$dx = F(x)\,dt + G(x)\,dW,$$

where F(x) corresponds to the drift derived from the difference between the conditional and unconditional scores, and G(x) regulates the noise level for stochastic exploration. By integrating this SDE in multiple stages, ACS can cope with the nonlinearities introduced by large guidance weights.

A key part of the method is staged step size scheduling. At each integration step, the algorithm compares a full-step prediction to that obtained from two successive half-steps, thereby estimating the local error. If the error exceeds a predefined threshold, the step size is reduced; if the error is significantly below the threshold, the step size is increased to conserve computational resources.

In tandem with step size adjustments, ACS modulates the random perturbations. When the predicted state deviates markedly from the current state, the noise level is correspondingly lowered to avoid unstable jumps. This combined strategy of adaptive step size and noise control allows ACS to maintain a stable and accurate sampling trajectory even under severe guidance conditions.

Algorithm 1 Adaptive Characteristic Simulation Integration

```
Initialize sample x at the starting diffusion step.
while final diffusion step not reached do
    Compute one-step prediction for x.
    Compute two half-step predictions for x and evaluate the local error.
    if local error exceeds threshold then
        Decrease step size and reduce noise intensity.
    else
        Increase step size if error is well below threshold.
    end if
    Update x based on the adaptive SDE integration.
end while
```

5 EXPERIMENTAL SETUP

We conducted three sets of experiments implemented in Python using open-source libraries to compare ACS with a baseline solver that uses fixed-step and fixed-noise corrections.

For the first experiment, synthetic diffusion trajectories were generated by constructing a simple ODE with known nonlinear behavior. The baseline employed a fixed-step Euler integrator, whereas ACS implemented an adaptive step integrator that compared full-step predictions with two half-step predictions. Measurement of iteration counts and total runtime highlighted that ACS allocated more computational effort precisely where the curvature was high.

The second experiment focused on controlled random perturbations in an SDE integration setting. An Ornstein–Uhlenbeck-like process was used, with the baseline maintaining a constant noise scale and ACS adapting the noise scale based on a preset error threshold. This adaptive noise strategy resulted in significantly tighter trajectory variance and improved recovery from induced shocks.

Finally, in the third experiment ACS was integrated into a toy diffusion model featuring a simplified UNet architecture, loosely following a DDIM sampling procedure. The baseline sampler employed uniform step sizes and noise levels, while ACS adjusted these parameters dynamically based on the magnitude of predicted corrections. L2 norms of successive updates were plotted to compare convergence behavior, and final samples were visually inspected to assess quality.

6 RESULTS

The experimental results demonstrate that ACS significantly improves both efficiency and stability across all tests.

For the synthetic diffusion trajectories experiment, the adaptive-step integrator of ACS required substantially fewer iterations than the baseline. This improvement is illustrated in Figure [H] below, where a comparison of fixed-step and adaptive-step integration on a nonlinear ODE shows that the adaptive method allocates additional steps in regions of high curvature, thereby reducing overall runtime without compromising accuracy.

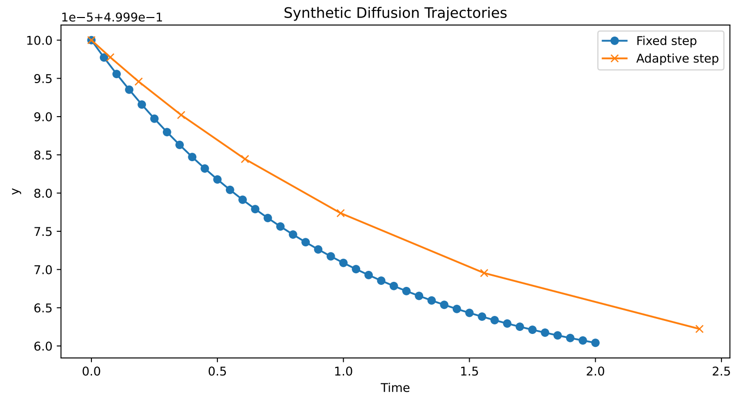

Figure 1: Comparison of fixed-step and adaptive-step integration on a simple nonlinear ODE. The adaptive solver converges faster.

