

Supplementary Materials for Submission 11223: TAG

Method	Deblur		Super-resolution		CIFAR10		ImageNet		Audio declipping		Audio inpainting	
	FID ↓	LPIPS ↓	FID ↓	LPIPS ↓	FID ↓	Acc. ↑	FID ↓	Acc. ↑	FAD ↓	DTW ↓	FAD ↓	DTW ↓
TFG	64.2	0.154	65.5	0.187	114.1	55.8	231.0	14.3	1.42	256	0.52	74
TFG + TAG (ours)	62.7	0.151	64.7	0.175	102.7	61.5	219.4	17.8	0.74	120	0.42	51
TCS [15]	96.5	0.350	188.7	0.518	160.5	63.7	297.9	15.1	20.03	549	6.25	446
Timestep Guidance [16]	469.8	0.951	483.8	0.973	371.5	11.3	536.5	25.0	33.67	112	21.96	900
Self-Guidance [17]	297.7	0.612	426.9	0.711	188.6	42.9	280.5	14.5	35.05	116	19.39	892

Method	Polarizability α		Dipole μ		Heat capacity C_v		ϵ_{HOMO}		ϵ_{LUMO}		Gap ϵ_{Δ}	
	MAE ↓	Stab. ↑	MAE ↓	Stab. ↑	MAE ↓	Stab. ↑	MAE ↓	Stab. ↑	MAE ↓	Stab. ↑	MAE ↓	Stab. ↑
TFG	8.91	19.2	2.41	26.3	2.65	96.2	0.55	14.6	1.33	10.8	1.40	16.1
TFG + TAG (ours)	4.46	43.6	1.28	94.3	2.67	96.7	0.43	93.9	0.89	92.5	0.78	82.8
TCS [15]	5.40	99.2	1.43	99.2	3.35	99.1	N/A	N/A	1.22	99.2	1.31	99.2
Timestep Guidance [16]	10.98	84.4	N/A	N/A	4.09	85.5	0.70	83.5	1.36	73.0	1.30	83.5
Self-Guidance [17]	7.66	80.2	32.54	80.3	3.80	80.3	N/A	N/A	1.32	80.3	1.27	80.4

Table R1: Comparison of TFG-based methods. The best result for each metric is highlighted in **bold**.

Method	FID ↓	Acc. ↑
DPS	217.1	57.5
TAG (ours)	190.4	63.2
TCS [15]	213.4	29.4
Timestep Guidance [16]	393.2	9.4
Self-Guidance [17]	205.4	51.6
Epsilon Scaling [10]	226.5	56.8
Time Shift Sampler [11]	247.7	56.4
Langevin Dynamics [13]	226.8	58.2

Table R2: Additional baselines when applying DPS on CIFAR-10.

Method	FID ↓	Acc. ↑
$\eta = 0$	332.0	28.5
$\eta = 0.05$	409.9	23.3
$\eta = 0.10$	376.6	25.4
$\eta = 0.15$	326.7	29.2

Table R3: Effect of Input perturbation on DPS, CIFAR-10.

Method	FID ↓	Acc. ↑
<i>512 samples</i>		
TFG	114.1	55.8
TFG + TAG (ours)	102.7	61.5
<i>50000 samples</i>		
TFG	77.5	54.3
TFG + TAG (ours)	47.1	84.4

Table R4: Evaluation with 50,000 samples on CIFAR-10. 100 inference steps.

