

Supplementary Material of On Exact Inversion of DPM-Solvers

Seongmin Hong¹, Kyeonghyun Lee¹, Suh Yoon Jeon¹, Hyewon Bae¹, Se Young Chun^{1,2,*}

¹Dept. of ECE, ²INMC & IPAI, Seoul National University, Republic of Korea

{smhongok, litiphysics, euniejeon, hyewon0309, sychun}@snu.ac.kr

Project page: <https://smhongok.github.io/inv-dpm.html>

S1. Convergence analysis

S1.1. Forward step method (Alg. 1)

Proposition S1 Convergence guarantee of Alg.1. *Let $\omega \geq 1$, t_{i-1} , C , and \emptyset be appropriate inputs for*

$$\mathbf{x}_\theta(\cdot, t_{i-1}) = \omega \bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, C) - (1 - \omega) \bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, \emptyset). \quad (\text{S1})$$

If $\bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, C)$ is monotone and L -Lipschitz with $L \leq \frac{1}{\omega} \frac{\sigma_{t_i}}{\sigma_{t_{i-1}} \alpha_{t_i} (e^{-h_i} - 1)}$, then the forward step method converges for all step size ρ such that

$$0 < \rho < 2 \frac{\sigma_{t_i}/\sigma_{t_{i-1}} - \alpha_{t_i} (e^{-h_i} - 1) \omega L}{(\sigma_{t_i}/\sigma_{t_{i-1}} + \alpha_{t_i} (e^{-h_i} - 1) (|\omega| + |1 - \omega|) L)^2}. \quad (\text{S2})$$

To prove Proposition S1, we use the following Lemma S1 from page 5 in [S4] and :

Lemma S1. *Let $a, b \in \mathbb{R}$. If $f, g : \mathcal{X} \rightarrow \mathcal{Y}$ be L_f, L_g -Lipschitz continuous, respectively, then $af + bg$ is $|a|L_f + |b|L_g$ -Lipschitz continuous.*

Now we start the proof of Proposition S1.

Proof of Proposition S1. Define $A : \mathbb{R}^D \rightarrow \mathbb{R}^D$ where

$$A(\mathbf{z}) := \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \mathbf{z} - \alpha_{t_i} (e^{-h_i} - 1) \mathbf{z}_\theta(\mathbf{z}, t_{i-1}) - \hat{\mathbf{z}}_{t_i} \quad (\text{S3})$$

for all feasible $\mathbf{z} \in \mathbb{R}^D$, so that the forward step method be written as

$$\hat{\mathbf{z}}_{t_{i-1}} = \hat{\mathbf{z}}_{t_{i-1}} - \rho A(\hat{\mathbf{z}}_{t_{i-1}}). \quad (\text{S4})$$

For all feasible \mathbf{z} and $\mathbf{z}' \in \mathbb{R}^D$,

$$\begin{aligned} \|A(\mathbf{z}) - A(\mathbf{z}')\| &= \left\| \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} (\mathbf{z} - \mathbf{z}') \right. \\ &\quad \left. - \alpha_{t_i} (e^{-h_i} - 1) (\mathbf{z}_\theta(\mathbf{z}, t_{i-1}) - \mathbf{z}_\theta(\mathbf{z}', t_{i-1})) \right\| \quad (\text{S5}) \\ &\leq \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \|\mathbf{z} - \mathbf{z}'\| \\ &\quad + \alpha_{t_i} (e^{-h_i} - 1) \|\mathbf{z}_\theta(\mathbf{z}, t_{i-1}) - \mathbf{z}_\theta(\mathbf{z}', t_{i-1})\|. \end{aligned}$$

holds by the triangle inequality. Using Lemma S1 and the assumption of Proposition S1, $\mathbf{z}_\theta(\cdot, t_{i-1})$ is $(|\omega| + |1 - \omega|)L$ -Lipschitz continuous. Thus, we have

$$\begin{aligned} \|A(\mathbf{z}) - A(\mathbf{z}')\| &\leq \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \|\mathbf{z} - \mathbf{z}'\| \\ &\quad + \alpha_{t_i} (e^{-h_i} - 1) (|\omega| + |1 - \omega|) L \|\mathbf{z} - \mathbf{z}'\| \\ &= \left(\frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} + \alpha_{t_i} (e^{-h_i} - 1) (|\omega| + |1 - \omega|) L \right) \|\mathbf{z} - \mathbf{z}'\|. \quad (\text{S6}) \end{aligned}$$