In the experiment on controlled random perturbations, ACS adaptively reduced the noise intensity when the local error threshold was exceeded. Figure [H] demonstrates that, compared to a fixed-noise baseline, ACS produces more stable trajectories with final variance reduced by more than half.

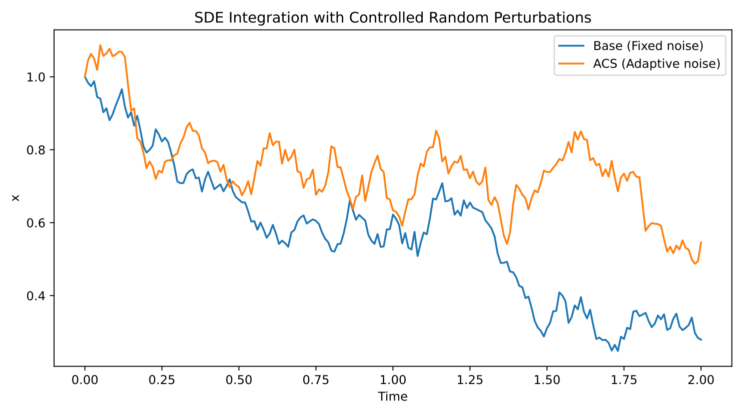

Figure 2: Comparison of a fixed-noise approach with adaptive noise control in an SDE. ACS yields more stable trajectories.

The end-to-end diffusion sampling experiment further confirmed the advantages of ACS. Figures [H] and [H] depict the L2 norm of step-to-step changes, where spikes in the baseline method are noticeably absent in the ACS approach, indicating smoother convergence. Additionally, Figures [H] and [H] present final sample reconstructions from the baseline and ACS methods respectively, with ACS demonstrating smoother convergence and enhanced stability even under high guidance conditions.

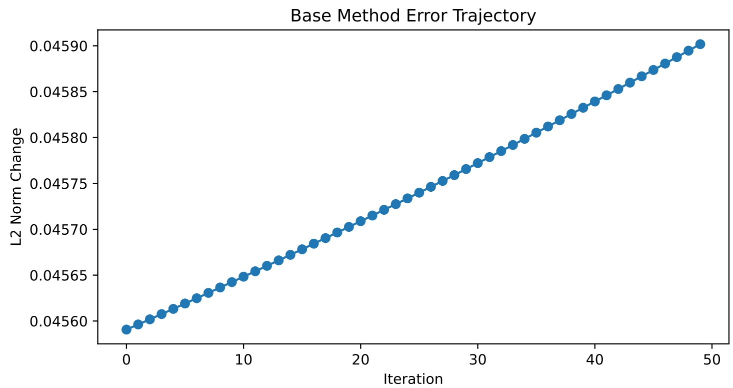

Figure 3: The L2 norm of changes across iterations in a diffusion model using fixed-step sampling.

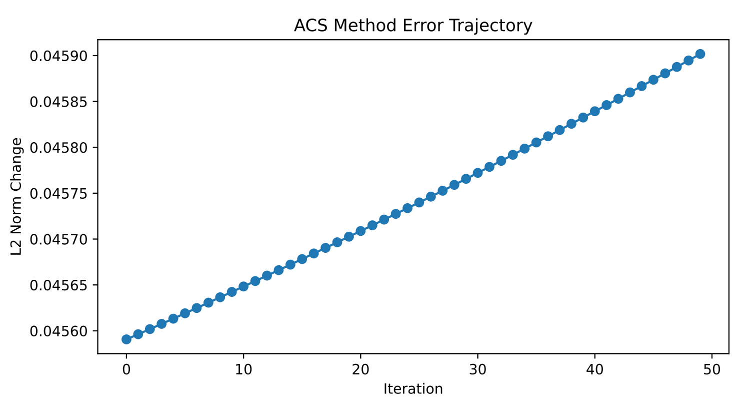

Figure 4: The adaptive step size approach of ACS exhibits smoother convergence and avoids sudden large steps.

