Modern AI for Inverse Problems (Data Driven Inverse Problems)

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August 7, 2024

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Motivation

Many success stories

Many success stories

Recently generative AI has achieved impressive performance

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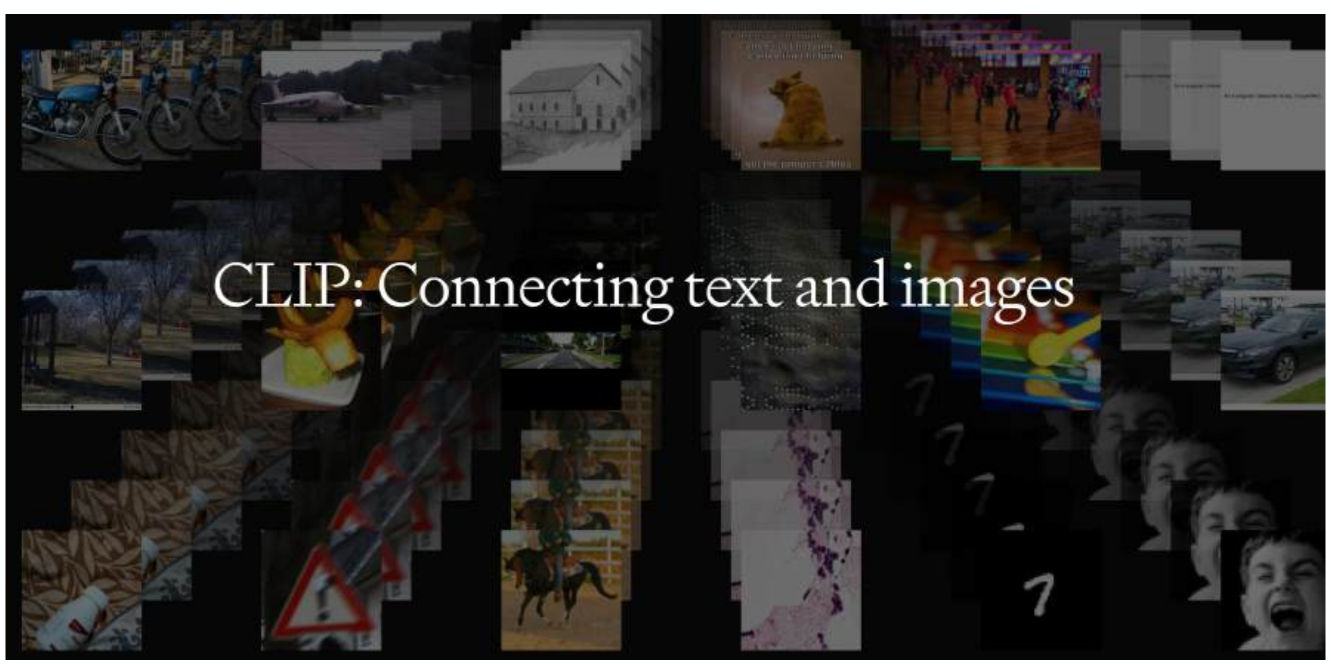

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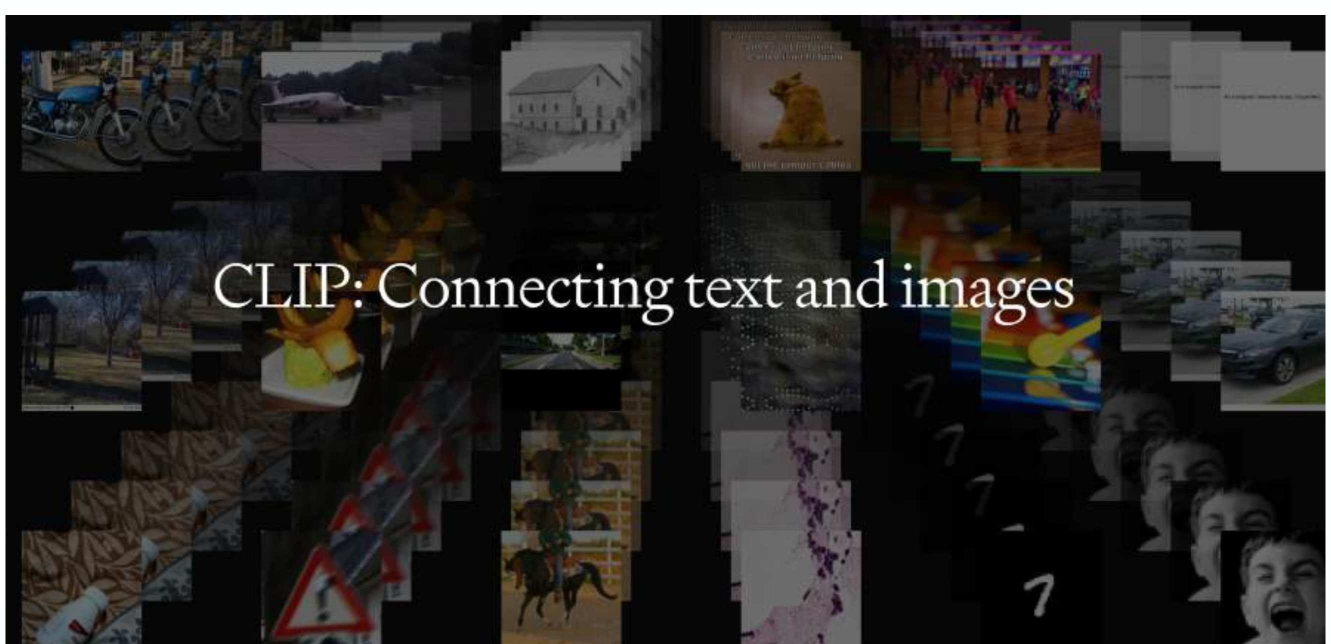

What about Inverse Problems?

AI for Comp Imaging/Inverse Problems

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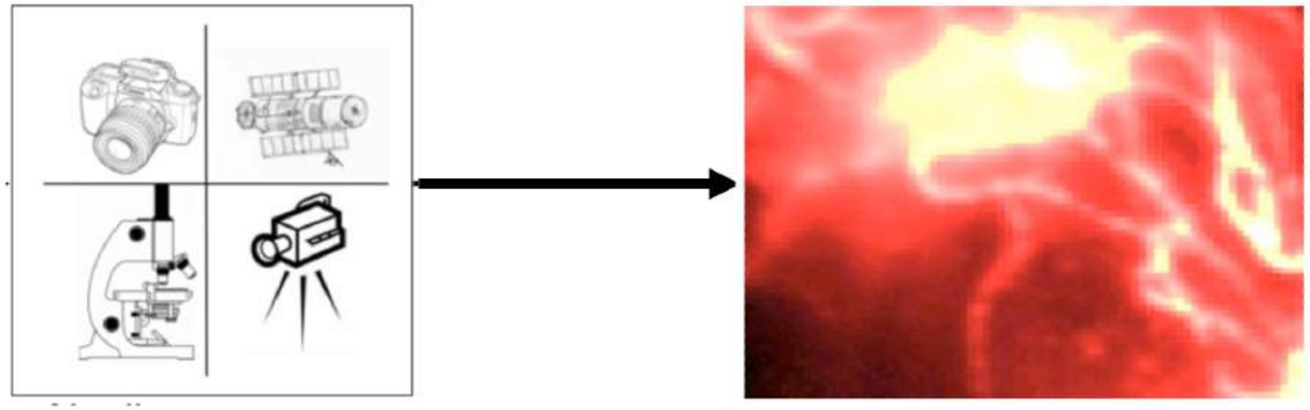

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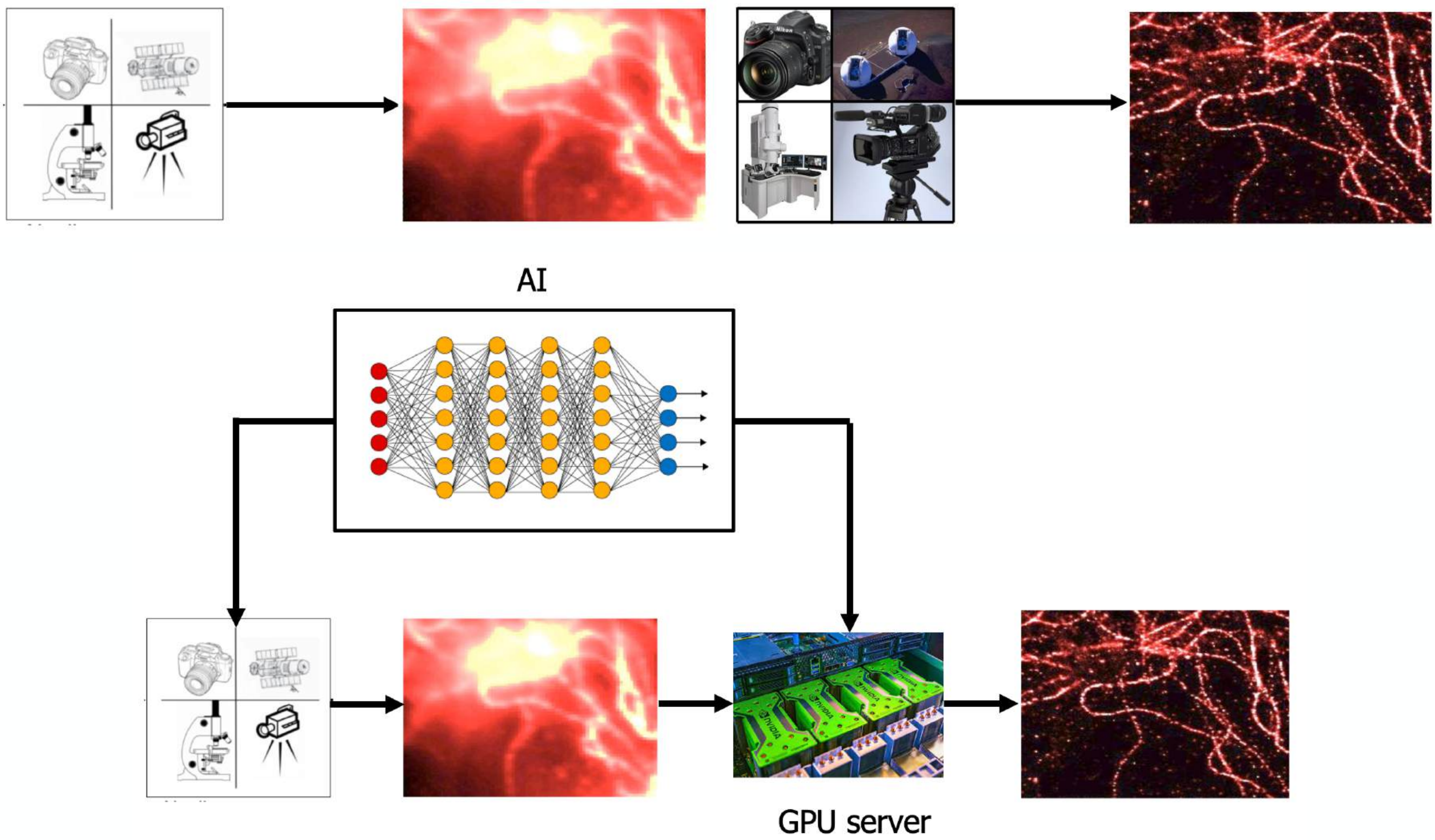

This Tutorial:
Opportunities and Challenges of AI for Inverse Problems

Inverse problems

- Formulation

$$y = \mathscr{A}(x) + \varepsilon$$

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Ground truth
(signal to be recovered)

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Forward operator (possibly non-linear)

Ground truth (signal to be recovered)

Noise

- Typically we have more unknowns than measurements
- Infinitely many solutions can be consistent with the observations

Common inverse problems (1)

