#### Yuanzhi Zhu

Supervisors: Dr. Kai Zhang, Jingyun Liang, Jiezhang Cao Principal Investigator: Prof. Luc Van Gool





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- <u>Preliminaries</u>
- <u>Methods</u>
- <u>Results</u>



**Forward Diffusion Process** 

$$q(x_{1:T}|x_0) := \prod_{t=1}^T q(x_t|x_{t-1})$$

Each Step

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \underbrace{\sqrt{1 - \beta_t} x_{t-1}, \beta_t \mathbf{I}}_{\text{norm invariant}}) \quad \text{or} \quad x_t = \sqrt{1 - \beta_t} x_{t-1} + \sqrt{\beta_t} \epsilon_{t-1}$$

noise schedule  $\beta_t$  controls the diffusion process

For arbitrary *t* 

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t} x_0, (1 - \bar{\alpha}_t)\mathbf{I}) \qquad \alpha_t = 1 - \beta_t \text{ and } \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

$$x_t = \sqrt{\bar{\alpha}_t} \boldsymbol{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot z_t$$

T



Negative Log Likelihood to Variational Lower Bound

$$-\log p_{\theta}(\mathbf{x}_{0}) \implies \mathbb{E}_{q}\left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0:T})}\right] \implies \sum_{t=2}^{T} \underbrace{D_{\mathrm{KL}}\left[q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})\right]}_{L_{t}} \|p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t})\right]$$

Explicit parameterization

$$p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \boldsymbol{\mu}_{\theta}(x_t, t), \boldsymbol{\Sigma}_{\theta}(x_t, t)) \quad \begin{cases} \boldsymbol{\mu}_{\theta}(x_t, t) &= \frac{1}{\sqrt{\alpha_t}} (x_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} z_{\theta}(x_t, t)) \\ \boldsymbol{\Sigma}_{\theta}(x_t, t) &= \sigma_t^2 \mathbf{I} \end{cases} \text{ two options}^{\dagger} \sigma^2 = \begin{cases} \beta_t \\ \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \beta_t \end{cases}$$

Model The Noise (Residual)

$$L_t^{\text{simple}} = \mathbb{E}_{x_0, z_t} \left[ \| z_t - z_\theta (\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} z_t, t) \|^2 \right] \qquad \hat{\mathbf{x}}_0^{(t)}(\mathbf{x}_t) = \frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \mathbf{z}_\theta^{(t)}(\mathbf{x}_t, t)}{\sqrt{\bar{\alpha}_t}}$$

<sup>†</sup> Covariance has analytical optimal form (Estimating the Optimal Covariance with Imperfect Mean in Diffusion Probabilistic Models)

- Known

$$x_0 \sim q(x_0) ~~~ q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-eta_t} x_{t-1}, eta_t I) ~~ ext{ or } q(x_{1:T}|x_0) = \prod_{t=1}^r q(x_t|x_{t-1})$$



| Algorithm 1 Training  | Algorithm 2 Sampling  |
|---|---|
| 1: repeat<br>2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$<br>3: $t \sim \text{Uniform}(\{1, \dots, T\})$<br>4: $\epsilon \sim \mathcal{N}(0, \mathbf{I})$<br>5: Take gradient descent step on | 1: $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$<br>2: for $t = T, \dots, 1$ do<br>3: $\mathbf{z} \sim \mathcal{N}(0, \mathbf{I})$ if $t > 1$ , else $\mathbf{z} = 0$<br>4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \mathbf{z}_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$ |
| $ abla_{	heta} \left\ oldsymbol{\epsilon} - \mathbf{z}_{oldsymbol{	heta}}(\sqrt{ar{lpha}_t}\mathbf{x}_0 + \sqrt{1 - ar{lpha}_t}oldsymbol{\epsilon},t) ight\ ^2$                         | 5: end for  |
| 6: <b>until</b> converged   | 6: return $\mathbf{x}_0$  |

T

$$x_{0} \sim q(x_{0}) \longrightarrow q(x_{t}|x_{t-1}) = \mathcal{N}(x_{t}; \sqrt{1-\beta_{t}}x_{t-1}, \beta_{t}I) \longrightarrow q(x_{1:T}|x_{0}) = \prod_{t=1}^{T} q(x_{t}|x_{t-1})$$

$$x_{0} \longrightarrow x_{t} = \int p(x_{T}) \prod_{t=1}^{T} p_{t}(x_{t}) + \int p_{t}($$

### DDIM: Denoising Diffusion Implicit Models\*

**Reverse Process:** deterministic given  $x_t, x_0$ , with  $\sigma_t = 0$ 

$$x_{t-1} = \sqrt{\bar{\alpha}_{t-1}} x_0 + \frac{\sqrt{1 - \bar{\alpha}_{t-1}}}{\sqrt{1 - \bar{\alpha}_t}} (x_t - \sqrt{\bar{\alpha}_t} x_0)$$

Sampling:

$$x_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \underbrace{\left(\frac{x_t - \sqrt{1 - \bar{\alpha}_t} z_{\theta}^{(t)}(x_t)}{\sqrt{\bar{\alpha}_t}}\right)}_{\text{"predicted } x_0\text{"}} + \underbrace{\sqrt{1 - \bar{\alpha}_{t-1}} \cdot z_{\theta}^{(t)}(x_t)}_{\text{"direction pointing to } x_t\text{"}}$$

