

Diffusion Models for Inverse Problems Done Right

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Conference on
Computational Science
and Engineering

**Generative Machine Learning Models for
Uncertainty Quantification**



UNIVERSITY OF MINNESOTA
*Driven to Discover*SM

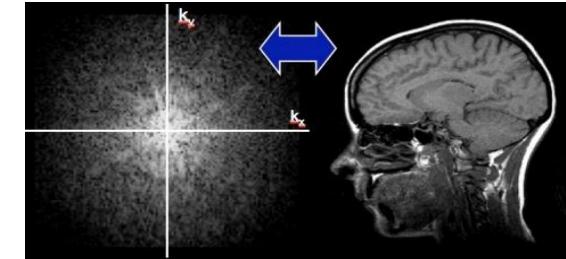
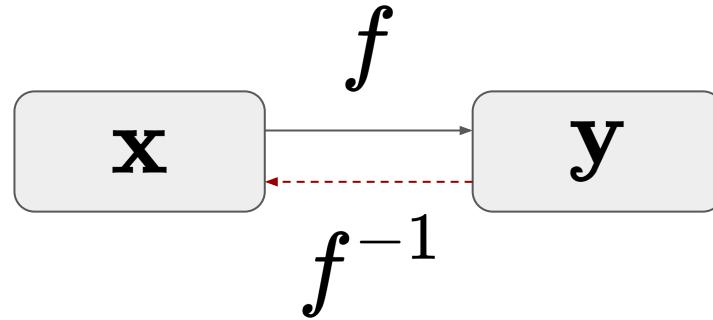
Inverse Problems

Inverse problems

Inverse problem: given $\mathbf{y} = f(\mathbf{x})$, recover \mathbf{x}



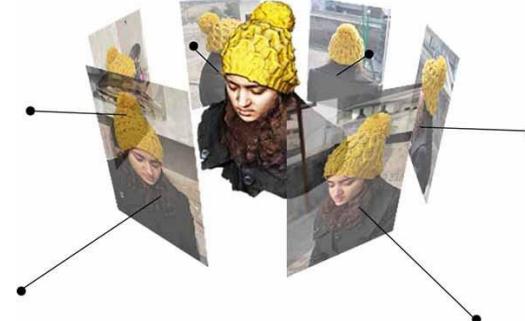
Image denoising



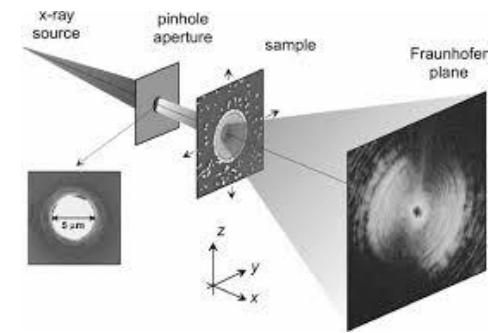
MRI reconstruction



Image super-resolution



3D reconstruction



Coherent diffraction imaging (CDI)

Traditional methods

Inverse problem: given $\mathbf{y} = f(\mathbf{x})$, recover \mathbf{x}

$$\min_{\mathbf{x}} \underbrace{\ell(\mathbf{y}, f(\mathbf{x}))}_{\text{data fitting}} + \lambda \underbrace{R(\mathbf{x})}_{\text{regularizer}}$$

RegFit

Questions

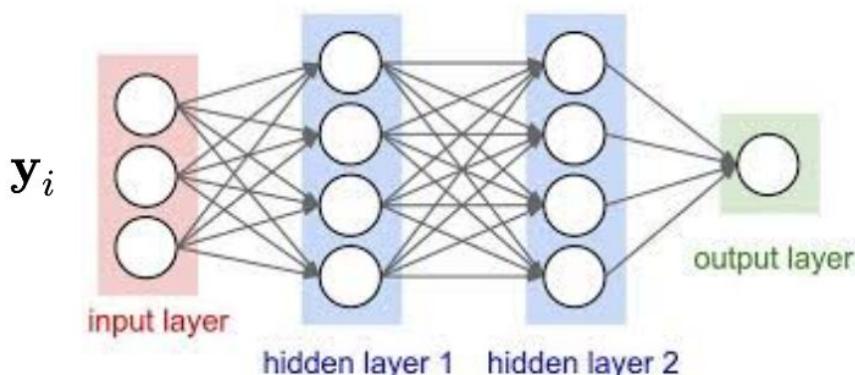
- Which ℓ ? (e.g., unknown/compound noise)
- Which R ? (e.g., structures not amenable to math description)
- Speed

Deep learning has changed everything

With paired datasets $\{(\mathbf{y}_i, \mathbf{x}_i)\}_{i=1,\dots,N}$

Direct inversion

Learn f^{-1} from $\{(\mathbf{y}_i, \mathbf{x}_i)\}_{i=1,\dots,N}$

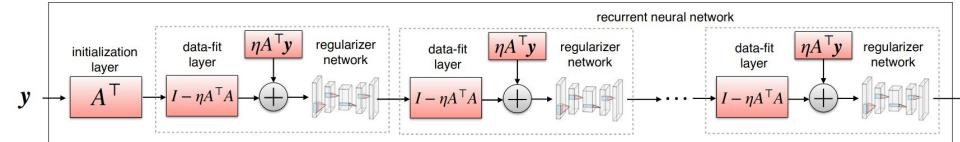


Algorithm unrolling

$$\min_{\mathbf{x}} \ell(\mathbf{y}, f(\mathbf{x})) + \lambda R(\mathbf{x})$$

$$\mathbf{x}^{k+1} = \mathcal{P}_R \left(\mathbf{x}^k - \eta \nabla^\top f(\mathbf{x}^k) \ell'(\mathbf{y}, f(\mathbf{x}^k)) \right)$$

