Accelerating diffusion models for inverse problems through stochastic contraction

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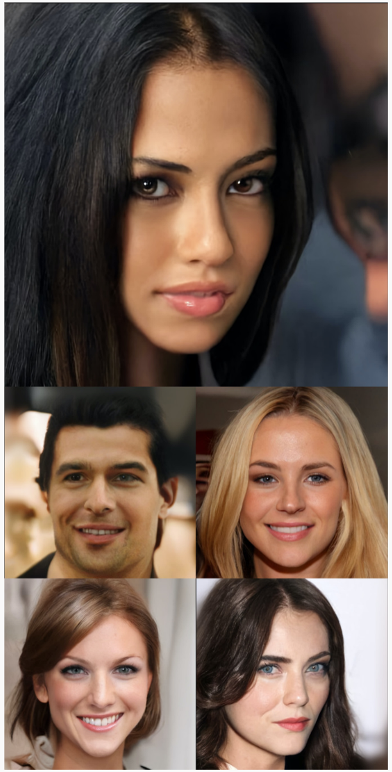
Diffusion-based Generative Models

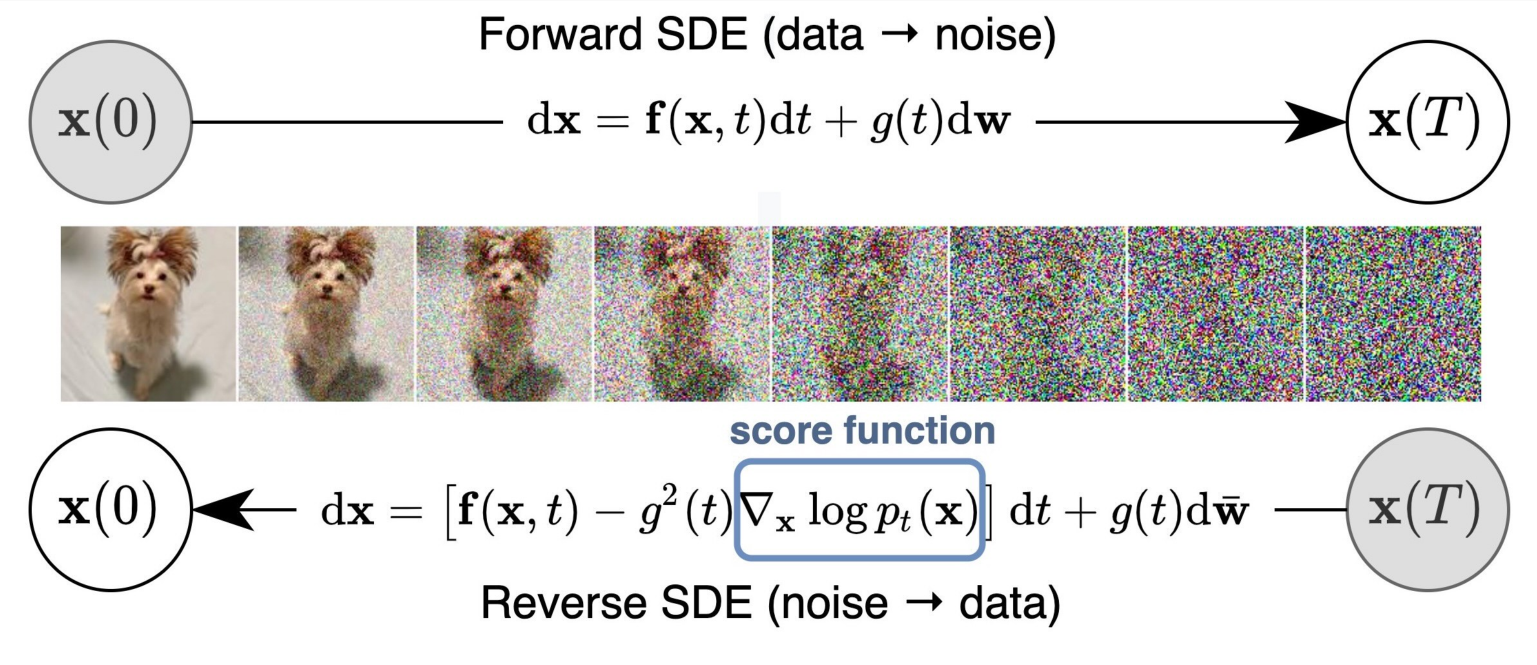
StyleGAN2-ADA
(Karras et al., 2020)

DDPM
(Ho et al., 2020)



Reverse SDE
(Song et al., 2020)

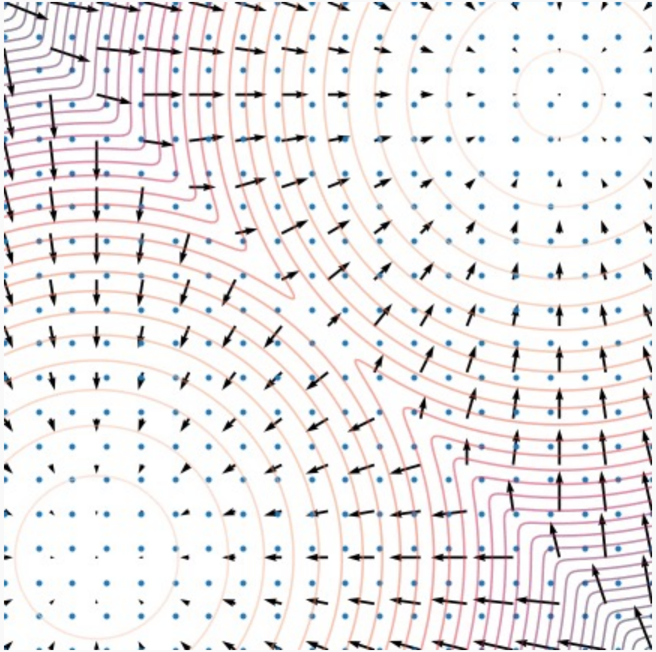
Score-based Generative Models through SDE



Yang Song et al, Generative modeling by estimating gradient of the data distributions, ICLR, 2021

http://yang-song.github.io/blog/2021/score/

Score-based Generative Models through SDE



- Once the score model is trained to optimality,
  - i.e. $s_\theta(\mathbf{x}) \simeq \nabla_{\mathbf{x}} p(\mathbf{x})$
- Use Langevin dynamics to draw samples

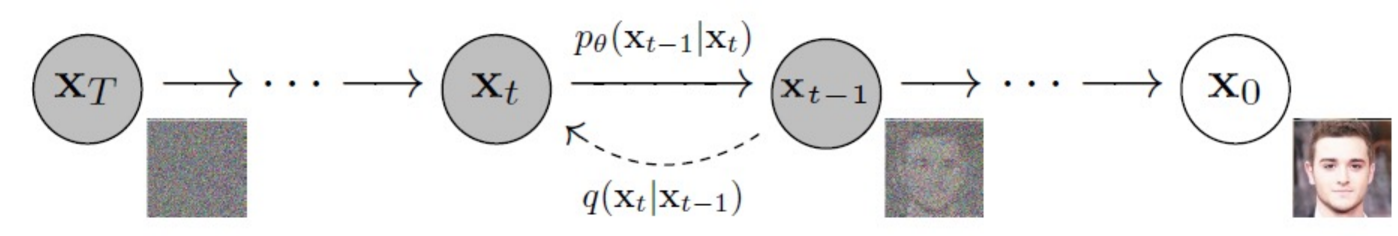
$$\mathbf{x}_{i+1} \leftarrow \mathbf{x}_i + \epsilon \nabla_{\mathbf{x}} \log p(\mathbf{x}) + \sqrt{2\epsilon}\mathbf{z}_i$$

$$i = 0, 1, \ldots, K$$

http://yang-song.github.io/blog/2021/score/

Diffusion Denoising Probabilistic Models (DDPMs)

Ho et al. *NeurIPS*, 2020



- **Train** with **variational lower bound**
- Follow the **reverse markov chain** at **inference**

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\epsilon}\left[\left\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)\right\|^2\right]$$

Diffusion Models Beat GANs on Image Synthesis

Dhariwal and Nichol, *NeurIPS*, 2021

Equivalence between the Two Approaches

Song et al. *ICLR* 2022

DDPM

- **Training objective:**

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right]$$

- **Inference:**

SGM

- **Training objective:**

$$\ell(\boldsymbol{\theta};\sigma) \triangleq \frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\mathbb{E}_{\tilde{\mathbf{x}}\sim\mathcal{N}(\mathbf{x},\sigma^2 I)}\left[\left\|\mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}},\sigma) + \frac{\tilde{\mathbf{x}}-\mathbf{x}}{\sigma^2}\right\|_2^2\right].$$

- **Inference:**

Reverse Diffusion Through Score-Matching

Noising

$$\mathrm{d}\boldsymbol{x} = \bar{\boldsymbol{f}}(\boldsymbol{x}, t)\, dt + \bar{g}(t)\mathrm{d}\boldsymbol{w}$$

Corresponding reverse SDE

Denoising

$$\mathrm{d}\boldsymbol{x} = [\bar{\boldsymbol{f}}(\boldsymbol{x}, t) - \bar{g}(t)^2 \nabla_x \log p_t(\boldsymbol{x})]dt + \bar{g}(t)\mathrm{d}\boldsymbol{w}$$

$$\simeq [\bar{\boldsymbol{f}}(\boldsymbol{x}, t) - \bar{g}(t)^2 s_\theta(\boldsymbol{x}, t)]dt + \bar{g}(t)\mathrm{d}\boldsymbol{w}$$

