# ENHANCING DIFFUSION POSTERIOR SAMPLING FOR INVERSE PROBLEMS BY INTEGRATING CRAFTED MEASUREMENTS

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## Abstract

Diffusion models have emerged as a powerful foundation model for visual generation. With an appropriate sampling process, it can effectively serve as a generative prior to solve general inverse problems. Current posterior sampling based methods take the measurement (i.e., degraded image sample) into the posterior sampling to infer the distribution of the target data (i.e., clean image sample). However, in this manner, we show that high-frequency information can be prematurely introduced during the early stages, which could induce larger posterior estimate errors during the restoration sampling. To address this issue, we first reveal that forming the log posterior gradient with the noisy measurement ( i.e., samples from a diffusion forward process) instead of the clean one can benefit the reverse process. Consequently, we propose a novel diffusion posterior sampling method DPS-CM, which incorporates a Crafted Measurement (i.e., samples generated by a reverse denoising process, compared to random sampling with noise in standard methods) to form the posterior estimate. This integration aims to mitigate the misalignment with the diffusion prior caused by cumulative posterior estimate errors. Experimental results demonstrate that our approach significantly improves the overall capacity to solve general and noisy inverse problems, such as Gaussian deblurring, super-resolution, inpainting, nonlinear deblurring, and tasks with Poisson noise, relative to existing approaches.

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## 1 INTRODUCTION

034 Diffusion models (Ho et al., 2020) have achieved remarkable generative performance on images (Amit et al., 2021; Baranchuk et al., 2021; Brempong et al., 2022), videos (Singer et al., 2022; Wu 035 et al., 2023), audios (Popov et al., 2021; Yang et al., 2023a), natural language (Austin et al., 2021; Hoogeboom et al., 2021; Li et al., 2022) and molecular generation (Hoogeboom et al., 2022; Jing 037 et al., 2022). Besides its strong modeling capacity for complex and high dimensional data, diffusion models have exhibited a strong generative prior to form the diffusion conditional sampling (Song et al., 2020) that can be harnessed for diffusion posterior sampling. In the context of noisy inverse 040 problems, this sampling process effectively approximates precise data distributions from noisy and 041 degraded measurements. Noisy inverse problems, such as super-resolution, inpainting, linear and 042 nonlinear deblurring, are targeted to restore an unknown image x from its noise corrupted mea-043 surement y given the corresponding forward measurement operators  $\mathcal{A}(\cdot): \mathbb{R}^n \to \mathbb{R}^m$ . Recently, 044 Diffusion models have been extensively utilized for these tasks (Zhu et al., 2023; Song et al., 2022; Wang et al., 2022), offering a robust framework for reconstructing high-quality images from degraded measurements. 046

Current diffusion-based methods generally employ two distinct strategies to solve inverse problems. The first strategy is to train problem-specialized diffusion models (Saharia et al., 2022; Whang et al., 2022; Luo et al., 2023; Chan et al., 2023) given measurements and clean image pairs. In contrast, methods of the second strategy only capitalize on problem-agnostic pre-trained diffusion models to benefit the zero-shot diffusion restoration sampling by posterior estimate (Song et al., 2023; Rout et al., 2024; Peng et al., 2024; Mardani et al., 2023) or enforcing data consistency (Chung et al., 2022b). In this paper, we concentrate on the second manner, posterior estimate for sampling, to solve noisy inverse problems universally. 054 Posterior estimate based methods enable controllable generations (Dhariwal & Nichol, 2021) via diffusion conditional reverse-time SDE (Song et al., 2020), such as classifier guidance (Dhariwal & 056 Nichol, 2021), loss-guided diffusion (Song et al., 2023b). Applying Bayesian, the gradient of log 057 posterior  $\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t \mid \boldsymbol{y})$  can be easily adopted into conditional reverse-time SDE sampling as a log likelihood gradient term  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \boldsymbol{x}_t)$  and an unconditional prior term  $\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t)$ . In the context of solving inverse problems, however,  $p(y | x_t)$  is an intractable distribution due to the unclear dependency between the measurement y and the diffusion generation  $x_t$  at time t. To tackle 060 this issue, existing posterior estimate methods for inverse problems, such as Diffusion Posterior 061 Sampling (DPS (Chung et al., 2022a)), form the measurement model  $p(\mathbf{y} \mid \hat{\mathbf{x}}_0)$  as the likelihood 062 estimate, where  $\hat{x}_0$  is the denoising prediction given diffusion intermediate output  $x_t$ . This process 063 maps  $\hat{x}_0$  into the measurement y's space, which can be interpreted as a reconstruction loss guidance 064 to push  $\mathcal{A}(\hat{x}_0)$  close to y, while narrowing the gap between  $x_t$  and the clean image x. 065

However, via empirical examples in Section 3.1, we show that solving inverse problems in the man-066 ner of diffusion posterior sampling follows a similar pattern of diffusion reverse process (Yang et al., 067 2023b), i.e., focusing on low-frequency recovery at first and posing increasing attention on high-068 frequency generation in the late stages. With such observation, the log posterior gradient estimate 069  $\nabla_{\boldsymbol{x}_{\star}} \log p(\boldsymbol{y} \mid \hat{\boldsymbol{x}}_{0})$  in DPS with sharp measurement  $\boldsymbol{y}$  will easily introduce abrupt high-frequency gradient signals for the subsequent step, which unfits the appropriate input pattern for the pre-trained 071 model  $s_{\theta}(x_t, t)$  during the early stages with large t. In fact, Song et al. (2023b) also note that DPS 072 significantly miscalculates the scale of the guidance term with different variance levels which re-073 sults in accumulated errors in posterior sampling. In Section 3.1, we have the similar observations 074 that DPS amplifies posterior sampling errors. We also find that applying the likelihood estimate 075  $p(y_t \mid \hat{x}_0)$  with randomly sampled **noisy measurement**  $y_t$  instead of the clean measurement y in DPS for each timestep t leads to a smaller approximation error during the early stages, and thus ben-076 efits the restoration generation. Posterior approximation with **noisy measurement**  $y_t$  at timestep t, 077 compared with the clean one, has the advantage that it adaptively matches the frequency pattern of 078 the diffusion model's generation at the timestep t. 079

080 Therefore, with this insight, we propose the posterior approximation that leads to less high-081 frequency signal recovery during the early stages. Specifically, we propose the Diffusion Posterior Sampling with Crafted Measurements (DPS-CM), which can introduce less biased posterior es-082 timate by combining crafted measurement  $y_t$ , the intermediate generation of another diffusion 083 reverse-time trajectory  $\{\mathbf{y}_t\}_{t=0}^T$  from posterior  $p(\mathbf{y}_t \mid \mathbf{y})$ . As  $\{\mathbf{y}_t\}_{t=0}^T$  shares a similar frequency 084 distribution pattern with the target generation trajectory  $\{x_t\}_{t=0}^T$ , i.e., low-frequency recovery at 085 first, the approximated log likelihood gradient  $\nabla_{x_t} \log p(\hat{y}_0 \mid \hat{x}_0)$  will bring in less high-frequency gradient signal and thus benefit the subsequent generations. Besides, leveraging crafted measure**ments**  $y_t$  brings the lower bias compared with directly using randomly sampled **noisy measure**-880 **ment**  $y_t$ . Our extensive experiments results on various noisy linear inverse problems, e.g. superresolution, random masked/fixed box inpainting, Gaussian/Motion deblurring, and nonlinear inverse 090 problems such as nonlinear deblurring, demonstrate that the proposed DPS-CM significantly outper-091 forms existing unsupervised methods on both FFHQ (Karras et al., 2019) and ImageNet (Deng et al., 092 2009) datesets while keeping the algorithm simplicity.