**Accelerated Generation Processes** 





- <u>Preliminaries</u>
- <u>Methods</u>
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Substitute degradation model  $\mathbf{y} = \mathcal{H}\mathbf{x} + \mathbf{n}$ :  $\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} \frac{1}{2\sigma_n^2} \|\mathbf{y} - \mathcal{H}(\mathbf{x})\|^2 + \lambda \mathcal{P}(\mathbf{x})$ prior term data term  $\hat{\mathbf{x}} = \underset{\mathbf{x}}{\operatorname{arg\,min}} \quad \frac{1}{2\sigma^2} \|\mathbf{y} - \mathcal{H}(\mathbf{x})\|^2 + \lambda \mathcal{P}(\mathbf{z}) \quad s.t. \quad \mathbf{z} = \mathbf{x}$ Introduce auxiliary variable **Z**:  $\mathcal{L}_{\mu}(\mathbf{x}, \mathbf{z}) = \frac{1}{2\sigma^2} \|\mathbf{y} - \mathcal{H}(\mathbf{x})\|^2 + \lambda \mathcal{P}(\mathbf{z}) + \frac{\mu}{2} \|\mathbf{z} - \mathbf{x}\|^2$ Lagrange multiplier:  $\begin{cases} \mathbf{z}_{k} = \arg\min_{\mathbf{z}} \underbrace{\frac{1}{2(\sqrt{\lambda/\mu})^{2}} \|\mathbf{z} - \mathbf{x}_{k}\|^{2}}_{\text{consistence}} \underbrace{\mathcal{P}(\mathbf{z})}_{\text{prior}} \\ \mathbf{x}_{k-1} = \arg\min_{\mathbf{x}} \underbrace{\|\mathbf{y} - \mathcal{H}(\mathbf{x})\|^{2}}_{\text{condition}} + \underbrace{\mu\sigma_{n}^{2} \|\mathbf{x} - \mathbf{z}_{k}\|^{2}}_{\text{consistence}} \end{cases}$ **Prior** Half Quadratic Splitting (**HQS**) algorithm: Data

$$\arg \min_{\mathbf{z}} \underbrace{\frac{1}{2(\sqrt{\lambda/\mu})^2} \|\mathbf{z} - \mathbf{x}_k\|^2}_{\text{consistence}} + \underbrace{\mathcal{P}(\mathbf{z})}_{\text{prior}} \qquad \underbrace{\mathbf{by definition}}_{\mathbf{x}_k = \mathbf{z}_k + \sqrt{\lambda/\mu\epsilon}} \mathbf{z}_k = Denoiser(\mathbf{x}_k, \sqrt{\lambda/\mu})$$

$$\operatorname{degradation models}$$

$$\operatorname{arg min}_{\mathbf{x}} \underbrace{\|\mathbf{y} - \mathcal{H}(\mathbf{x})\|^2}_{\text{condition}} + \underbrace{\mu\sigma_n^2 \|\mathbf{x} - \mathbf{z}_k\|^2}_{\text{consistence}} \left\{ \begin{array}{c} \text{Inpainting } \mathbf{x}_{k-1} = \frac{\mathbf{M} \odot \mathbf{y} + \rho_k \mathbf{z}_k}{\mathbf{M} + \rho_k} & \mathbf{y} = \mathbf{M} \odot \mathbf{x} \\ \\ \text{Deblurring } \mathbf{x}_{k-1} = \mathcal{F}^{-1} \left( \frac{\overline{\mathcal{F}(\mathbf{k})} \mathcal{F}(\mathbf{y}) + \rho_k \mathcal{F}(\mathbf{z}_k)}{\overline{\mathcal{F}(\mathbf{k})} \mathcal{F}(\mathbf{k}) + \rho_k} \right) & \mathbf{y} = \mathbf{x} \otimes \mathbf{k} + \mathbf{n} \\ \\ \mathbf{SR} \quad \mathbf{x}_{k-1} = \mathcal{F}^{-1} \left( \frac{1}{\rho_k} \left( \mathbf{d} - \overline{\mathcal{F}(\mathbf{k})} \odot_s \frac{(\mathcal{F}(\mathbf{k})\mathbf{d}) \Downarrow_s}{(\overline{\mathcal{F}(\mathbf{k})} \mathcal{F}(\mathbf{k})) \Downarrow_s + \rho_k} \right) \right) & \mathbf{y} = \mathbf{x} \downarrow_{sf}^{bicubic} + \mathbf{n} \\ \mathbf{d} = \overline{\mathcal{F}(\mathbf{k})} \mathcal{F}(\mathbf{y} \uparrow_{sf}) + \rho_k \mathcal{F}(\mathbf{z}_k) \\ \end{aligned}$$

Previous Iterative Approaches:

- Empirically chosen *schedules* 😕
- Discriminative denoisers 😕



Introduce Diffusion Models:

- Well-defined sampling schedules/trajectories 😳
- *Generative* prior 🙂

Sampling as Optimization

$$dx_t = -\nabla V(x_t)dt + \sqrt{2}dB_t$$

But where does the generative power come from?