- **Solve reverse SDE numerically: Image generation (denoising)**

Song et al. *ICLR* 2022

SCORE-BASED DIFFUSION MODELS FOR INVERSE PROBLEMS

Chung et al, Medical Image Analysis (in revision), 2022

A General Score-based Formula for Inverse Problems

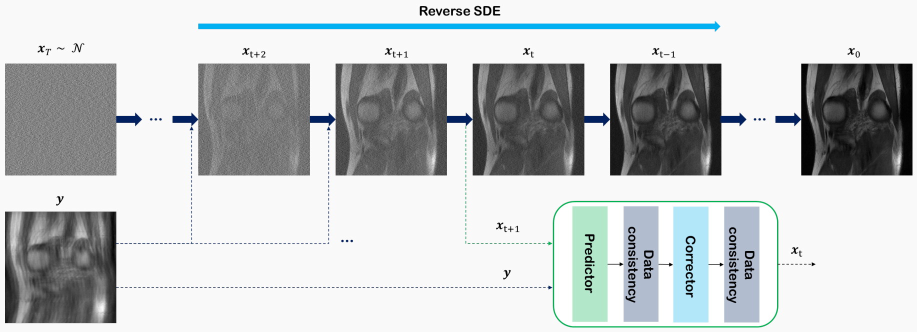
$$\boxed{\min_{\mathbf{x}} \|y - A\mathbf{x}\|^2}$$

$$\boldsymbol{x}_i \leftarrow \boldsymbol{x}_{i+1} + \epsilon_i \boldsymbol{s}_\theta(\boldsymbol{x}_{i+1}, \sigma_{i+1}) + \sqrt{2\epsilon_i}\boldsymbol{z}$$

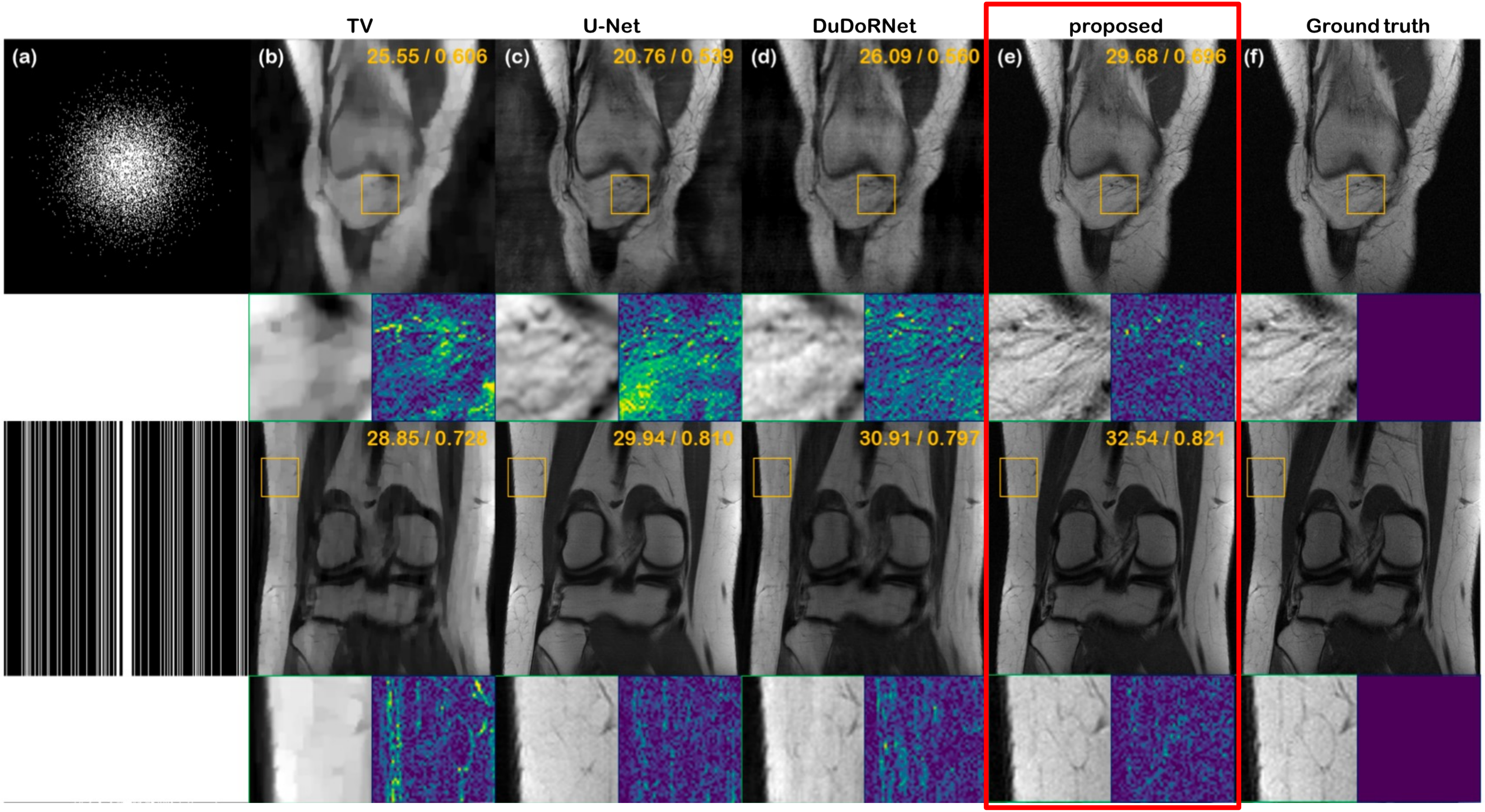
$$\boldsymbol{x}_i \leftarrow \boldsymbol{x}_i + \lambda A^*(y - A\boldsymbol{x}_i),$$

Denoising step (reverse SDE)

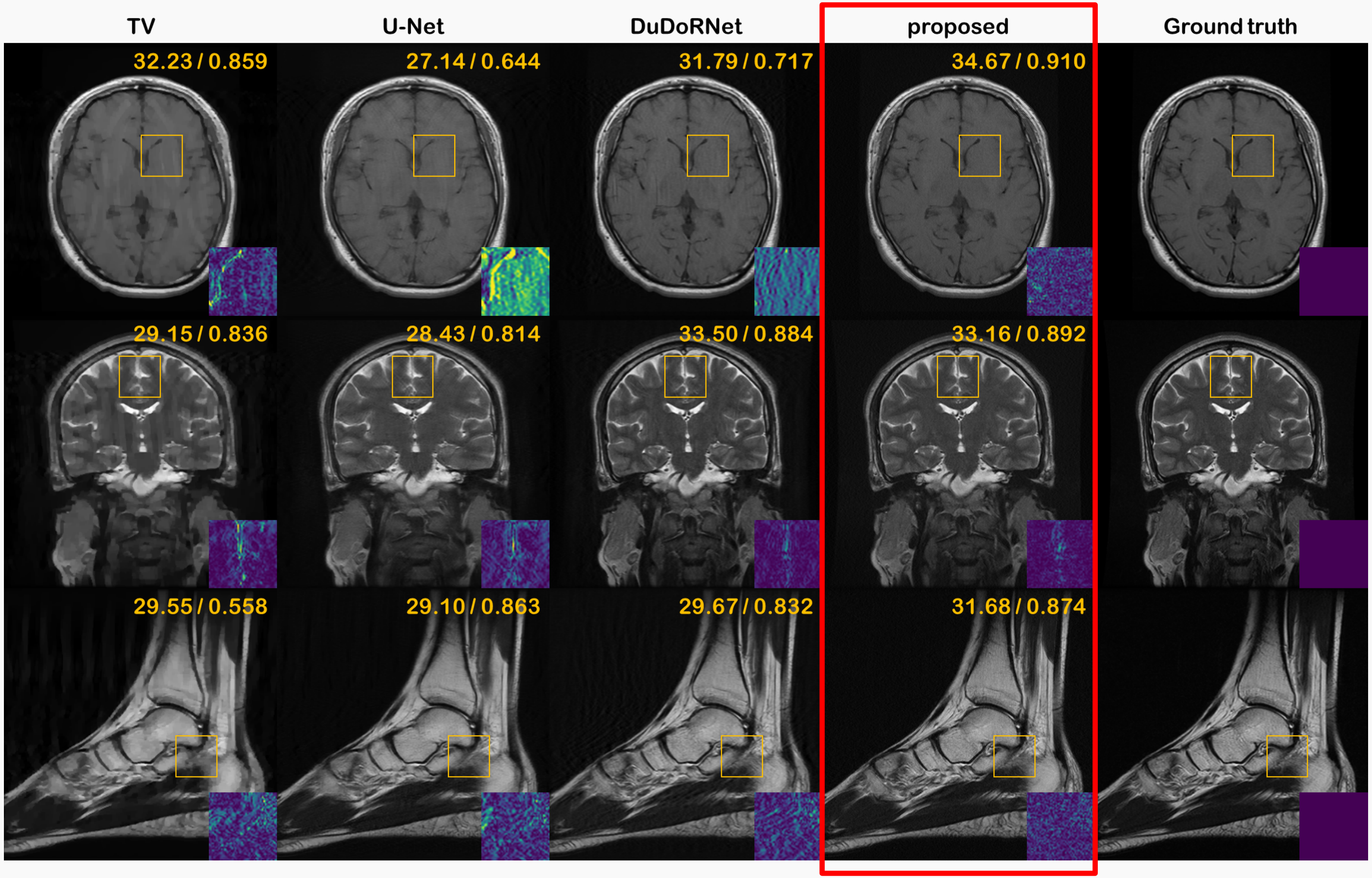
Data consistency step (e.g. GD, POCS)