- Denoising

$$A = I, \qquad y = x + \varepsilon$$

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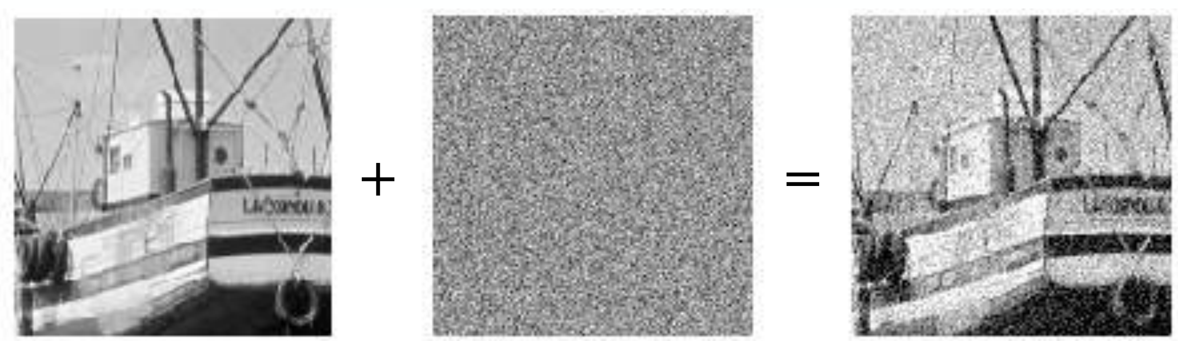
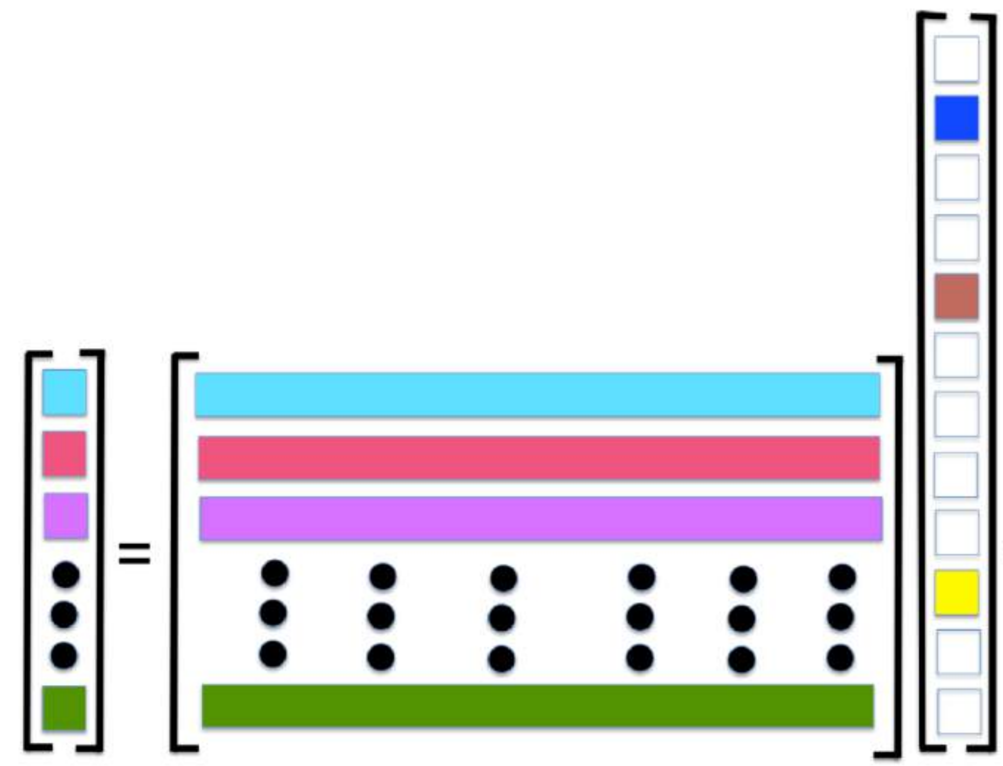


Common inverse problems (2)

- Compressed sensing

$$A = \begin{cases} \text{DFT + subsampling} \\ \text{Gaussian ensemble} \\ \text{Bernoulli ensemble} \end{cases}$$



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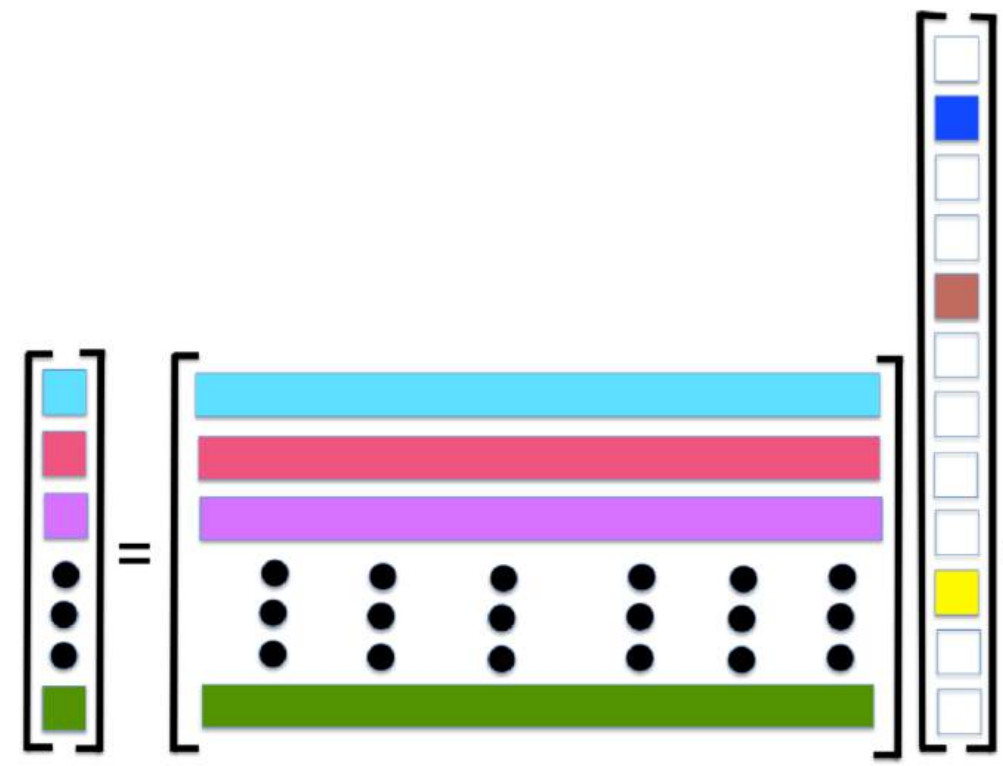

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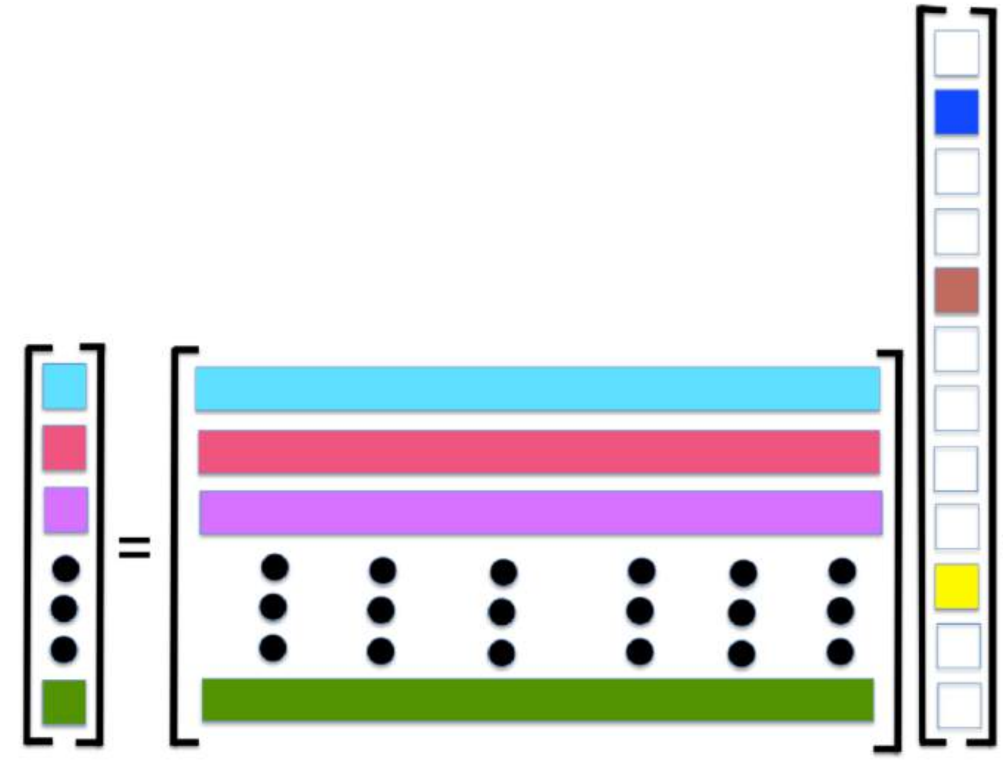

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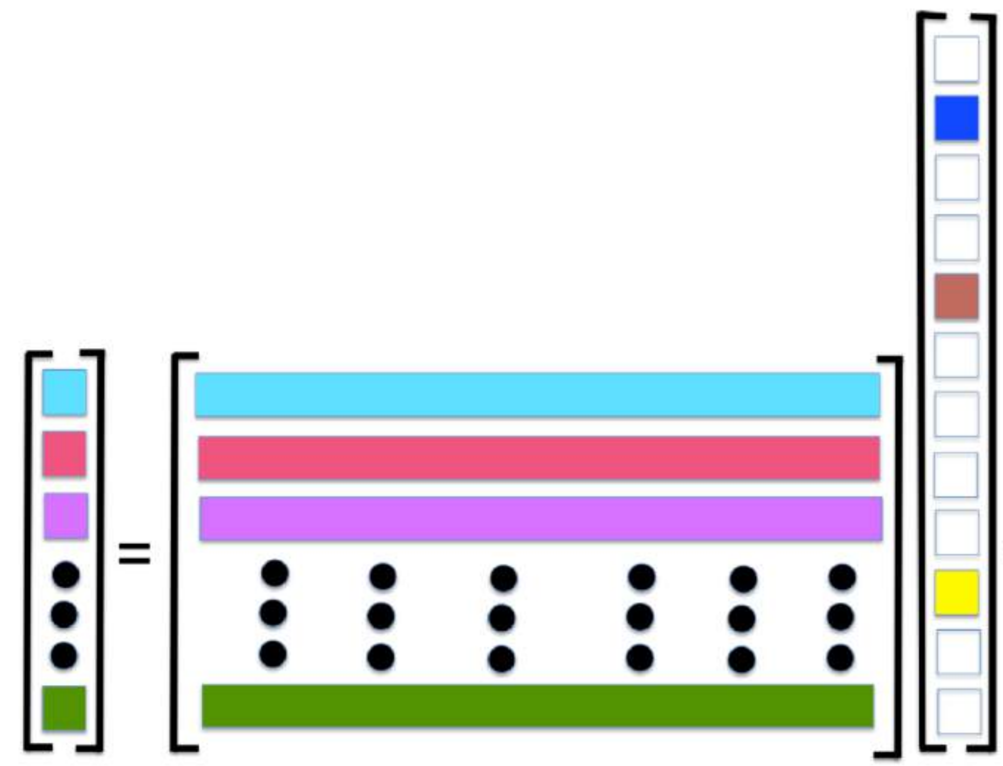

- nice theoretical guarantees on recovery
- exploiting sparsity in transform domain
- special case: MRI reconstruction

Common inverse problems (3)