Image from: cszn/USRNet: Deep Unfolding Network for Image Super-Resolution (CVPR, 2020) (PyTorch) (github.com)

$$x_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \underbrace{\left(\frac{x_t - \sqrt{1 - \bar{\alpha}_t}\epsilon_{\theta}^{(t)}(x_t)}{\sqrt{\bar{\alpha}_t}}\right)}_{\text{"predicted } x_0\text{"}} + \underbrace{\sqrt{1 - \bar{\alpha}_{t-1}} \cdot \epsilon_{\theta}^{(t)}(x_t)}_{\text{"direction pointing to } x_t\text{"}}$$
One iteration **HQS**  $\rightarrow$  estimate  $\hat{\mathbf{x}}_0^{(t)}(\mathbf{x}_t, \mathbf{y})$ 

$$\begin{cases} \mathbf{x}_0^{(t)} = \arg\min_{\mathbf{z}} \frac{1}{2\bar{\sigma}_t^2} \|\mathbf{z} - \mathbf{x}_t\|^2 + \mathcal{P}(\mathbf{z}) \\ \hat{\mathbf{x}}_0^{(t)} = \arg\min_{\mathbf{x}} \|\mathbf{y} - \mathcal{H}(\mathbf{x})\|^2 + \rho_t \|\mathbf{x} - \mathbf{x}_0^{(t)}\|^2 \end{cases}$$
Calculate the predicted conditional noise
$$\hat{\epsilon}(\mathbf{x}_t, \mathbf{y}) = \frac{1}{\sqrt{1 - \bar{\alpha}_t}} (\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \hat{\mathbf{x}}_0^{(t)}(\mathbf{x}_t, \mathbf{y}))$$

Finish one sampling step by adding noise back

$$\mathbf{x}_{t-1} = \sqrt{\bar{\alpha}_{t-1}} \mathbf{\hat{x}}_0^{(t)}(\mathbf{x}_t, \mathbf{y}) + \sqrt{1 - \bar{\alpha}_{t-1}} (\sqrt{1 - \zeta} \mathbf{\hat{\epsilon}}(\mathbf{x}_t, \mathbf{y}) + \sqrt{\zeta} \epsilon_t)$$

$$\hat{\mathbf{x}}_{0}(\mathbf{x}_{t}, \mathbf{y}) = \frac{1}{\sqrt{\bar{\alpha}_{t}}} (\mathbf{x}_{t} + (1 - \bar{\alpha}_{t})\mathbf{s}_{\theta}(\mathbf{x}_{t}, y)) = \frac{1}{\sqrt{\bar{\alpha}_{t}}} (\mathbf{x}_{t} + (1 - \bar{\alpha}_{t})(\mathbf{s}_{\theta}(\mathbf{x}_{t}) + \nabla_{\mathbf{x}_{t}}\log p_{t}(\mathbf{y}|\mathbf{x}_{t})) = \hat{\mathbf{x}}_{0}(\mathbf{x}_{t}) + \frac{1 - \bar{\alpha}_{t}}{\sqrt{\bar{\alpha}_{t}}} \nabla_{\mathbf{x}_{t}}\log p_{t}(\mathbf{y}|\mathbf{x}_{t}).$$

In this page we use  $\epsilon_{\theta}$  instead  $z_{\theta}$  to avoid confusion





Approximately  $\hat{\mathbf{x}}_{0}^{(t)} \approx \mathbf{x}_{0}^{(t)} - \frac{\bar{\sigma}_{t}^{2}}{2\lambda\sigma_{n}^{2}} \nabla_{\mathbf{x}_{0}^{(t)}} \|\mathbf{y} - \mathcal{H}(\mathbf{x}_{0}^{(t)})\|^{2}$ 

But where does the generative power come from?







Can skip this part!

# Ablation Study: Sampling Steps & Start Timestep

#### **Effect of sampling steps**



#### **Effect of start sampling timestep**



# Ablation Study: Effect of Hyperparameters

- $\lambda < 1$   $\rightarrow$  the noise is amplified
- $\lambda > 1000 \rightarrow$  more *unconditional*
- $\zeta \sim 1$   $\rightarrow$  more blurry





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# Quantitative Results

| FFHQ      |                   | Deblur (Gaussian)       |                 |                    | <b>Deblur</b> (motion) |                 |                    | <b>SR</b> (×4) |                 |                    |  |
|-----------|-------------------|-------------------------|-----------------|--------------------|------------------------|-----------------|--------------------|----------------|-----------------|--------------------|--|
| Method    | NFEs $\downarrow$ | $\mathbf{PSNR}\uparrow$ | $FID\downarrow$ | LPIPS $\downarrow$ | <b>PSNR</b> ↑          | $FID\downarrow$ | LPIPS $\downarrow$ | <b>PSNR</b> ↑  | $FID\downarrow$ | LPIPS $\downarrow$ |  |
| DiffPIR   | 100               | 27.36                   | 59.65           | 0.236              | 26.57                  | 65.78           | 0.255              | 26.64          | 65.77           | 0.260              |  |
| DPS [8]   | 1000              | 25.46                   | 65.57           | 0.247              | 23.31                  | 73.31           | 0.289              | 25.77          | 67.01           | 0.256              |  |
| DDRM [29] | 20                | 25.93                   | 101.89          | 0.298              | -                      | -               | -                  | 27.92          | 89.43           | 0.265              |  |
| DPIR [52] | >20               | 27.79                   | 123.99          | 0.450              | 26.41                  | 146.44          | 0.467              | 28.03          | 133.39          | 0.456              |  |
|           |                   |                         |                 |                    |                        |                 |                    |                |                 |                    |  |
| ImageNet  |                   | Deblur (Gaussian)       |                 |                    | <b>Deblur</b> (motion) |                 |                    | <b>SR</b> (×4) |                 |                    |  |
| Method    | NFEs $\downarrow$ | $\mathbf{PSNR}\uparrow$ | $FID\downarrow$ | LPIPS $\downarrow$ | PSNR ↑                 | $FID\downarrow$ | LPIPS $\downarrow$ | PSNR ↑         | $FID\downarrow$ | LPIPS $\downarrow$ |  |
| DiffPIR   | 100               | 22.80                   | 93.36           | 0.355              | 24.01                  | 124.63          | 0.366              | 23.18          | 106.32          | 0.371              |  |
| DPS [8]   | 1000              | 19.58                   | 138.80          | 0.434              | 17.75                  | 184.45          | 0.491              | 22.16          | 114.93          | 0.383              |  |
| DDRM [29] | 20                | 22.33                   | 160.73          | 0.427              | -                      | -               | -                  | 23.89          | 118.55          | 0.358              |  |
| DPIR [52] | >20               | 23.86                   | 180.02          | 0.476              | 23.60                  | 210 31          | 0 / 80             | 23.00          | 204 83          | 0.475              |  |