State-of-the-art Performance



Generalization Capability



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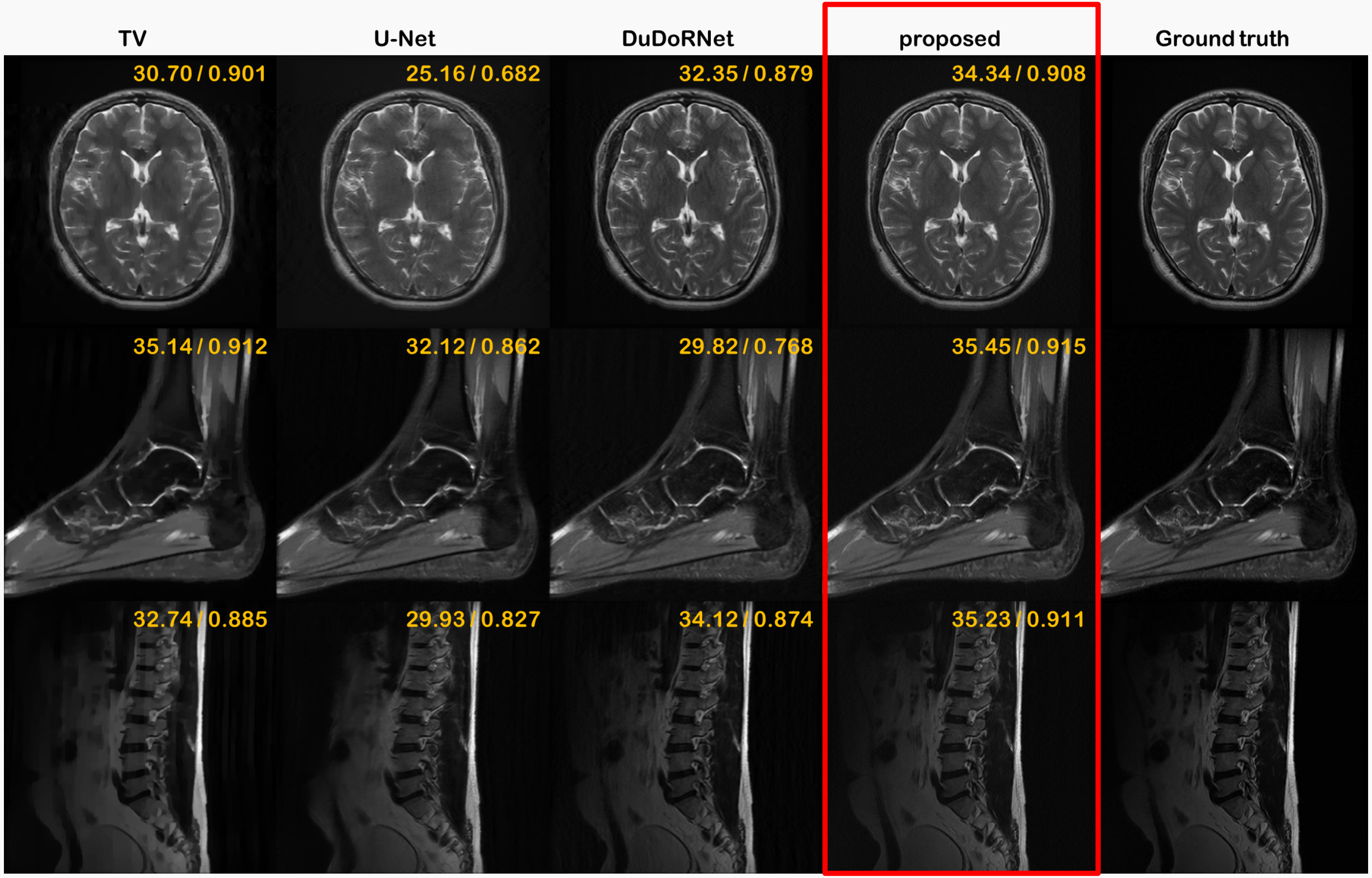
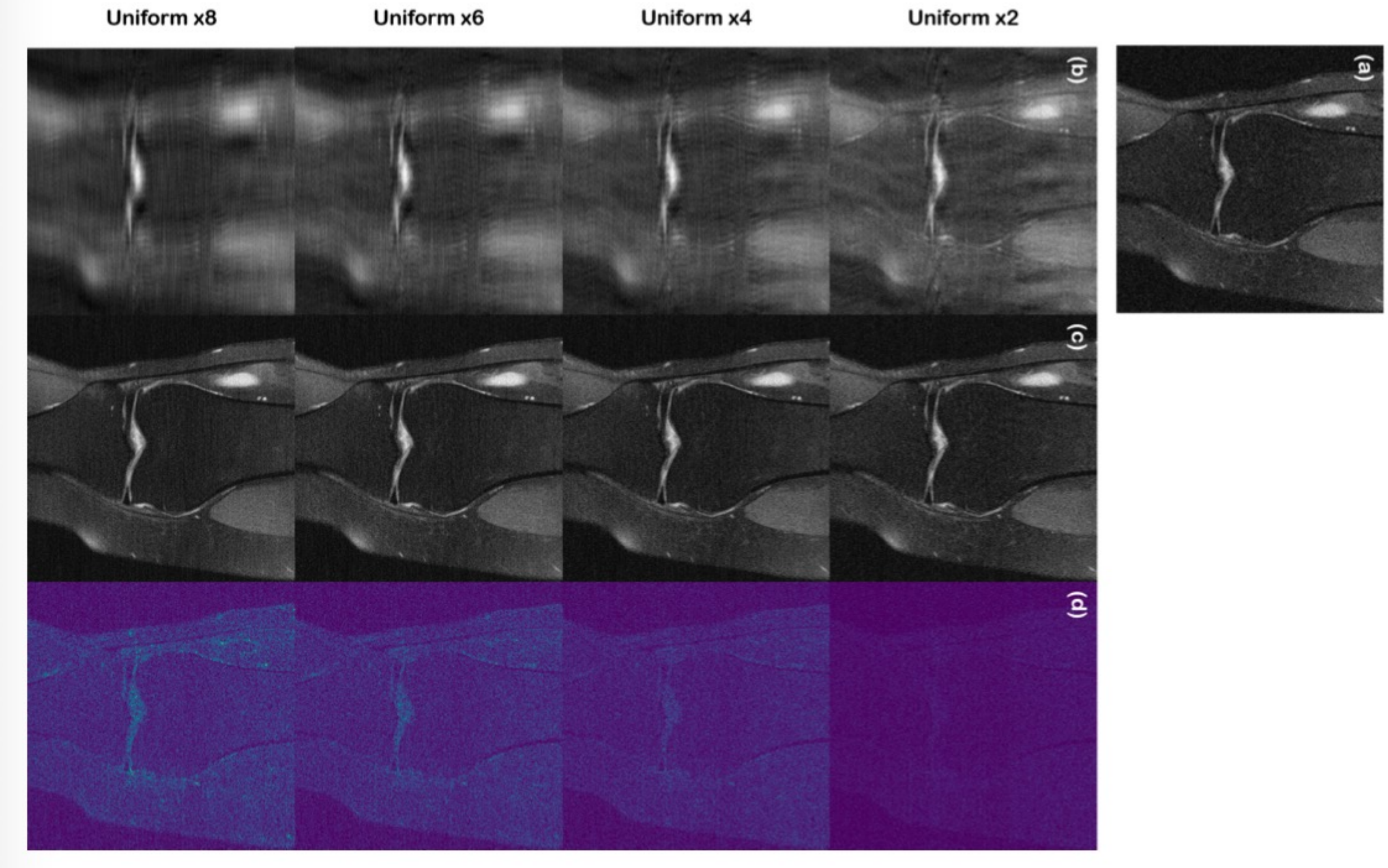
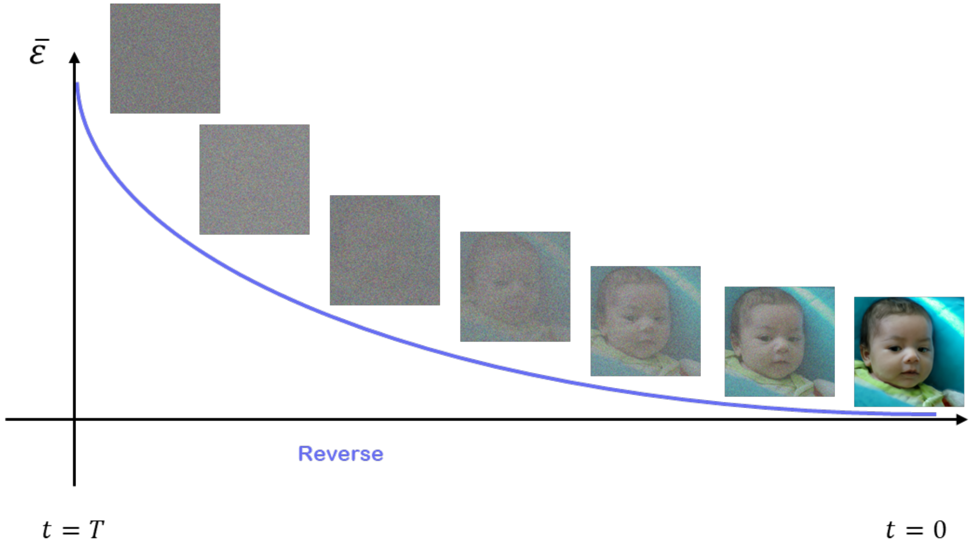
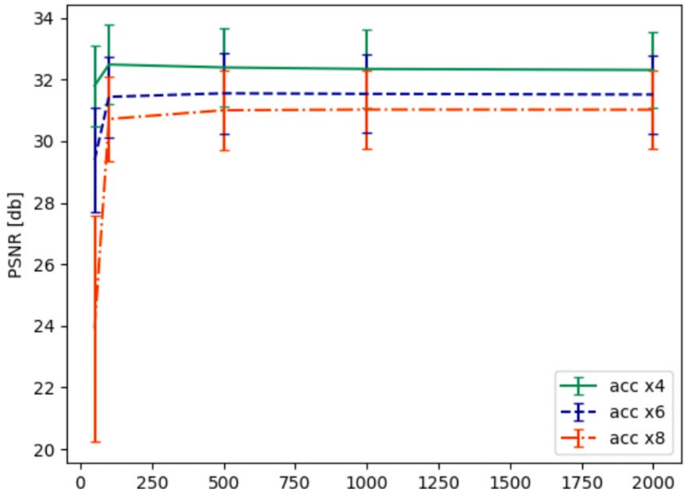