Equation (S4) converges if A is β -cocoercive and $\rho \in (0, 2\beta)$ [page 39 in [S4]]. So we should check the cocoercivity of A as follows:

$$\begin{aligned} \langle A(\mathbf{z}) - A(\mathbf{z}'), \mathbf{z} - \mathbf{z}' \rangle &= \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \|\mathbf{z} - \mathbf{z}'\|_2^2 \\ &\quad - \alpha_{t_i} (e^{-h_i} - 1) \left(\right. \\ &\quad \left. \omega \langle \bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, C) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, C), \mathbf{z} - \mathbf{z}' \rangle \right. \\ &\quad \left. + (1 - \omega) \langle \bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, \emptyset) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, \emptyset), \mathbf{z} - \mathbf{z}' \rangle \right). \quad (\text{S7}) \end{aligned}$$

Since $\bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, C)$ is monotone, $\langle \bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, C) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, C), \mathbf{z} - \mathbf{z}' \rangle \geq 0$ and $\langle \bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, \emptyset) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, \emptyset), \mathbf{z} - \mathbf{z}' \rangle \geq 0$ holds. Because $\omega \geq 1$,

$$\begin{aligned} \langle A(\mathbf{z}) - A(\mathbf{z}'), \mathbf{z} - \mathbf{z}' \rangle &\geq \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \|\mathbf{z} - \mathbf{z}'\|_2^2 - \alpha_{t_i} \\ &\quad \cdot (e^{-h_i} - 1) \omega \langle \bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, C) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, C), \mathbf{z} - \mathbf{z}' \rangle. \quad (\text{S8}) \end{aligned}$$

*Corresponding author

By the Cauchy-Schwarz inequality,

$$\begin{aligned} & \langle \bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, C) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, C), \mathbf{z} - \mathbf{z}' \rangle \\ & \leq \|\mathbf{z} - \mathbf{z}'\|_2 \|\bar{\mathbf{x}}_\theta(\mathbf{z}, t_{i-1}, C) - \bar{\mathbf{x}}_\theta(\mathbf{z}', t_{i-1}, C)\|_2 \quad (\text{S9}) \\ & \leq L \|\mathbf{z} - \mathbf{z}'\|_2^2, \end{aligned}$$

where the second inequality holds because $\bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, C)$ is L -Lipschitz. Merging Eq. (S6), Eq. (S8) and Eq. (S9), we have

$$\begin{aligned} & \langle A(\mathbf{z}) - A(\mathbf{z}'), \mathbf{z} - \mathbf{z}' \rangle \\ & \geq \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \|\mathbf{z} - \mathbf{z}'\|_2^2 - \alpha_{t_i} (e^{-h_i} - 1) \omega L \|\mathbf{z} - \mathbf{z}'\|_2^2 \\ & = \left(\frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} - \alpha_{t_i} (e^{-h_i} - 1) \omega L \right) \|\mathbf{z} - \mathbf{z}'\|_2^2 \\ & \geq \frac{\left(\frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} - \alpha_{t_i} (e^{-h_i} - 1) \omega L \right) \|A(\mathbf{z}) - A(\mathbf{z}')\|_2^2}{\left(\frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} + \alpha_{t_i} (e^{-h_i} - 1) (|\omega| + |1 - \omega|) L \right)^2}, \quad (\text{S10}) \end{aligned}$$

which indicates A is $\frac{\sigma_{t_i}/\sigma_{t_{i-1}} - \alpha_{t_i}(e^{-h_i} - 1)\omega L}{(\sigma_{t_i}/\sigma_{t_{i-1}} + \alpha_{t_i}(e^{-h_i} - 1)(|\omega| + |1 - \omega|)L)^2}$ -cocoercive. \square

S1.2. Notes on instability of fixed point iteration in large classifier-free guidance

In Section 4.1 of the main paper, we explained why the fixed point iteration (FPI)-based method [S2] loses stability in the context of large classifier-free guidance. Here, we formulate and prove this as Proposition S2. Proposition S2 suggests that FPI may not converge when the classifier-free guidance is large.