Table 1. Noisy quantitative results on FFHQ (top) and ImageNet (bottom). We compute the average PSNR (dB), FID and LPIPS of different methods on Gaussian deblurring, motion deblurring and  $4 \times$  SR.

# Quantitative Results

| FFHQ                   |                   | Inpai                 | nt (box)              | Inpa                  | int (rand                | lom)                  | Debl                  | ur (Gaus                 | ssian)                | Deb            | lur (mot                 | ion)                  |                       | <b>SR</b> (×4)           |                       |
|------------------------|-------------------|-----------------------|-----------------------|-----------------------|--------------------------|-----------------------|-----------------------|--------------------------|-----------------------|----------------|--------------------------|-----------------------|-----------------------|--------------------------|-----------------------|
| Method                 | NFEs $\downarrow$ | $FID\downarrow$       | LPIPS $\downarrow$    | PSNR ↑                | $\mathrm{FID}\downarrow$ | LPIPS $\downarrow$    | PSNR ↑                | $\mathrm{FID}\downarrow$ | LPIPS $\downarrow$    | PSNR ↑         | $\mathrm{FID}\downarrow$ | LPIPS $\downarrow$    | PSNR ↑                | $\mathrm{FID}\downarrow$ | LPIPS $\downarrow$    |
| DiffPIR<br>DiffPIR     | 20<br>100         | 35.72<br><b>25.64</b> | 0.117<br><b>0.107</b> | 34.03<br><b>36.17</b> | 30.81<br><b>13.68</b>    | 0.116<br><b>0.066</b> | 30.74<br><b>31.00</b> | 46.64<br><b>39.27</b>    | 0.170<br><b>0.152</b> | 37.03<br>37.53 | 20.11<br><b>11.54</b>    | 0.084<br><b>0.064</b> | 29.17<br>29.52        | 58.02<br><b>47.80</b>    | 0.187<br><b>0.174</b> |
| DPS [8]                | 1000              | 43.49                 | 0.145                 | 34.65                 | 33.14                    | 0.105                 | 27.31                 | 51.23                    | 0.192                 | 26.73          | 58.63                    | 0.222                 | 27.64                 | 59.06                    | 0.209                 |
| DDRM [29]<br>DPIR [52] | 20 > 20           | 37.05                 | 0.119                 | 31.83                 | 56.60<br>-               | 0.164                 | 28.40<br>30.52        | 67.99<br>96.16           | 0.238<br>0.350        | 38.39          | 27.55                    | 0.233                 | 30.09<br><b>30.41</b> | 68.59<br>96.16           | 0.188<br>0.362        |

Table 2. Noiseless quantitative results on FFHQ. We compute the average PSNR (dB), FID and LPIPS of different methods on inpainting, deblurring, and SR.

### Qualitative Results: Noisy 4x SR



# Qualitative Results: Noisy Motion Deblurring



\*All methods used the same diffusion model as denoiser

# Diverse Reconstruction: Inpainting



# Diverse Reconstruction: Super Resolution



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# Thank You!

# Additional Slides on Diffusion Models for IR

#### **Sampling from the Posterior**



#### SDE-based Generative Models: A Unified Framework\*



#### SDE-based Generative Models: A Unified Framework

Training Objective (DSM)  $\theta^* = \arg \min \mathbb{E}_{t \sim U(0,T)} \left\{ \lambda(t) \mathbb{E}_{x(0)} \mathbb{E}_{x(t)|x(0)} [||s_{\theta}(x(t), t) - \nabla_{x(t)} \log p_{0t}(x(t)|x(0))||_2^2] \right\}$ known Gaussian when f(x, t) if affine

Discretizations

dx = f(x, t)dt + g(t)dw

| SDE Form                               | Discrete Markov Chain  | SDE Expression  |
|--|--|---|
| Variance Exploding (VE) SDE<br>(NCSN)  | $x_i = x_{i-1} + \sqrt{\sigma_i^2 - \sigma_{i-1}^2} z_{i-1}$ | $\mathrm{d}x = \sqrt{\frac{\mathrm{d}[\sigma^2(t)]}{\mathrm{d}t}}\mathrm{d}w$ |
| Variance Preserving (VP) SDE<br>(DDPM) | $x_i = \sqrt{1 - \beta_i} x_{i-1} + \sqrt{\beta_i} z_{i-1}$  | $\mathrm{d}x = \frac{1}{2}\beta(t)x\mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}w$  |