Uncertainty Quantification



Very Slow Convergence

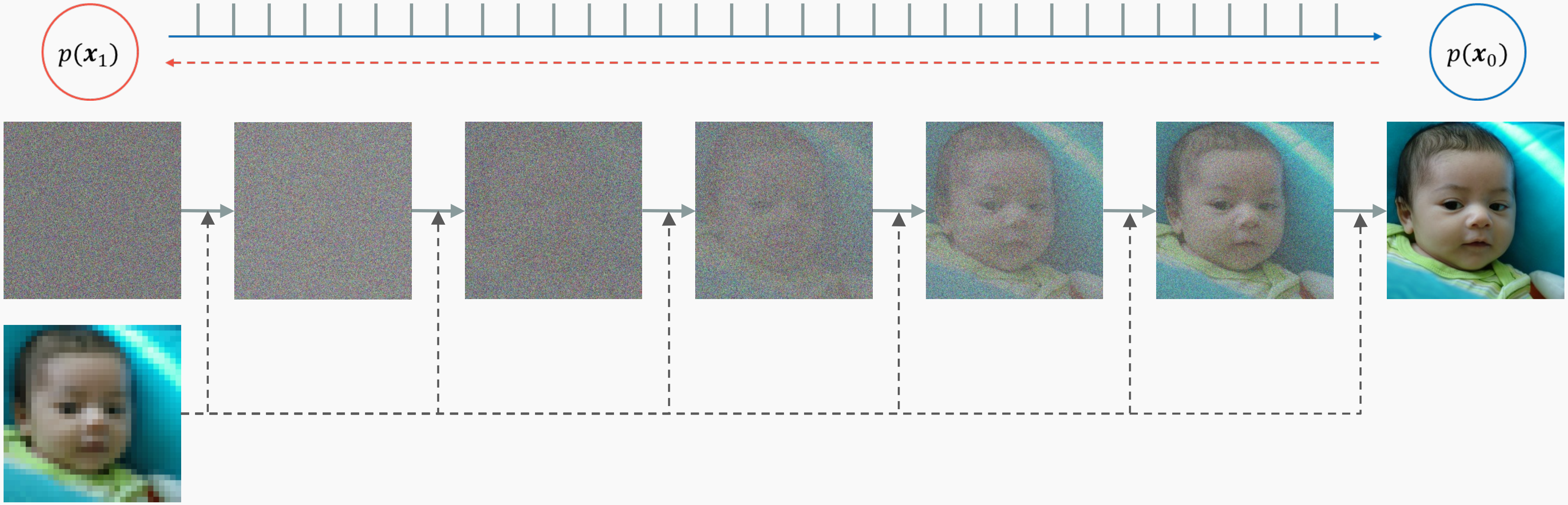




CCDF: COME CLOSER, DIFFUSE FASTER

Chung et al, CVPR, 2022

Intuition: Why use the whole process?



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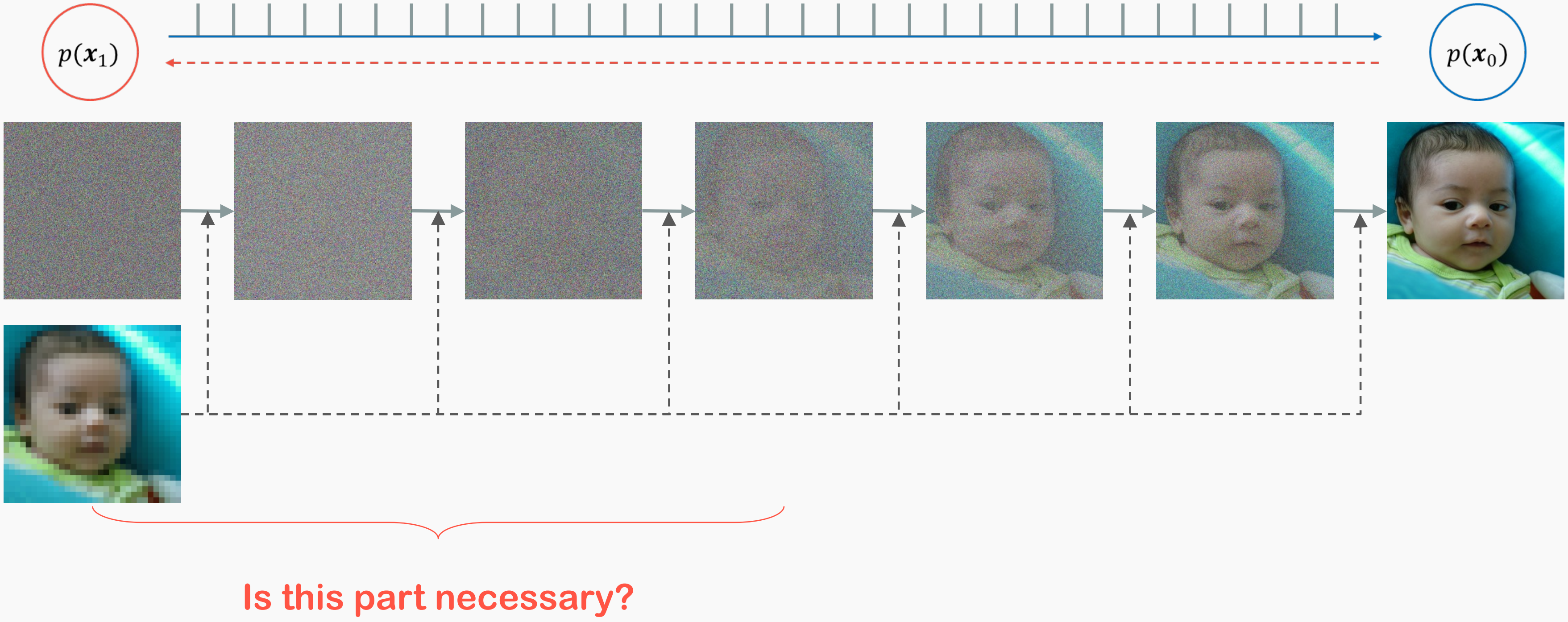
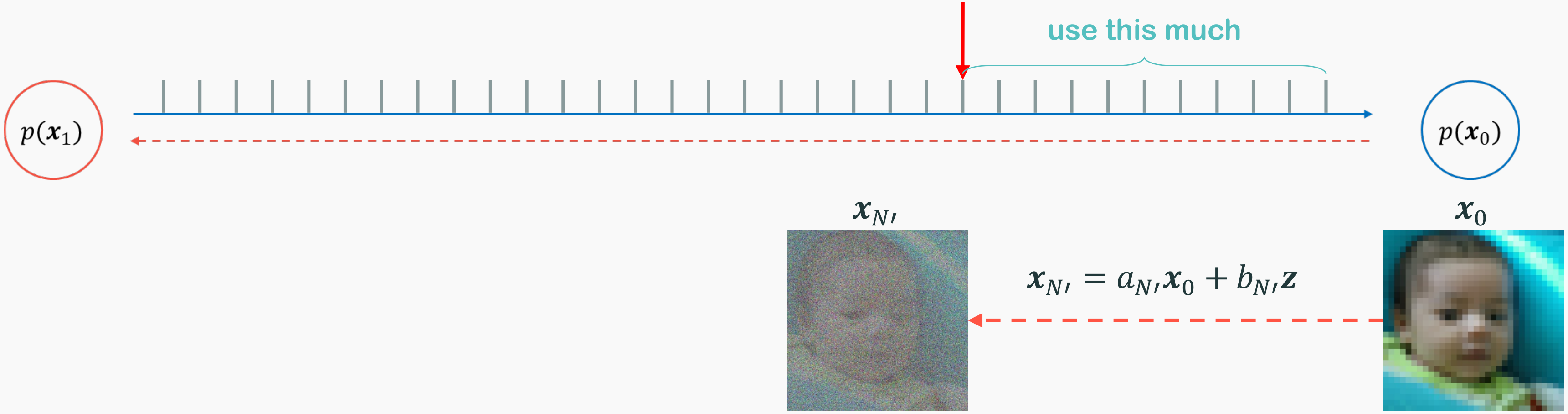


Intuition: Why use the whole process?