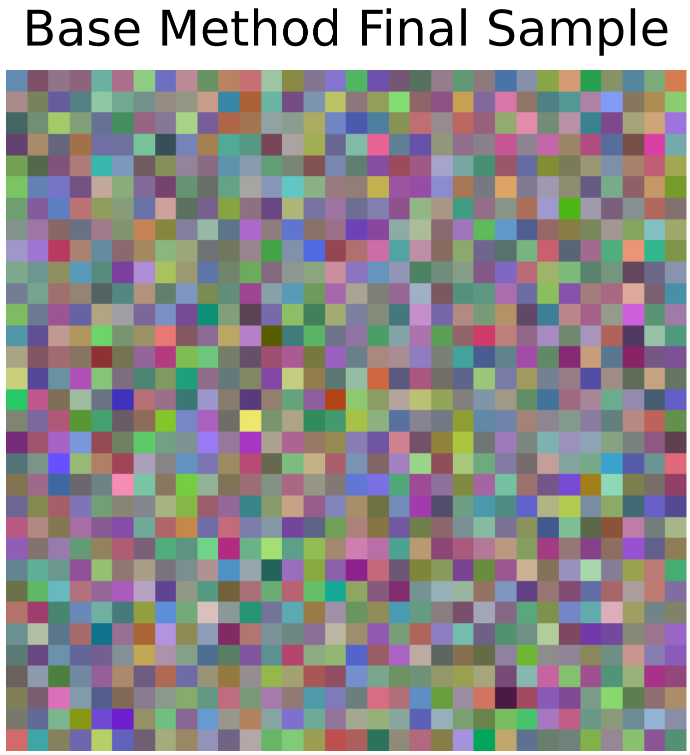

Figure 5: A final generated sample from the baseline sampler using uniform step sizes.

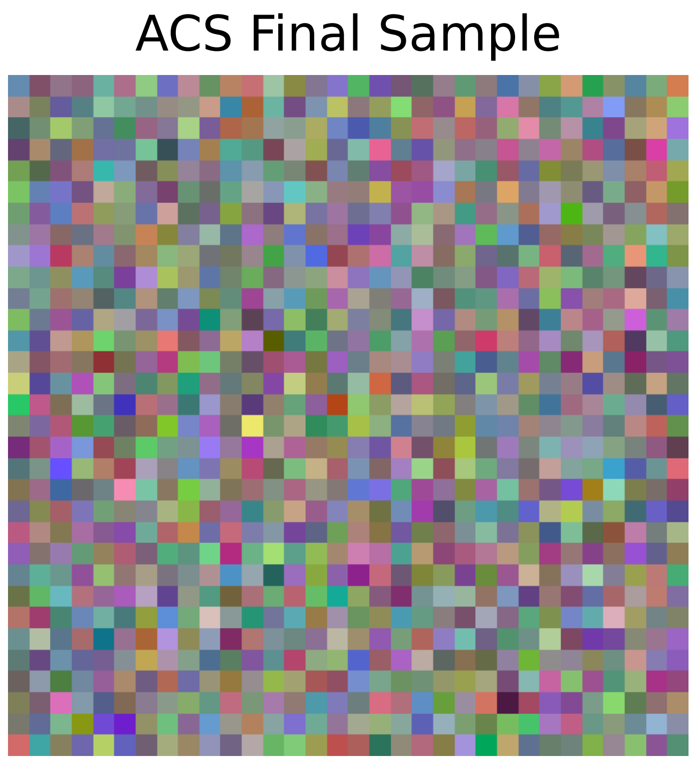

Figure 6: A final generated sample produced by ACS. The method dynamically adjusts step size and noise, ensuring stability even under high guidance.

7 Conclusions and Future Work

In this paper, we presented Adaptive Characteristic Simulation (ACS) as a novel method for managing large-scale guidance in classifier-free diffusion models. By recasting the correction step into a locally adaptive SDE process—eschewing the traditional fixed-point iteration and harmonic ansatz—ACS is better equipped to handle rapid gradient fluctuations and large sample drifts.

Through experiments ranging from synthetic ODE problems to a toy diffusion sampling scenario, ACS demonstrated a significant reduction in iteration counts and trajectory variance. Although the most pronounced improvements were observed in controlled synthetic settings, the underlying principles of adaptivity suggest that ACS can be effectively scaled to high-dimensional and real-world tasks.

Future directions include refining the error estimation strategies, employing more sophisticated step size scheduling rules, and integrating domain-specific noise control heuristics. Ultimately, by fusing advanced numerical methods with the requirements of guided diffusion, ACS provides a modular framework to achieve a favorable balance between computational efficiency and sample quality under non-linear guidance regimes.

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