- Deconvolution

$$\mathscr{A}(x) = h * x$$

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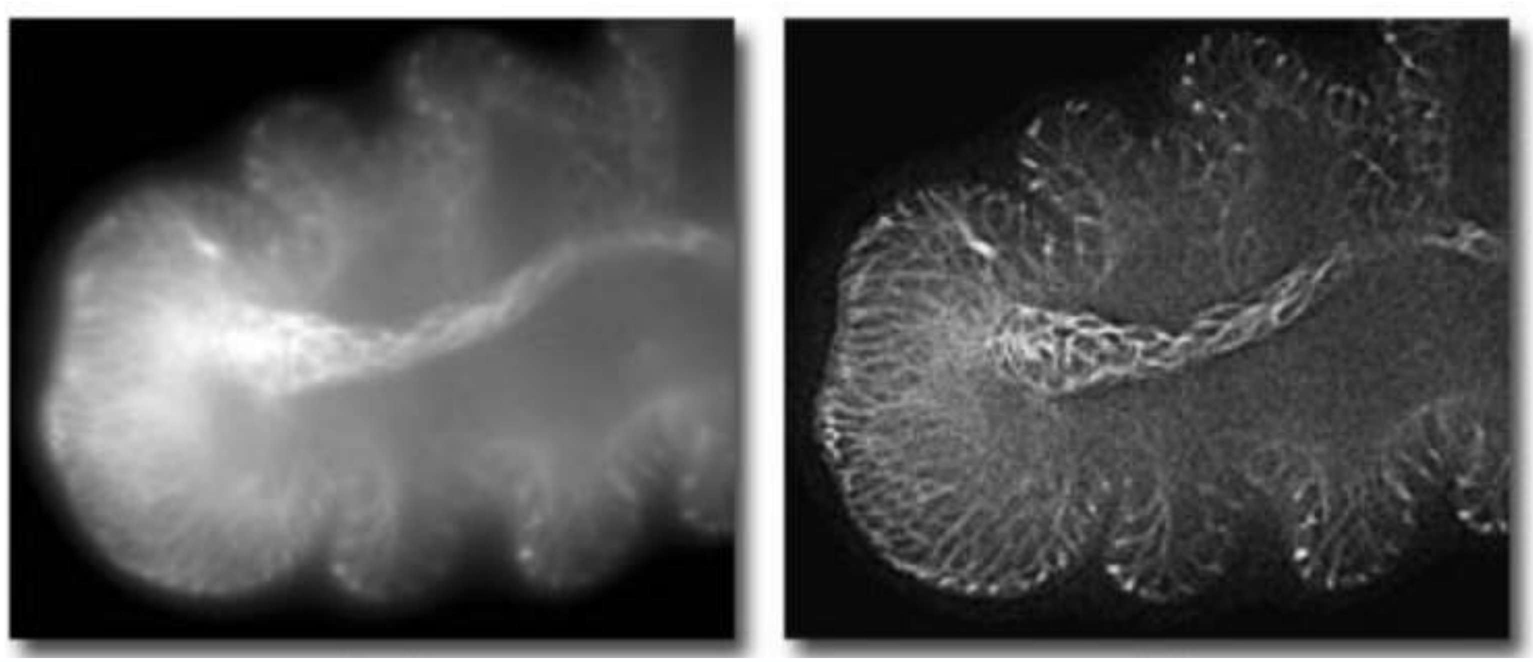

Common inverse problems (4)

- Inpainting

$$A = S \quad \text{diagonal operator, with} \quad S_{ii} = \begin{cases} 1 & \text{,if } x_i \text{ is sampled} \\ 0 & \text{,otherwise} \end{cases}$$

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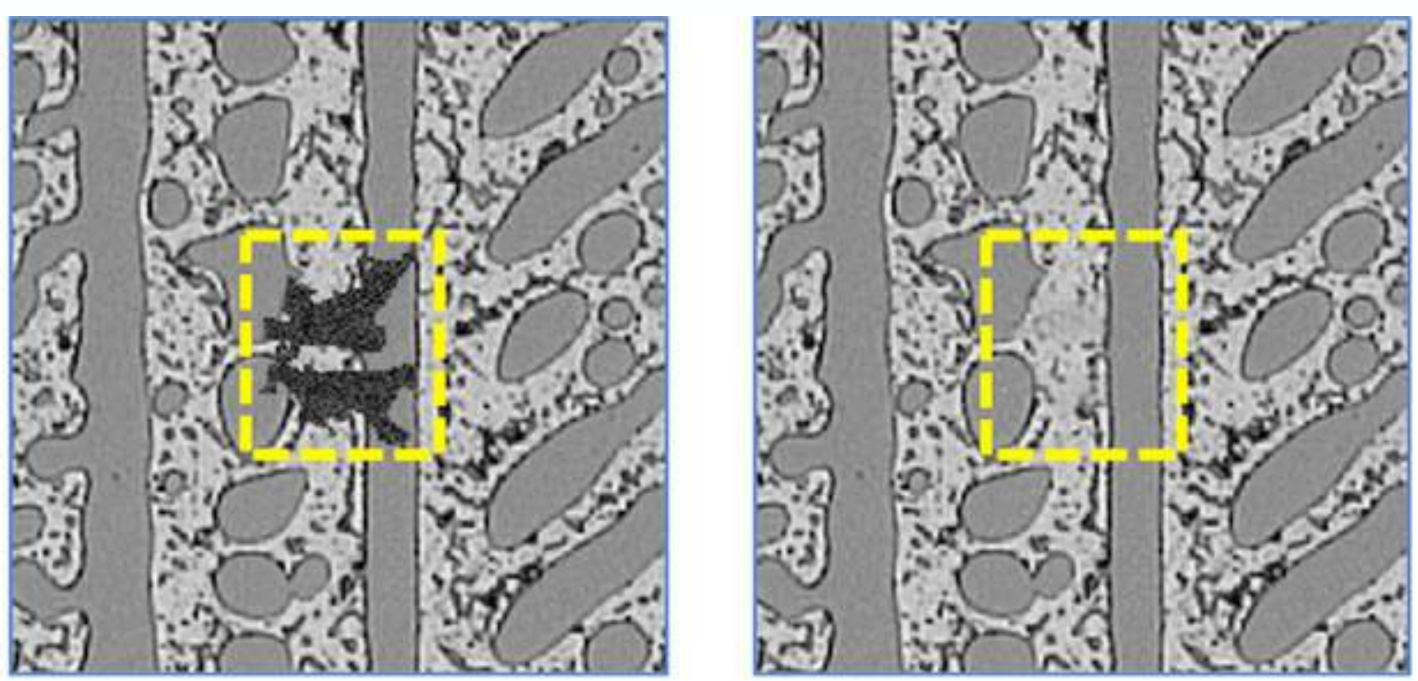

Damaged image *Restored image*

Common inverse problems (5)

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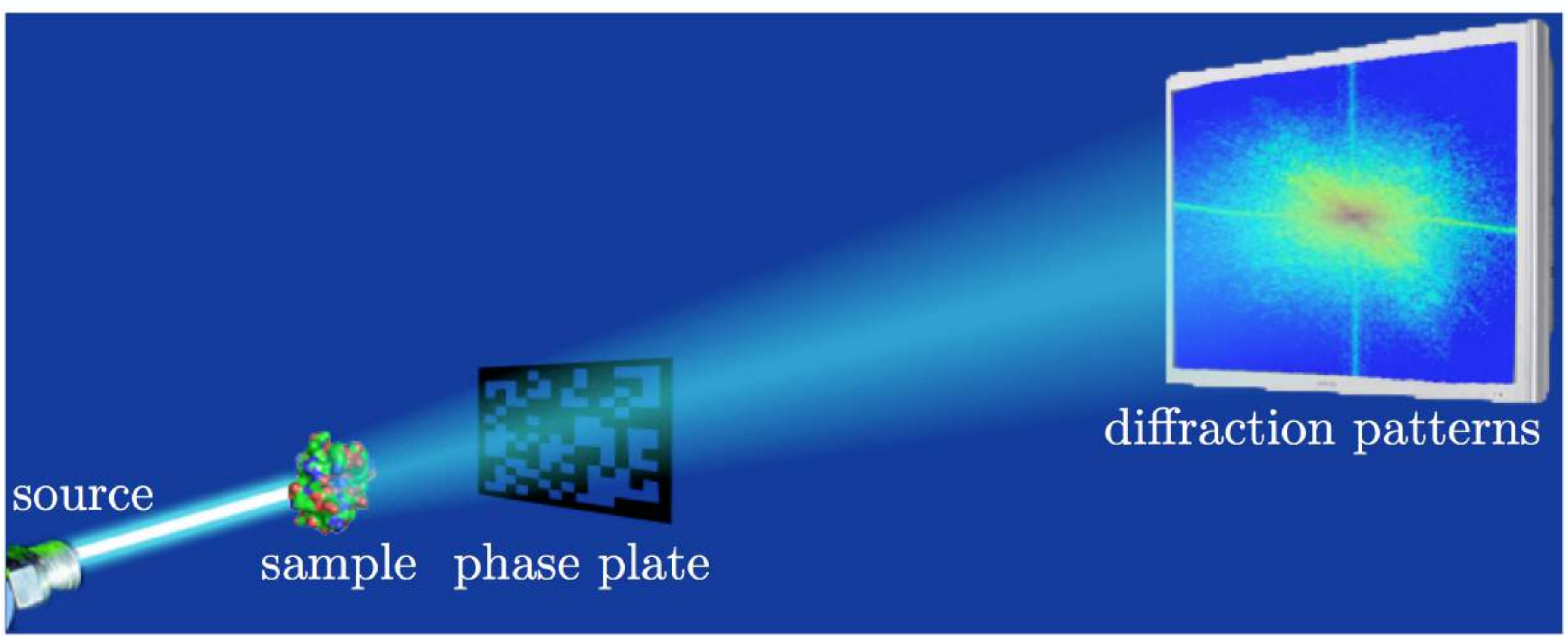
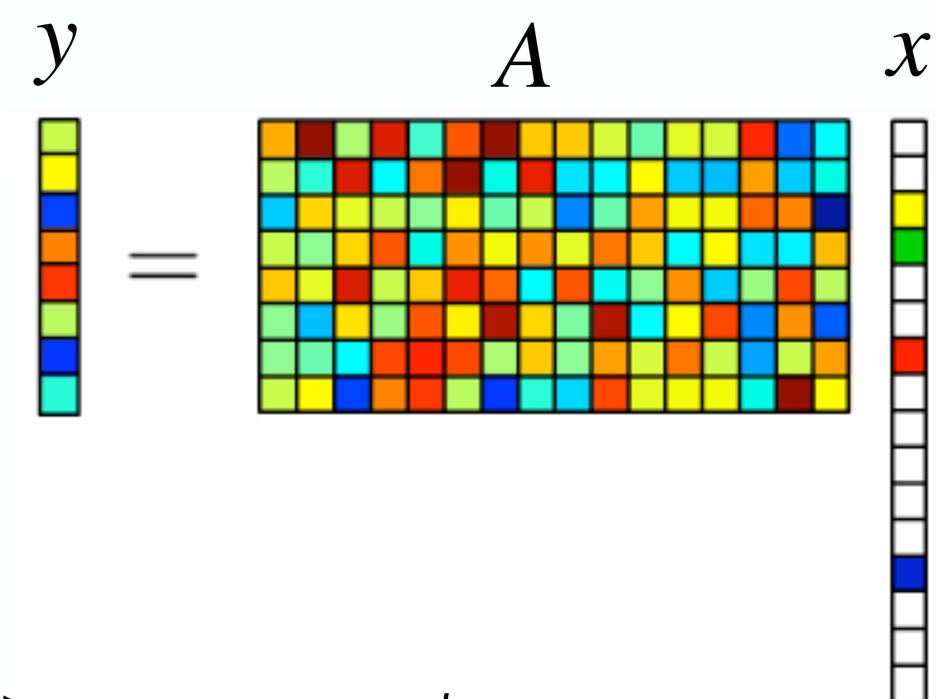


Tackling inverse problems (1)