- $t_0 = 0.3$
- $N' = t_0 N = 300$



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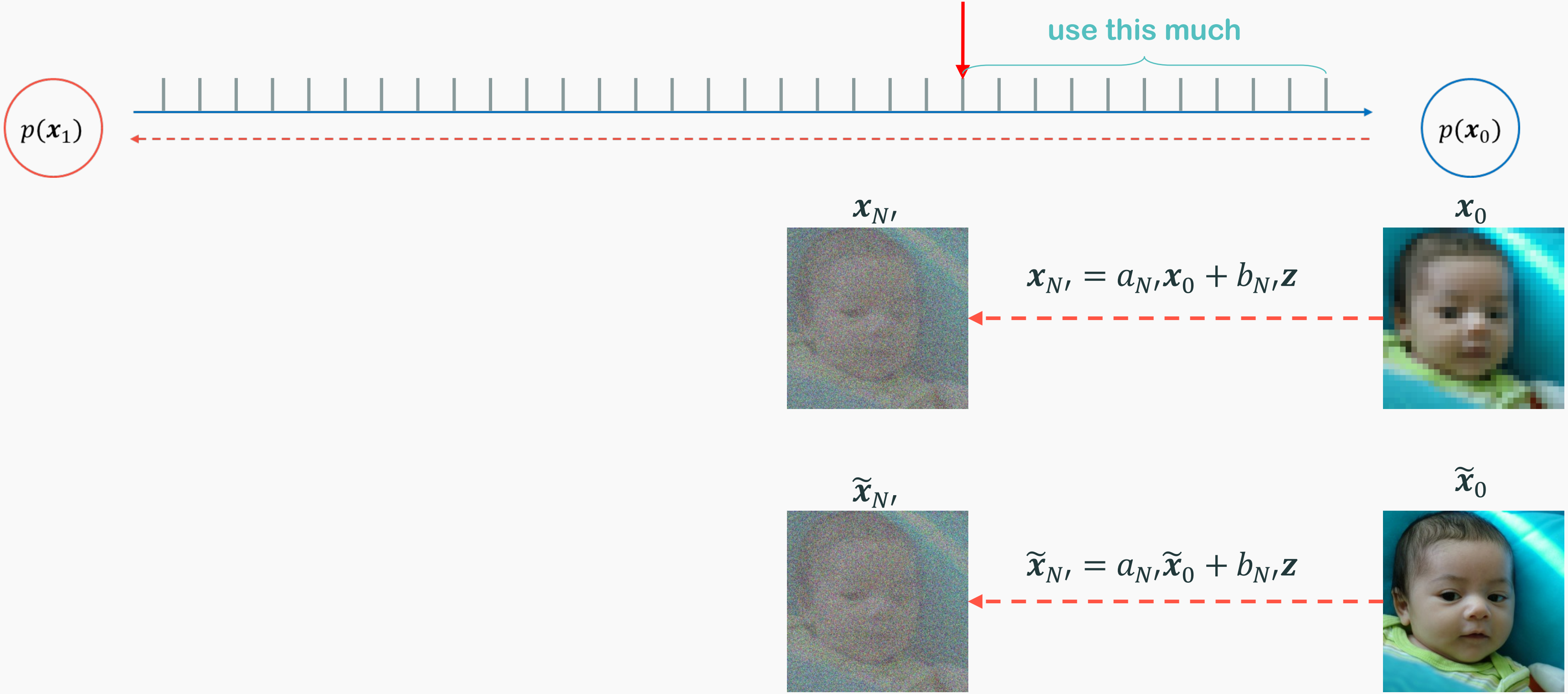

Intuition of CCDF

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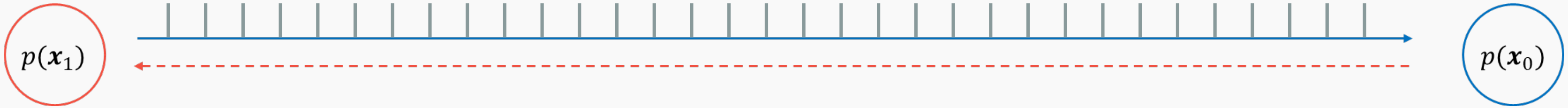
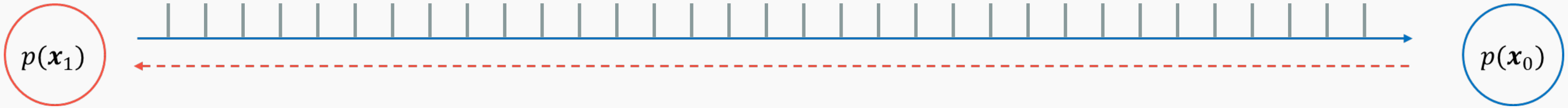
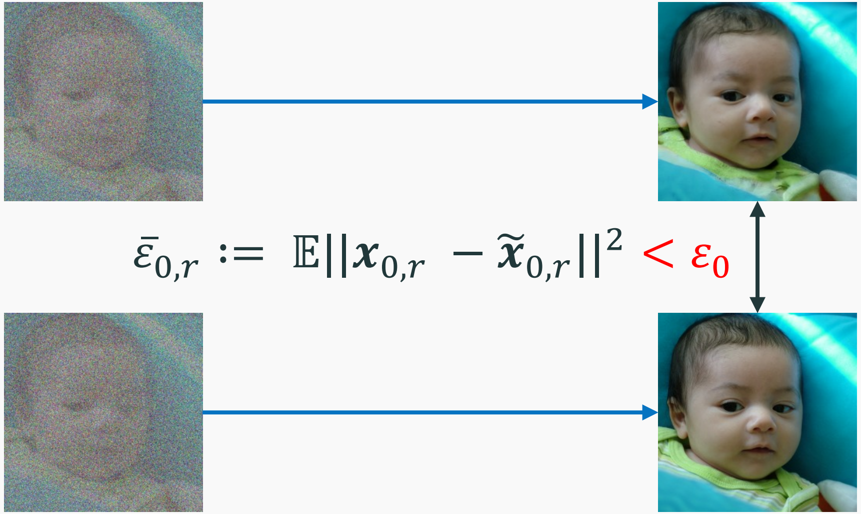


$$\bar{\varepsilon}_{N'} := \mathbb{E}||\boldsymbol{x}_{N'} - \tilde{\boldsymbol{x}}_{N'}||^2$$

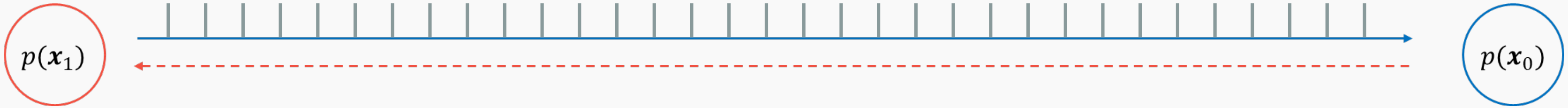
Intuition of CCDF





$$\bar{\varepsilon}_{0,r} := \mathbb{E}||\boldsymbol{x}_{0,r} - \tilde{\boldsymbol{x}}_{0,r}||^2 < \varepsilon_0$$

CCDF: The Algorithm



Algorithm 1 Accelerated Super-resolution / inpainting (VP, Markov)

Require: $\boldsymbol{x}_0, \hat{\boldsymbol{x}}_0, N', \{\alpha_i\}_{i=1}^{N'}, \{\sigma_i\}_{i=1}^{N'}, \boldsymbol{s}_\theta$

$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$

$\boldsymbol{x}_{N'} \leftarrow \sqrt{\bar{\alpha}_{N'}}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_{N'}}\boldsymbol{z}$ ▷ Forward diffusion

for $i = N'$ to 1 **do** ▷ Reverse diffusion

$\quad \boldsymbol{x}'_{i-1} \leftarrow \frac{1}{\sqrt{\alpha_i}}(\boldsymbol{x}_i + (1-\alpha_i)\boldsymbol{s}_\theta(\boldsymbol{x}_i, i))$

$\quad \boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$

$\quad \boldsymbol{x}_{i-1} \leftarrow \boldsymbol{x}'_{i-1} + \sigma_i \boldsymbol{z}$ ▷ Unconditional update

$\quad \boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$

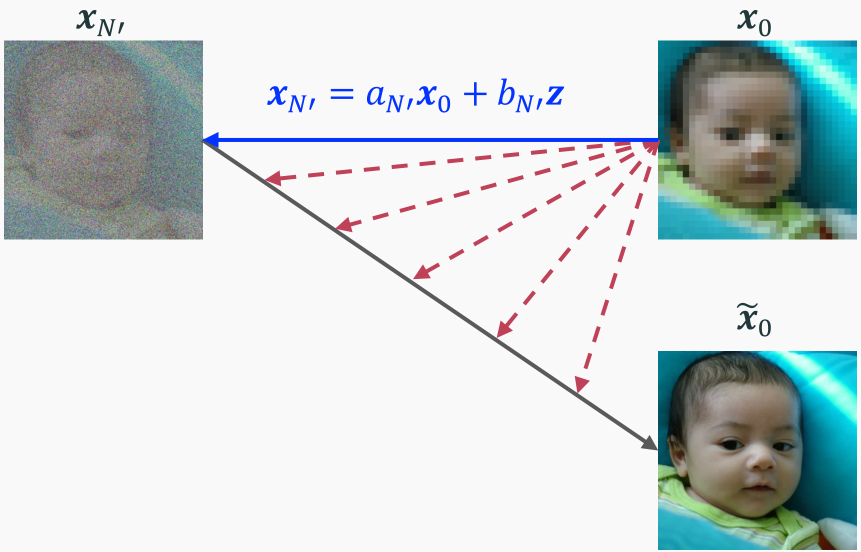
$\quad \hat{\boldsymbol{x}}_i \leftarrow \sqrt{\bar{\alpha}_i}\hat{\boldsymbol{x}}_0 + \sqrt{1-\bar{\alpha}_i}\boldsymbol{z}$