Idea: make \mathcal{P}_R trainable



With paired datasets $\{(\mathbf{y}_i, \mathbf{x}_i)\}_{i=1,\dots,N}$

Conditional generation & regularization

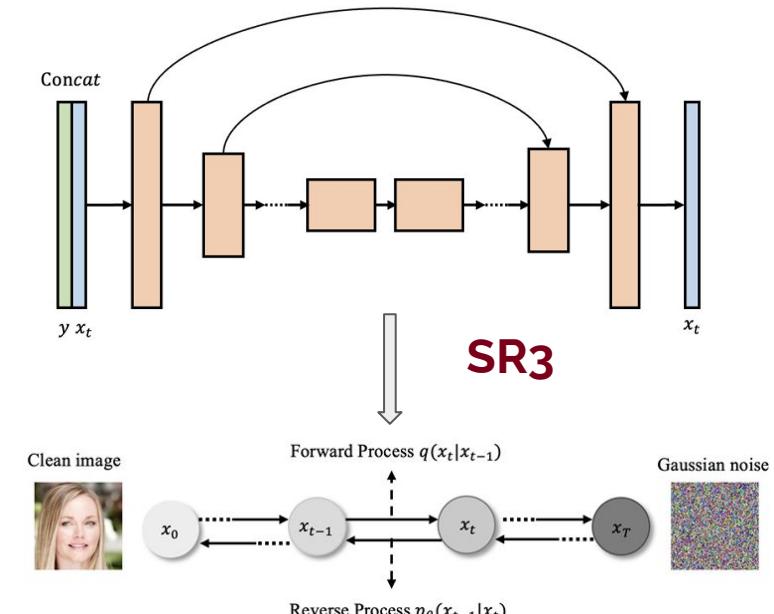
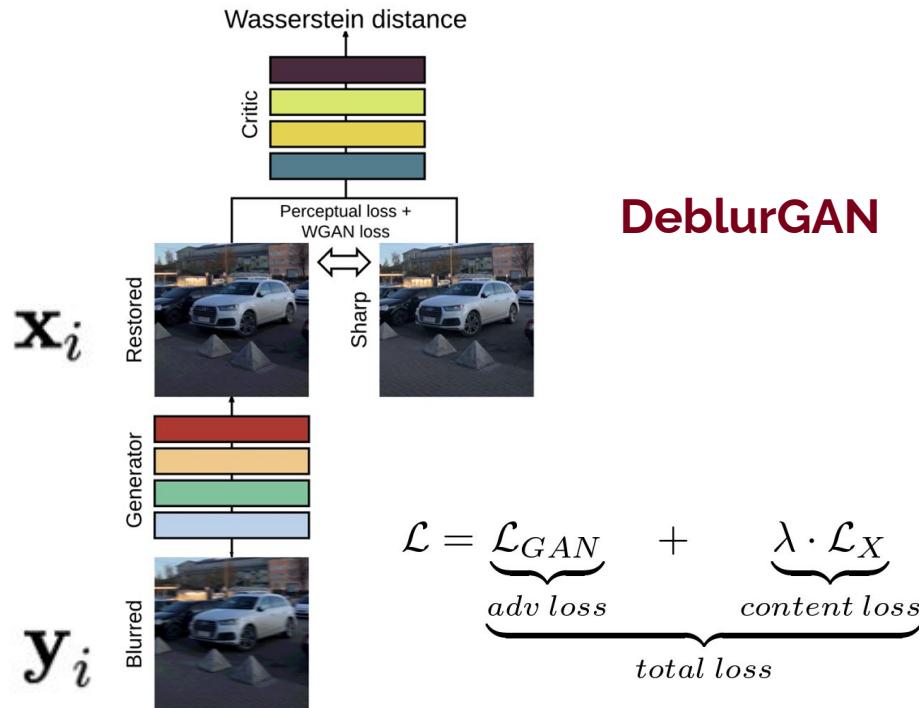


Image credit: <https://arxiv.org/abs/2308.09388>

With object datasets only $\{x_i\}_{i=1,\dots,N}$

**Model the distribution of the objects first, and then plug the prior in
GAN Inversion**

Pretraining: $x_i \approx G_\theta(z_i) \quad \forall i$

Deployment: $\min_z \ell(y, f \circ G_\theta(z)) + \lambda R \circ G_\theta(z)$

Interleaving pretrained diffusion models

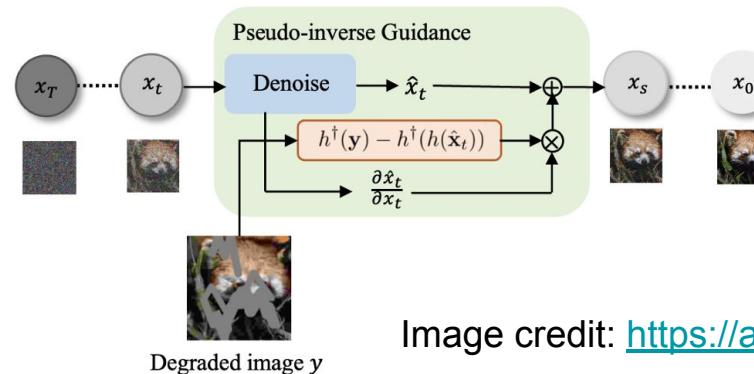


Image credit: <https://arxiv.org/abs/2308.09388>

Without datasets? Single-instance methods

Deep image prior (DIP) $\mathbf{x} \approx G_{\theta}(\mathbf{z})$ G_{θ} (and \mathbf{z}) trainable

$$\min_{\mathbf{x}} \underbrace{\ell(\mathbf{y}, f(\mathbf{x}))}_{\text{data fitting}} + \lambda \underbrace{R(\mathbf{x})}_{\text{regularizer}}$$

↓

$$\min_{\mathbf{z}} \ell(\mathbf{y}, f \circ G_{\theta}(\mathbf{z})) + \lambda R \circ G_{\theta}(\mathbf{z})$$

No extra training data!

Neural implicit representation (NIR)

$\mathbf{x} \approx \mathcal{D} \circ \bar{\mathbf{x}}$ \mathcal{D} : discretization $\bar{\mathbf{x}}$: continuous function

Physics-informed neural networks (PINN)

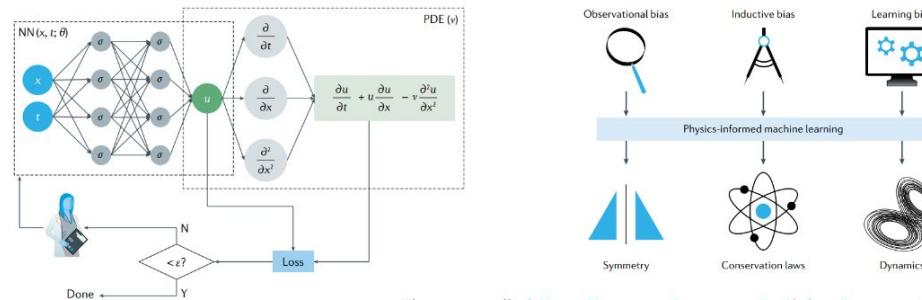


Figure credit: <https://www.nature.com/articles/s42254-021-00314-5>

Other specialized surveys

Algorithm Unrolling: Interpretable, Efficient Deep Learning for Signal and Image Processing

Vishal Monga, *Senior Member, IEEE*, Yuelong Li, *Member, IEEE*, and Yonina C. Eldar, *Fellow, IEEE*

Focused on alg. unrolling

Untrained Neural Network Priors for Inverse Imaging Problems: A Survey

Deep Internal Learning:

Understanding Untrained Deep Models for Inverse Problems: Algorithms and Theory

Tom Tirer *Member,*

Focused on single-instance methods

Ismail Alkhouri, Evan Bell, Avraijit Ghosh, Shijun Liang, Rongrong Wang,

Theoretical Perspectives on Deep Learning Methods in Inverse Problems

Jonathan Scarlett, Reinhard Heckel, Miguel R. D. Rodrigues, Paul Hand, and Yonina C. Eldar