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## 2 BACKGROUND

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## 2.1 DIFFUSION MODELS

Diffusion models (Ho et al., 2020; Song et al., 2020) comprise two processes: a forward noising process in which the noise is progressively injected into the sample and a reverse denoising process for generation. Specifically, the forward process of Denoising Diffusion Probabilistic Models (DDPM) (Ho et al., 2020) can be formulated by the variance preserving stochastic differential equation (VP-SDE) (Song et al., 2020):

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 $d\boldsymbol{x} = -\frac{\beta_t}{2}\boldsymbol{x}dt + \sqrt{\beta_t}d\boldsymbol{w}, \quad t \in [0,T],$ (1)

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where  $\{\beta_t\}_{t=0}^T$  is the designed noise schedule which is monotonically increased and w is the standard Wiener process. To generate samples of targeted data distribution from Gaussian noise

108  $x_T \sim \mathcal{N}(\mathbf{0}, I)$ , corresponding reverse SDE of Eq. 1 is formulated as:

$$d\boldsymbol{x} = \left[-\frac{\beta_t}{2}\boldsymbol{x} - \beta_t \nabla_{\boldsymbol{x}_t} \log p\left(\boldsymbol{x}_t\right)\right] dt + \sqrt{\beta_t} d\bar{\boldsymbol{w}},\tag{2}$$

where  $d\bar{w}$  is the reverse standard Wiener process and  $\nabla_{x_t} \log p(x_t)$  is the score function of denoised sample at time t. Approximating this score function is the key to solving the reverse generative process, which can be done by training a parameterized model  $s_{\theta}(x_t, t)$  by denoising score matching (Song & Ermon, 2019) expected on samples from the forward diffusion process:

$$\boldsymbol{x}_t = \sqrt{\bar{\alpha}_t} \boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{z}, \quad \boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I}).$$
 (3)

117 With trained score model  $s_{\theta}$ , applying Tweedie's formula (Efron, 2011; Dunn & Smyth, 2005), we 118 are able to approximate the mean  $\hat{x}_0$  of posterior  $p(x_0 | x_t)$  for the above case (VP-SDE) as:

$$\hat{\boldsymbol{x}}_{0} := \mathbb{E}\left[\boldsymbol{x}_{0} \mid \boldsymbol{x}_{t}\right] \simeq \frac{1}{\sqrt{\bar{\alpha}(t)}} \left(\boldsymbol{x}_{t} + (1 - \bar{\alpha}(t))\boldsymbol{s}_{\theta}\left(\boldsymbol{x}_{t}, t\right)\right). \tag{4}$$

## 2.2 SOLVING NOISY INVERSE PROBLEMS WITH DIFFUSION MODELS

Given a clean image  $x_0$  and a forward measurement operator  $\mathcal{A}(\cdot)$ , the general form of the noisy inverse problem can be stated as:

$$oldsymbol{y} = \mathcal{A}\left(oldsymbol{x}_{0}
ight) + oldsymbol{\eta}_{1}$$

127 where an i.i.d. noise  $\eta \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$  is added in  $\mathcal{A}(\mathbf{x}_0)$  in the case of Gaussian noise to formulate 128 the noisy inverse problem. Given measurements  $\mathbf{y} \in \mathbb{R}^m$  and a known forward measurement opera-129 tor  $\mathcal{A}(\cdot) : \mathbb{R}^n \to \mathbb{R}^m$ , the target is to restore the unknown signal  $\mathbf{x}_0 \in \mathbb{R}^n$ . Replacing unconditional 130 score  $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$  in Eq. 2 with the conditional score  $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y})$  paves the way for solving 131 inverse problems using diffusion models. Applying the Bayesian rule on the gradient of posterior 132  $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y})$ , the reverse-time SDE of the posterior sampling is given by:

$$d\boldsymbol{x} = \left[-\frac{\beta_t}{2}\boldsymbol{x} - \beta_t \left(\nabla_{\boldsymbol{x}_t} \log p\left(\boldsymbol{x}_t\right) + \nabla_{\boldsymbol{x}_t} \log p\left(\boldsymbol{y} \mid \boldsymbol{x}_t\right)\right)\right] dt + \sqrt{\beta_t} d\bar{\boldsymbol{w}}.$$
 (5)

However, the gradient of the log likelihood  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \boldsymbol{x}_t)$  in Eq. 5 is intractable given  $\boldsymbol{y} = \mathcal{A}(\boldsymbol{x}_0) + \boldsymbol{\eta}$ . DDRM (Kawar et al., 2022) addresses this issue by forming the conditional sampling in the spectral space without dealing with  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \boldsymbol{x}_t)$ , but with the restriction to handle complex inverse problems due to the SVD computation efficiency. DPS (Chung et al., 2022a) provides a universal posterior approximation approach to deal with the intractable likelihood term  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \boldsymbol{x}_t)$ . Given mean estimate  $\hat{\boldsymbol{x}}_0$  of posterior  $\mathbb{E}[\boldsymbol{x}_0 \mid \boldsymbol{x}_t]$  by applying Eq.4, DPS assumes:

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$$p(\boldsymbol{y} \mid \boldsymbol{x}_t) = \mathbb{E}_{\boldsymbol{x}_0 \sim p(\boldsymbol{x}_0 \mid \boldsymbol{x}_t)} \left[ p(\boldsymbol{y} \mid \boldsymbol{x}_0) \right]$$
$$\simeq p(\boldsymbol{y} \mid \hat{\boldsymbol{x}}_0).$$

As the production, they form the gradient of the posterior as:

$$abla_{oldsymbol{x}_t} \log p_t\left(oldsymbol{x}_t \mid oldsymbol{y}
ight) \simeq oldsymbol{s}_{ heta^*}\left(oldsymbol{x}_t,t
ight) - 
ho 
abla_{oldsymbol{x}_t} \left\|oldsymbol{y} - \mathcal{A}\left(\hat{oldsymbol{x}}_0
ight)
ight\|_2^2$$

Although DPS provides a straightforward and task-independent approximation, many existing works, such as Peng et al. (2024); Song et al. (2023b), point out this posterior estimate is biased.

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# 3 METHOD: DIFFUSION POSTERIOR SAMPLING WITH CRAFTED MEASUREMENTS

152 We propose DPS-CM, which perform diffusion posterior sampling from  $p(\mathbf{x}_t | \mathbf{y}_t)$  with **Crafted Measurement**  $\mathbf{y}_t$  belonging to another diffusion reverse trajectory  $\{\mathbf{y}_t\}_{t=0}^T$  instead of the vanilla 153 154 input y. Specifically, applying Eq.4 on  $x_t$  and  $y_t$ , we incorporate the tractable  $p(\hat{y}_0 | \hat{x}_0)$  as the 155 likelihood approximation of  $p(\mathbf{y}_t \mid \mathbf{x}_t)$  to enable the posterior sampling from  $p(\mathbf{x}_t \mid \mathbf{y}_t)$ . DPS-156 CM can be interpreted as pushing the bond between two noisy approximation  $\hat{y}_0$  and  $\hat{x}_0$  as the 157 measurement model  $\hat{\mathbf{y}}_0 = \mathcal{A}(\hat{x}_0)$ . While  $\hat{\mathbf{y}}_0$  is progressively recovered to the input measurement y 158 via its diffusion denoising process,  $\hat{x}_0$  is expected to develop into the target ground truth x gradually 159 during the synchronous reverse process with the measurement bond  $\hat{\mathbf{y}}_0 = \mathcal{A}(\hat{\mathbf{x}}_0)$ . In Section 3.1, we explore the advantage of posterior sampling utilizing noisy measurements  $y_t$  sampled from the 160 diffusion forward process over using the clean input y in reducing intermediate generation errors in 161 diffusion posterior sampling. In Section 3.2, we formulate the DPS-CM in detail.

## 3.1 DPS AMPLIFY POSTERIOR SAMPLING ERRORS



Figure 1: (a) mean magnitude ratio between high- and low-frequency area at timestep t; (b)  $\epsilon$ prediction error ratio:  $\frac{DPS_{y_t}}{DPS}$  and  $\frac{DPS-CM}{DPS}$  at timestep t; (c) reconstruction error between target x and intermediate  $\hat{x}_0(x_t)$  at timestep t. These results are achieved by performing Gaussian Deblurring on 10 FFHQ images.

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Our claim is that solving inverse problems in the posterior sampling manner follows the similar frequency dynamics with the regular denoising process that it recovers the low-frequency (structural, domain-independent) components at first and the high-frequency (details, domain-dependent) components later. The posterior sampling from  $p_t(x_t | y)$  in DPS is inevitable adding high-frequency signals from the gradient of the approximate log likelihood  $\nabla_{x_t} \log p_t(y | \hat{x}_0)$  during the early stages due to the frequency and noise discrepancy between the sharp measurement y and intermediate noisy reconstruction  $\hat{x}_0$ . It will create a distorted frequency dynamic which leads to the larger posterior sampling error.