- Simplest case



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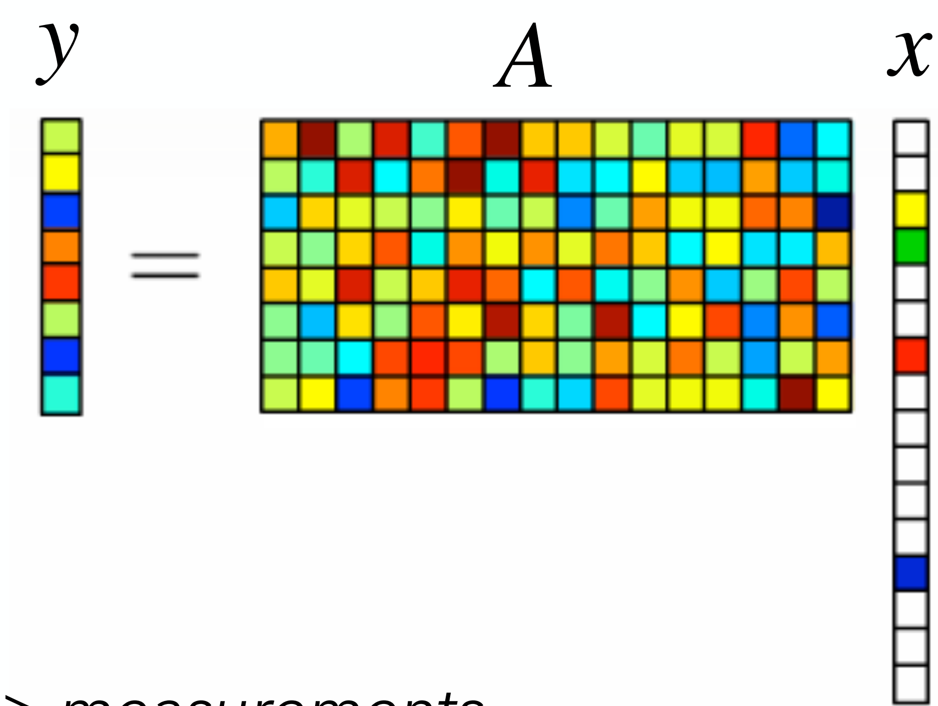

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Minimum norm solution: $\hat{x} = A^T(AA^T)^{-1}y$

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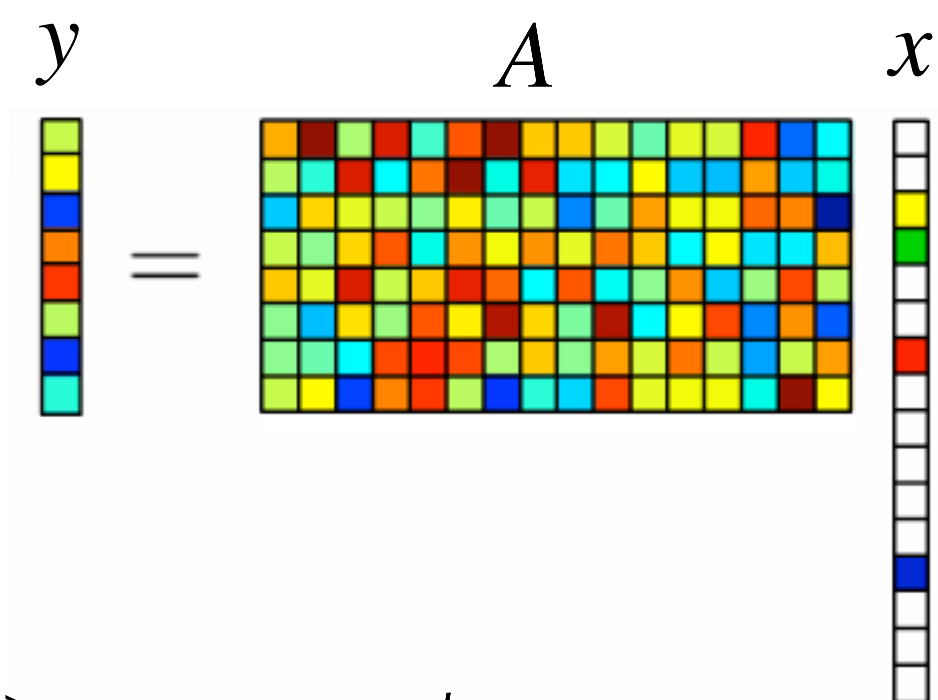

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Can we do better by leveraging side-information?

Tackling inverse problems (2)

- Compressed sensing formulation

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$$\min_x \|\mathscr{A}(x) - y\|^2 + \mathscr{R}(x)$$

data consistency

prior knowledge

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$$\min_x \underbrace{\|\mathscr{A}(x) - y\|^2}_{\text{data consistency}} + \underbrace{\mathscr{R}(x)}_{\text{prior knowledge}}$$

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  - Most often: sparsity in some transform domain (Fourier, Wavelet)
  - Solution: numerical, iterative algorithms

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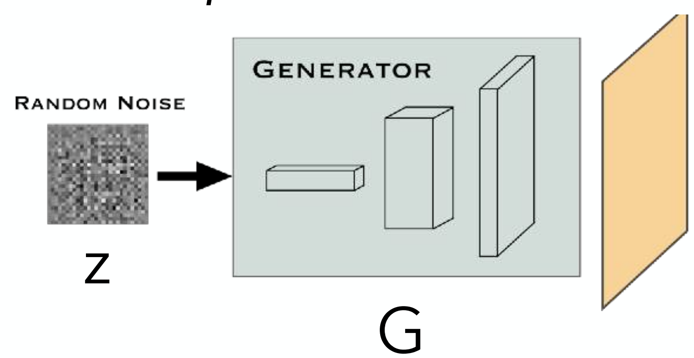

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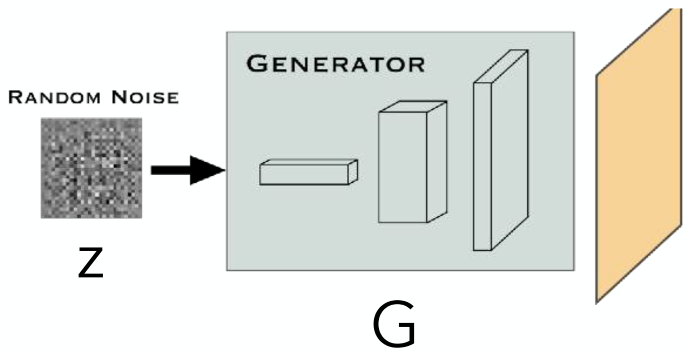

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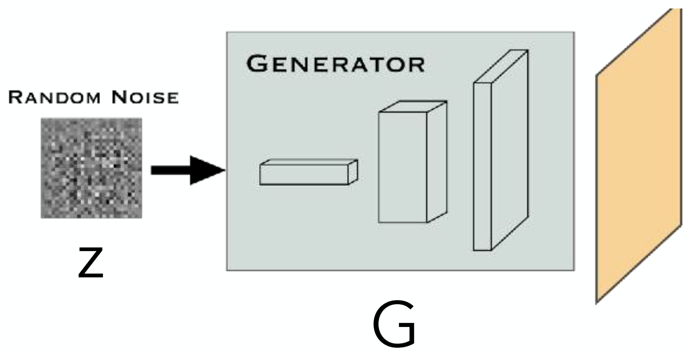

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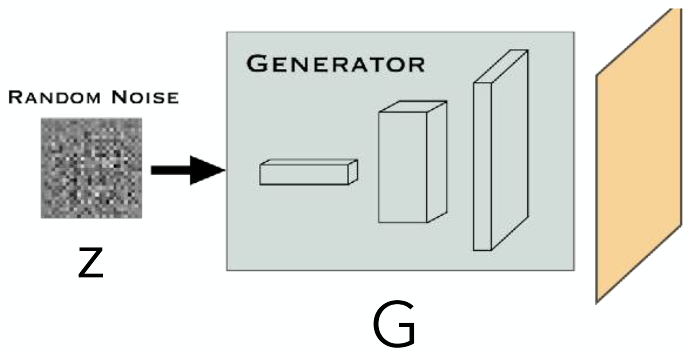

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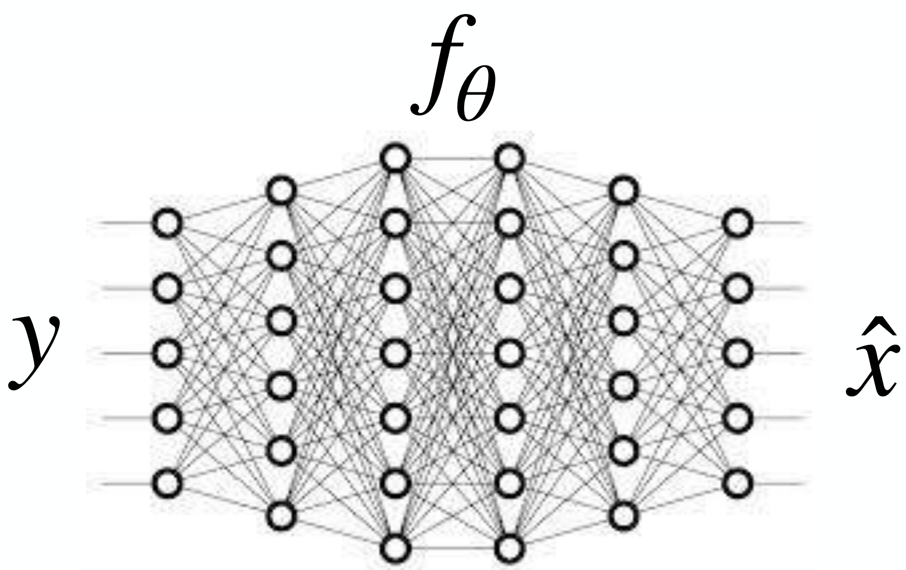

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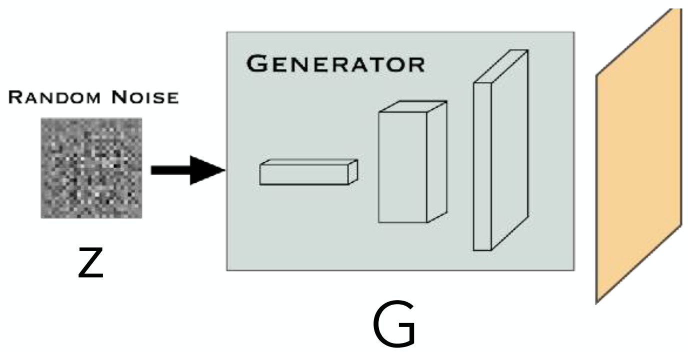

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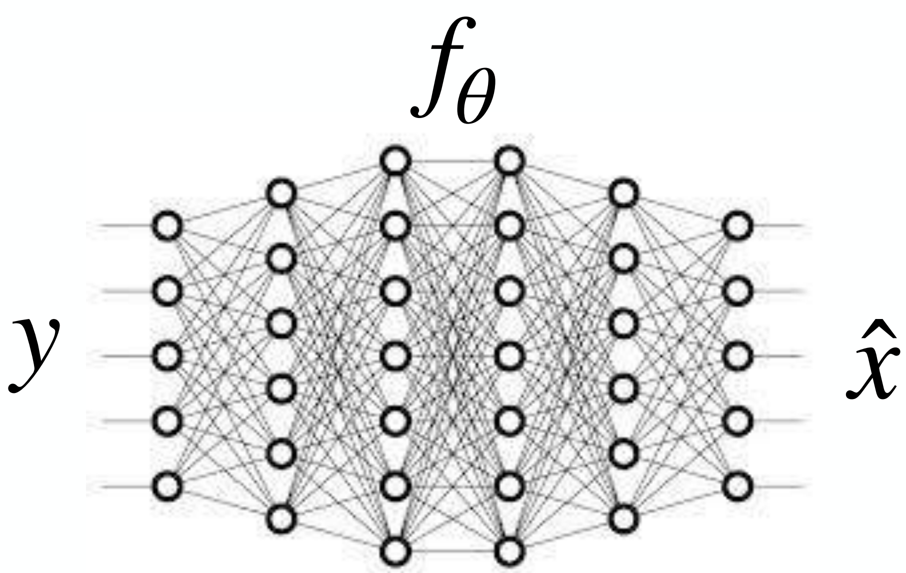