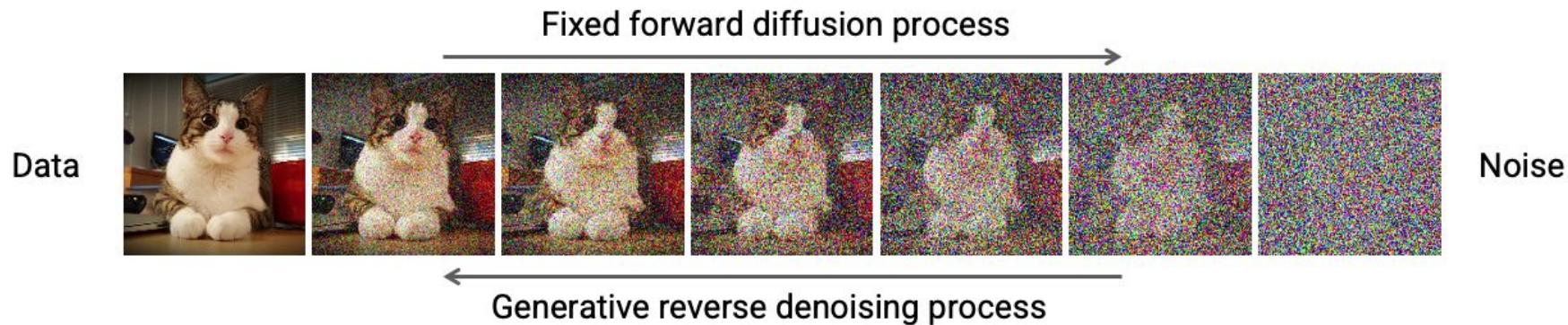
Focused on theories for linear IPs

This talk:

Solving Inverse Problems (IPs)
Using Pretrained Diffusion Models

Diffusion models

$$d\mathbf{x} = -\beta_t/2 \cdot \mathbf{x} dt + \sqrt{\beta_t} d\mathbf{w},$$

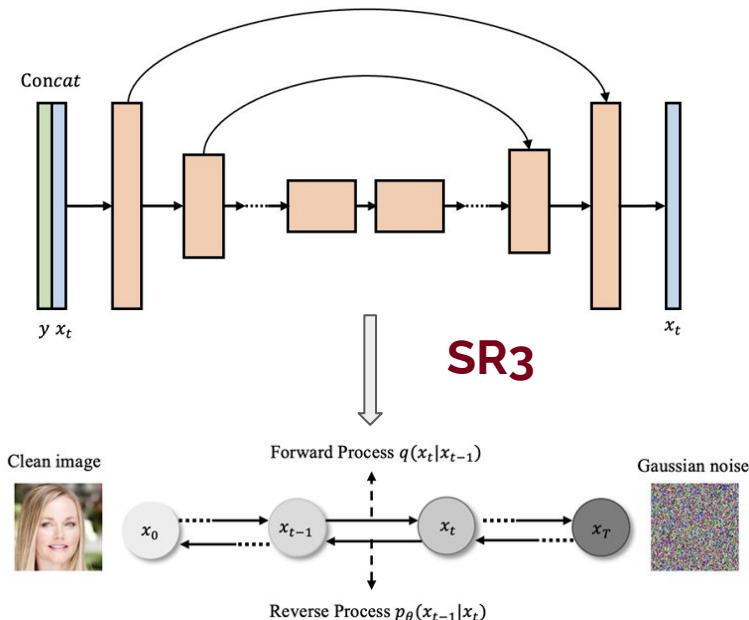


$$d\mathbf{x} = -\beta_t [\mathbf{x}/2 + \boxed{\nabla_{\mathbf{x}} \log p_t(\mathbf{x})}] dt + \sqrt{\beta_t} d\mathbf{w}.$$

$$\approx \epsilon_{\theta}^{(t)}(\mathbf{x})$$

Diffusion models for inverse problems (IPs)

Supervised



Zero-shot

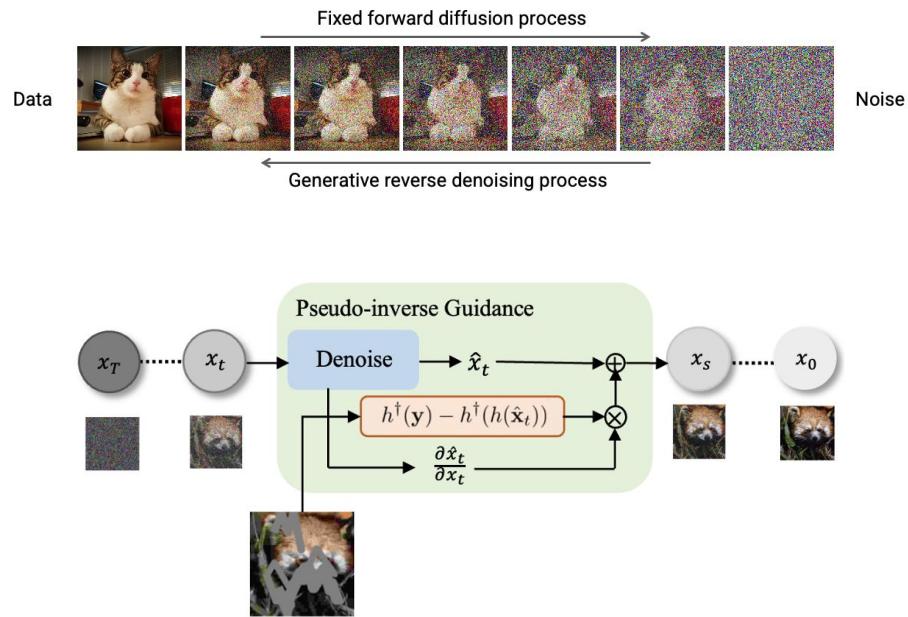


Image credit: <https://arxiv.org/abs/2308.09388>

Focus: IPs with pretrained diffusion models

(Reverse SDE for DDPM) $d\mathbf{x} = -\beta_t [\mathbf{x}/2 + \nabla_{\mathbf{x}} \log p_t(\mathbf{x})] dt + \sqrt{\beta_t} d\bar{\mathbf{w}}$



Think of **conditional score function**

$$\nabla_{\mathbf{x}} \log p_t(\mathbf{x}|\mathbf{y}) = \nabla_{\mathbf{x}} \log p_t(\mathbf{x}) + \nabla_{\mathbf{x}} \log p_t(\mathbf{y}|\mathbf{x})$$



Conditional reverse SDE

$$d\mathbf{x} = [-\beta_t/2 \cdot \mathbf{x} - \beta_t (\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) + \nabla_{\mathbf{x}} \log p_t(\mathbf{y}|\mathbf{x}))] dt + \sqrt{\beta_t} d\bar{\mathbf{w}}$$

Coping with conditional score function

$$\nabla_{\mathbf{x}} \log p_t(\mathbf{x}|\mathbf{y}) = \boxed{\nabla_{\mathbf{x}} \log p_t(\mathbf{x})} + \boxed{\nabla_{\mathbf{x}} \log p_t(\mathbf{y}|\mathbf{x})}$$
$$\approx \varepsilon_{\theta}^{(t)}(\mathbf{x})$$

$$p_t(\mathbf{y}|\mathbf{x}(t))$$
$$\cong p_t(\mathbf{y}|\hat{\mathbf{x}}(0)[\mathbf{x}(t)])$$

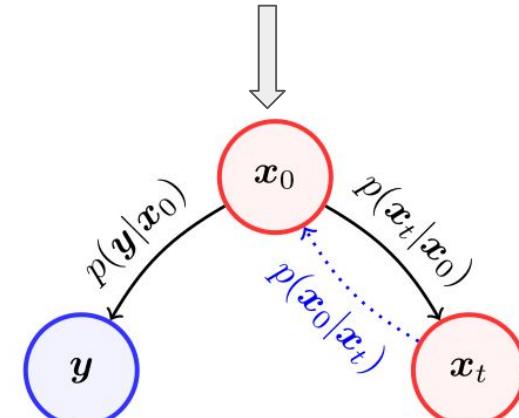


Figure 2: Probabilistic graph. Black solid line: tractable, blue dotted line: intractable in general.