To verify our assumption, we conduct frequency dynamic analysis of different posterior sampling methods for solving inverse problems in Fig.1a. Afterward, the posterior sampling error is illustrated via the visualization of the  $\epsilon$ -prediction error and intermediate reconstruction error dynamics in Fig.1b and Fig.1c respectively. We conduct the diffusion posterior sampling from  $p_t(x_t \mid y_t)$  with noisy measurement DPS<sub>yt</sub> in comparison with DPS to illustrate the advantage of the likelihood approximation with less high-frequency elements.

194 **Diffusion posterior sampling with the noisy measurement DPS**<sub> $y_t$ </sub>. Given the noisy measurement 195  $y_t$  constructed by the diffusion forward process starting from the clean measurement y as in Eq. 196 3, we replace y with  $y_t$  to form DPS<sub> $y_t$ </sub> with the posterior sampling from  $p_t(x_t | y_t)$ . The corre-197 sponding likelihood approximation  $p_t(y_t | \hat{x}_0) \simeq p_t(y_t | x_t)$  involves  $y_t$  and  $x_t$  with the similar 198 frequency pattern and noise level.

Frequency dynamic of diffusion posterior sampling. We verify our assumption on frequency dynamic of diffusion posterior sampling by transforming the gradient of log posterior (i.e.,  $\nabla_{x_t} \log p(x_t | y)$  in the case of DPS) into spectral space as the gradient of log posterior serving as the main update for each posterior sampling step in Eq.5. We split the low-frequency and highfrequency areas in the spectral space of the gradient with the low-high cut-off frequency of 32Hz and visualize the mean magnitude ratio between them of each t shown in Fig.1a.

205  $\epsilon$ -prediction error and intermediate reconstruction error. Since there exists no ground truth for 206 the intermediate generation of diffusion posterior sampling for inverse problems, we measure the 207 posterior sampling error implicitly by computing  $\epsilon$ -prediction error and intermediate reconstruction 208 error at timestep t. Given intermediate  $x_t$  and the posterior mean  $\hat{x}_0$  by applying Eq.4, the  $\epsilon$ prediction error is formulated as  $\|\epsilon_{\theta}(\mathbf{x}'_{t},t) - \epsilon\|_{2}^{2}$ , where  $\mathbf{x}'_{t} = \sqrt{\bar{\alpha}_{t}}\hat{\mathbf{x}}_{0} + \sqrt{1-\bar{\alpha}_{t}}\epsilon, \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 209 210 and  $\epsilon_{\theta}(\boldsymbol{x}'_{t},t) = -\sqrt{1-\bar{\alpha}_{t}}\boldsymbol{s}_{\theta}(\boldsymbol{x}'_{t},t)$  by applying Tweedie's formula.  $\epsilon$ -prediction error at timestep 211 t can reflect how accurately the posterior sampling recovers at t. We compare different posterior 212 sampling with DPS by computing their ratio of  $\epsilon$ -prediction error at each timestep shown in Fig.1b, 213 where a ratio below 1 indicates a smaller  $\epsilon$ -prediction error than DPS, and above 1 means a larger one. Besides, the reconstruction error formed as  $MSE(x, \hat{x}_0)$  is shown in Fig.1c to evaluate how 214 well the the intermediate reconstruction  $\hat{x}_0(x_t)$  converges to the target x utilizing the mean squared 215 error.



Figure 2: Qualitative example of Gaussian Deblurring on FFHQ dataset including  $DPS_{y_t}$ . All measurements are corrupted by additional Gaussian noise with a variance of  $\sigma_u = 0.05$ .

226 **Observations.** From Fig.1a, the frequency dynamic of both DPS's  $\nabla_{x_t} \log p(x_t \mid y)$  (purple) and 227  $DPS_{y_t}$ 's  $\nabla_{x_t} \log p(x_t \mid y_t)$  (red) are focusing on low-frequency components and gradually recover-228 ing more on high-frequency components, but  $DPS_{y_t}$  maintains larger attention on the low-frequency 229 recovery throughout all timesteps. This difference arises from the discrepancy between y and  $y_t$  and 230 leads to their contrast in  $\epsilon$ -prediction and reconstruction error. From timestep 1000 to 600 (around) 231 as the early stages of diffusion posterior sampling,  $DPS_{y_t}$  prohibits a smaller  $\epsilon$ -prediction error than DPS (the red curve of Fig.1b). Consistently accompanying with it, the reconstruction error of 232  $DPS_{y_t}$  is smaller and converges faster before t = 600 by comparing DPS (purple) and  $DPS_{y_t}$  (red) 233 in Fig.1c. 234

235 Such observations verify our claim that the gradient of log likelihood  $\nabla_{x_t} \log p(y \mid \hat{x}_0)$  involved 236 in DPS introduces more high-frequency signals during early stages which poses negative effects on early time low-frequency recovery reflecting from the larger posterior sampling error shown in DPS. 237 The success of  $DPS_{y_t}$  in early stages arises from the similar noise and frequency level between  $y_t$ 238 and  $\hat{x}_0$  which brings less biased guidance for low-frequency generations before t = 600. However, 239 from t = 600 to 0, when the diffusion model gradually transfers it focus from low-frequency to 240 high-frequency restoration shown in Fig.1a, the random noise u in  $y_t$  brings guidance mismatching 241 the real details, which leads  $DPS_{y_t}$  with larger posterior sampling error than DPS shown in Fig.1b 242 and 1c. Further, in Figure 2, DPS  $y_t$ 's generation lacks details and looks ambiguous compared with 243 DPS. 244

The proposed DPS-CM preserves the advantage of DPS<sub>y<sub>t</sub></sub> at the early stages of sampling but still keeps accurate high-frequency generations during the later period. DPS-CM leverages the crafted measurement y<sub>t</sub> instead of random sampled y<sub>t</sub> to perform preciser posterior sampling from  $\nabla_{x_t} \log p(x_t | y_t)$ , while y<sub>t</sub> is sampled from another diffusion denoising process with the posterior p(y<sub>t</sub> | y). We will formulate DPS-CM in detail and discuss its advantages in Section 3.2.

## 3.2 ENHANCING POSTERIOR SAMPLING BY INTEGRATING CRAFTED NOISY MEASUREMENTS

253 DPS<sub>yt</sub> introduced in Section 3.1 fits the diffusion model  $\epsilon_{\theta}(\cdot, t)$  adaptively and produces smaller  $\epsilon$ -254 prediction error, but fails to recover high-frequency components (details, domain-dependent signals) 255 during the late denoising stage. Besides the random noise obstructing the generation of real details, 256 this failure also origins from the intractable likelihood term  $p(y_t | x_t)$  in Eq.7:

$$\nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{x}_{t} \mid \boldsymbol{y}_{t}\right) = \nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{x}_{t}\right) + \nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{y}_{t} \mid \boldsymbol{x}_{t}\right). \tag{7}$$

Apparently, there exists no explicit dependency between the noisy measurement  $y_t$  and  $x_t$  nor  $\hat{x}_0$ applying Eq.4 given the measurement model. Thus,  $\nabla_{x_t} \log p(y_t | \hat{x}_0)$  is an inadequate estimate for  $\nabla_{x_t} \log p(x_t | y_t)$ . In order to leverage the advantage of DPS $_{y_t}$  while exploiting the tractable measurement model  $p(y_0 | x_0)$  into approximation, the gradient of log posterior in DPS $_{y_t}$  can be factorized as:

$$egin{aligned} 
abla_{oldsymbol{x}_t} \log p\left(oldsymbol{x}_t \mid oldsymbol{y}_t
ight) &= 
abla_{oldsymbol{x}_t} \log \int p\left(oldsymbol{x}_t \mid oldsymbol{y}_0, oldsymbol{y}_t
ight) p\left(oldsymbol{y}_0 \mid oldsymbol{y}_t
ight) doldsymbol{y}_0 \ &= 
abla_{oldsymbol{x}_t} \log \int p\left(oldsymbol{x}_t \mid oldsymbol{y}_0
ight) p\left(oldsymbol{y}_0 \mid oldsymbol{y}_t
ight) doldsymbol{y}_0 \end{aligned}$$