#### SDE-based Generative Models: A Unified Framework

Model: DDPM and SDE point of views

Score in score-based model is affine transformation of predicted noise in DDPM

$$oldsymbol{x}_{t} = \sqrt{ar{lpha}_{t}} oldsymbol{x}_{0} + \sqrt{1 - ar{lpha}_{t}} \cdot oldsymbol{arepsilon}$$
 Equivalent one step forward  
 $oldsymbol{s}_{ heta}(oldsymbol{x}_{t},t) \approx 
abla_{oldsymbol{x}_{t}} \log p(oldsymbol{x}_{t} | oldsymbol{x}_{0})$  Denoising score matching  
 $= -rac{oldsymbol{x}_{t} - \sqrt{ar{lpha}_{t}} oldsymbol{x}_{0}}{1 - ar{lpha}_{t}}$  Gaussian assumption  
 $= -rac{oldsymbol{arepsilon}}{\sqrt{1 - ar{lpha}_{t}}}$   $\displaystyle lpha_{oldsymbol{arepsilon}}$   $\displaystyle = -rac{oldsymbol{arepsilon}}{\sqrt{1 - ar{lpha}_{t}}}$ 

#### SDE-based Generative Models: A Unified Framework

**Controllable Generation** 

$$dx = [f(x,t) - g(t)^{2} \nabla_{x} \log p_{t}(x|y)] dt + g(t) d\bar{w}$$
  

$$\int \text{Bayesian}$$
  

$$dx = \{f(x,t) - g(t)^{2} [\nabla_{x} \log p_{t}(x) + \nabla_{x} \log p_{t}(y|x)] \} dt + g(t) d\bar{w}$$
  
unconditional model



# ILVR: Conditioning Method for DDPM\*



#### \*[2108.02938] ILVR: Conditioning Method for Denoising Diffusion Probabilistic Models (arxiv.org)

#### RePaint: Inpainting using Denoising Diffusion Probabilistic Models\*

Same idea but different downstream tasks from ILVR



Algorithm 1 Inpainting using our RePaint approach.

1:  $x_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 2: for t = T, ..., 1 do for  $u = 1, \ldots, U$  do 3:  $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$  if t > 1, else  $\epsilon = \mathbf{0}$ 4: unconditional  $x_{t-1}^{\text{known}} = \sqrt{\bar{\alpha}_t} x_0 + (1 - \bar{\alpha}_t) \epsilon$ 5:  $z \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$  if t > 1, else  $\mathbf{z} = \mathbf{0}$ 6:  $x_{t-1}^{\text{unknown}} = \frac{1}{\sqrt{\alpha_t}} \left( x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(x_t, t) \right) + \sigma_t \boldsymbol{z}$ 7:  $x_{t-1} = m \odot x_{t-1}^{\text{known}} + (1-m) \odot x_{t-1}^{\text{unknown}}$ 8: if u < U and t > 1 then 9:  $x_t \sim \mathcal{N}(\sqrt{1-\beta_{t-1}}x_{t-1}, \beta_{t-1}\mathbf{I})$ 10: end if 11: 12: end for 13: end for 14: return  $x_0$ 

#### Diffusion Posterior Sampling for General Noisy Inverse Problems\*

General forward model  $\ m{y} = \mathcal{A}(m{x}_0) + m{n}, \quad m{y}, m{n} \in \mathbb{R}^n, \ m{x} \in \mathbb{R}^d$ 

→ S<sub>A</sub>\*

Algorithm 2 DPS - Gaussian [8] **Require:** *N*, *y*,  $\{\zeta_i\}_{i=1}^N, \{\tilde{\sigma}_i\}_{i=1^N}$ 1:  $x_N \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 2: for i = N - 1 to 0 do 3:  $\hat{s} \leftarrow s_{\theta}(x_i, i)$ 4:  $\hat{x}_0 \leftarrow \frac{1}{\sqrt{\bar{\alpha}_i}} (x_i + \sqrt{1 - \bar{\alpha}_i} \hat{s})$ 5:  $z \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 6:  $x'_{i-1} \leftarrow \frac{\sqrt{\alpha_i}(1-\bar{\alpha}_{i-1})}{1-\bar{\alpha}_i} x_i + \frac{\sqrt{\bar{\alpha}_{i-1}}\beta_i}{1-\bar{\alpha}_i} \hat{x}_0 + \tilde{\sigma}_i z$ 7:  $x_{i-1} \leftarrow x'_{i-1} - \zeta_i \nabla_{x_i} \| y - \mathscr{A}(\hat{x}_0) \|_2^2$ 8: **return** *x*<sub>0</sub>

$$\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t | \boldsymbol{y}) = \nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t) + \nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{y} | \boldsymbol{x}_t)$$
$$\nabla_{\boldsymbol{x}_t} \log p_t(\boldsymbol{x}_t | \boldsymbol{y}) \simeq \boldsymbol{s}_{\theta^*}(\boldsymbol{x}_t, t) - \rho \nabla_{\boldsymbol{x}_t} \| \boldsymbol{y} - \mathcal{A}(\hat{\boldsymbol{x}}_0) \|_2^2$$

#### HQS as one diffusion step

$$\begin{cases} \hat{\mathbf{x}}_t = \operatorname*{arg\,min}_{\mathbf{x}_t} \|\mathbf{y} - \mathcal{H}(\mathbf{x}_t)\|^2 + \mu \sigma_n^2 \|\mathbf{x}_t - \hat{\mathbf{z}}_t\|^2 \\ \hat{\mathbf{z}}_t = \operatorname*{arg\,min}_{\mathbf{z}_t} \frac{1}{2(\sqrt{\lambda/\mu})^2} \|\mathbf{z}_t - \hat{\mathbf{x}}_t\|^2 + \mathcal{P}(\mathbf{z}_t) \end{cases}$$