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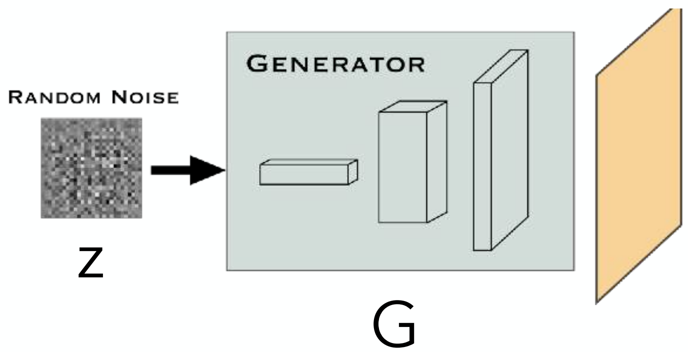

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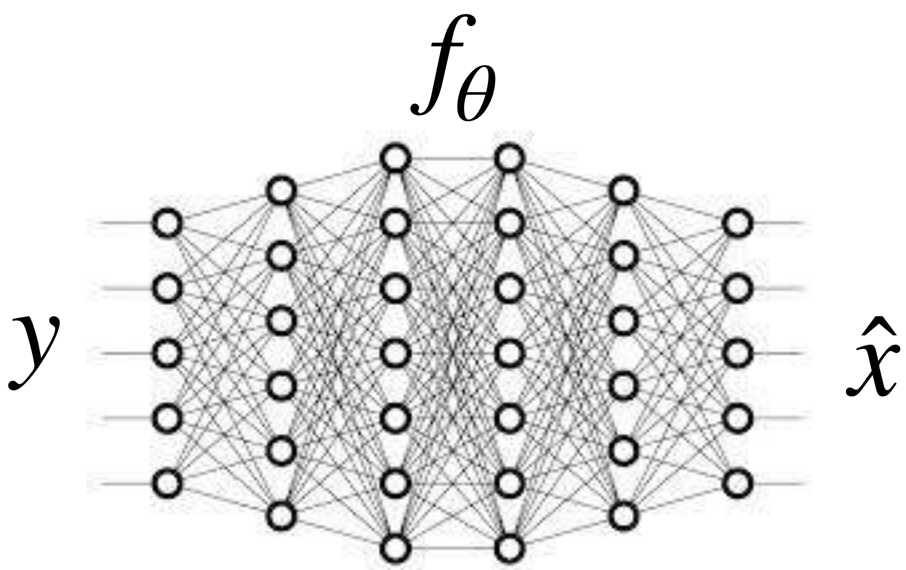

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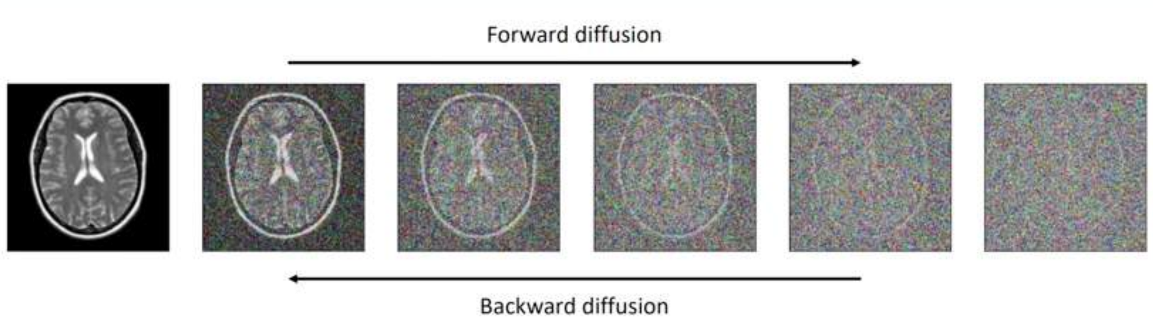
  - *Diffusion solvers*



Deep Generative Models
In Inverse Problems

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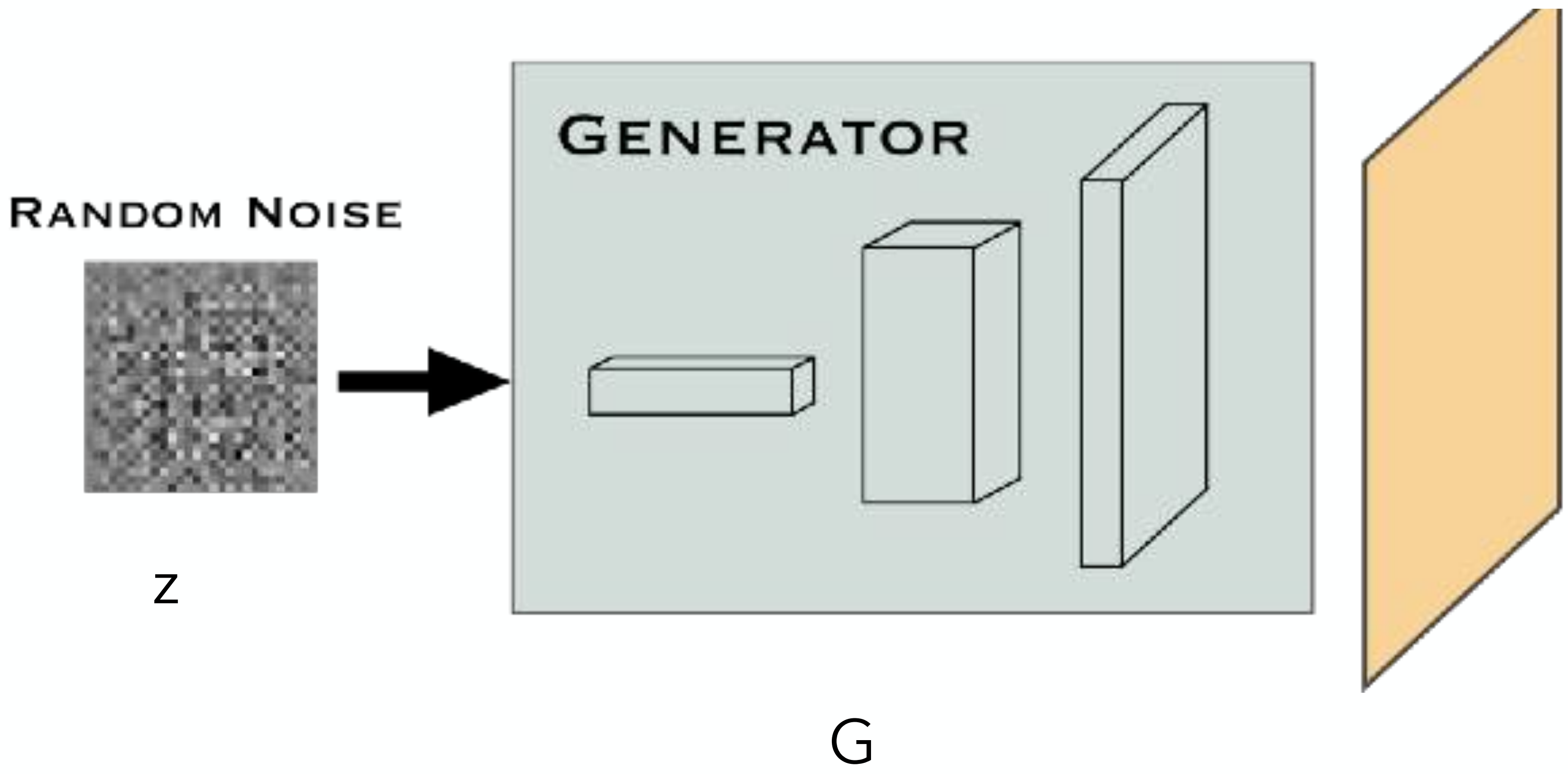

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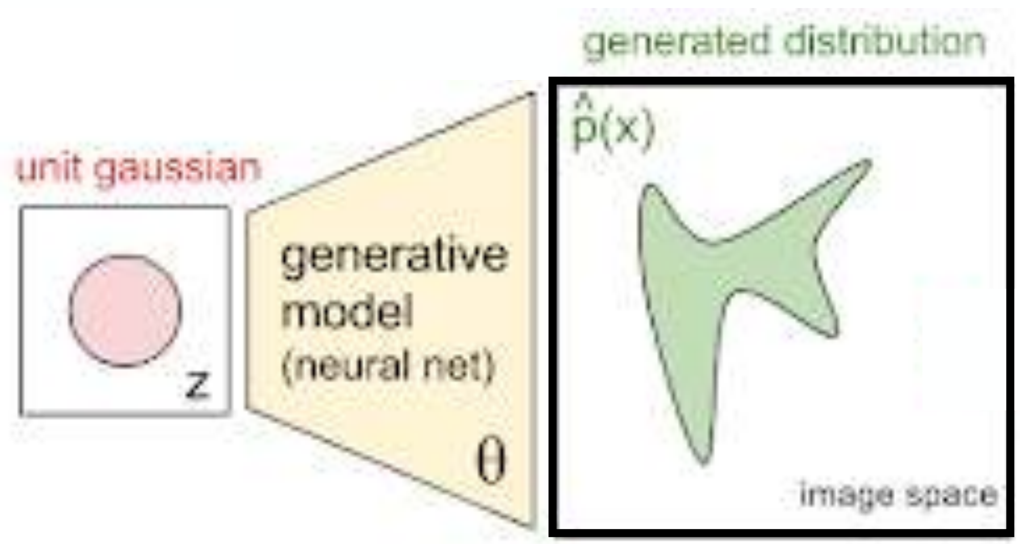

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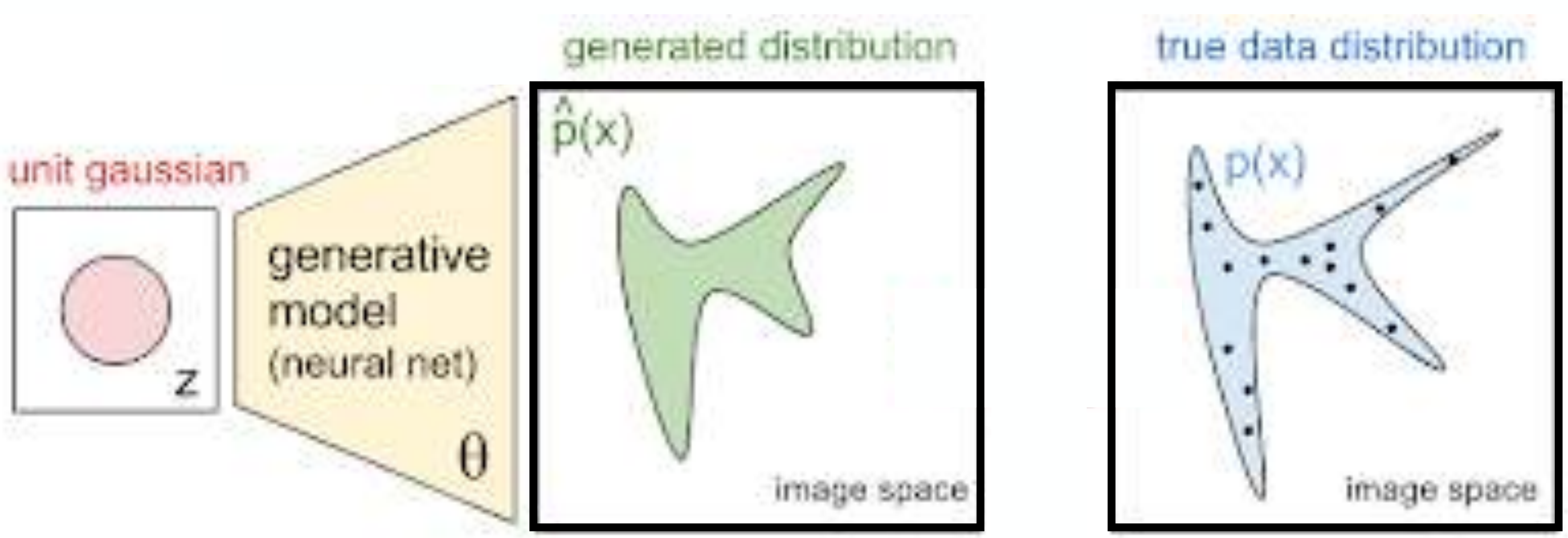