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$$= \nabla_{\boldsymbol{x}_t} \log \mathbb{E}_{\boldsymbol{y}_0 \sim p(\boldsymbol{y}_0 | \boldsymbol{y}_t)} \left[ p\left(\boldsymbol{x}_t \mid \boldsymbol{y}_0\right) \right]$$

$$= \nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{x}_{t}\right) + \nabla_{\boldsymbol{x}_{t}} \log \mathbb{E}_{\boldsymbol{y}_{0} \sim p\left(\boldsymbol{y}_{0} \mid \boldsymbol{y}_{t}\right)} \left[ p\left(\boldsymbol{y}_{0} \mid \boldsymbol{x}_{t}\right) \right].$$

With the similar factorization on the posterior  $p(y_0 | x_t)$ , we have:

273 274  $\nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{x}_{t} \mid \boldsymbol{y}_{t}\right) = \nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{x}_{t}\right) + \nabla_{\boldsymbol{x}_{t}} \log \mathbb{E}_{\boldsymbol{y}_{0} \sim p\left(\boldsymbol{y}_{0} \mid \boldsymbol{y}_{t}\right)} \left[p\left(\boldsymbol{y}_{0} \mid \boldsymbol{x}_{t}\right)\right] \\ = \nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{x}_{t}\right) + \nabla_{\boldsymbol{x}_{t}} \log \mathbb{E}_{\boldsymbol{y}_{0} \sim p\left(\boldsymbol{y}_{0} \mid \boldsymbol{y}_{t}\right)} \left[\mathbb{E}_{\boldsymbol{x}_{0} \sim p\left(\boldsymbol{x}_{0} \mid \boldsymbol{x}_{0}\right)} \left[p\left(\boldsymbol{y}_{0} \mid \boldsymbol{x}_{0}\right)\right]\right].$ (8)

The gradient of log likelihood  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y}_t | \boldsymbol{x}_t)$  represented as the second term in Eq.8 enables us to exploit the tractable measurement model  $p(\boldsymbol{y}_0 | \boldsymbol{x}_0)$  for the target posterior sampling. Applying the posterior mean approximation of  $p(\boldsymbol{x}_0 | \boldsymbol{x}_t)$  in Eq.4, we can have  $\hat{\boldsymbol{x}}_0$  in the estimate of  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y}_t | \boldsymbol{x}_t)$  as:

$$\nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{y}_{t} \mid \boldsymbol{x}_{t}\right) = \nabla_{\boldsymbol{x}_{t}} \log \mathbb{E}_{\boldsymbol{y}_{0} \sim p\left(\boldsymbol{y}_{0} \mid \boldsymbol{y}_{t}\right)} \left[\mathbb{E}_{\boldsymbol{x}_{0} \sim p\left(\boldsymbol{x}_{0} \mid \boldsymbol{x}_{t}\right)} \left[p\left(\boldsymbol{y}_{0} \mid \boldsymbol{x}_{0}\right)\right]\right]$$
$$\simeq \nabla_{\boldsymbol{x}_{t}} \log \mathbb{E}_{\boldsymbol{y}_{0} \sim p\left(\boldsymbol{y}_{0} \mid \boldsymbol{y}_{t}\right)} \left[p\left(\boldsymbol{y}_{0} \mid \hat{\boldsymbol{x}}_{0}\right)\right].$$
(9)

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The approximated mean of the posterior  $p(y_0 | y_t)$  is left here because the crucial selection affects the generation quality. Here,  $DPS_{y_t}$  treats the random sampled  $y_t$  as the noisy approximated mean for  $p(y_0 | y_t)$  at t. For the case of DPS, applying  $y = \mathbb{E}[y_0 | y_t]$  makes the same gradient  $\nabla_{x_t} \log p(x_t | y_t) = \nabla_{x_t} \log p(x_t | y)$ . According to the discussion in Section.3.1, both cases are flawful: DPS increases posterior errors during early stages and DPS<sub>yt</sub> produces biased highfrequency recovery in the later period. To retain their benefits while eliminating the drawbacks, we integrate crafted measurements  $y_t$  into posterior sampling as follows.

290 Integrate crafted measurements  $\mathbf{y}_t$ . Since Eq.9 gives us a closer estimate of  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y}_t \mid \boldsymbol{x}_t)$ , the random sampled  $y_t$  within the DPS $_{y_t}$ 's likelihood approximation  $p(y_t \mid \hat{x}_0)$  is a rough esti-291 mate for the intractable  $p(y_0 | y_t)$  and induces random noise that impacts negatively on the crisp 292 reconstructions during the late stages. To form a tractable posterior approximation while keeping 293 the advantage of DPS<sub> $u_t$ </sub> discussed in Section 3.1, we introduce another DDPM reverse trajectory as  $\{\mathbf{y}_t\}_{t=T}^0$  along with the restoration trajectory of  $x_t$ . This crafted measurement trajectory  $\{\mathbf{y}_t\}_{t=T}^0$  is 295 constructed by the intermediate generation  $y_t$  of a diffusion posterior sampling process with the pos-296 terior distribution  $p(\mathbf{y}_t \mid \mathbf{y})$ . In the case of Gaussian noise,  $\{\mathbf{y}_t\}_{t=T}^0$  is formed as line 3-6 iteratively 297 in Algorithm 1. Throughout the trajectory,  $y_t$  is gradually remedied to the vanilla measurement 298 y. Besides,  $\{\mathbf{y}_t\}_{t=T}^0$  shares the same diffusion model  $s_{\theta}(\cdot, t)$  with restoration trajectory  $\{x_t\}_{t=T}^0$ 299 because x and y lie on close manifolds in most typical inverse problems. We incorporate  $y_t$  into 300 the posterior distribution  $p(x_t | y_t)$  to form DPS-CM. Unlike the random sampled  $y_t$  in DPS<sub>4</sub>, 301 the gradually denoised crafted measurement  $\mathbf{y}_t$  will not cause information loss but inject signals 302 adaptively from low-frequency to high-frequency matching the restoration denoising trajectory of x with the close model distribution. Thus, we can estimate the posterior mean  $\mathbb{E}[\mathbf{y}_0 \mid \mathbf{y}_t]$  of  $\mathbf{y}_0$  in 303 Eq.9 as  $\hat{\mathbf{y}}_0$  by applying Eq.4. Replacing  $y_t$  with  $\mathbf{y}_t$ , the log likelihood gradient  $\nabla_{x_t} \log p\left(\mathbf{y}_t \mid x_t\right)$ 304 is estimated as: 305

$$\nabla_{\boldsymbol{x}_t} \log p\left(\mathbf{y}_t \mid \boldsymbol{x}_t\right) \simeq \nabla_{\boldsymbol{x}_t} \log \mathbb{E}_{\mathbf{y}_0 \sim p(\mathbf{y}_0 \mid \mathbf{y}_t)} \left[ p\left(\mathbf{y}_0 \mid \hat{\boldsymbol{x}}_0\right) \right]$$
$$\simeq \nabla_{\boldsymbol{x}_t} \log p\left(\hat{\mathbf{y}}_0 \mid \hat{\boldsymbol{x}}_0\right).$$

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Given this tractable approximation  $\nabla_{\boldsymbol{x}_t} \log p(\hat{\boldsymbol{y}}_0 \mid \hat{\boldsymbol{x}}_0)$ , leveraging the measurement model, it is clear to construct  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t \mid \boldsymbol{y}_t)$  in the case of Gaussian noise as follows:

$$\nabla_{\boldsymbol{x}_t} \log p_t \left( \boldsymbol{x}_t \mid \boldsymbol{y}_t \right) \simeq \boldsymbol{s}_{\theta} \left( \boldsymbol{x}_t, t \right) - \zeta_t \nabla_{\boldsymbol{x}_t} \left\| \hat{\boldsymbol{y}}_0 - \mathcal{A} \left( \hat{\boldsymbol{x}}_0 \right) \right\|_2^2.$$
(10)

313 We perform the posterior sampling incorporating the estimate in Eq.10 with crafted measurements 314 on Gaussian deblurring and visualize the frequency pattern and sampling error in Fig.1. Shown in 315 Fig.1a, DPS-CM (blue) concentrates more on the low-frequency recovery in the early stages com-316 pared with DPS and DPS<sub> $y_t$ </sub> and adjusts itself to high-frequency components better than DPS<sub> $y_t$ </sub> dur-317 ing the late period. Besides, in Fig.1b and 1c, DPS-CM (blue) has the overall smallest  $\epsilon$ -prediction 318 error and achieves the best final generation closest to ground truth with the smallest reconstruction 319 error. Empirically, combining DPS with DPS-CM leads to even better results and benefits the sam-320 pling to jump out of the plateau in the early stages of sampling. Thus, we integrate the approximated 321 gradient of log likelihood  $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{y} \mid \hat{\boldsymbol{x}}_0)$  of DPS with our proposed  $\nabla_{\boldsymbol{x}_t} \log p(\hat{\boldsymbol{y}} \mid \hat{\boldsymbol{x}}_0)$  to facilitate the inverse problem solving. The final diffusion reverse sampling of x's restoration in DPS-CM 322 is shown as line 7-10 in Algorithm 1. In Appendix C, DPS-CM for measurements with Poisson 323 noise is shown in Algorithm 2.