Algorithm 2 Extended Sampling I: DPS $y_t$ Require:  $\mathbf{s}_{\theta}, T, \mathbf{y}, \sigma_n, \{\sigma_t\}_{t=1}^T, \lambda$ 1: Initialize  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 2: for t = T to 1 do 3:  $\epsilon_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 4:  $\mathbf{z}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_{\theta}(\mathbf{x}_t, t) \right) + \sqrt{\beta_t} \epsilon_t // \text{ one step}$ reverse diffusion sampling 5:  $\mathbf{x}_{t-1} = \mathbf{z}_{t-1} - \frac{\sigma_t^2}{2\lambda\sigma_n^2} \nabla_{\mathbf{z}_{t-1}} ||\mathbf{y}_{t-1} - \mathcal{H}(\mathbf{z}_{t-1})||^2 // \text{ Solving}$ data proximal subproblem

- 6: **end for**
- 7: return  $\mathbf{x}_0$

$$\arg_{\mathbf{x}_{t}} \min ||\mathbf{y} - \mathcal{H}(\mathbf{x}_{t})||^{2} + \mu \sigma_{n}^{2} ||\mathbf{x}_{t} - \hat{\mathbf{z}}_{t}||^{2}$$
$$\mathbf{\hat{x}}_{t} \approx \hat{\mathbf{z}}_{t} - \frac{\sigma_{t}^{2}}{2\lambda \sigma_{n}^{2}} \nabla_{\mathbf{z}_{t}} ||\mathbf{y} - \mathcal{H}(\mathbf{z}_{t})||^{2}$$

$$\nabla_{\mathbf{x}_{t}} \log p(\mathbf{y} \mid \mathbf{x}_{t}) \simeq \nabla_{\mathbf{x}_{t}} \log \tilde{p}(\mathbf{y} \mid \mathbf{x}_{t})$$
$$= \frac{1}{\sqrt{\bar{\alpha}_{t}}} \mathbf{A}^{T} \left( \sigma^{2} \mathbf{I} + \frac{1 - \bar{\alpha}_{t}}{\bar{\alpha}_{t}} \mathbf{A} \mathbf{A}^{T} \right)^{-1} \left( \mathbf{y} - \frac{1}{\sqrt{\bar{\alpha}_{t}}} \mathbf{A} \mathbf{x}_{t} \right)$$

A itself is row-orthogonal

$$[\nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{y} \mid \mathbf{x}_t)]_m = \frac{\mathbf{a}_m^T \left( \mathbf{y} - \frac{1}{\sqrt{\bar{\alpha}_t}} \mathbf{A} \mathbf{x}_t \right)}{\sigma^2 \sqrt{\bar{\alpha}_t} + \frac{1 - \bar{\alpha}_t}{\sqrt{\bar{\alpha}_t}} \|\mathbf{a}_m\|_2^2}$$

#### efficient computation via SVD

$$\nabla_{\mathbf{x}_{t}} \log p(\mathbf{y} \mid \mathbf{x}_{t}) \simeq \nabla_{\mathbf{x}_{t}} \log \tilde{p}(\mathbf{y} \mid \mathbf{x}_{t})$$
$$= \frac{1}{\sqrt{\bar{\alpha}_{t}}} \mathbf{V} \mathbf{\Sigma} \left( \sigma^{2} \mathbf{I} + \frac{1 - \bar{\alpha}_{t}}{\bar{\alpha}_{t}} \mathbf{\Sigma}^{2} \right)^{-1} \left( \mathbf{U}^{T} \mathbf{y} - \frac{1}{\sqrt{\bar{\alpha}_{t}}} \mathbf{\Sigma} \mathbf{V}^{T} \mathbf{x}_{t} \right),$$
(12)

Algorithm 1: DMPS: DM based posterior sampling Input: y, A,  $\sigma^2$ ,  $\{\tilde{\sigma}_t\}_{t=1}^T, \lambda$ Initialization:  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 1 for t = T to 1 do Draw  $\mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 2  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) \right) + \tilde{\sigma}_t \mathbf{z}_t$ 3 Compute  $\nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{y} \mid \mathbf{x}_t)$  as (12) 4 5  $\mathbf{x}_{t-1} = \mathbf{x}_{t-1} + \lambda \frac{1-\alpha_t}{\sqrt{\alpha_t}} \nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{y} \mid \mathbf{x}_t)$ **Output:**  $\mathbf{x}_0$ 

#### 2343] Diffusion Model Based Posterior Sampling for Noisy Linear Inverse Problems (arxiv.org)

# Denoising Diffusion Restoration Models (DDRM)\*



[H = Diagonal with 0 and 1's]

$$\mathbf{U} = H\mathbf{x}_0 + \mathbf{z}$$
  $\Longrightarrow$   $\mathbf{U}^{\top}\mathbf{y} = \mathbf{\Sigma}(\mathbf{V}^{\top}\mathbf{x}_0) + \mathbf{U}^{\top}\mathbf{z}$ 

\*[2201.11793] Denoising Diffusion Restoration Models (arxiv.org)