$\quad \boldsymbol{x}_{i-1} = (\boldsymbol{I} - \boldsymbol{P})\boldsymbol{x}_{i-1} + \hat{\boldsymbol{x}}_i$

▷ Measurement consistency

end for

return $\boldsymbol{x}_0$



CCDF: The Algorithm

General form

$$\boldsymbol{x}_{N'} = a_{N'}\boldsymbol{x}_0 + b_{N'}\boldsymbol{z}$$

: 1-step noising

$$\boldsymbol{x}'_{i-1} = \boldsymbol{f}(\boldsymbol{x}_i, i) + \boldsymbol{g}(\boldsymbol{x}_i, i)\boldsymbol{z}_i$$

$$\boldsymbol{x}_{i=1} = \boldsymbol{A}\boldsymbol{x}'_{i-1} + \boldsymbol{b}$$

: Iterative denoising

- **Denoising step** (reverse SDE)
- **Data consistency step** (e.g. GD, POCS)

Constraint

$$\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}\boldsymbol{x}'\| \le \|\boldsymbol{x} - \boldsymbol{x}'\| \ \forall \boldsymbol{x}, \boldsymbol{x}'$$

- **Non-expansive mapping**

Key Idea: Stochastic Contraction

Contraction on $\mathbb{R}^n$

A function $\boldsymbol{f}: \mathbb{R}^n \mapsto \mathbb{R}^n$ contraction mapping ,

if there exists $0 \leq \lambda < 1$ s.t. $\forall\, \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$

$$\|\boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{y})\| \leq \lambda \|\boldsymbol{x} - \boldsymbol{y}\|$$

$$\sigma_{\max}\left(\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right) \leq \lambda < 1$$

Theorem A.1. (Pham et al. 2008)

$$\boldsymbol{x}_{i+1} = f(\boldsymbol{x}_i, i) + g(\boldsymbol{x}_i, i)\boldsymbol{z}$$

- $\boldsymbol{f}$ is contracting with λ
- $\mathrm{Tr}\big(g(\boldsymbol{x}, i)\boldsymbol{I}g(\boldsymbol{x}, i)\big) \leq C \quad \forall \boldsymbol{x}, i$

Then,

$$\mathbb{E}\|x_i - \tilde{x}_i\|^2 \leq \frac{2C}{1 - \lambda^2} + \lambda^{2i}\mathbb{E}\|x_0 - \tilde{x}_0\|^2$$

Reverse SDE is Contracting!

Proof of Theorem 1. (VE-SDE; SMLD)

Forward $\boldsymbol{x}_i = \boldsymbol{x}_0 + \sigma_i z$

Reverse SDE $\boldsymbol{x}'_{i-1} = \underbrace{\boxed{\boldsymbol{x}_i + \left(\sigma_i^2 - \sigma_{i-1}^2\right) s_\theta(\boldsymbol{x}_i, i)}}_{f(x_i, i)} + \sqrt{\sigma_i^2 - \sigma_{i-1}^2}\,\boldsymbol{z}$ **: Stochastically contracting**

Proof.

$$\frac{\partial \boldsymbol{f}^T(\boldsymbol{x}_i, i)}{\partial \boldsymbol{x}_i} = I + \left(\sigma_i^2 - \sigma_{i-1}^2\right) \frac{\partial s_\theta(\boldsymbol{x}_i, i)}{\partial \boldsymbol{x}_i} = \frac{\sigma_{i-1}^2 - \sigma_0^2}{\sigma_i^2 - \sigma_0^2} \boldsymbol{I}$$

$$\lambda = \max_{i \in [N']} \frac{\sigma_{i-1}^2 - \sigma_0^2}{\sigma_i^2 - \sigma_0^2} < 1$$

$$C = \max_{i \in [N']} \sigma_i^2 - \sigma_{i-1}^2$$

Non-expansiveness is Sufficient!

Corollary 1.

$$\boldsymbol{x}'_{i+1} = f(\boldsymbol{x}_i, i) + g(\boldsymbol{x}_i, i)\boldsymbol{z}_i$$

$$\boldsymbol{x}_{i+1} = \underbrace{\boldsymbol{A}}_{\text{Non-expansive mapping}}\boldsymbol{x}'_{i+1} + \boldsymbol{b}$$

$$\mathbb{E}\|x_i - \tilde{x}_i\|^2 \le \frac{2C\tau}{1 - \lambda^2} + \lambda^{2i}\mathbb{E}\|x_0 - \tilde{x}_0\|^2$$

$$\tau = \frac{\mathrm{Tr}(\boldsymbol{A}^T\boldsymbol{A})}{n}$$

Proof.

$$\boldsymbol{x}_{i+1} = \underbrace{\boldsymbol{A}f(x_i, i) + \boldsymbol{b}}_{\tilde{\boldsymbol{f}}(\boldsymbol{x}_i, i)} + \sigma(\boldsymbol{x}_i, i)\boldsymbol{A}\boldsymbol{z}_i$$

$$\sigma_{\max}\left(\frac{\partial\tilde{\boldsymbol{f}}(\boldsymbol{x}, i)}{\partial\boldsymbol{x}}\right) \le \sigma_{\max}(A)\sigma_{\max}\left(\frac{\partial\boldsymbol{f}(\boldsymbol{x}, i)}{\partial\boldsymbol{x}}\right) \le \lambda$$

$$\mathrm{Tr}\big(g(\boldsymbol{x}, i)\boldsymbol{A}^T\boldsymbol{A}g(\boldsymbol{x}, i)\big) = g(\boldsymbol{x}, i)^2\mathrm{Tr}(\boldsymbol{A}^T\boldsymbol{A}) = C\tau$$

Theoretical Findings

Theorem 1.

$$\bar{\varepsilon}_{0,r} \le \frac{2C\tau}{1-\lambda^2} + \lambda^{2N'}\,\bar{\varepsilon}_{N'}$$

Error decreases exponentially with reverse diffusion!

$$\lambda = \begin{cases} \max\limits_{i\in[N']} \sqrt{\alpha_i}\left(\frac{1-\bar{\alpha}_{i-1}}{1-\bar{\alpha}_i}\right) & (DDPM) \\ \max\limits_{i\in[N']} \frac{\sigma_{i-1}^2-\sigma_0^2}{\sigma_i^2-\sigma_0^2} & (SMLD) \\ \max\limits_{i\in[N']} \frac{\sigma_{i-1}}{\sigma_i} & (DDIM) \end{cases}$$

$$C = \begin{cases} n(1-\alpha_N) & (DDPM) \\ n \max\limits_{i\in[N']} \sigma_i^2 - \sigma_{i-1}^2 & (SMLD) \\ 0 & (DDIM) \end{cases}$$

$$\tau = \frac{\mathrm{Tr}(\boldsymbol{A}^T\boldsymbol{A})}{n}$$

Theoretical Findings

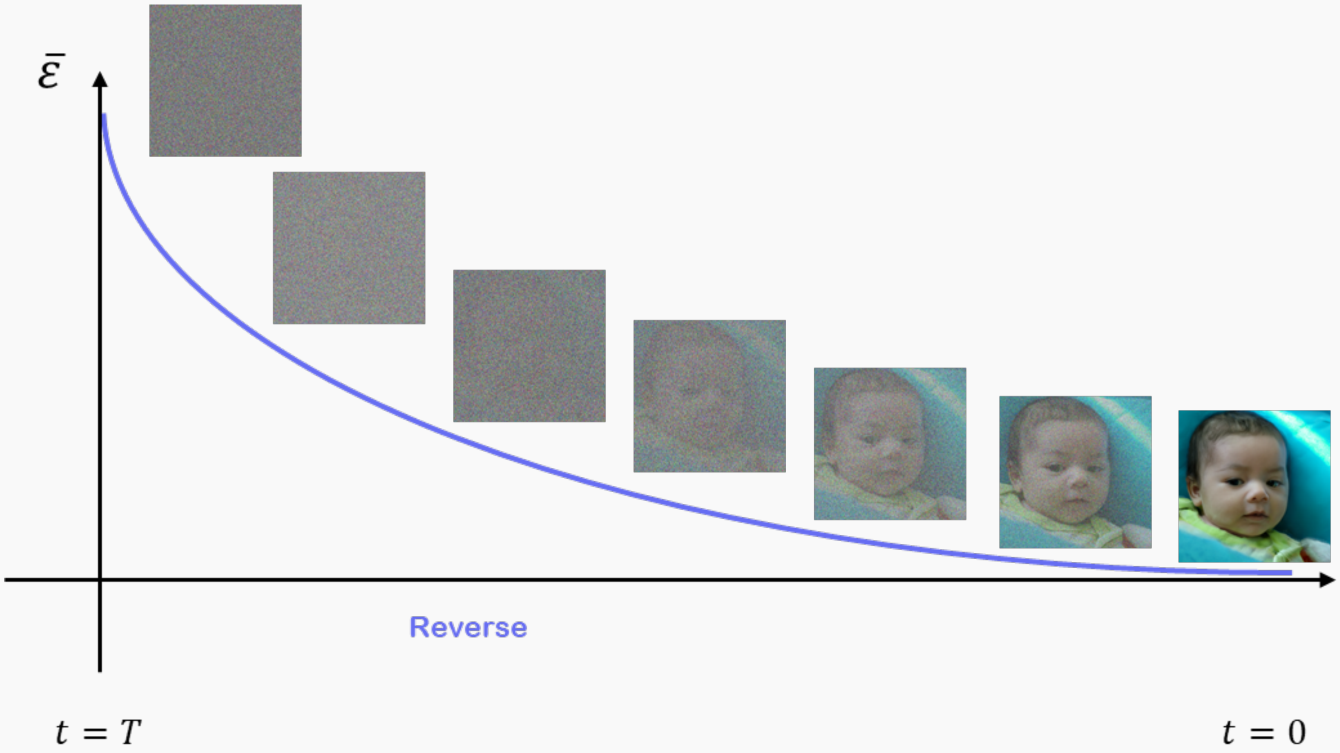
Theorem 2. (shortcut path)

- For any $0 < \mu \leq 1$, there exists a **minimum** N' s.t.