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Requ {	<b>tire:</b> Forward operator $\mathcal{A}(\cdot)$ , <i>T</i> , Measurement $\zeta_t \}_{t=1}^{T}$ , Hyperparameter $\mu \in [0, 1]$ for integrating $\chi_T \sim \mathcal{N}(0, \mathbf{I}), \mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$	$\{x, y\}$ , Step size for $y$ : $\{\omega_t\}_{t=1}^t$ , Step size for $x$ : ion control, Score function $s_{\theta}(\cdot, t)$
2: <b>f</b>	or $t = T - 1$ to 1 do	
3:	$oldsymbol{s_v} \leftarrow oldsymbol{s_{ extbf{v}}}(\mathbf{y}_t,t)$	⊳ Start of y trajectory
4:	$\hat{\mathbf{y}}_0 \leftarrow \frac{1}{\sqrt{\bar{\sigma}_t}} \left( \mathbf{y}_t + (1 - \bar{\alpha}_t)  \boldsymbol{s}_{\mathbf{y}} \right)$	$\triangleright$ Mean Estimate of $\mathbb{E} [\mathbf{y}_0 \mid \mathbf{y}_t]$
5:	$\mathbf{y}_{t-1}' \leftarrow \frac{1}{\sqrt{1-\beta}} \left( \mathbf{y}_t + \beta_t \mathbf{s}_{\mathbf{y}} \right) + \sigma_t z_{\mathbf{y}}$	▷ Unconditional DDPM Sampling of y
6:	$\mathbf{y}_{t-1} \leftarrow \mathbf{y}_{t-1}^{1-eta_t} - \omega_t  abla_{\mathbf{y}_t} \  \hat{\mathbf{y}}_0 - oldsymbol{y} \ _2$	Reconstruction Loss Guidance
7:	$oldsymbol{s_x} \leftarrow oldsymbol{s_ heta}(oldsymbol{x}_t,t)$	$\triangleright$ Start of $x$ trajectory
8:	$\hat{\boldsymbol{x}}_{0} \leftarrow \frac{1}{\sqrt{\bar{\alpha}_{\star}}} \left( \boldsymbol{x}_{t} + (1 - \bar{\alpha}_{t}) \boldsymbol{s}_{\boldsymbol{x}} \right)$	$\triangleright$ Mean Estimate of $\mathbb{E}[\mathbf{x}_0 \mid \mathbf{x}_t]$
9:	$oldsymbol{x}_{t-1}' \leftarrow rac{1}{\sqrt{1-eta_t}} \left(oldsymbol{x}_t + eta_t oldsymbol{s}_{oldsymbol{x}} ight) + \sigma_t z_{oldsymbol{x}}$	$\triangleright$ Unconditional DDPM Sampling of $x$
10:	$oldsymbol{x}_{t-1} \leftarrow oldsymbol{x}_{t-1}' \stackrel{arphi_t}{\leftarrow} \zeta_t  abla_{oldsymbol{x}_t}(\mu \  \hat{oldsymbol{y}}_0 - \mathcal{A}\left(\hat{oldsymbol{x}}_0 ight) \ _2 + oldsymbol{x}_t$	$(1-\mu) \  \boldsymbol{y} - \mathcal{A}(\hat{\boldsymbol{x}}_0) \ _2) \triangleright$ Integrate Crafted $\hat{\boldsymbol{y}}_0$
11: <b>r</b>	eturn $\mathbf{x}_0$	

#### **EXPERIMENTS** 4

#### 4.1 EXPERIMENTAL SETTINGS



(a) Gaussian Deblurring



Figure 3: Qualitative results of deblurring tasks on ImageNet dataset. All measurements are corrupted by additional Gaussian noise with a variance of  $\sigma_{u} = 0.05$ .

360 Evaluation datasets and baselines. We evaluate our proposed posterior sampling method DPS-CM 361 on the validation set of FFHQ  $256 \times 256$  and ImageNet  $256 \times 256$  datasets applying DDPM sampling 362 with 1000 timesteps. For the diffusion prior, the pre-trained diffusion models for FFHQ and Ima-363 geNet are taken from DPS (Chung et al., 2022a) and ablated diffusion model (ADM) (Dhariwal & Nichol, 2021) respectively. Detailed hyperparameter  $\{\zeta_t, \omega_t, \mu\}$  settings of DPS-CM are shown in 364 Appendix A.1. We compare our method with several recent state-of-the-art approaches including DPS (Chung et al., 2022a), Denoising Diffusion Restoration Models (DDRM) (Kawar et al., 2022), 366 DiffPIR (Zhu et al., 2023), Optimal Posterior Covariance (OPC) (Peng et al., 2024), and also latent 367 diffusion-based methods: Posterior Sampling with Latent Diffusion (PSLD) (Rout et al., 2024) and 368 ReSample (Song et al., 2023a). We also compare DPS-CM with FPS-SMC (Dou & Song, 2023) 369 and LGD-MC (Song et al., 2023b) for ablation study in Section.4.3 as they also improve posterior 370 sampling with augmented  $y_t$  or x. Although FPS-SMC relies on the separable Gaussian kernel for 371 deblurring and LGD-MC is applied for more general tasks, they are still worthy of comparison in 372 investigating the effect from different posterior estimate designs. We utilize the same pre-trained 373 models used in DPS-CM for baselines DPS, DDRM, OPC, DiffPIR, FPS-SMC, and LGD-MC. For 374 PSLD, Stable Diffusion v-1.5 (Rombach et al., 2022) is applied. For ReSample, we use the VQ-4 375 autoencoder and the FFHQ-LDM with CelebA-LDM from latent diffusion (Rombach et al., 2022). For OPC, we report the performance of the convert posterior covariance version with Type I guid-376 ance, as this version has the best and most stable performance among all variants. We assume that 377 all the measurements are injected in Gaussian noise with standard deviation  $\sigma = 0.05$ . For mea-



(a) Box Inpainting

(b) Random Inpainting

Figure 4: Qualitative results of inpainting tasks on ImageNet dataset. All measurements are corrupted by additional Gaussian noise with a variance of  $\sigma_{u} = 0.05$ .

surements with Poisson noise, the noise level is  $\lambda = 1.0$ . We run our experiments on a single GPU Nvidia A6000. We list the baseline settings in detail in Appendix A.2.

Experimental setting for forward operators. The forward measurement operators are mostly fol-394 lowing Chung et al. (2022a): (1) for random inpainting, 70 percent of image pixels are masked in 395 all channels; (2) for box inpainting, a box region with size  $128 \times 128$  in an image is masked; (3) 396 for Gaussian blur, we use the same operator implemented in DPS (Chung et al., 2022a) with kernel 397 size 61×61 and standard deviation value 3.0; (4) We take the implementation from LeviBorodenko 398 (2019) to form motion blur operator with kernel size  $61 \times 61$  and intensity value 0.5; (5) For  $4 \times$ super-resolution, we consider bicubic downsampling method; (6) For nonlinear deblurring, we uti-400 lize the approximated forward model in Tran et al. (2021) to simulate the real-world blur.

401 **Evaluation metrics.** We report the average performance of 100 validation samples of 4 metrics: 402 peak signal-to-noise ratio (PSNR), structural similarity index (SSIM), Learned Perceptual Patch 403 Similarity (LPIPS) (Dosovitskiy & Brox, 2016), and Fréchet Inception Distance (FID) (Heusel et al., 404 2017) for comprehensive evaluations.