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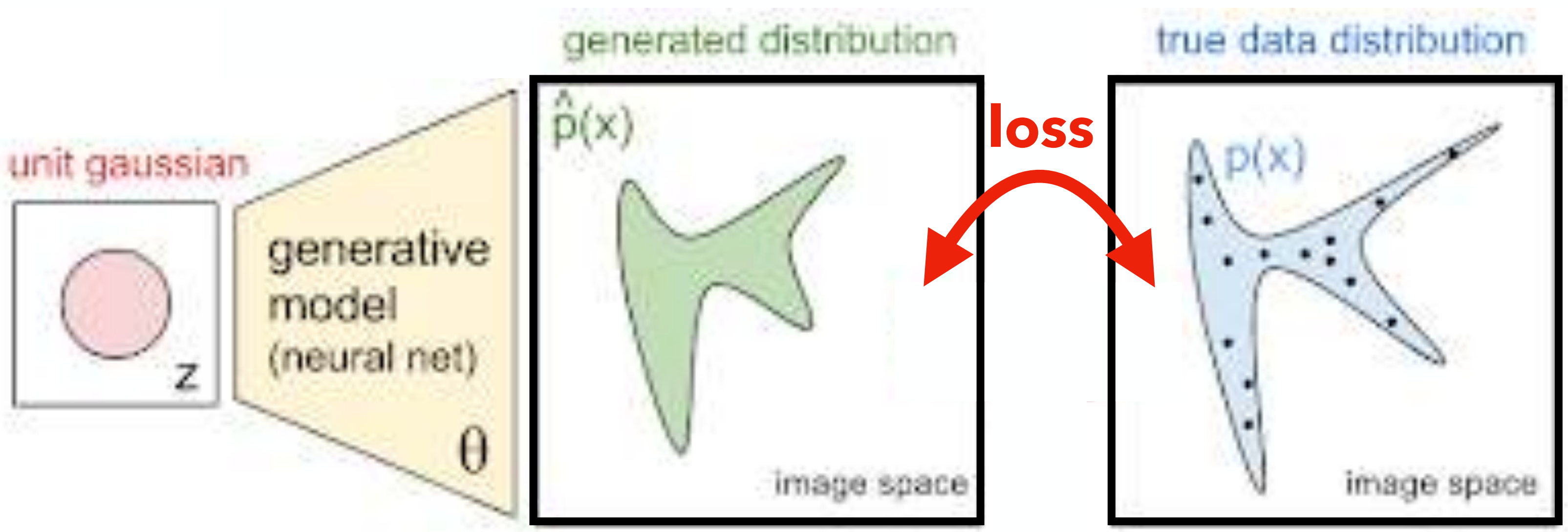

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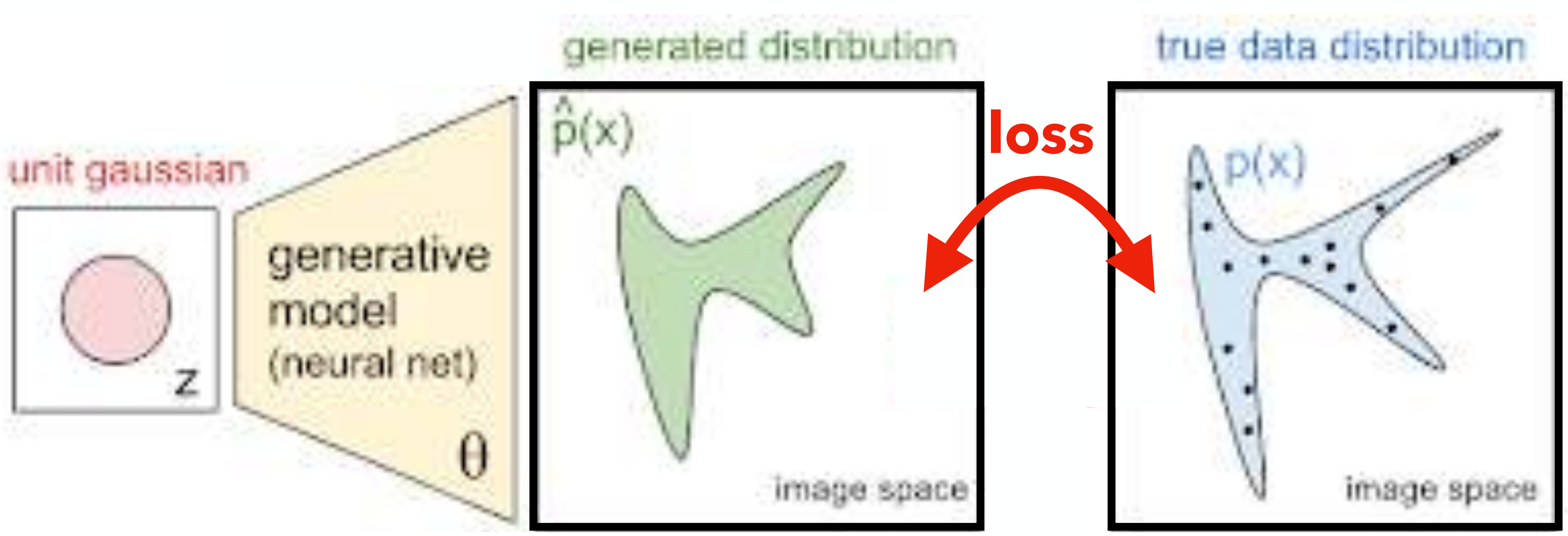

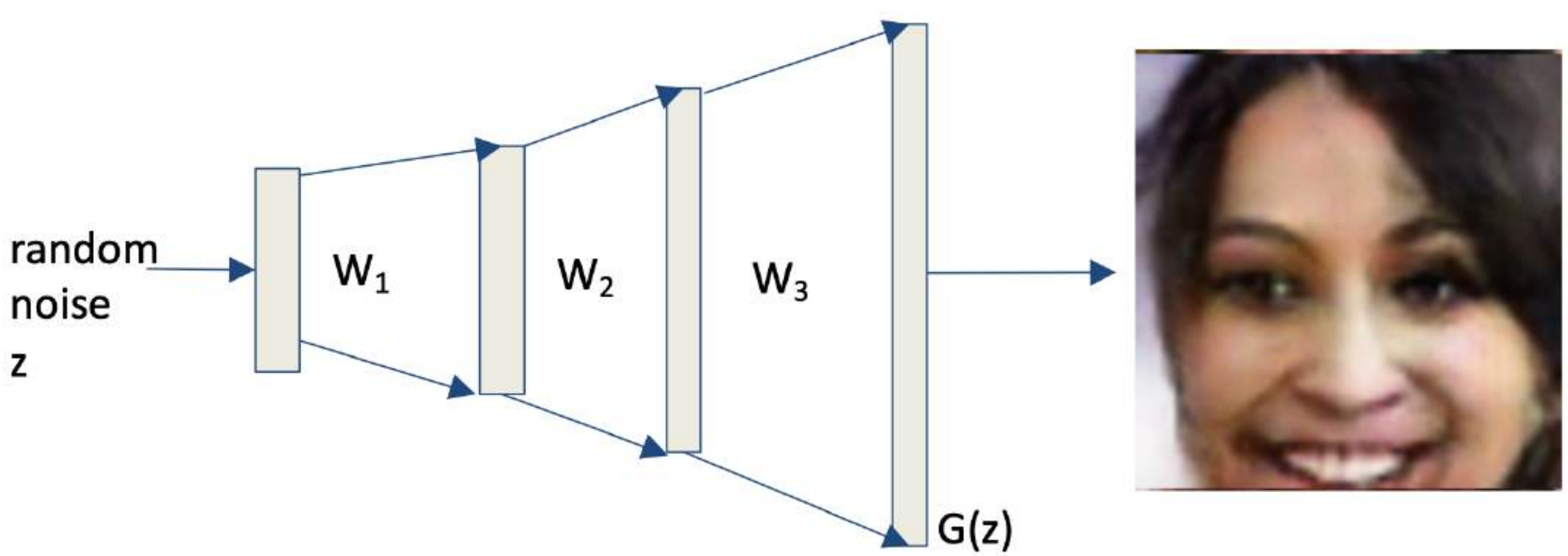

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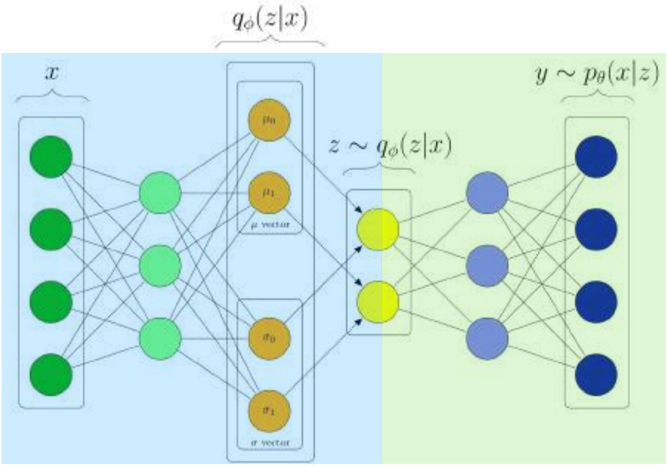

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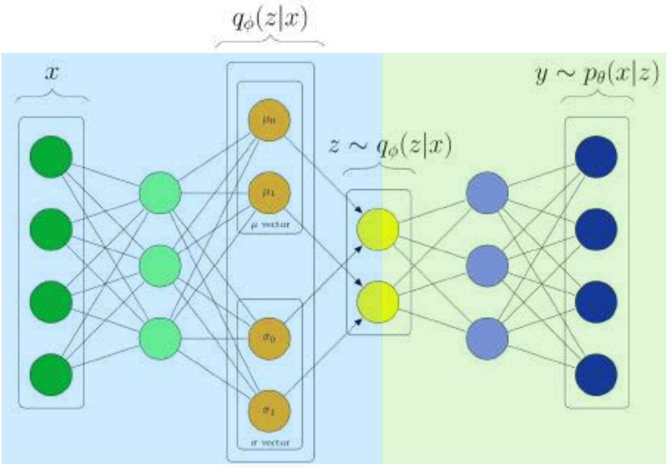

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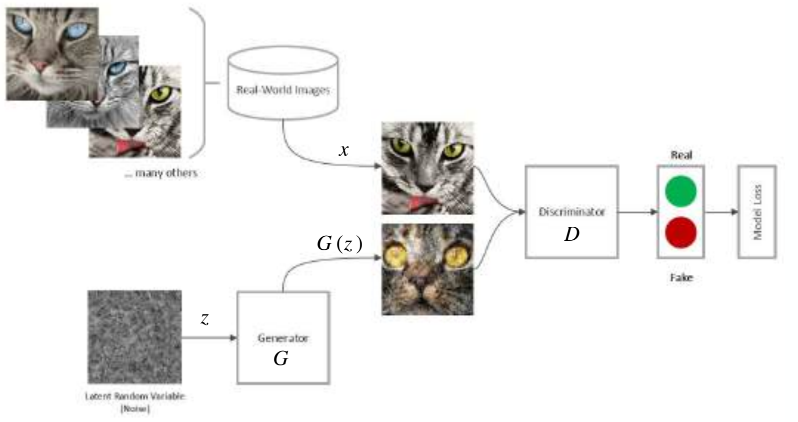