Proposition S2 Instability of FPI in large classifier-free guidance. Let $\omega \geq 1$, t_{i-1} , C , and \emptyset be appropriate inputs for

$$\mathbf{x}_\theta(\cdot, t_{i-1}) = \omega \bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, C) - (1 - \omega) \bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, \emptyset). \quad (\text{S11})$$

If $\bar{\mathbf{x}}_\theta(\cdot, t_{i-1}, C)$ is Lipschitz continuous with the constant

$$\frac{1}{|\omega| + |1 - \omega|} \cdot \frac{\sigma_{t_i}}{\sigma_{t_{i-1}} \alpha_{t_i} (e^{-h_i} - 1)}, \quad (\text{S12})$$

then

$$F(\cdot) := \frac{\sigma_{t_{i-1}}}{\sigma_{t_i}} \alpha_{t_i} (e^{-h_i} - 1) \mathbf{x}_\theta(\cdot, t_{i-1}) + \frac{\sigma_{t_{i-1}}}{\sigma_{t_i}} \hat{\mathbf{x}}_{t_i} \quad (\text{S13})$$

is nonexpansive (i.e., 1-Lipschitz continuous).

Proof of Proposition S2. By the assumption, Eq. (S11) and Lemma S1, $\mathbf{x}_\theta(\cdot, t_{i-1})$ is $\frac{\sigma_{t_i}}{\sigma_{t_{i-1}} \alpha_{t_i} (e^{-h_i} - 1)}$ -Lipschitz continuous. By Eq. (S13) and Lemma S1, $F(\cdot)$ is nonexpansive. \square

Proposition S1 also suggests our method has more generous Lipschitz condition for converge than [20]: $\frac{1}{\omega} \frac{\sigma_{t_i}}{\sigma_{t_{i-1}} \alpha_{t_i} (e^{-h_i} - 1)} > \frac{1}{|\omega| + |1 - \omega|} \frac{\sigma_{t_i}}{\sigma_{t_{i-1}} \alpha_{t_i} (e^{-h_i} - 1)}$.

S2. Algorithm 2

Algorithm 2 Inversion of DPM-Solver++(2M)

Require: initial value \mathbf{x}_0 , time steps $\{t_i\}_{i=0}^M$, data prediction model \mathbf{z}_θ , UPDATE, \mathcal{D}^\dagger in ??.

- 1: Denote $h_i := \lambda_{t_i} - \lambda_{t_{i-1}}$ and $r_i := \frac{h_i - 1}{h_i}$ for $i = 1, \dots, M$.
 - 2: $\hat{\mathbf{z}}_{t_M} \leftarrow \mathcal{D}^\dagger(\mathbf{x}_0)$ **if** LDM **else** \mathbf{x}_0
 - 3: **for** $i \leftarrow M$ **to** 2 **do** $\hat{\mathbf{y}}_{t_i} \leftarrow \hat{\mathbf{z}}_{t_i}$
 - 4: **for** $j \leftarrow 1$ **to** $2J$ **do**
 - 5: $\hat{\mathbf{y}}_{t_{i-j/J}} \leftarrow \frac{\sigma_{t_{i-j/J}}}{\sigma_{t_{i-(j-1)/J}}} (\hat{\mathbf{y}}_{t_{i-j/J}} + \alpha_{t_{i-j/J}} (e^{-h_{i-j/J}} - 1) \mathbf{z}_\theta(\hat{\mathbf{y}}_{t_{i-(j-1)/J}, t_{i-j/J}}))$
 - 6: **end for**
 - 7: $\hat{\mathbf{z}}_{t_{i-1}} \leftarrow \hat{\mathbf{y}}_{t_{i-1}}$
 - 8: **repeat**
 - 9: $\mathbf{d}'_i \leftarrow \mathbf{z}_\theta(\hat{\mathbf{z}}_{t_{i-1}}, t_{i-1}) + \frac{1}{2r_i} (\mathbf{z}_\theta(\hat{\mathbf{y}}_{t_{i-1}}, t_{i-1}) - \mathbf{z}_\theta(\hat{\mathbf{y}}_{t_{i-2}}, t_{i-2}))$
 - 10: $\mathbf{z}'_{t_i} \leftarrow \frac{\sigma_{t_i}}{\sigma_{t_{i-1}}} \hat{\mathbf{z}}_{t_{i-1}} - \alpha_{t_i} (e^{-h_i} - 1) \mathbf{d}'_i$
 - 11: UPDATE($\hat{\mathbf{z}}_{t_{i-1}}; \hat{\mathbf{z}}_{t_i}, \mathbf{z}'_{t_i}$)
 - 12: **until** converged
 - 13: **end for**
 - 14: $\hat{\mathbf{z}}_{t_0} \leftarrow \frac{\sigma_{t_0}}{\sigma_{t_1}} (\hat{\mathbf{z}}_{t_1} + \alpha_{t_1} (e^{-h_1} - 1) \mathbf{z}_\theta(\hat{\mathbf{z}}_{t_1}, t_0))$
 - 15: **repeat**
 - 16: $\mathbf{z}'_{t_1} \leftarrow \frac{\sigma_{t_1}}{\sigma_{t_0}} \hat{\mathbf{z}}_{t_0} - \alpha_{t_1} (e^{-h_1} - 1) \mathbf{z}_\theta(\hat{\mathbf{z}}_{t_0}, t_0)$
 - 17: UPDATE($\hat{\mathbf{z}}_{t_0}; \hat{\mathbf{z}}_{t_1}, \mathbf{z}'_{t_1}$)
 - 18: **until** converged
 - 19: **return** $\hat{\mathbf{z}}_{t_0}$
-