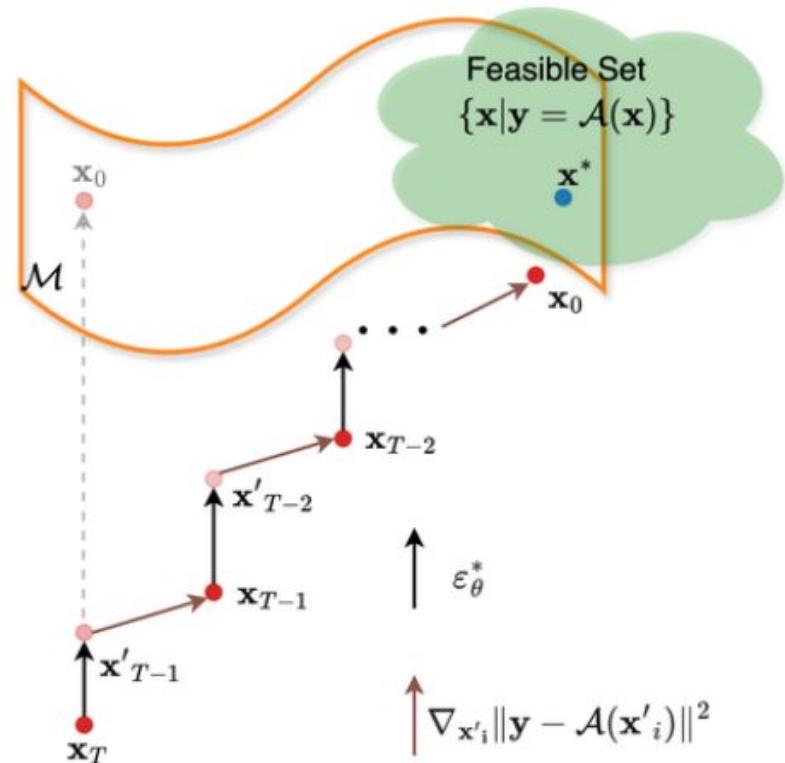
Interleaving methods

Algorithm 1 Template for interleaving methods

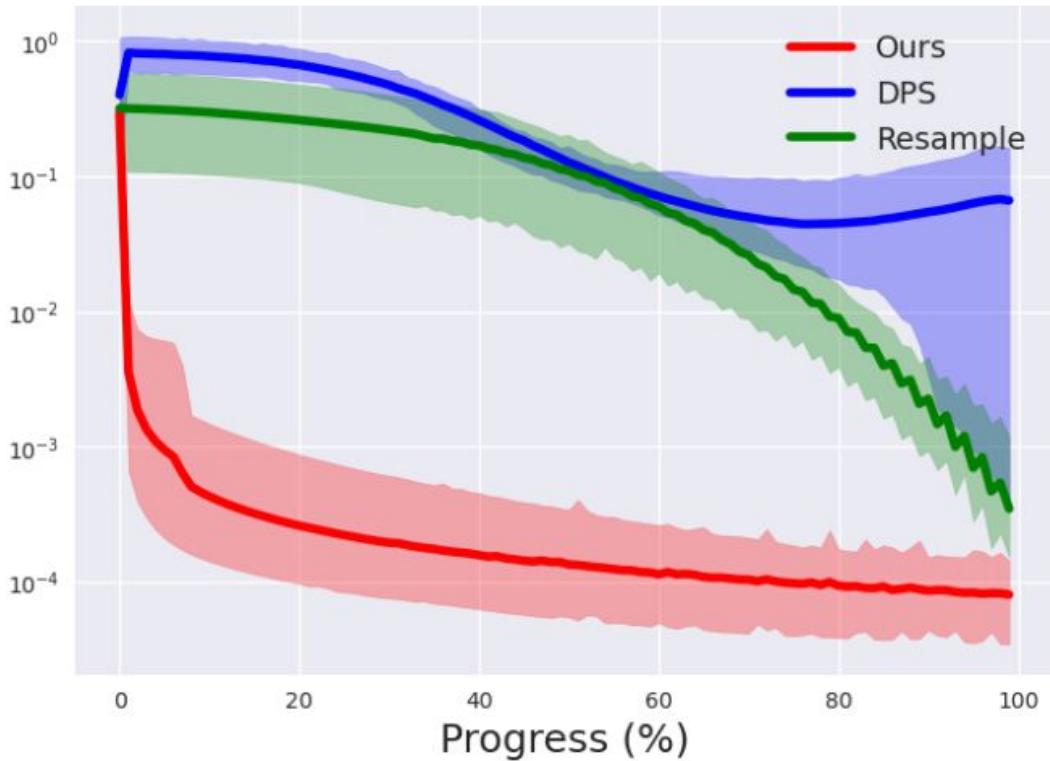
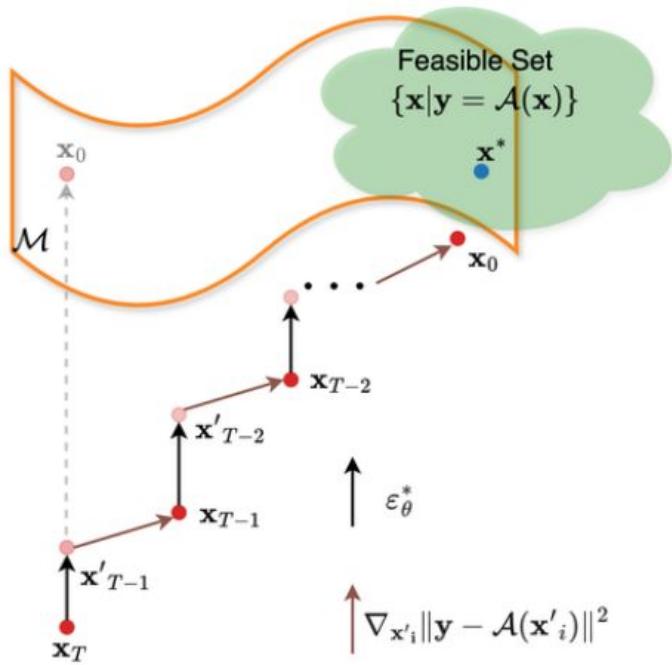
Input: # Diffusion steps T , measurement \mathbf{y}

```
1:  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
2: for  $i = T - 1$  to 0 do
3:    $\hat{\mathbf{s}} \leftarrow \varepsilon_{\theta}^{(i)}(\mathbf{x}_i)$ 
4:    $\hat{\mathbf{x}}_0 \leftarrow \frac{1}{\sqrt{\bar{\alpha}_i}}(\mathbf{x}_i - \sqrt{1 - \bar{\alpha}_i}\hat{\mathbf{s}})$ 
5:    $\mathbf{x}'_{i-1} \leftarrow \text{DDIM reverse with } \hat{\mathbf{x}}_0 \text{ and } \hat{\mathbf{s}}$ 
6:    $\mathbf{x}_{i-1} \leftarrow \text{(Approximately) Projection [39, 30, 33, 32, 40, 41, 34] or gradient update [20, 28, 19, 21, 29, 27, 26]} \text{ with } \hat{\mathbf{x}}_0 \text{ and } \mathbf{x}'_{i-1} \text{ to get closer to } \{\mathbf{x} | \mathbf{y} = \mathcal{A}(\mathbf{x})\}$ 
7: end for
```