### Denoising Diffusion Restoration Models (DDRM)\*

\*[2201.11793] Denoising Diffusion Restoration Models (arxiv.org)

These equations in DDRM are in VESDE form

#### Zero-Shot Image Restoration Using Denoising Diffusion Null-Space Model\*

Decouple 
$$\mathbf{x} \equiv \mathbf{A}^{\dagger} \mathbf{A} \mathbf{x} + (\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \mathbf{x}$$
  
range-space of  $\mathbf{A}$  null-space of  $\mathbf{A}$   
Consistency:  $\mathbf{A} \hat{\mathbf{x}} \equiv \mathbf{y}$ , Realness:  $\hat{\mathbf{x}} \sim q(\mathbf{x})$   
Reconstruction  $\hat{\mathbf{x}} = \mathbf{A}^{\dagger} \mathbf{y} + (\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \bar{\mathbf{x}}$  find a proper  $\bar{\mathbf{x}}$  that makes the null-space term  
is in harmony with the range-space term  
Diffusion Models  $\hat{\mathbf{x}}_{0|t} = \mathbf{A}^{\dagger} \mathbf{y} + (\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \mathbf{x}_{0|t}$   
 $\mathbf{X}_{T} + \cdots + \mathbf{X}_{t}$   $\underbrace{\mathbf{x}_{0|t}}_{(\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \mathbf{x}_{0|t}}_{(\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \mathbf{x}_{0|t}}$ 

\*[2212.00490] Zero-Shot Image Restoration Using Denoising Diffusion Null-Space Model (arxiv.org)

 $-- - A^{\dagger} A - + (T - A^{\dagger} A) -$ 

| Algorithm 1 Sampling of DDNM   | Algorithm 2 Sampling of DDNM <sup>+</sup>   |
|--|---|
| $\begin{array}{ll} 1: \ \mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I}) \\ 2: \ \mathbf{for} \ t = T,, 1 \ \mathbf{do} \end{array}$   | $ \frac{1: \mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})}{2: \text{ for } t = T, \dots, 1 \text{ do}} $  |
| 3: $\mathbf{x}_{0 t} = \frac{1}{\sqrt{\bar{\alpha}_t}} \left( \mathbf{x}_t - \mathcal{Z}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) \sqrt{1 - \bar{\alpha}_t} \right)$   | 5: $L = \min\{T - t, t\}$ 4: $\mathbf{x}_{t+L} \sim q(\mathbf{x}_{t+L}   \mathbf{x}_t)$ 5: $\mathbf{for} \ j = L,, 0 \ \mathbf{do}$ 6: $\mathbf{x}_{0 t+j} = \frac{1}{\sqrt{\bar{\alpha}_{t+j}}} \left(\mathbf{x}_{t+j} - \mathcal{Z}_{\boldsymbol{\theta}}(\mathbf{x}_{t+j}, t+j)\sqrt{1 - \bar{\alpha}_{t+j}}\right)$ |
| 4: $\hat{\mathbf{x}}_{0 t} = \mathbf{A}^{\dagger} \mathbf{y} + (\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \mathbf{x}_{0 t}$<br>5: $\mathbf{x}_{t-1} \sim p(\mathbf{x}_{t-1}   \mathbf{x}_t, \hat{\mathbf{x}}_{0 t})$<br>6: return $\mathbf{x}_0$ | 7: $\hat{\mathbf{x}}_{0 t+j} = \mathbf{x}_{0 t+j} - \mathbf{\Sigma}_{t+j} \mathbf{A}^{\dagger} (\mathbf{A} \mathbf{x}_{0 t+j} - \mathbf{y})$<br>8: $\mathbf{x}_{t+j-1} \sim \hat{p}(\mathbf{x}_{t+j-1}   \mathbf{x}_{t+j}, \hat{\mathbf{x}}_{0 t+j})$<br>9: return $\mathbf{x}_0$                                       |

#### **IIGDM:** Pseudoinverse-Guided Diffusion Models for Inverse Problems\*



\*Pseudoinverse-Guided Diffusion Models for Inverse Problems | OpenReview

On Equivalence of Diffusion Posterior Sampling Strategies

DPS 
$$\hat{\mathbf{x}}_t \approx \mathbf{x}_t - \zeta_t \nabla_{\mathbf{x}_t} \log p(\mathbf{y} | \mathbf{x}_t)$$
  
 $\nabla_{\mathbf{x}_t} \log p(\mathbf{y} | \mathbf{x}_t) \simeq \nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{y} | \mathbf{x}_t)$   
 $= \frac{1}{\sqrt{\bar{\alpha}_t}} \mathbf{A}^T \left( \sigma^2 \mathbf{I} + \frac{1 - \bar{\alpha}_t}{\bar{\alpha}_t} \mathbf{A} \mathbf{A}^T \right)^{-1} \left( \mathbf{y} - \frac{1}{\sqrt{\bar{\alpha}_t}} \mathbf{A} \mathbf{x}_t \right)$   
Some coefficient  
DDNM  $\hat{\mathbf{x}}_{0|t} = \mathbf{A}^{\dagger} \mathbf{y} + (\mathbf{I} - \mathbf{A}^{\dagger} \mathbf{A}) \mathbf{x}_{0|t}$   
 $= \mathbf{x}_{0|t} - (\mathbf{A}^{\dagger} \mathbf{A} \mathbf{x}_{0|t} - \mathbf{A}^{\dagger} \mathbf{y})$   
 $= \mathbf{x}_{0|t} - \mathbf{A}^{\dagger} (\mathbf{A} \mathbf{x}_{0|t} - \mathbf{y})$ 