S3. Experimental details

S3.1. Reconstruction

S3.1.1 Pixel-space DPM

For pixel-space DPM, we used gradient descent without momentum, with l_2 loss and a learning rate of 0.1. To dynamically adjust the learning rate, when the minimum loss for the last 5 iterations did not improve, the learning rate was halved, but not below a minimum of 0.001. The number of iterations was a maximum of 500. The convergence criterion was $\|\mathbf{x}'_{t_i} - \hat{\mathbf{x}}_{t_i}\|_2 < 10^{-3}$. The original model operates in half float (i.e., 16-bit), so it was used as is during gradient descent. We used $J = 100$ in Algorithm 2. We experimented with 100 images.

S3.1.2 Latent diffusion model (LDM)

For LDM, we generated images with classifier-free guidance of 3.0, and the same prompt was employed for the inversion process. We used the forward step method, with l_2 loss. The initial step size was set as 0.5 for Algorithm 1, and $10/t$ for Algorithm 2 except for the first step ($t = 0$) where it was 1. To dynamically adjust the step size, when the minimum loss for the last 20 iterations did not improve,

the step size was halved. For numerical stability, we applied a 20-step warmup (*i.e.*, linearly increasing the step size from 0). We used $J = 10$ in Algorithm 2. The number of iterations was a maximum of 500. The convergence criterion was $\|z'_{t_i} - \hat{z}_{t_i}\|_2 < 10^{-3}$. Every operation was held in float (*i.e.*, 32-bit). We experimented with 100 images.

Decoder inversion We applied decoder inversion for every method for a fair comparison, including naïve DDIM inversion and [S2]. We used Adam with l_2 loss and a learning rate of 0.1. For improved convergence, we applied a cosine learning rate scheduler with 10-step warmup within a total of 100 iterations.

S3.2. Application: Tree-ring watermark

The work of tree-ring watermark in [S5] injects a watermark in the frequency domain of noise and then generates an image with noise obtained by inverse transformation. We tested on detection of watermarks by generating various types of watermarks with the same radius and calculated l_1 difference between the original watermark and the watermark obtained by inversion. The radius was set the same to make the comparison consistent and detection difficult. We tested on three watermarks with the shape of a tree-ring and a radius of 6 pixels. For watermark creation, we set a constant and designated pixel values to be random but close to constant to make the difference scale reliable.

S3.3. Application: Background-preserving editing

In this experiment, we employed the open-source code of [S3] to compare Algorithm 1 with three other methods: (i) The original code utilizing the latents stored during the generating process (*i.e.*, oracle), (ii) the naïve DDIM inversion, and (iii) the naïve DDIM inversion with decoder inversion. We used classifier-free guidance of 7.5 and for decoder inversion, we applied a cosine learning rate scheduler with 50-step warmup within a total of 500 iterations. All other experimental settings remained identical to those of LDM.

S4. Additional results

S4.1. Reconstruction

In Sec. 5.1 of the main paper, we performed the reconstruction of noise and image to evaluate the exact invertibility of the proposed methods. We provide more qualitative results in Fig. S1. In Fig. S1, we additionally provide the FPI-based method of Pan et al. [S2], namely AIDI-E.

S4.2. Application: Tree-ring watermark

In Sec. 5.2 of the main paper, we demonstrated the improved detection of watermarks [S5] by employing our algorithm, even when the images were generated using high-order DPM-solvers. We provide an additional example of

watermark detection / classification in Figs. Fig. S2 and Fig. S3. We experimented with different shaped watermarks and prompts from the main paper.

S4.3. Application: Background-preserving editing

In Sec. 5.3 of the main paper, we experimentally demonstrated our proposed methods enable the background-preserving editing, without the need for the original latents. In Figs. S4 and S5, we show additional results with different prompts.