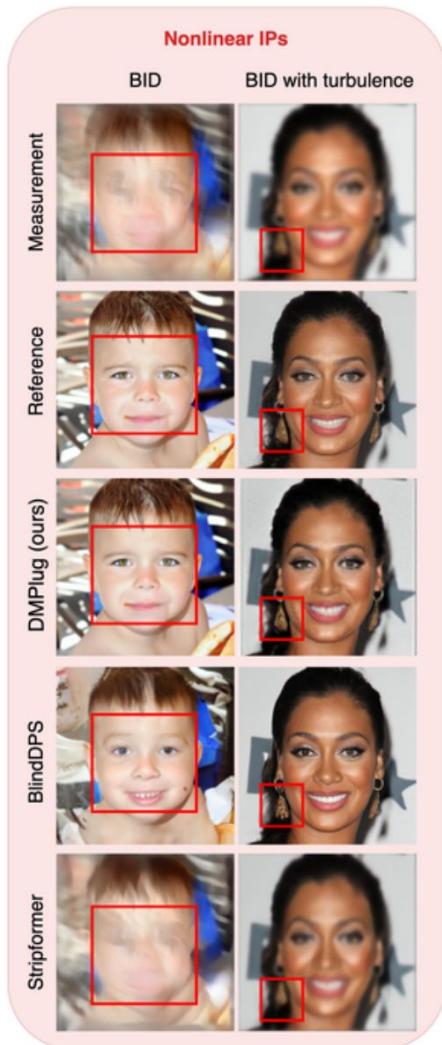
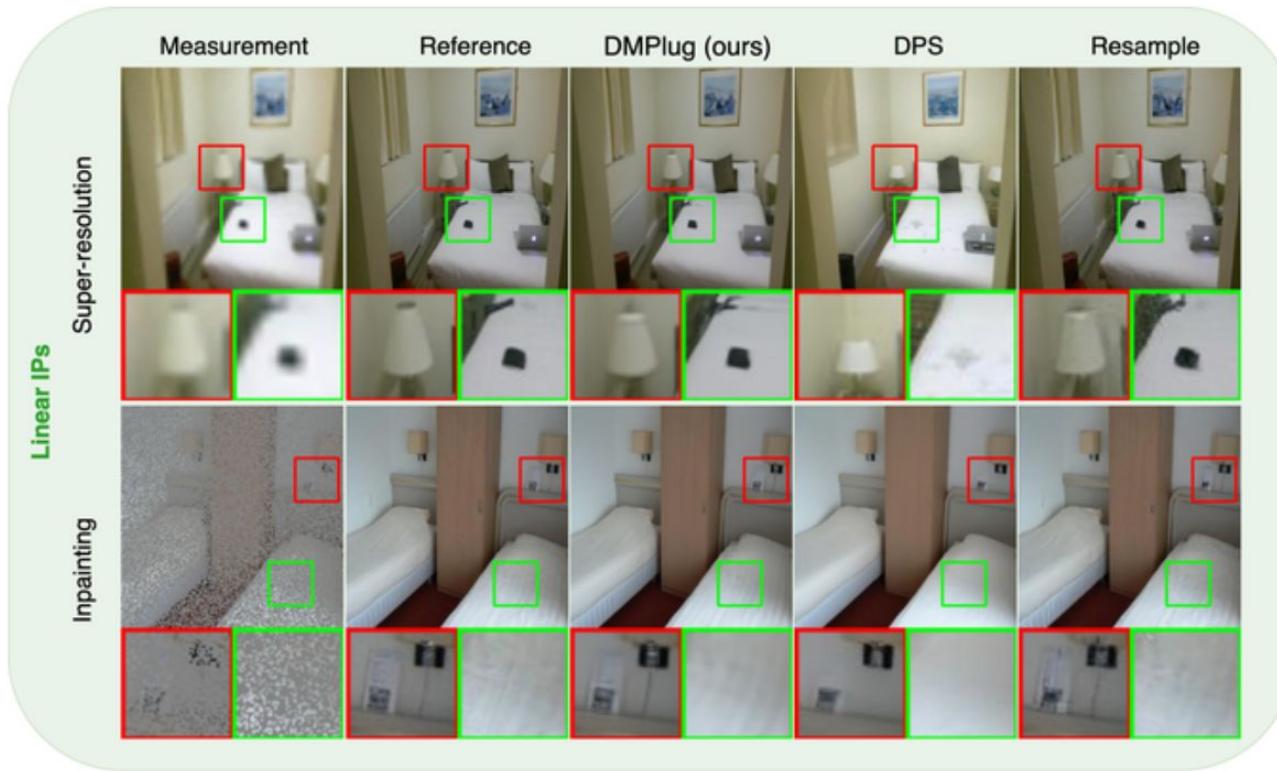
Output: Recovered object \mathbf{x}_0



Issue I: Measurement feasibility



Issue 2: Manifold feasibility



Issue 3: Robustness to unknown noise

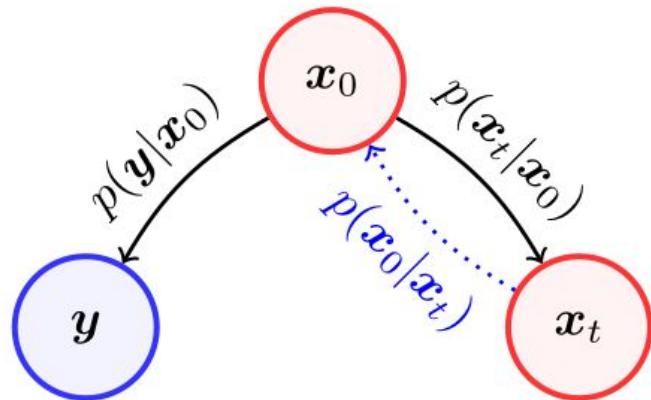


Figure 2: Probabilistic graph. Black solid line: tractable, blue dotted line: intractable in general.