#### Solving Image Restoration Tasks Iteratively (Traditional PnP Methods)

Image Restoration by Iterative Denoising and Backward Projections

Algorithm 2 Iterative Denoising and Backward Projections (IDBP)

Input:  $H, y, \sigma_e$ , denoising operator  $\mathcal{D}(\cdot; \sigma)$ , stopping criterion. y = Hx + e, such that  $e \sim \mathcal{N}(\mathbf{0}, \sigma_e^2 \mathbf{I}_m)$  and x is an unknown signal whose prior model is specified by  $\mathcal{D}(\cdot; \sigma)$ . Output:  $\hat{x}$  an estimate for x. Initialize:  $\tilde{y}_0$  = some initialization, k = 0,  $\delta$  approx. satisfying (12). while stopping criterion not met do  $\begin{vmatrix} k = k + 1; \\ \tilde{x}_k = \mathcal{D}(\tilde{y}_{k-1}; \sigma_e + \delta); \\ \tilde{y}_k = H^{\dagger}y + (\mathbf{I}_n - H^{\dagger}H)\tilde{x}_k; \end{vmatrix}$ end  $\hat{x} = \tilde{x}_k;$ 

#### What are the advantages of diffusion sampling framework?

In our experiment all methods use the same diffusion model checkpoints

Plug-and-Play Image Restoration with Deep Denoiser Prior

**Algorithm 1:** Plug-and-play image restoration with deep denoiser prior (DPIR).

**Input** : Deep denoiser prior model, degraded image  $\mathbf{y}$ , degradation operation  $\mathcal{T}$ , image noise level  $\sigma$ ,  $\sigma_k$  of denoiser prior model at *k*-th iteration for a total of *K* iterations, trade-off parameter  $\lambda$ .

**Output:** Restored image  $\mathbf{z}_K$ .

- 1 Initialize  $\mathbf{z}_0$  from  $\mathbf{y}$ , pre-calculate  $\alpha_k \triangleq \lambda \sigma^2 / \sigma_k^2$ .
- 2 for  $k = 1, 2, \cdots, K$  do
- 3  $\mathbf{x}_k = \arg\min_{\mathbf{x}} \|\mathbf{y} \mathcal{T}(\mathbf{x})\|^2 + \alpha_k \|\mathbf{x} \mathbf{z}_{k-1}\|^2$ ; // Solving data subproblem
- 4  $\mathbf{z}_k = Denoiser(\mathbf{x}_k, \sigma_k)$ ; // Denoising with deep DRUNet denoiser and periodical geometric self-ensemble

5 end

- $\rightarrow$  well-defined path connecting two distributions
- $\rightarrow$  schedule is all you need!!

#### Sampling from Langevin Dynamics?

[2103.04715] Bayesian imaging using Plug & Play priors: when Langevin meets Tweedie (arxiv.org)

Algorithm 1 PnP-ULA

**Require:**  $n \in \mathbb{N}, y \in \mathbb{R}^m, \varepsilon, \lambda, \alpha, \delta > 0, \mathbb{C} \subset \mathbb{R}^d$  convex and compact **Ensure:**  $2\lambda(2L_y + \alpha L/\varepsilon) \leq 1$  and  $\delta < (1/3)(L_y + 1/\lambda + \alpha L/\varepsilon)^{-1}$  **Initialization:** Set  $X_0 \in \mathbb{R}^d$  and k = 0. **for** k = 0 : N **do**   $Z_{k+1} \sim \mathcal{N}(0, \mathrm{Id})$   $X_{k+1} = X_k + \delta \nabla \log(p(y|X_k)) + (\alpha \delta/\varepsilon)(D_{\varepsilon}(X_k) - X_k) + (\delta/\lambda)(\Pi_{\mathsf{C}}(X_k) - X_k) + \sqrt{2\delta}Z_{k+1}$  **end for return**  $\{X_k : k \in \{0, \dots, N+1\}\}$ 

[1611.02862] The Little Engine that Could: Regularization by Denoising (RED) (arxiv.org) An Interpretation Of Regularization By Denoising And Its Application With The Back-Projected Fidelity Term

$$egin{aligned} oldsymbol{x}_{k+1} &=& oldsymbol{x}_k - \mu \left( 
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Metropolis-adjusted Langevin algorithm (MALA) sampler

$$\begin{aligned} x_{t+1} &= x_t + \epsilon_1 \frac{\partial \log p(x_t)}{\partial x_t} + \epsilon_2 \frac{\partial \log p(y = y_c | x_t)}{\partial x_t} + N(0, \epsilon_3^2) \\ & \frac{\partial \log p(x)}{\partial x} \approx \frac{R_x(x) - x}{\sigma^2} \quad \text{Denoising AutoEncoder output as score} \\ h_{t+1} &= h_t + \epsilon_1 (R_h(h_t) - h_t) + \epsilon_2 \frac{\partial \log C_c(G(h_t))}{\partial G(h_t)} \frac{\partial G(h_t)}{\partial h_t} \quad + N(0, \epsilon_3^2) \\ & \text{latent} \qquad \text{prior} \qquad \text{condition} \qquad \text{noise} \\ & realistic \qquad \text{e.g. class-specific} \qquad diverse \end{aligned}$$

\*[1612.00005] Plug & Play Generative Networks: Conditional Iterative Generation of Images in Latent Space (arxiv.org)