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#### 4.2 **QUANTITATIVE RESULTS**

The quantitative results of DPS-CM and baselines on these noisy linear and nonlinear inverse prob-409 lems are shown in Table 1, 2 and Table 3. Besides, the performance of DPS-CM for measure-410 ments with Poisson noise is shown in Appendix C. We can observe that DPS-CM can achieve the 411 overall best performance over four metrics when solving deblurring and super-resolution problems 412 and significantly outperform baselines on random/box inpainting problems. While the performance 413 and stability of DPS will significantly drop when performing Gaussian/Motion deblurring on the 414 ImageNet dataset, DPS-CM with the crafted measurements can instead form more precise and ro-415 bust posterior sampling reflected from the consistent performance over these two datasets. Optimal 416 Posterior Covariance (OPC), an improved posterior estimate by constructing the optimal posterior 417 covariance instead of improving over the expectation, is no better than DPS-CM but still achieves comparable performance with our method. For latent diffusion-based baselines PSLD and Resam-418 ple, It is interesting that they can handle the more challenging inverse problems on the ImageNet 419 better than the FFHQ dataset, which exhibits the advantage of latent diffusion capturing on more 420 complex visual distributions and semantic patterns. Remarkably, our method exceeds baselines with 421 different diffusion priors when solving motion deblurring problems, shown in examples of Figure 422 3b. Besides, DPS-CM outperforms DPS in solving ill-posed problems, such as nonlinear blurring 423 and inverse problems with Poisson noise as shown in Table 3 and Appendix C. In Fig.3, 4 and 5a, 424 compared with baselines on different noisy linear inverse problems, DPS-CM shows high-quality 425 reconstructions with mild distortion and precise detail recovery. For example, DPS-CM has better 426 letter recovery on the keyboards in Fig.3b and signature recovery (under the car) in Fig.4b. In super-427 resolution and box inpainting, DPS-CM displays fewer missing details and provides reconstructions 428 suited to the natural background and masked objects. For nonlinear deblurring in Fig.5b, DPS recon-429 structs measurements to the target to some extent but with extra noise and distortions injected, and DPS-CM can capture the realistic details close to the target in this nonlinear task. Additional visual 430 examples of DPS-CM and baselines on different inverse problems with Gaussian/Poisson noise are 431 shown in Appendix E.



(a) Super-resolution

(b) Nonlinear Deblurring

Figure 5: Qualitative results of super-resolution on ImageNet and nonlinear deblurring on FFHQ. All measurements are corrupted by additional Gaussian noise with a variance of  $\sigma_u = 0.05$ .

Dataset	Method		Gaussia	ı Deblur			Motion	Deblur		sup	oer-resol	ution (4×	()
		$\overline{\text{PSNR}\uparrow}$	$\text{SSIM} \uparrow$	LPIPS $\downarrow$	$\overline{\text{FID}}\downarrow$	$\overline{\text{PSNR}\uparrow}$	$\text{SSIM} \uparrow$	LPIPS $\downarrow$	$\mathrm{FID}\downarrow$	$\overline{\text{PSNR}\uparrow}$	$\text{SSIM} \uparrow$	LPIPS $\downarrow$	FID ↓
	DPS-CM (Ours)	27.45	0.7819	0.2059	56.04	30.31	0.8585	0.1609	42.58	27.81	0.7942	0.2008	51.72
	DDRM	25.20	0.7289	0.2976	105.06	-	-	-	-	26.89	0.7821	0.2667	95.23
FELIO	DPS	26.35	0.7533	0.2178	65.20	27.84	0.8023	0.2129	70.10	27.55	<u>0.7886</u>	0.2077	<u>57.20</u>
ггпү	OPC	27.06	0.7651	0.2196	61.76	26.20	0.7371	0.2535	<u>66.63</u>	26.90	0.7637	0.2400	76.33
	DiffPIR	24.13	0.6649	0.2919	76.96	26.35	0.7394	0.2487	64.25	25.74	0.7143	0.2711	67.19
	PSLD	28.45	0.7689	0.3019	99.90	26.19	0.6779	0.3667	137.88	27.91	0.7783	0.2783	87.82
	ReSample	26.10	0.6441	0.3361	100.21	28.26	0.7221	0.2937	89.80	23.23	0.4517	0.5061	151.20
	DPS-CM (Ours)	22.73	0.6147	0.3397	128.92	24.36	0.6814	0.3163	97.54	23.78	0.6450	0.3242	97.38
	DDRM	21.48	0.5527	0.4948	242.38	-	-	-	-	22.72	0.6225	0.4252	196.32
ImagaNat	DPS	16.36	0.3449	0.5041	208.49	17.41	0.3970	0.4920	204.27	21.17	0.5404	0.3668	106.71
imagemet	OPC	18.93	0.4254	0.4579	132.38	18.43	0.3782	0.4989	174.44	19.44	0.4113	0.4836	169.71
	DiffPIR	20.62	0.4753	0.4445	154.12	23.38	0.6285	0.3711	120.58	22.97	0.5985	0.3840	119.66
	PSLD	23.45	0.6089	0.3419	131.90	23.18	0.5688	0.4206	167.57	23.79	0.6371	0.3346	120.68
	ReSample	22.79	0.5147	0.4355	172.17	23.95	0.5723	0.3929	125.33	21.04	0.3973	0.5001	203.56

Table 1: Quantitative results for delur and super-resolution on FFHQ and ImageNet dataset. dicate the best and second best results, respectively.

### 4.3 ABLATION STUDIES

Influence of hyperparameter  $\mu$ . Here, we want to investi-gate the influence of hyperparameter  $\mu \in [0, 1]$ , which controls the proportion of proposed  $\nabla_{\boldsymbol{x}_t} \log p_t (\boldsymbol{y}_t \mid \mathbf{x}_t)$  in the sampling of DPS-CM. When  $\mu = 0.0$ , it falls into DPS. Specifically, we can observe the performance (PSNR) of DPS-CM on box inpainting on ImageNet with different  $\mu$  in Figure 6. DPS-CM achieves the best results when  $\mu = 0.5$  which indicates the benefits of the interplay between  $\nabla_{\boldsymbol{x}_t} \log p_t \left( \mathbf{y}_t \mid \mathbf{x}_t \right)$  and  $\nabla_{\boldsymbol{x}_t} \log p_t (\boldsymbol{y} \mid \mathbf{x}_t)$ . Besides, pure DPS-CM with  $\mu = 1.0$ leads to a better log posterior gradient estimate and outper-forms DPS-CM with  $\mu = 0.0$ .





**Compare crafted measurements with other augmented posterior estimate methods.** Here, we further validate the effect of our crafted measurements  $\{\mathbf{y}_t\}_{t=T}^0$  compared with DPS<sub>yt</sub>, where  $y_t$ in the posterior is an i.i.d sample from the forward process  $p(y_t | y_0)$  same as Eq.3, LGD-MC (Song et al., 2023b), which is a loss guided diffusion with  $x^{(i)}$  i.i.d. sampled from  $p(\mathbf{x}_0 | \mathbf{x}_t)$  for the posterior estimate, and FPS-SMC which incorporates the  $\mathbf{y}_{t-1}$  sampled from the non-parametric forward/reverse process given  $\mathbf{y}$ . Specifically, in the inverse problem setting, the gradient of the log likelihood LGD-MC is approximated as:

$$\mathrm{MC}_{n}\left(\mathbf{x}_{t},\mathbf{y}\right) = \rho \nabla_{\mathbf{x}_{t}} \log \left(\frac{1}{n} \sum_{i=1}^{n} \left\| \boldsymbol{y} - \mathcal{A}\left(\hat{\boldsymbol{x}}_{0}^{(i)}\right) \right\|_{2}^{2}\right),$$