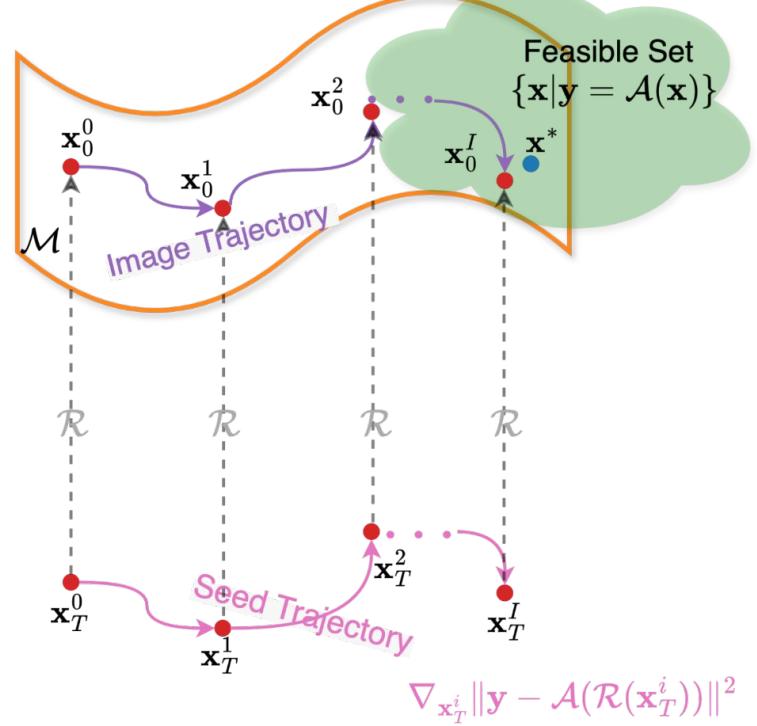
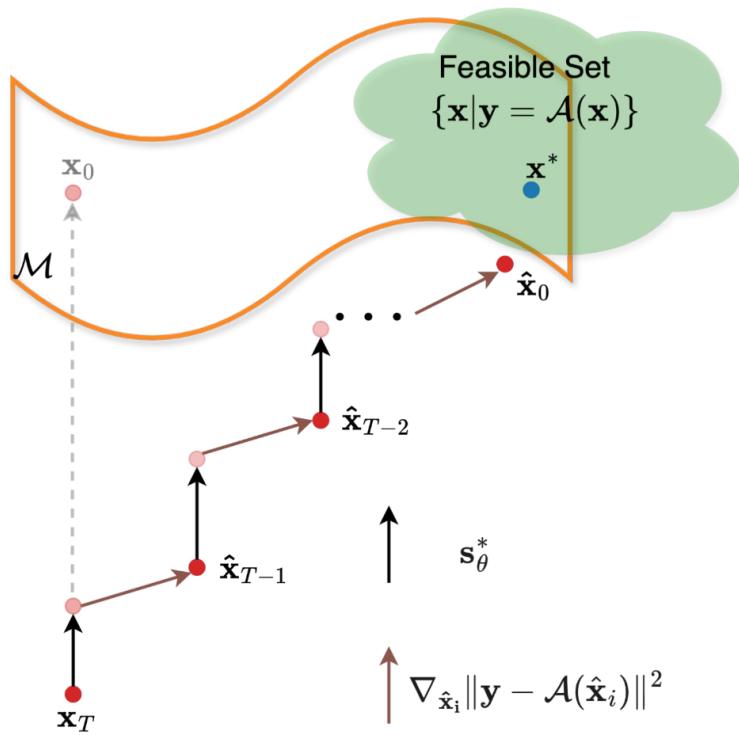
Algorithm 1 DPS - Gaussian

Require: $N, \mathbf{y}, \{\zeta_i\}_{i=1}^N, \{\tilde{\sigma}_i\}_{i=1}^N$

```
1:  $\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
2: for  $i = N - 1$  to 0 do
3:    $\hat{\mathbf{s}} \leftarrow \mathbf{s}_\theta(\mathbf{x}_i, i)$ 
4:    $\hat{\mathbf{x}}_0 \leftarrow \frac{1}{\sqrt{\bar{\alpha}_i}}(\mathbf{x}_i + (1 - \bar{\alpha}_i)\hat{\mathbf{s}})$ 
5:    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
6:    $\mathbf{x}'_{i-1} \leftarrow \frac{\sqrt{\alpha_i}(1 - \bar{\alpha}_{i-1})}{1 - \bar{\alpha}_i}\mathbf{x}_i + \frac{\sqrt{\bar{\alpha}_{i-1}}\beta_i}{1 - \bar{\alpha}_i}\hat{\mathbf{x}}_0 + \tilde{\sigma}_i \mathbf{z}$ 
7:    $\mathbf{x}_{i-1} \leftarrow \mathbf{x}'_{i-1} - \zeta_i \nabla_{\mathbf{x}_i} \|\mathbf{y} - \mathcal{A}(\hat{\mathbf{x}}_0)\|_2^2$ 
8: end for
9: return  $\hat{\mathbf{x}}_0$ 
```

depending on noise level

Our solution: DMPlug

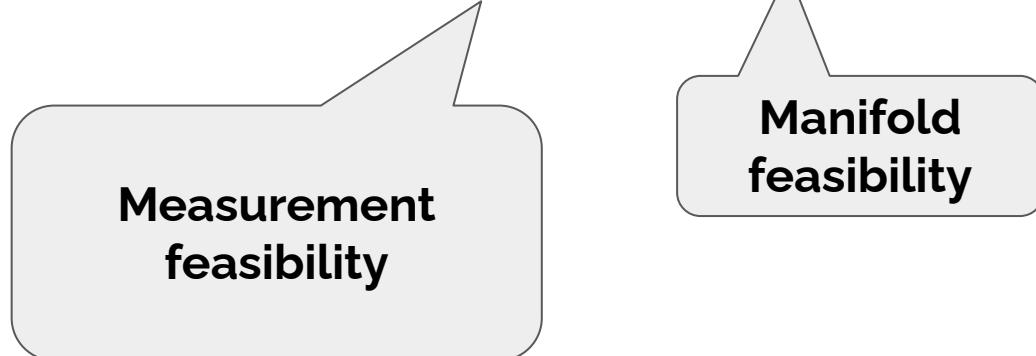


Our solution: DMPlug

Viewing the reverse process as a function \mathcal{R}

$$\mathcal{R} = g_{\varepsilon_\theta^{(0)}} \circ g_{\varepsilon_\theta^{(1)}} \circ \cdots \circ g_{\varepsilon_\theta^{(T-2)}} \circ g_{\varepsilon_\theta^{(T-1)}}. \quad (\circ \text{ means function composition})$$

$$(\textbf{DMPlug}) \ z^* \in \arg \min_z \ell(\mathbf{y}, \mathcal{A}(\boxed{\mathcal{R}(z)})) + \Omega(\mathcal{R}(z)), \quad x^* = \mathcal{R}(z^*).$$