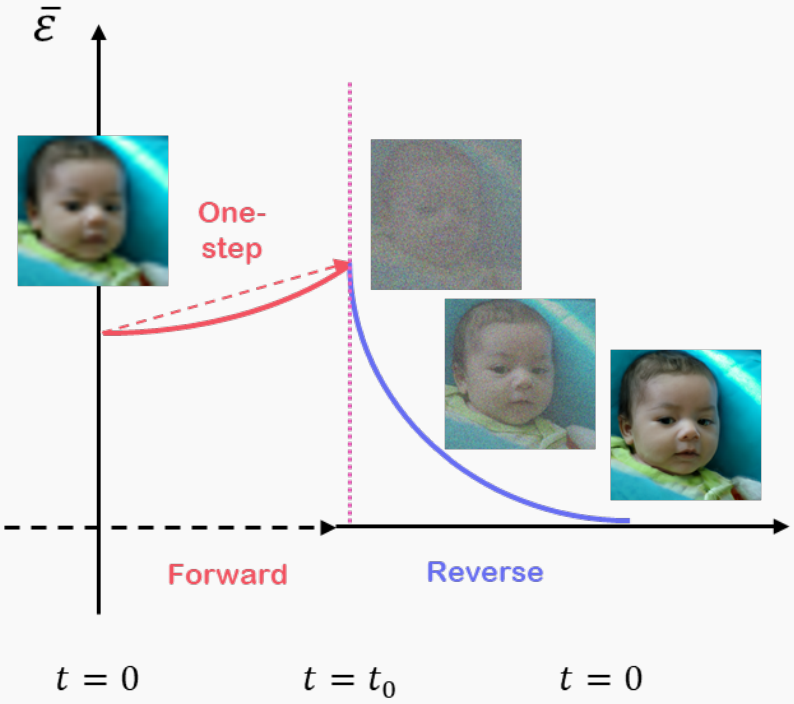
$$\bar{\varepsilon}_{0,r} \leq \mu\varepsilon_0$$

- Optimal N' **decreases** as ε_0 **gets smaller**

Come Closer, Diffuse Faster

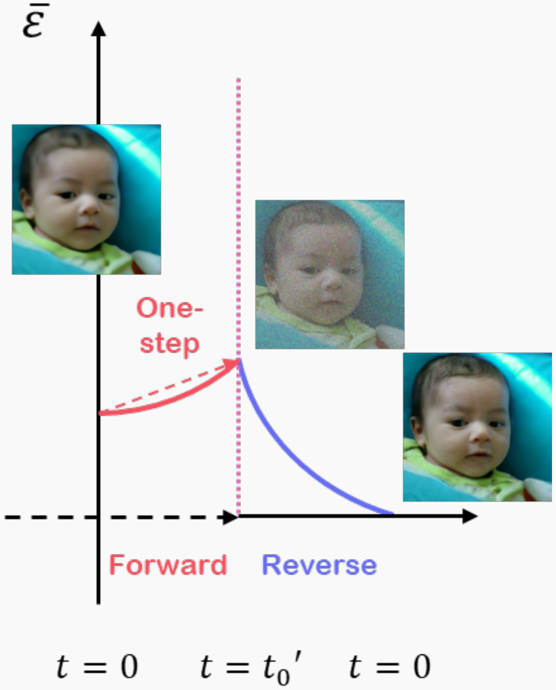


Come Closer, Diffuse Faster

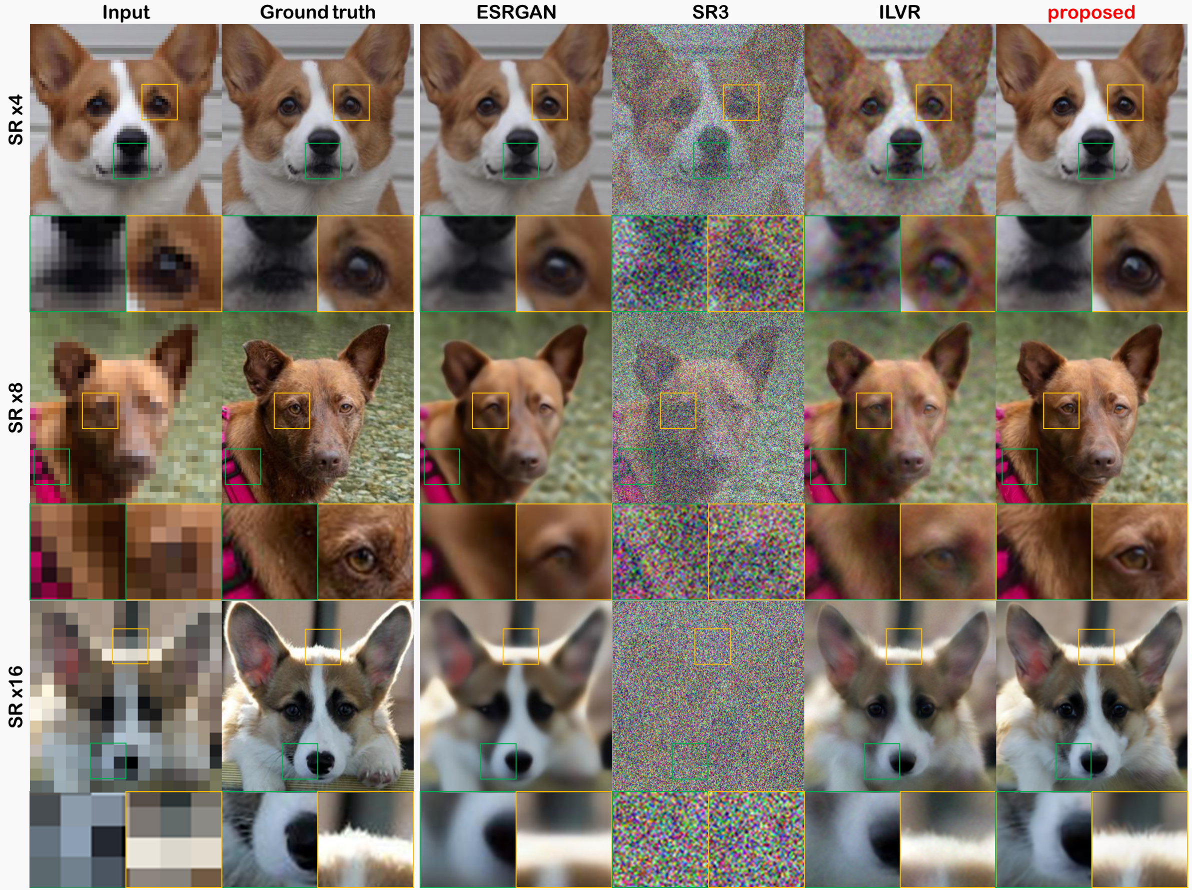


Come Closer, Diffuse Faster

Feed-forward network correction



Experimental Results: SR



20 step diffusion

- **ILVR, SR3**

  $N = 20, \quad t_0 = 1.0$

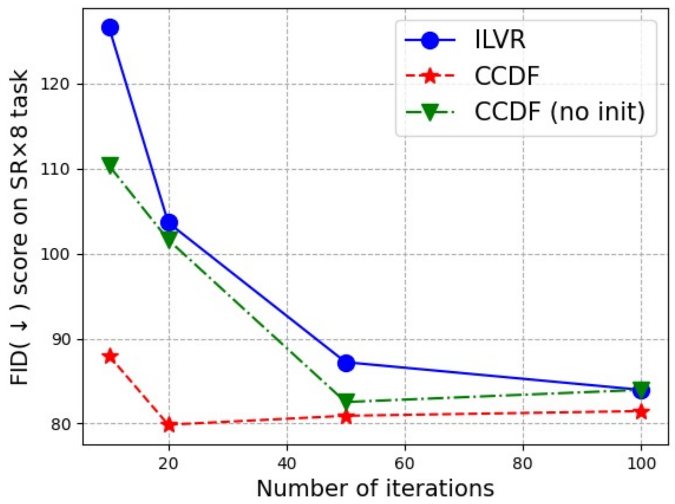
- **proposed**

  $N = 100, \quad t_0 = 0.2$

t_0	0.05	0.1	0.2	0.5	0.75	1.0 [5]
SR $\times 4$	63.90	**60.90**	<u>60.91</u>	64.04	64.14	63.31
SR $\times 8$	85.21	78.13	**75.76**	79.34	79.67	<u>77.34</u>
SR $\times 16$	116.37	101.79	92.59	**88.09**	92.12	<u>88.49</u>

Table 1. FID(↓) scores on FFHQ test set for SR task with $N = 1000$, and varying t_0 values. $t_0 = 1.0$ is the baseline method without any acceleration used in [5]. Numbers in boldface, and underline indicate the best, and the second best scores.