References

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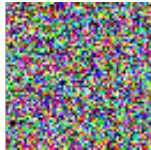
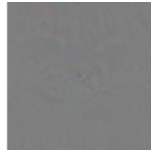
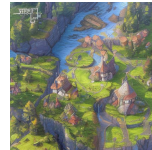
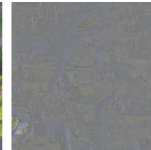
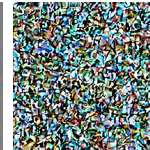
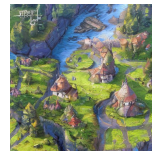
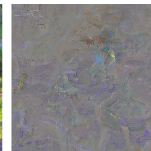
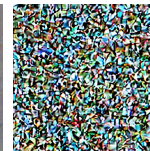
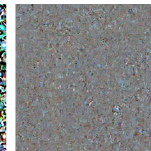




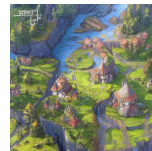
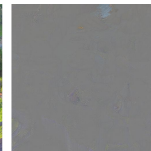
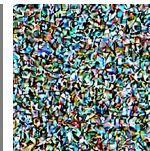
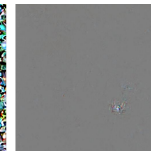


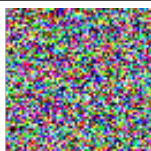
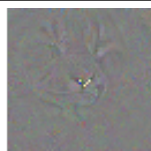
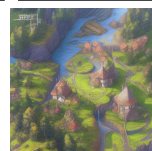
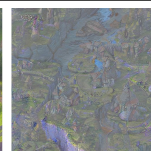
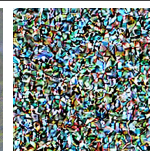
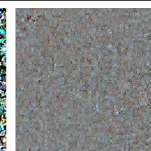



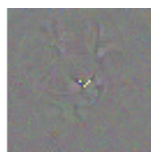
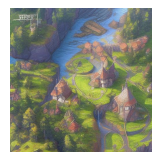
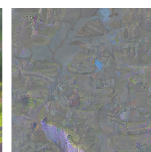
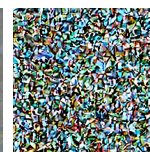
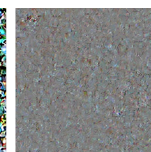

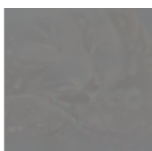

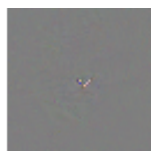
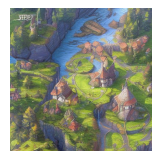
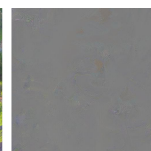

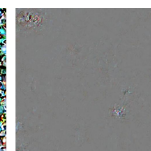
Generation Inversion	Pixel-space DPM				LDM			
	Image (Recon. / Error $\times 2$)		Noise (Recon. / Error $\times 2$)		Image (Recon. / Error $\times 3$)		Noise (Recon. / Error $\times 2$)	
	DDIM 50 steps naïve / 1000							
DDIM 50 steps FPI [S2] / 50								
Alg. 1 / 50								
DPM-Solver++(2M) 10 steps naïve / 1000								
DPM-Solver++(2M) 10 steps Alg. 1 / 50								
DPM-Solver++(2M) 10 steps Alg. 2 / 10								

Figure S1. Our Algs. 1 and 2 significantly reduce reconstruction errors, whether it's for images or noise, DDIM or high-order DPM-solvers, or pixel-space DPM or LDM. The generation / inversion method varies for each row, *e.g.*, 'naïve / 1000' indicates that we performed the naïve DDIM inversion for 1000 steps. 'Alg. 1 / 50' and 'Alg. 2 / 10' attempt exact inversion with 50 steps of DDIM and 10 steps of DPM-Solver++(2M), respectively. Achieving exact inversion in LDM is challenging due to information loss from the autoencoder and instability caused by a classifier-free guidance of 3.0. Nonetheless, our algorithm produces good results (extremely low residual error in Alg. 1 for DDIM on the 3rd row and in Alg. 2 for DPM-solver++(2M) on the 6th row) also in LDM.