Dataset	Method	In	painting	(Randon	1)	Inpainting (Box)				
Dutuset		$\overline{\text{PSNR}\uparrow}$	SSIM ↑	LPIPS $\downarrow$	$FID\downarrow$	$\overline{\text{PSNR}\uparrow}$	SSIM $\uparrow$	LPIPS $\downarrow$	FID 、	
	DPS-CM (Ours)	31.20	0.8903	0.1233	28.05	23.87	0.8470	0.1331	35.52	
	DDRM	25.49	0.7727	0.2702	101.26	20.40	0.8005	0.2265	65.12	
EEUO	DPS	29.74	0.8136	0.1397	43.12	21.54	0.8127	0.1514	50.69	
ггпү	OPC	29.84	0.8709	0.1615	50.49	22.69	0.8222	0.1569	48.0	
	DiffPIR	29.40	0.8425	0.2275	83.09	21.95	0.7253	0.2484	63.40	
	PSLD	28.52	0.7756	0.3165	101.04	21.07	0.6894	0.3761	128.2	
	ReSample	29.65	0.8367	0.2024	61.44	19.69	0.7837	0.2452	136.8	
	DPS-CM (Ours)	26.71	0.8121	0.1684	37.92	20.05	0.7880	0.2270	111.0	
	DDRM	21.89	0.6204	0.4162	230.95	18.32	0.7373	0.3003	142.9	
ImagaNat	DPS	26.61	0.8060	0.1824	<u>39.92</u>	18.04	0.7626	0.2201	119.8	
imagervei	OPC	23.46	0.6517	0.3063	88.47	16.46	0.6412	0.2910	168.2	
	DiffPIR	25.79	0.7470	0.2873	106.79	18.08	0.6030	0.3326	160.9	
	PSLD	25.46	0.6841	0.3509	104.99	18.17	0.5469	0.4701	220.9	
	ReSample	25.01	0.7201	0.2825	98.45	17.50	0.6862	0.3346	225.5	

Table 2: Quantitative results for inpainting on FFHQ and ImageNet dataset. We use **bold** and <u>underline</u> to indicate the best and second best results, respectively.

where  $x_0^{(i)} \sim p(x_0 \mid x_t)$ . DPS<sub>y</sub> with multiple Monte-Carlo samples can be formed as:

$$\nabla_{\boldsymbol{x}_{t}} \log p\left(\boldsymbol{y}_{t} \mid \boldsymbol{x}_{t}\right) = \rho \nabla_{\boldsymbol{x}_{t}} \log \left(\frac{1}{n} \sum_{i=1}^{n} \left\|\boldsymbol{y}_{t}^{(i)} - \mathcal{A}\left(\hat{\boldsymbol{x}}_{0}\right)\right\|_{2}^{2}\right),$$

where  $\boldsymbol{y}_{t}^{(i)} \sim p(\boldsymbol{y}_{t} \mid \boldsymbol{y}_{0})$ . And the estimate in FPS-SMC is  $p_{\boldsymbol{\theta}}(\mathbf{y}_{t-1} \mid \mathbf{x}_{t-1})$  given sampled  $\mathbf{y}_{t-1}$ . We conduct experiments on  $4 \times$  super-resolution to demonstrate the superiority of our crafted mea-surements  $\mathbf{y}_t$  over these augmented posterior estimate methods. The Monte Carlo sample number is set as 10 for all of them (M = 10 for FPS-SMC). Shown in Table 4, DPS-CM shows the best results on perception oriented metrics (LPIPS and FID) and comparable performance on the standard met-rics (PSNR and SSIM) with FPS-SMC. DPS-MC is 50% more efficient than FPS-SMC as shown in the running time report in Appendix B, which validates the design in this work can keep the details and promote posterior approximation at the same time. 

						Method	super-resolution (4×)				
	]	Nonlinea	r Deblur		_		$PSNR \uparrow$	$\text{SSIM} \uparrow$	LPIPS $\downarrow$	$\text{FID}\downarrow$	
Method	PSNR ↑	SSIM ↑	LPIPS ↓	$\mathrm{FID}\downarrow$	_	DPS-CM (Ours)	$\frac{27.81}{22.40}$	0.7942	0.2008	<b>51.72</b> 96.34	
DPS-CM (Ours)	<b>22.66</b>	0.6465	0.3626	122.64		LGD-MC	26.35 28.12	0.7674	0.2359	61.98	
DFS	21.21	0.0191	0.3640	150.80	_	rps-smc	28.12	0.8055	0.2140	<u>60.22</u>	

Table 3: Quantitative results for nonlinear deblurring on FFHQ.

Table 4: Ablation study results on FFHQ comparing crafted measurements in DPS-CM with other augmented posterior estimate methods.

## 5 CONCLUSION

This work introduces Diffusion Posterior Sampling with Crafted Measurements to solve general and noisy inverse problems. DPS-CM leverages an additional diffusion reverse process to form a crafted measurement trajectory  $\{\mathbf{y}_t\}_{t=T}^0$  with extensive noise levels to perform a frequency-adaptive and less biased diffusion posterior sampling with the log posterior gradient  $\nabla_{x_t} \log p(x_t \mid y_t)$  incorporating  $y_t$ . Via experimental results, we show that our DPS-CM can generate improved high-quality restorations compared with recent state-of-the-art and also latent diffusion approaches. For the po-tential future works, following the idea of DPS-CM, improved design on forming more beneficial crafted measurement, e.g., additional inverse problem-related guidance for  $y_t$  diffusion sampling besides the reconstruction loss guidance, is a crucial direction to explore. We discuss the limitation of DPS-CM and solutions in Appendix D.

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# A EXPERIMENTAL DETAILS

## A.1 IMPLEMENTATION SETTINGS OF DPS-CM

Hyperparameter  $\{\zeta_t, \omega_t, \mu\}$  for DPS-CM are fixed during the 1000 DDPM denoising steps. Detailed settings in the case of Gaussian and Poisson noise are shown in Table 5 and 6 respectively.

	Gaussian Deblur	Motion Deblur	super-resolution	Inpainting(Random)	Inpainting(Box)	Nonlinear Deblur
FFHQ	$\{1.8, 13.0, 0.5\}$	$\{1.7, 11.0, 0.5\}$	$\{2.2, 8.0, 0.5\}$	$\{3.1, 19.0, 0.285\}$	$\{1.7, 13.0, 0.5\}$	$\{1.6, 10.0, 0.5\}$
ImageNet	$\{1.8, 13.0, 0.7\}$	$\{1.4, 11.0, 0.5\}$	$\{1.7, 7.0, 0.5\}$	$\{2.4, 19.0, 0.285\}$	$\{1.8, 13.0, 0.5\}$	-

Table 5: Hyperparameter settings of DPS-CM for measurements with Gaussian noise

	Gaussian Deblur	Motion Deblur	super-resolution
FFHQ	$\{0.5, 6.0, 0.5\}$	$\{0.4, 6.0, 0.5\}$	$\{0.4, 3.0, 0.5\}$

Table 6: Hyperparameter settings of DPS-CM for measurements with Poisson noise

A.2 IMPLEMENTATION SETTINGS OF BASELINES

**DPS**: we follow all the default  $\rho$  settings in Appendix D.1 in their paper with 1000 DDPM steps.

**DDRM**: the number of steps we used is 20. DDRM with 100 steps sometimes has better results on PSNR and SSIM but worse on LPIPS and FID. The overall performance between different step schedules is very similar. For hyperparameter  $\{\eta, \eta_b\}$ , we follow the default setting  $\{0.85, 1\}$ .

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 OPC: we compare their different variants and report the Convert version with their defined Type I guidance which has the overall best performance with 50 EDM steps.

**DiffPIR**: we follow the hyperparameter settings in Appendix B.1 with 100 timesteps.

**FPS-SMC**: particle size M is 10 and the c value is followed the setting in their Table 8.

**LGD-MC**: LGD-MC is performed with n = 10. The loss function follows the settings in Appendix B.2 with  $r_t = 0.05$ , loss coefficient  $\lambda = 10^{-3}$  and 1000 timesteps.

**PSLD**: we follow the default hyperparameter setting  $\{\eta = 1, \gamma = 0.1\}$  and sample for 1000 DDIM steps.

**ReSample**: we implement it with default settings of their paper and codebase:  $\{\tau = 10^{-4}, \gamma = 40\}$ , conducting latent optimization with maximum 500 iterations and sampling for 500 DDIM steps.

# B RUNNING TIME OF DPS-CM AND BASELINES

Methods	Running Time(in seconds)	NFEs
DPS-CM	123.22	2000
DDRM	0.54	20
DPS	64.70	1000
OPC	9.69	50
DiffDIR	3.92	100
LGD-MC	66.45	1000
FPS-SMC	182.67	1000
PSLD	517.47	1000
ReSample	639.51	500

Table 7: Implementation details of DPS-CM

#### С ALGORITHM: DPS-CM FOR MEASUREMENTS WITH POISSON NOISE

DPS-CM is applied in the case of the measurements with Poisson noise in Algorithm 2. Its performance on the deblurring and super-resolution is shown in Tab.8.