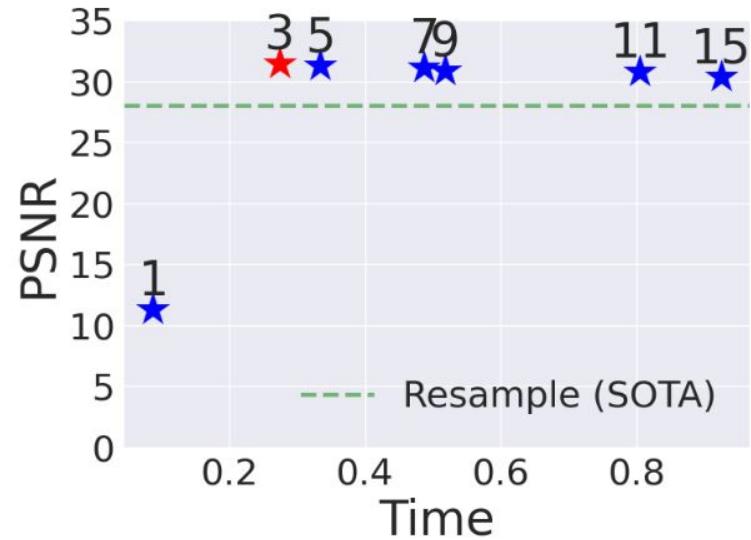


Overcoming the computational bottleneck

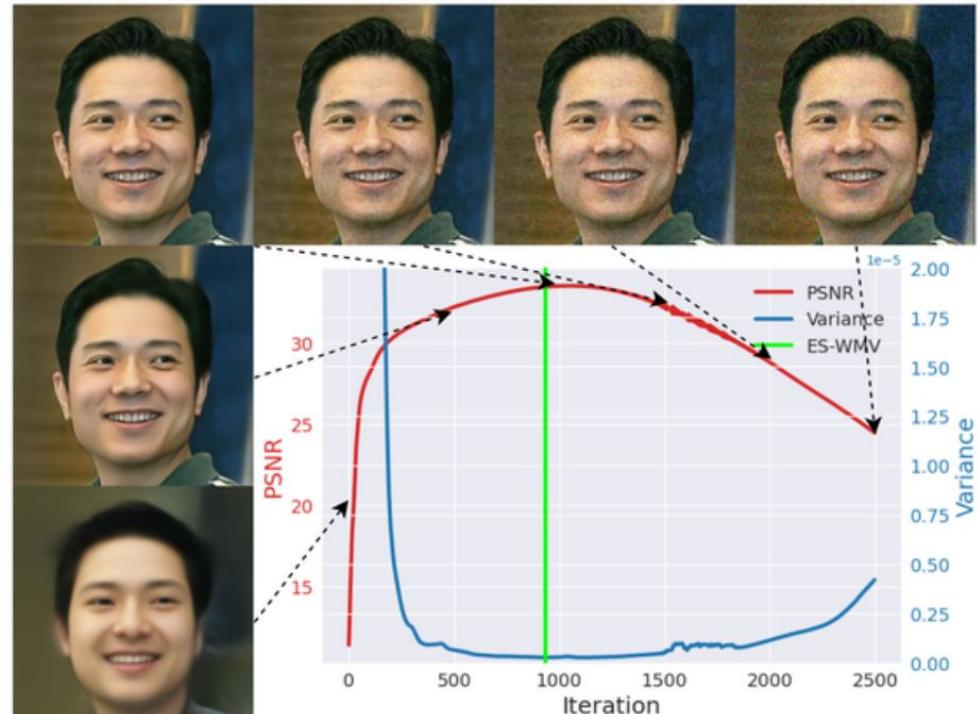
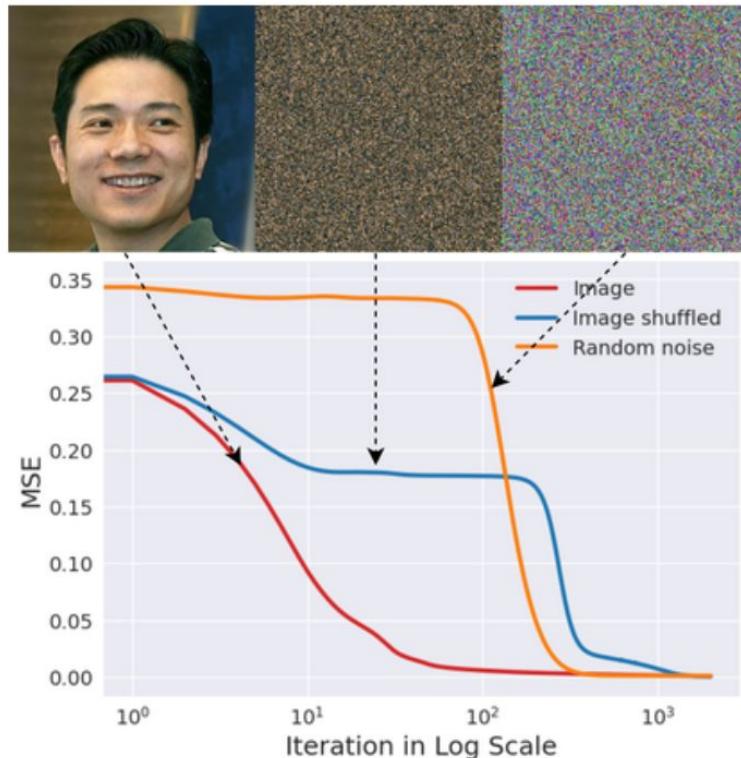
$$\mathcal{R} = g_{\varepsilon_\theta^{(0)}} \circ g_{\varepsilon_\theta^{(1)}} \circ \cdots \circ g_{\varepsilon_\theta^{(T-2)}} \circ g_{\varepsilon_\theta^{(T-1)}}. \quad (\circ \text{ means function composition})$$

$$(\textbf{DMPlug}) \ z^* \in \arg \min_z \ \ell(y, \mathcal{A}(\mathcal{R}(z))) + \Omega(\mathcal{R}(z)), \quad x^* = \mathcal{R}(z^*).$$

Issue: T blocks of DNNs involved, and we have to back-propagate through it



How to achieve robustness to unknown noise?