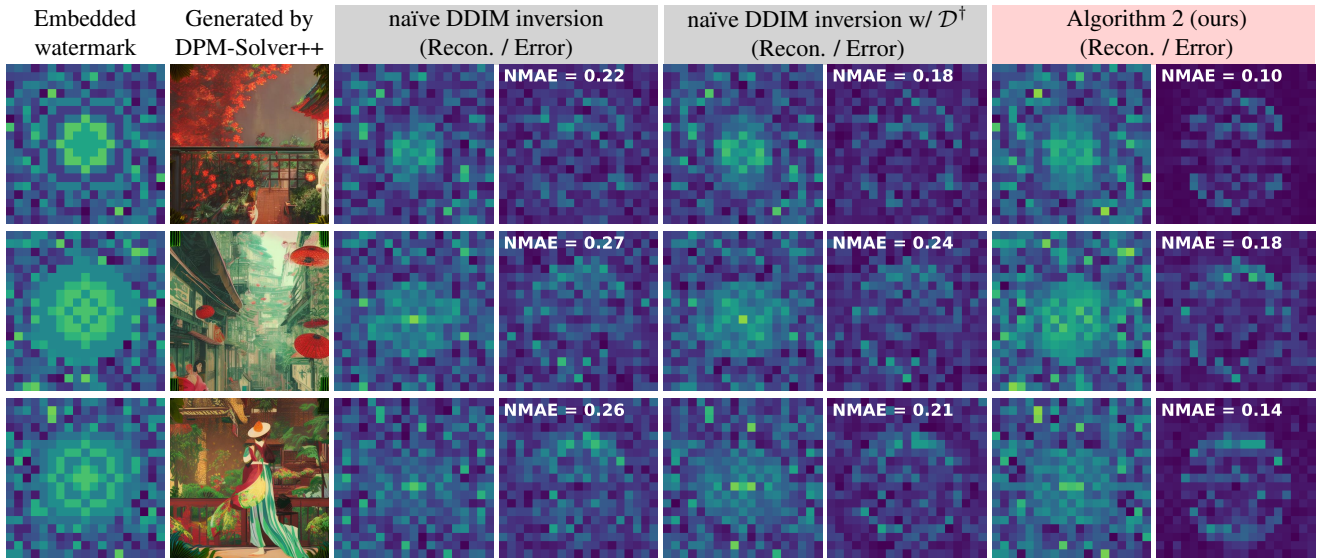


Figure S2. Our Algorithm 2 enables accurate reconstruction of Tree-ring watermarks [S5] in the Fourier space of the initial noise (z_T). The Tree-ring watermark is embedded in the Fourier space of the initial noise in the shape of tree-rings and can be utilized for copyright tracing (column 1). Then, the image is generated starting from the watermarked noise. The practical approach is to accelerate image generation using methods like DPM-Solver++(2M) [S1] (column 2). NMAEs are shown on each error map. Using Algorithm 2 (columns 7-8) for watermark reconstruction results in lower errors compared to employing naïve DDIM inversion (columns 3-6), achieving nearly 50% reduction in NMAE.

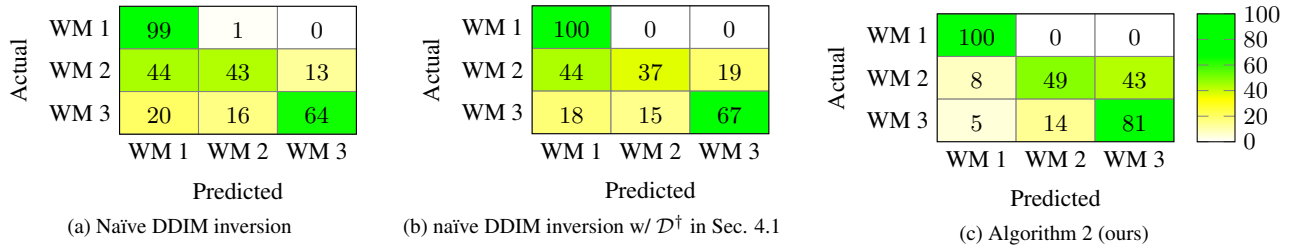


Figure S3. Our algorithm’s strong reconstruction performance allows for the classification of tree-ring watermarks as well. For copyright tracing, it is possible to generate images by embedding different unique watermarks. Three distinct watermarks (WM 1,2, and 3) are displayed in the first column of Fig. S2. In the confusion matrices, ‘Predicted’ corresponds to the watermark with the smallest l_1 difference among the three watermarks. In Figs. S3a and S3b, the naïve DDIM inversion encounters difficulties in detecting WM 2. In contrast (Fig. S3c), our Algorithm 2 performs well in detecting WM 2.