## Algorithm 2 DPS-CM (Poisson)

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**Require:** Forward operator  $\mathcal{A}(\cdot)$ , T, Measurement  $\boldsymbol{y}$ , Step size for  $\mathbf{y}$ :  $\{\omega_t\}_{t=1}^T$ , Step size for  $\boldsymbol{x}$ : 764  $\{\zeta_t\}_{t=1}^T$ , Hyperparameter  $\mu \in [0, 1]$  for integration control, Score function  $s_{\theta}(\cdot, t)$ 1:  $\mathbf{y}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 2: for t = T - 1 to 1 do 766  $\begin{aligned} \mathbf{s}_{\mathbf{y}} &\leftarrow \mathbf{s}_{\theta}(\mathbf{y}_{t}, t) \\ \hat{\mathbf{y}}_{0} &\leftarrow \frac{1}{\sqrt{\bar{\alpha}_{t}}} \left( \mathbf{y}_{t} + (1 - \bar{\alpha}_{t}) \, \mathbf{s}_{\mathbf{y}} \right) \\ \mathbf{y}_{t-1}' &\leftarrow \frac{1}{\sqrt{1 - \beta_{t}}} \left( \mathbf{y}_{t} + \beta_{t} \mathbf{s}_{\mathbf{y}} \right) + \sigma_{t} z_{\mathbf{y}} \\ \mathbf{y}_{t-1} &\leftarrow \mathbf{y}_{t-1}' - \omega_{t} \nabla_{\mathbf{y}_{t}} \left\| \hat{\mathbf{y}}_{0} - \mathbf{y} \right\|_{\mathbf{\Lambda}} \end{aligned}$ ▷ Start of y trajectory 3: 4:  $\triangleright$  Mean Estimate of  $\mathbb{E} [\mathbf{y}_0 \mid \mathbf{y}_t]$ 5: ▷ Unconditional DDPM Sampling of y 772 6: Reconstruction Loss Guidance  $\begin{aligned} & \boldsymbol{s_x} \leftarrow \boldsymbol{s_\theta}(\boldsymbol{x}_t, t) \\ & \hat{\boldsymbol{x}}_0 \leftarrow \frac{1}{\sqrt{\bar{\alpha}_t}} \left( \boldsymbol{x}_t + (1 - \bar{\alpha}_t) \, \boldsymbol{s_x} \right) \end{aligned}$ 774 7:  $\triangleright$  Start of x trajectory 8:  $\triangleright$  Mean Estimate of  $\mathbb{E}[x_0 \mid x_t]$ 775  $\begin{aligned} \mathbf{x}_{0}^{(\mathbf{x}_{t})} & \leftarrow \mathbf{x}_{t}^{(\mathbf{x}_{t})} + (\mathbf{1} - \alpha_{t}) \mathbf{s}_{\mathbf{x}}) \\ \mathbf{x}_{t-1}^{'} & \leftarrow \frac{1}{\sqrt{1-\beta_{t}}} \left( \mathbf{x}_{t} + \beta_{t} \mathbf{s}_{\mathbf{x}} \right) + \sigma_{t} z_{\mathbf{x}} \qquad \triangleright \text{ Unconditional DI} \\ \mathbf{x}_{t-1}^{'} & \leftarrow \mathbf{x}_{t-1}^{'} - \zeta_{t} \nabla_{\mathbf{x}_{t}} \left( \mu \left\| \hat{\mathbf{y}}_{0} - \mathcal{A} \left( \hat{\mathbf{x}}_{0} \right) \right\|_{\mathbf{\Lambda}} + (1-\mu) \left\| \mathbf{y} - \mathcal{A} \left( \hat{\mathbf{x}}_{0} \right) \right\|_{\mathbf{\Lambda}} \end{aligned}$ 776  $\triangleright$  Unconditional DDPM Sampling of x9: 10: ▷ Integrating 778 Crafted  $\hat{\mathbf{y}}_0$ 779 11: return  $\mathbf{x}_0$ 780

Dataset	Method	Gaussian Deblur		Motion Deblur			super-resolution (4 $\times$ )						
Dutuset		PSNR ↑	SSIM $\uparrow$	LPIPS $\downarrow$	$\mathrm{FID} \downarrow$	$\overline{\text{PSNR}\uparrow}$	$\text{SSIM} \uparrow$	LPIPS $\downarrow$	$\mathrm{FID} {\downarrow}$	$PSNR \uparrow$	$\text{SSIM} \uparrow$	LPIPS $\downarrow$	FID ↓
FFHQ	DPS-CM (Ours) DPS	<b>26.23</b> 25.22	<b>0.7368</b> 0.7184	<b>0.2348</b> 0.2391	<b>66.61</b> 71.82	<b>27.53</b> 27.01	<b>0.7687</b> 0.7608	<b>0.2208</b> 0.2213	<b>53.19</b> 58.78	<b>26.40</b> 25.17	<b>0.7417</b> 0.6708	<b>0.2552</b> 0.3391	<b>72.97</b> 106.53

Table 8: Quantitative results for deblurring and super-resolution on FFHQ with Poisson noise. We use **bold** for the best.

#### D LIMITATIONS

792 As the high-quality generations of DPS-CM benefit from the interplay between two posterior sam-793 pling processes for the crafted measurement's generation and x's restoration, the running time of 794 DPS-CM is nearly twice of DPS's sampling as shown in Tabel 7. However, DPS-CM shows better or comparable performance compared with latent diffusion based methods such as PSLD, Resample, and methods with Monte Carlo such as FPS-SMC and LGD-MC with less running time. Besides, we 796 try to improve the efficiency of DPS-CM by setting  $\mu = 0$  after t during the late stages of sampling 797 as the posterior sampling with crafted measurements shows similar  $\epsilon$ -prediction errors with DPS 798 during the late stages in Fig. 1b. We set the t as 400 and conduct an experiment for random inpaint-799 ing on FFHQ dataset. From Table 9, the accelerated variant achieves comparable performance and 800 has the over 20% efficiency improvement. Besides, the core idea of DPS-CM is based on insight-801 ful observations in posterior sampling methods. We can potentially combine crafted measurements 802 with a more efficient method, such as DiffPIR, to achieve high-quality reconstructions and maintain 803 efficiency. Another concern for DPS-CM is how it deals with the inverse problems with the targets 804 and measurements from very different modalities, such as phrase retriever. In this case, utilizing 805 the same pre-trained diffusion model to construct the crafted measurements for DPS-CM sampling 806 can not generate stable restorations. One solution is to train a smaller diffusion model on the mea-807 surement modality for crated measurements. It should be noted that most of the current zero-shot methods are designed for typical inverse problems in which the target and measurement lie on the 808 close manifold and perform unstably on tasks similar to phrase retriever. Thus, fitting a small model to facilitate DPS-CM for such tasks is acceptable and reasonable.

	Method	super-resolution (4×)				
Running Third		$\overline{\text{PSNR}\uparrow}$	SSIM $\uparrow$	LPIPS $\downarrow$	FID ↓	
123.22	DPS-CM	31.20	0.8903	0.1233	28.05	
98.14	DPS-CM (accelerated)	30.98	0.8906	0.1349	36.64	
64.70	DPS	29.74	0.8136	0.1397	43.12	

Table 9: Quantitative results for random inpainting on FFHQ with Gaussian noise of **accelerated** DPS-CM

# E ADDITIONAL VISUAL RESULTS

Additional visual examples are shown here to to compare with baselines on different tasks with Gaussian noise ( $\sigma = 0.05$ ) from Fig. 7 to Fig. 13 and with Poisson noise ( $\lambda = 1.0$ ) from Fig. 14 to Fig. 16.



Figure 7: Additional Qualitative Results on Gaussian Deblur with Gaussian Noise.



Figure 8: Additional Qualitative Results on Motion Deblurring with Gaussian Noise.



Figure 9: Additional Qualitative Results on super-resolution with Gaussian Noise.



Figure 10: Additional Qualitative Results on Box Inpainting with Gaussian Noise.



Figure 11: Additional Qualitative Results on Random Inpainting with Gaussian Noise.



Figure 12: Additional Qualitative Results on Nonlinear Deblurring with Gaussian Noise.



Figure 13: Additional Qualitative Results on Super-resolution with Gaussian noise compared with FPS-SMC (M = 10).



Figure 14: Additional Qualitative Results on Gaussian Deblurring with Poisson noise.



Figure 15: Additional Qualitative Results on Motion Deblurring with Poisson noise.



Figure 16: Additional Qualitative Results on Super-resolution with Poisson noise.