Method	FID ↓	Acc. ↑
<i>Original Update Order</i>		
DPS + TAG	190.4	63.2
TFG + TAG	102.7	61.5
<i>Changed Update Order</i>		
DPS + TAG	203.5	60.1
TFG + TAG	116.4	54.1

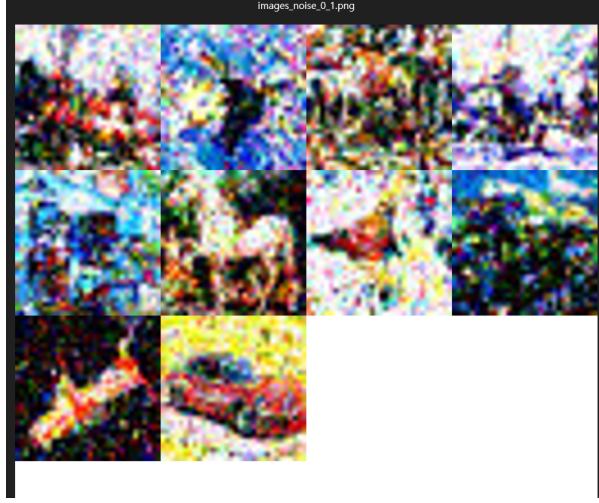
Table R5: Effect of original vs. changed update order for Algorithm 1 (TAG) on CIFAR-10.

	Training Steps	
	10K	30K
FID ↓	116.0	102.7
Acc. ↑	55.3	61.5

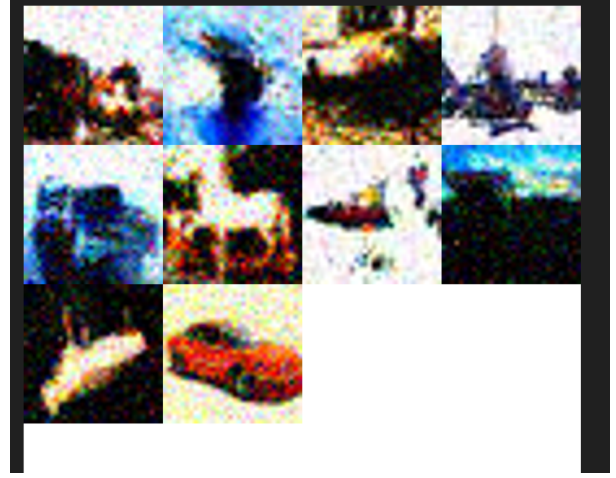
Table R6: Quantitative evaluation of TFG+TAG for varying training steps on CIFAR10.

Layers	W1 distance ↓
0 (No TAG)	6.458
1	1.716
2	1.681
3	1.975
4	1.714
5	1.713
6	1.788

Table R7: Robustness of time classifier network on toy experiment.



(a) Original images of corrupted reverse process.



(b) Images after applying TAG.

Figure R1: Comparison of images with different noise levels.

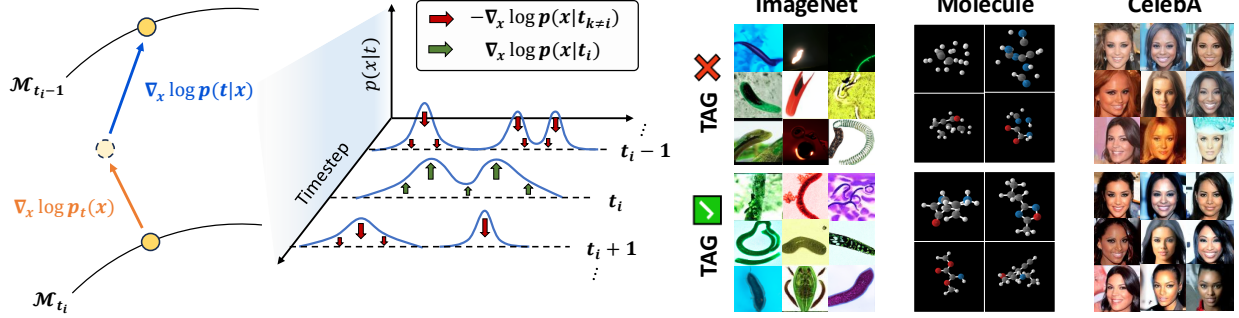


Figure R2: Overview of TAG algorithm. In the left figure, we specifically visualized the decomposition of $\nabla_x \log p(t_i|x)$ according to Eq. 11 in Lemma 3.3.