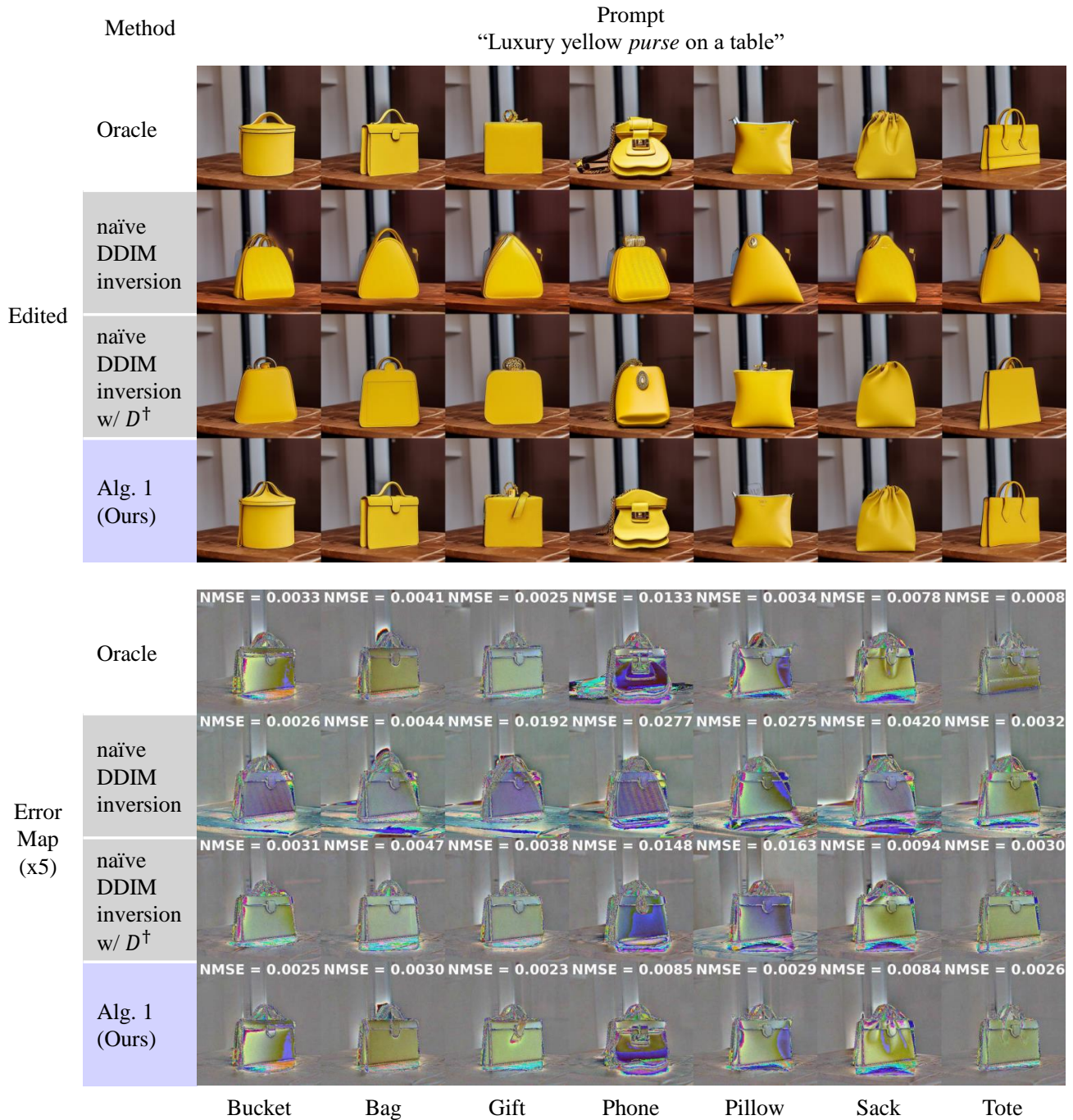


Figure S4. Additional experiment result on background-preserving editing. The *emphasized* word indicates the object changed in the generated image, replaced with different words at the bottom of the figure (e.g., *purse* becomes ‘bucket’). Our Alg. 1 preserves the background and allows diverse editing, even when the original image’s path is unknown (i.e., $(z_t)_{i=0}^M$). The first row (Oracle) shows results with the full trajectory, while subsequent rows use only the generated image (i.e., x_0). In these cases, we estimate the trajectory through each inversion method and edit based on the inversion results. Estimating the original trajectory using the basic DDIM inversion (rows 2-3) fails to keep the background (background in the error map is not gray) compared to the Oracle and doesn’t consistently edit the ‘purse’ as prompted. In contrast, using our Alg. 1 (row 4) preserves the background similarly to the Oracle (with the background in the error map being gray) while consistently editing the ‘purse’ as prompted. Background NMSEs are inset.