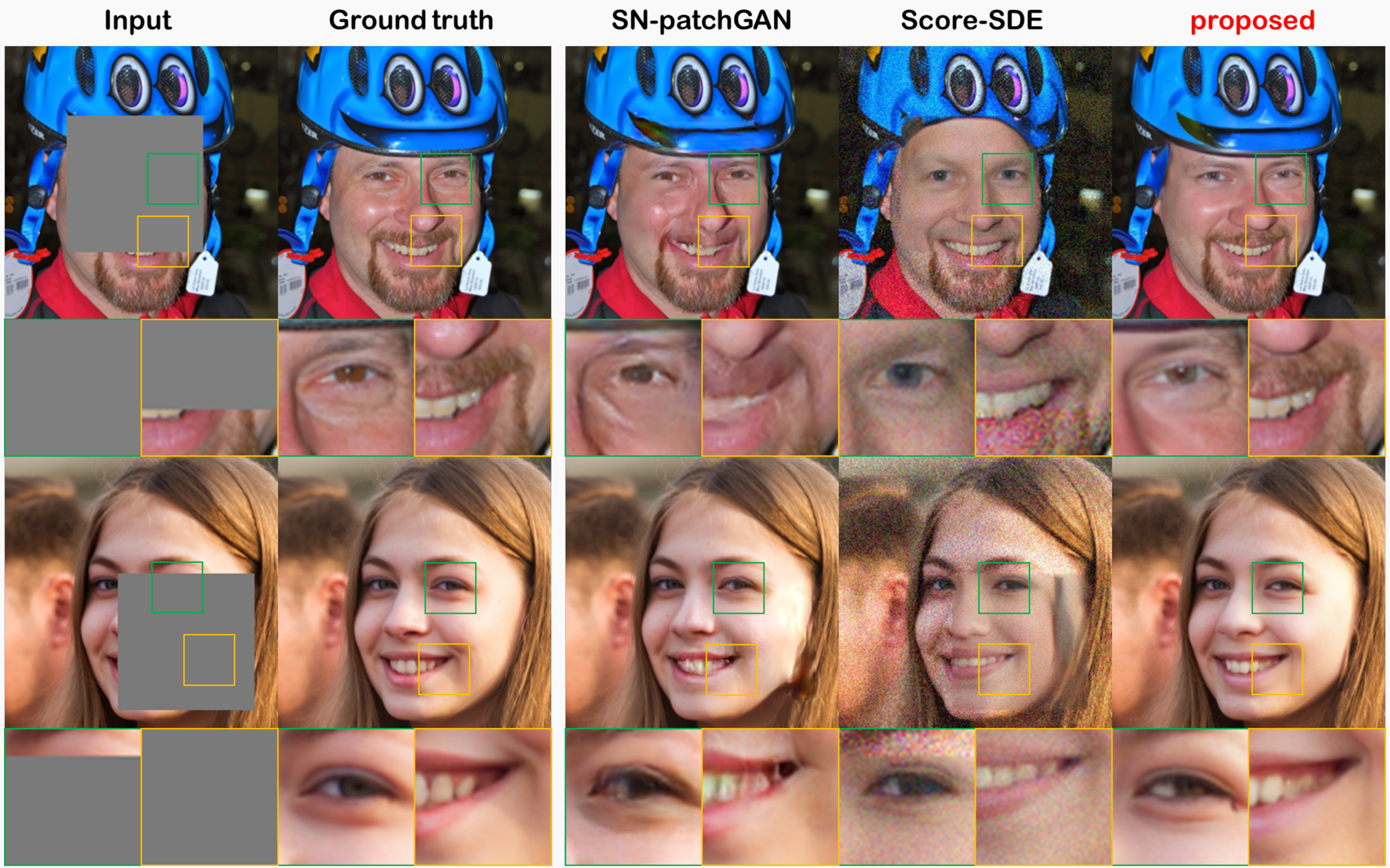
Experimental Results: SR



	SR factor	ESRGAN [36]	SR3* [25]	ILVR [5]	CCDF (ours)
FFHQ	×4	81.14	66.79	63.14	**60.90**
	×8	108.96	80.27	81.85	**75.76**
	×16	143.80	99.46	92.32	**88.39**
AFHQ	×4	24.52	20.68	18.70	**15.53**
	×8	51.84	30.23	34.85	**32.30**
	×16	98.22	60.76	**47.28**	48.77

Table 2. Comparison of FID(↓) scores on FFHQ and AFHQ test set. t_0 values used for the proposed method is $0.1, 0.2, 0.3$ for $\times 4$, $\times 8$, $\times 16$ SR, respectively. Numbers in boldface represent the best results among the row. (*unofficial re-implementation)

Experimental Results: Inpainting



20 step diffusion

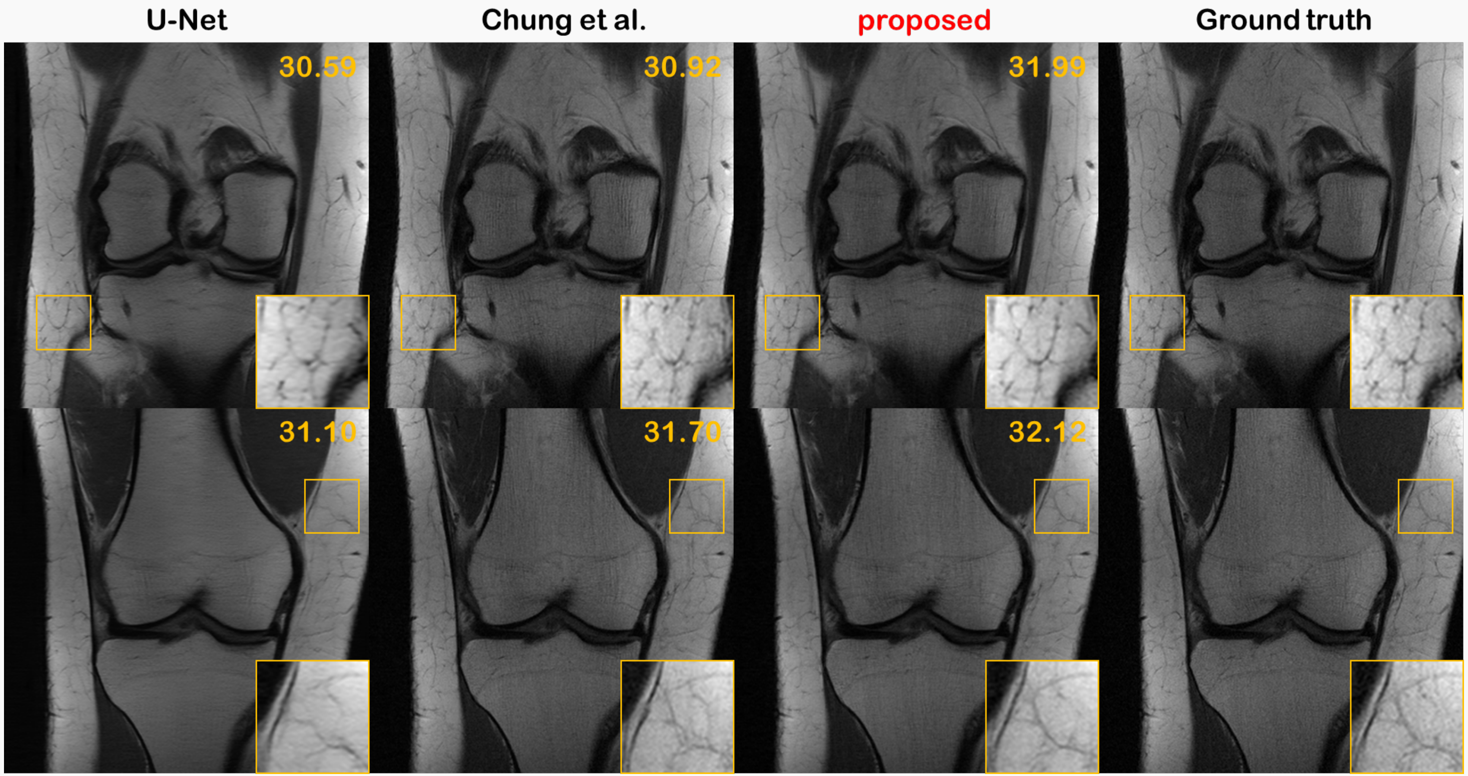
- Score-SDE

  $N = 20, \qquad t_0 = 1.0$

- proposed

  $N = 100, \qquad t_0 = 0.2$

Experimental Results: Fast MRI



20 step diffusion

- Chung et al.

  $N = 1000, \quad t_0 = 1.0$

- proposed

  $N = 1000, \quad t_0 = 0.02$

Summary

- Diffusion models: Exciting new path for solving inverse problems
- Universal solver without knowledge about the problem a priori
- Great generalization capacity
- Acceleration through stochastic contraction theory

Questions?