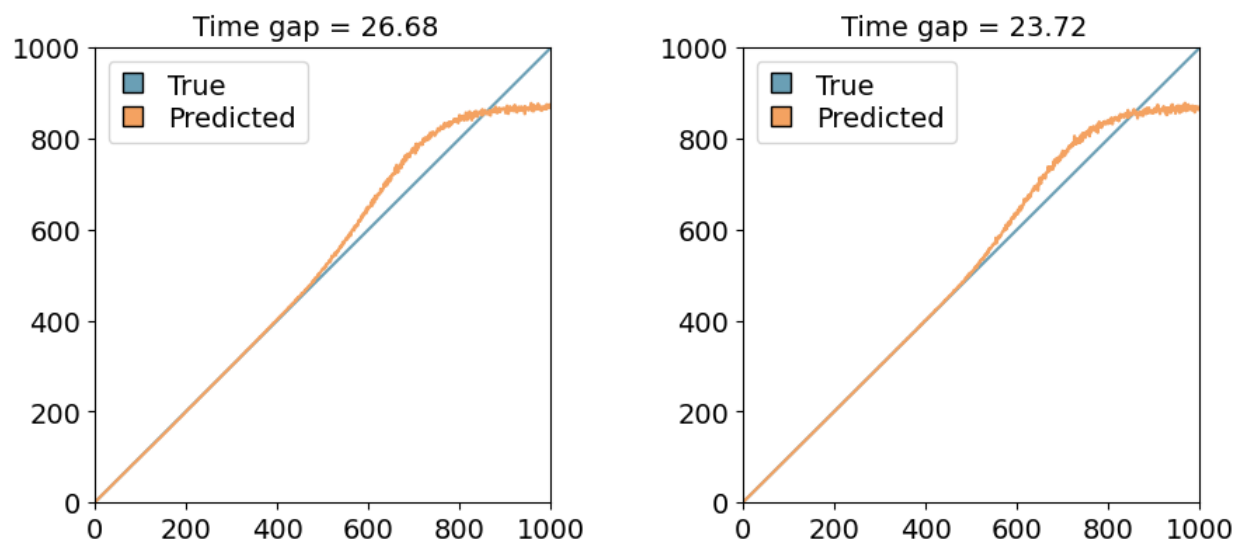


Figure R3: Time gap in CIFAR10. Training iterations are 10K (left) and 30K (right), respectively.