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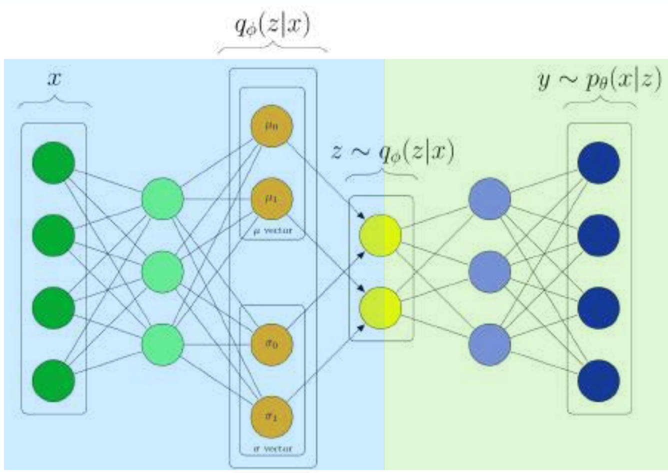

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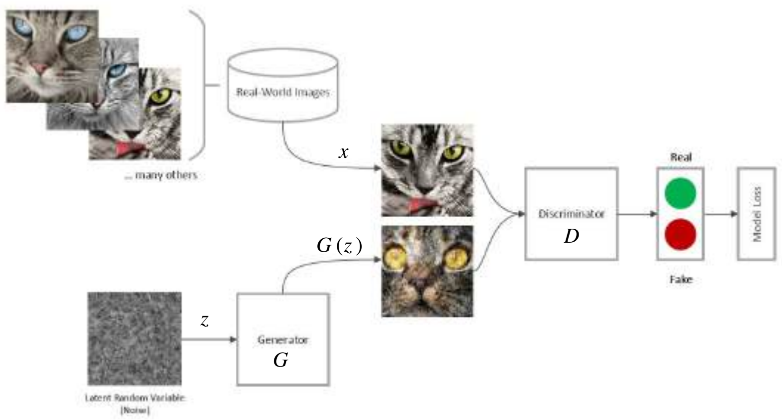
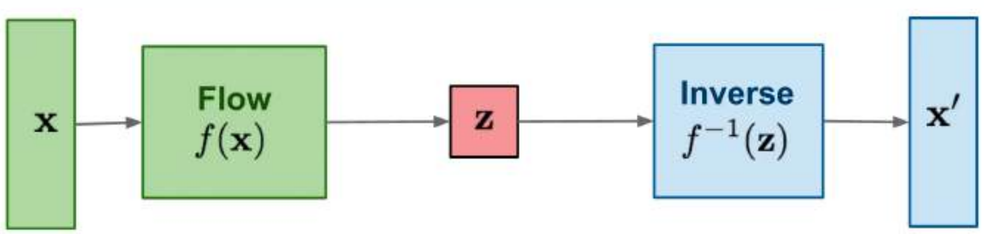


- Normalizing Flow Models (2015)



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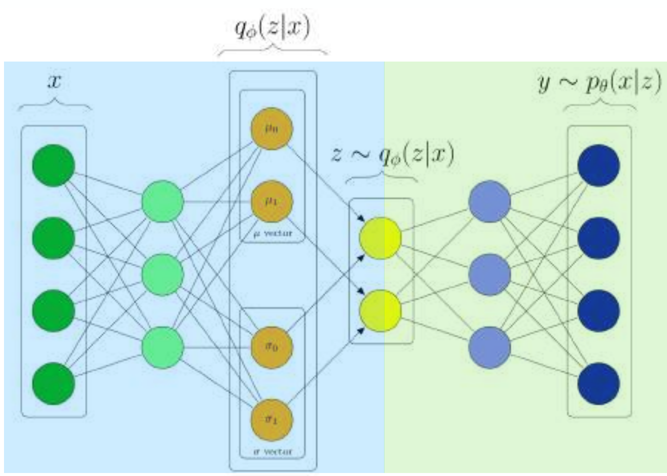

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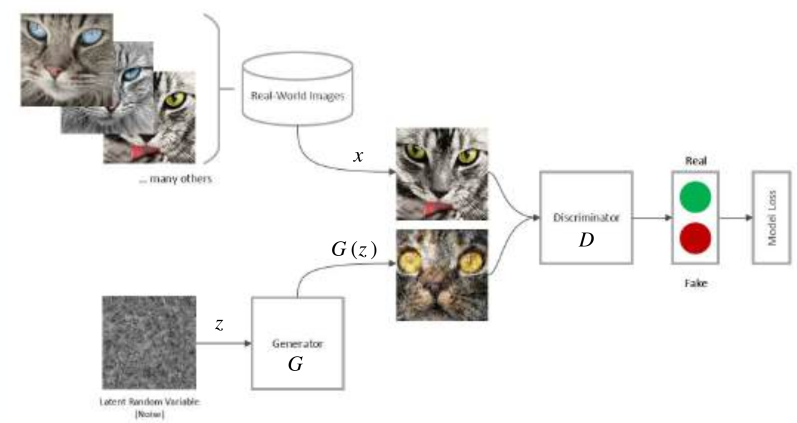

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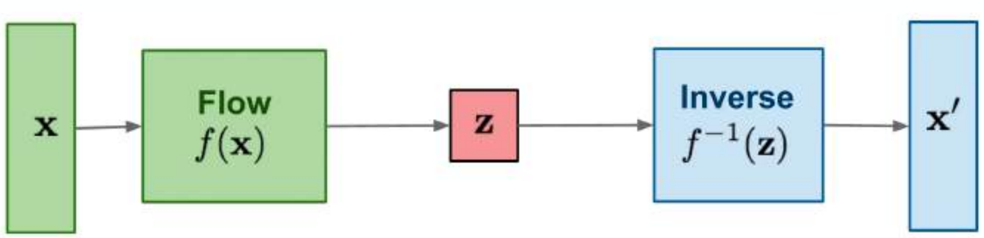
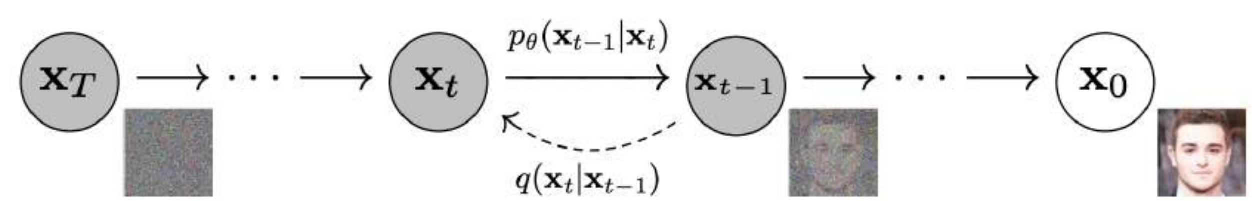


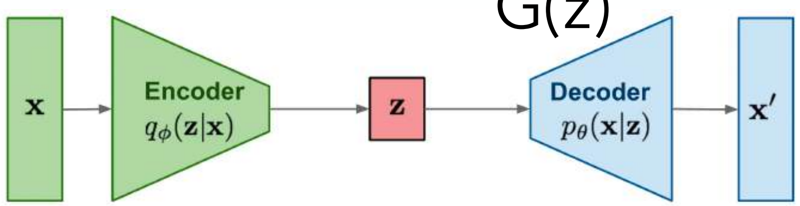
- Diffusion Models (2015, dominantly since 2020)



Compressed Sensing using Generative Models

Step 1: Pre-train generator on available training data

G(z)



VAE (example)

$$\min_{\theta} \quad \sum_{i=1}^{n} \|G_\theta(\mathbf{z}_i) - x_i\|_{\ell_2}^2$$

Bora, A., Jalal, A., Price, E. and Dimakis, A.G., 2017, July. Compressed sensing using generative models. In *International Conference on Machine Learning* (pp. 537-546). PMLR.

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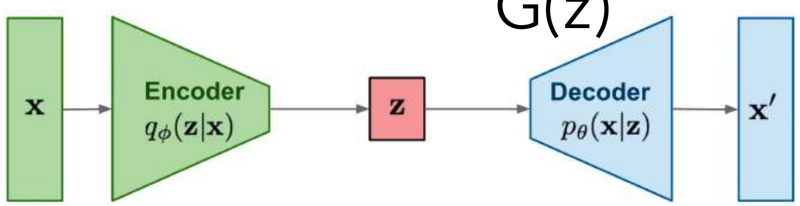

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Step 2: Leverage generative prior for reconstruction

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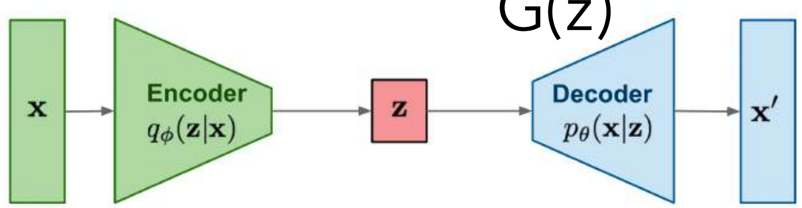

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- find vector in latent space of a generator

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Compressed Sensing using Generative Models

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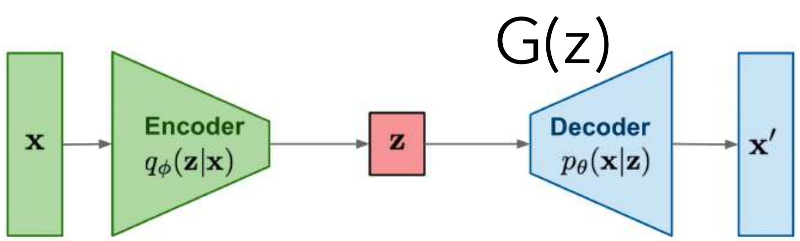

VAE (example)

$$\min_{\theta} \sum_{i=1}^{n} \|G_\theta(\mathbf{z}_i) - x_i\|_{\ell_2}^2$$

Step 2: Leverage generative prior for reconstruction

$$\min_{z} ||AG_\theta(z) - y||^2$$

- find vector in latent space of a generator
- such that corresponding sample in data space

Bora, A., Jalal, A., Price, E. and Dimakis, A.G., 2017, July. Compressed sensing using generative models. In *International Conference on Machine Learning* (pp. 537-546). PMLR.

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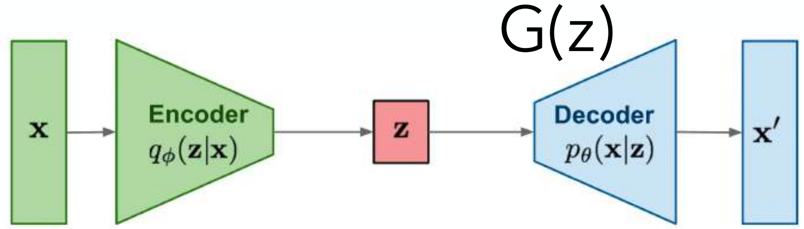
G(z)



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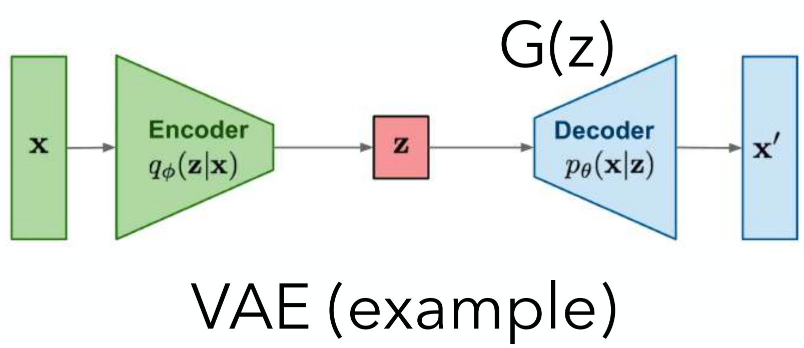

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For given MSE, 5-10x less measurements than classical sparsity-based methods!