Early-learning-then-overfitting (OLTO)

Algorithm 3 DMPlug+ES–WMV for solving general IPs

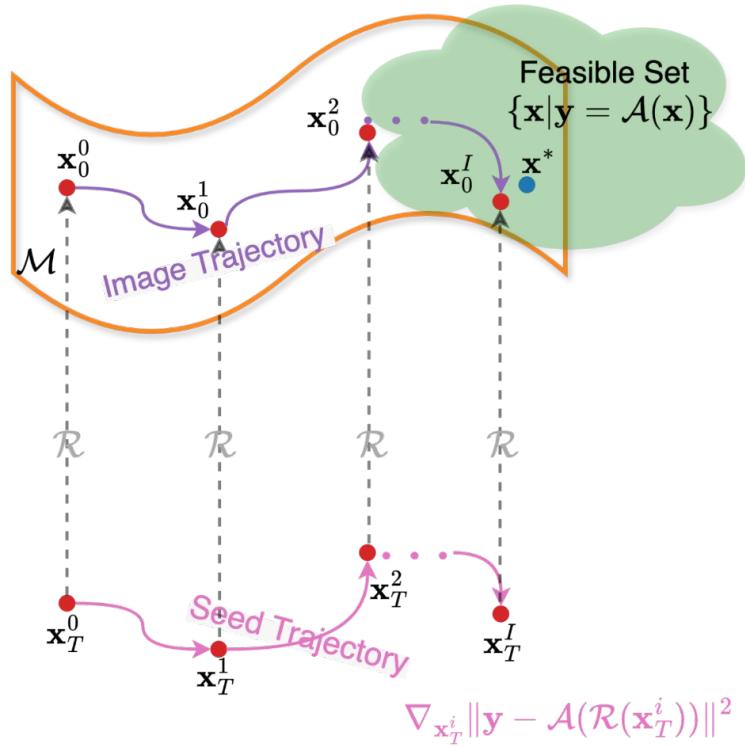
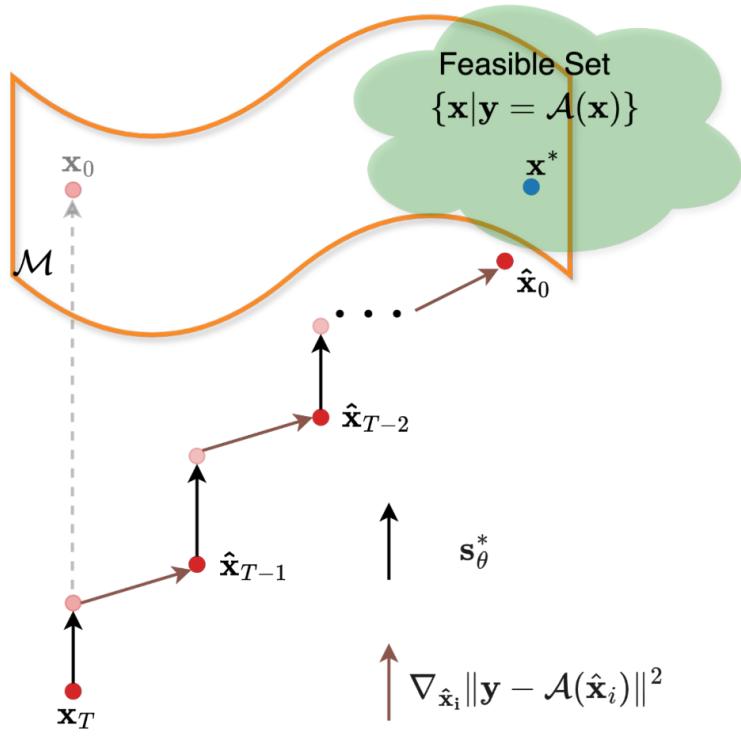
Input: # diffusion steps T , \mathbf{y} , window size W , patience P , empty queue \mathcal{Q} ,
iteration counter $e = 0$, $\text{VAR}_{\min} = \infty$

```
1: while not stopped do
2:   for  $i = T - 1$  to 0 do
3:      $\hat{\mathbf{s}} \leftarrow \varepsilon_{\theta}^{(i)}(\mathbf{z}_i^e)$ 
4:      $\hat{\mathbf{z}}_0^e \leftarrow \frac{1}{\sqrt{\bar{\alpha}_i}}(\mathbf{z}_i^e - \sqrt{1 - \bar{\alpha}_i}\hat{\mathbf{s}})$ 
5:      $\mathbf{z}_{i-1}^e \leftarrow \text{DDIM reverse with } \hat{\mathbf{z}}_0^e, \hat{\mathbf{s}}$ 
6:   end for
7:   Update  $\mathbf{z}_T^{e+1}$  from  $\mathbf{z}_T^e$  via a gradient update for Eq. (7)
8:   push  $\mathcal{R}(\mathbf{z}_T^{e+1})$  to  $\mathcal{Q}$ , pop queue if  $|\mathcal{Q}| > W$ 
9:   if  $|\mathcal{Q}| = W$  then
10:    compute VAR of elements in  $\mathcal{Q}$  via Eq. (15)
11:    if VAR <  $\text{VAR}_{\min}$  then
12:       $\text{VAR}_{\min} \leftarrow \text{VAR}$ ,  $\mathbf{z}^* \leftarrow \mathbf{z}_T^{e+1}$ 
13:    end if
14:    if  $\text{VAR}_{\min}$  stagnates for  $P$  iterations then
15:      stop and return  $\mathbf{z}^*$ 
16:    end if
17:  end if
18:   $e = e + 1$ 
19: end while
```

Output: Recovered object $\mathcal{R}(\mathbf{z}^*)$

Early stopping
based on
running
variance

DMPlug to get everything right



The paper (NeurIPS'24)

[Submitted on 27 May 2024]

DMPlug: A Plug-in Method for Solving Inverse Problems with Diffusion Models

Hengkang Wang, Xu Zhang, Taihui Li, Yuxiang Wan, Tiancong Chen, Ju Sun

Pretrained diffusion models (DMs) have recently been popularly used in solving inverse problems (IPs). The existing methods mostly interleave iterative steps in the reverse diffusion process and iterative steps to bring the iterates closer to satisfying the measurement constraint. However, such interleaving methods struggle to produce final results that look like natural objects of interest (i.e., manifold feasibility) and fit the measurement (i.e., measurement feasibility), especially for nonlinear IPs. Moreover, their capabilities to deal with noisy IPs with unknown types and levels of measurement noise are unknown. In this paper, we advocate viewing the reverse process in DMs as a function and propose a novel plug-in method for solving IPs using pretrained DMs, dubbed DMPlug. DMPlug addresses the issues of manifold feasibility and measurement feasibility in a principled manner, and also shows great potential for being robust to unknown types and levels of noise. Through extensive experiments across various IP tasks, including two linear and three nonlinear IPs, we demonstrate that DMPlug consistently outperforms state-of-the-art methods, often by large margins especially for nonlinear IPs. The code is available at [this https URL](https://arxiv.org/abs/2405.16749).

<https://arxiv.org/abs/2405.16749>

Train diffusion models in small-data regime?



(a) Full Gaussian (ambient dimension $d = 12288$)



(a) Full Gaussian (ambient dimension $d = 16384$, FID-50K=5.09)



(b) Restricted Gaussian (subspace dimension $k = 2048$)



(b) Restricted Gaussian (subspace dimension $k = 8192$, FID-50K=3.21)

Luo et al. **Small-Data Flow Matching**. Forthcoming, 2025