References

- [1] Han, D., et al. (2024). Understanding training-free diffusion guidance: Mechanisms and limitations. *arXiv:2403.12404*.
- [2] Ho, J., & Salimans, T. (2022). Classifier-Free Diffusion Guidance. *arXiv:2207.12598*.
- [3] He, Y., et al. (2024). CFG++: Manifold-constrained classifier-free guidance for diffusion models. *arXiv:2406.08070*.
- [4] Lin, C. H., et al. (2025). Diffusion models without classifier-free guidance. *arXiv:2502.12154*.
- [5] Shi, J., et al. (2023). Language-driven scene synthesis using multi-conditional diffusion model. *arXiv:2310.15948*.
- [6] Schneuing, A., et al. (2024). Inverse molecular design with multi-conditional diffusion guidance. *arXiv:2401.13858*.
- [7] Inference-time diffusion model distillation. (n.d.). *arXiv:2412.08871*.
- [8] Li, J., et al. (2023). On error propagation of diffusion models. *arXiv:2308.05021*.
- [9] Ning, Z., Li, W., He, D., & Zhang, L. (2023). Input perturbation reduces exposure bias in diffusion models. In *Proceedings of the International Conference on Machine Learning (ICML)* (arXiv:2301.11706).
- [10] Ning, Z., Li, W., He, D., & Zhang, L. (2024). Elucidating the exposure bias in diffusion models. In *Proceedings of the International Conference on Learning Representations (ICLR)* (arXiv:2308.15321).
- [11] Li, Z., Liu, J., & Zhang, L. (2024). Alleviating exposure bias in diffusion models through sampling with shifted time steps. In *Advances in Neural Information Processing Systems*.
- [12] Le, N. A. K., Nguyen, T., & Tran, A. T. (2024). Classification diffusion models: Revitalizing density ratio estimation. In *Proceedings of the Neural Information Processing Systems (NeurIPS)* (arXiv:2402.10095).
- [13] Song, Y., & Ermon, S. (2019). Generative modeling by estimating gradients of the data distribution. In *Proceedings of the Neural Information Processing Systems (NeurIPS)* (arXiv:1907.05600).
- [14] Ye, H., et al. (2024). TFG: Unified training-free guidance for diffusion models. *arXiv:2409.15761*.
- [15] Jung, H., Park, Y., Schmid, L., Jo, J., Lee, D., Kim, B., Yun, S.-Y., & Shin, J. (2024). Conditional synthesis of 3D molecules with time correction sampler. In *Advances in Neural Information Processing Systems*, 37.
- [16] Sadat, S., Kansy, M., Hilliges, O., & Weber, R. M. (2024). No training, no problem: Rethinking classifier-free guidance for diffusion models. *arXiv:2407.02687*.
- [17] Li, T., Luo, W., Chen, Z., Ma, L., & Qi, G. J. (2024). Self-guidance: Boosting flow and diffusion generation on their own. *arXiv:2412.05827*.

- [18] Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., & Poole, B. (2021). Score-based generative modeling through stochastic differential equations. In *Proceedings of the International Conference on Learning Representations (ICLR)*.
- [19] Zhang, L., & Agrawala, M. (2023). Adding conditional control to text-to-image diffusion models. In *Proceedings of the IEEE/CVF International Conference on Computer Vision (ICCV)*.
- [20] Chung, H., et al. (2022). Diffusion posterior sampling for general noisy inverse problems. *arXiv:2209.14687*.
- [21] Bhat, S. F., Mitra, N., & Wonka, P. (2024). Loosecontrol: Lifting ControlNet for generalized depth conditioning. In *ACM SIGGRAPH 2024 Conference Papers*, 1–11.
- [22] Lin, H., Cho, J., Zala, A., & Bansal, M. (2024). Ctrl-adapter: An efficient and versatile framework for adapting diverse controls to any diffusion model. *arXiv:2404.09967*.
- [23] Yang, J., Zhao, J., Wang, P., Wang, Z., & Liang, Y. (2025). Meta ControlNet: Enhancing task adaptation via meta learning. In *Proceedings of The Second Conference on Parsimony and Learning (Proceedings Track)*. Available at <https://openreview.net/forum?id=ju63pUpq0N>.
- [24] Rout, L., et al. (2025). RB-modulation: Training-free personalization of diffusion models using stochastic optimal control. In *Proceedings of the International Conference on Learning Representations (ICLR)* (arXiv:2405.17401).
- [25] Bar-Tal, O., et al. (2023). MultiDiffusion: Fusing diffusion paths for controlled image generation. In *Proceedings of the International Conference on Machine Learning (ICML)*.
- [26] Yu, J., Wang, Y., Zhao, C., Ghanem, B., & Zhang, J. (2023). FreeDoM: Training-free energy-guided conditional diffusion model. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*.
- [27] He, Y., Murata, N., Lai, C. H., Takida, Y., Uesaka, T., Kim, D., Liao, W. H., Mitsufuji, Y., Kolter, J. Z., Salakhutdinov, R., & Ermon, S. (2024). Manifold preserving guided diffusion (MPGD). In *Proceedings of the International Conference on Learning Representations (ICLR)*.
- [28] Du, Y., Mao, J., & Tenenbaum, J. B. (2024). Learning iterative reasoning through energy diffusion. *arXiv preprint arXiv:2406.11179*.