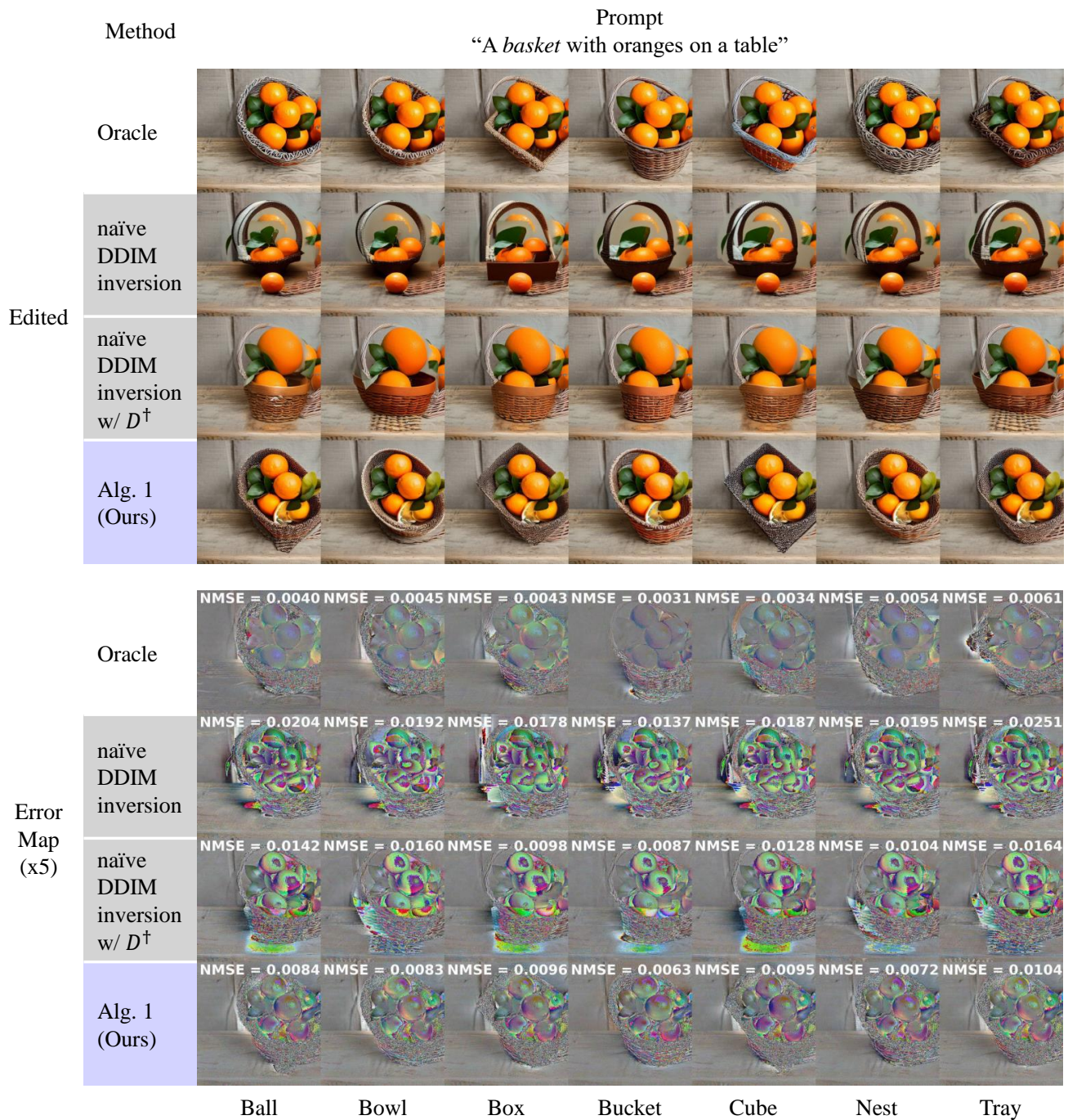


Figure S5. Additional experiment result on background-preserving editing using prompt "A basket with oranges on a table". This experiment has the same setting with Fig. S4. As we attempt to edit the *basket*, the oranges should be treated as part of the background and should not be changed. Our Alg. 1 (row 4) preserves the oranges well, similar to the Oracle (row 1). In contrast, the naïve DDIM inversion indicates significant changes to the appearance of oranges (rows 2-3).