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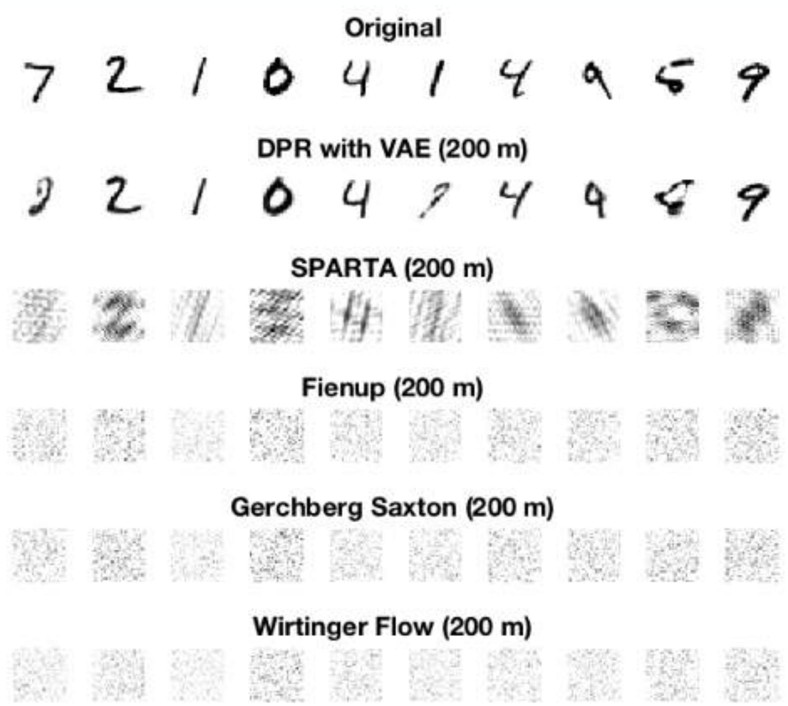
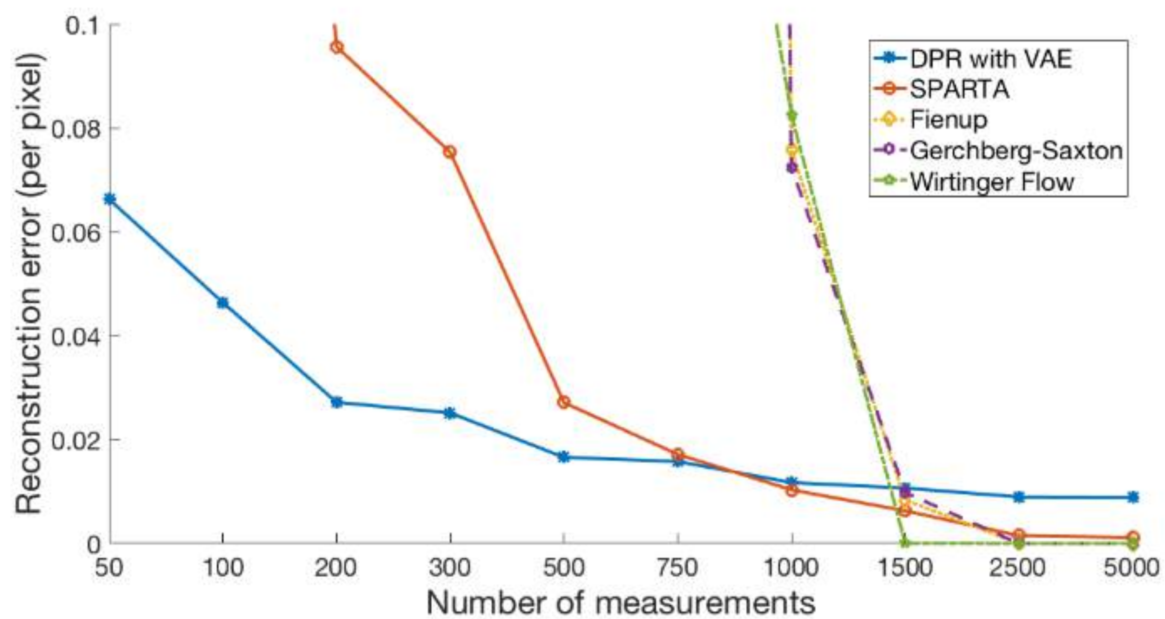
DGM in Phase Retrieval





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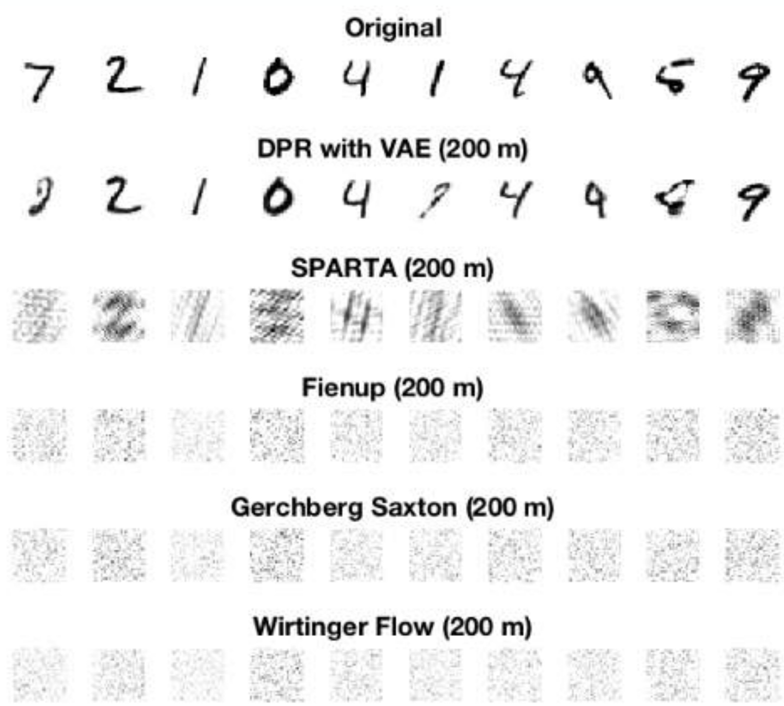

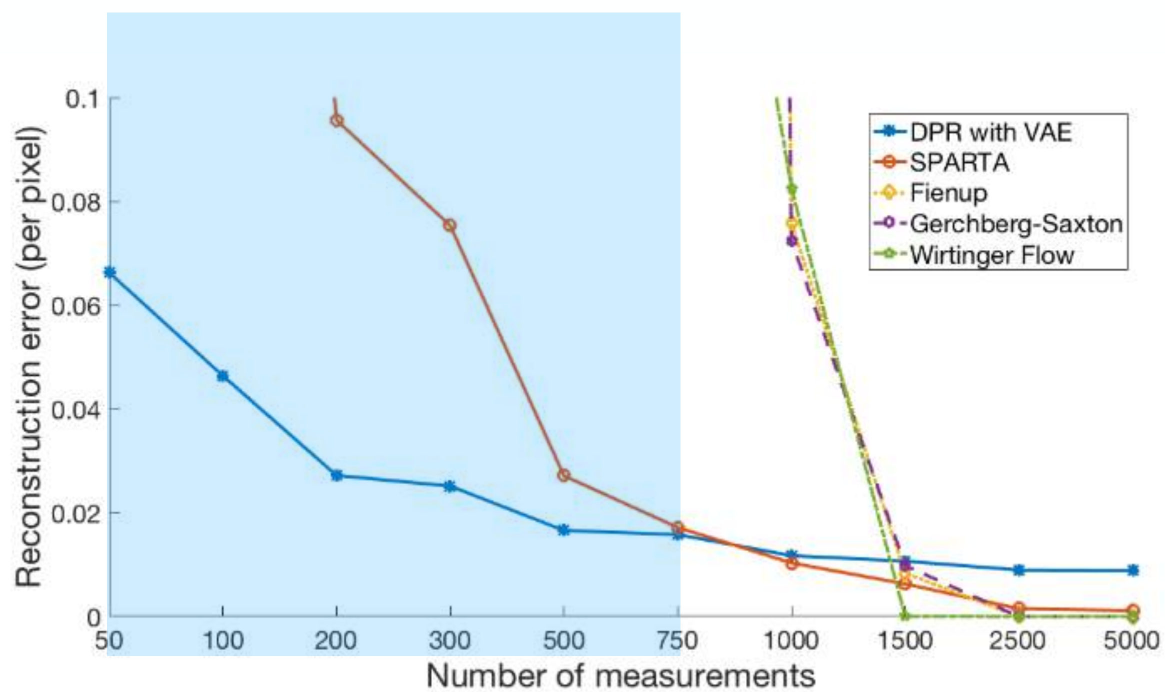

Best performance with low # of observations

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Existing Barrier to using DGM in Inverse Problems

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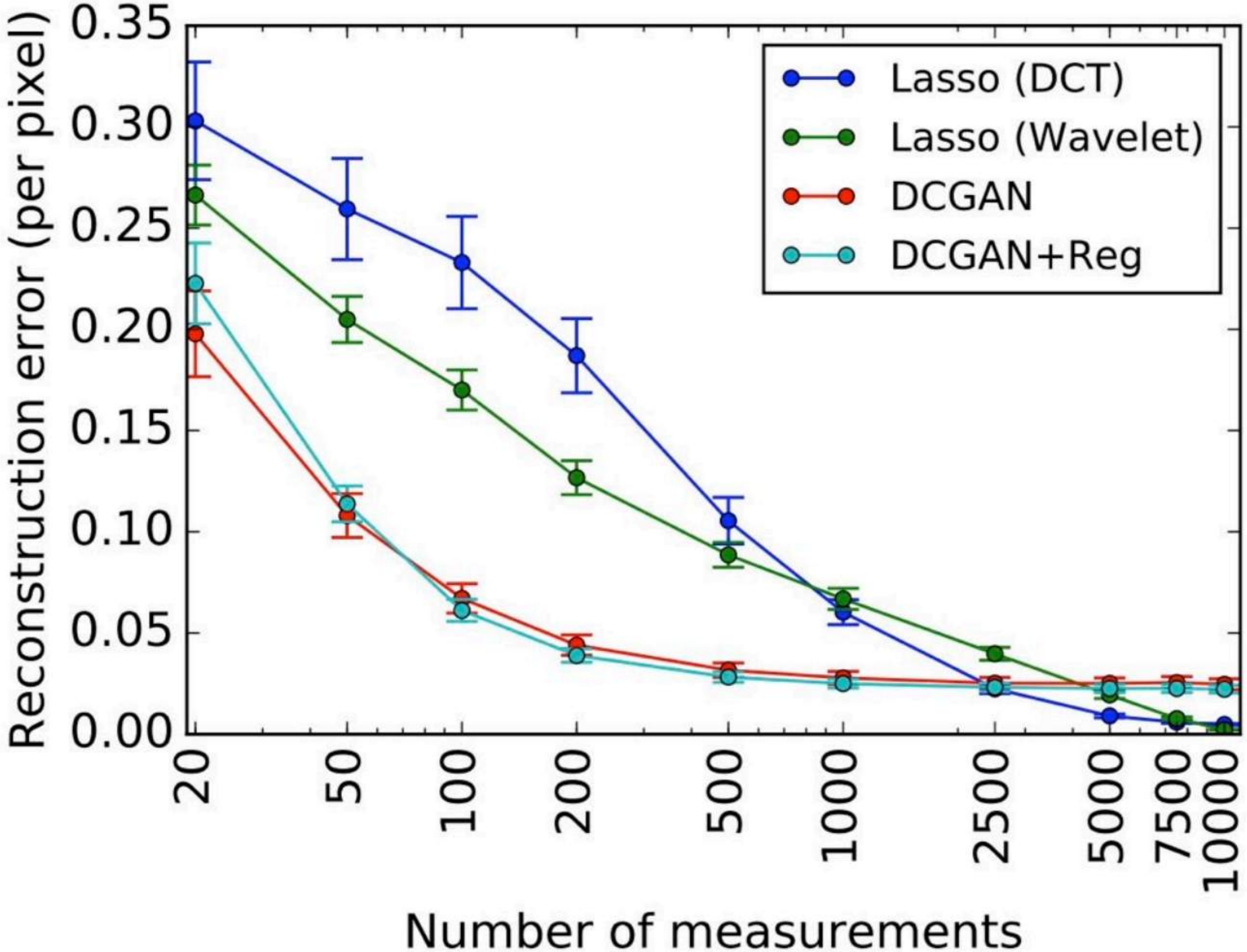

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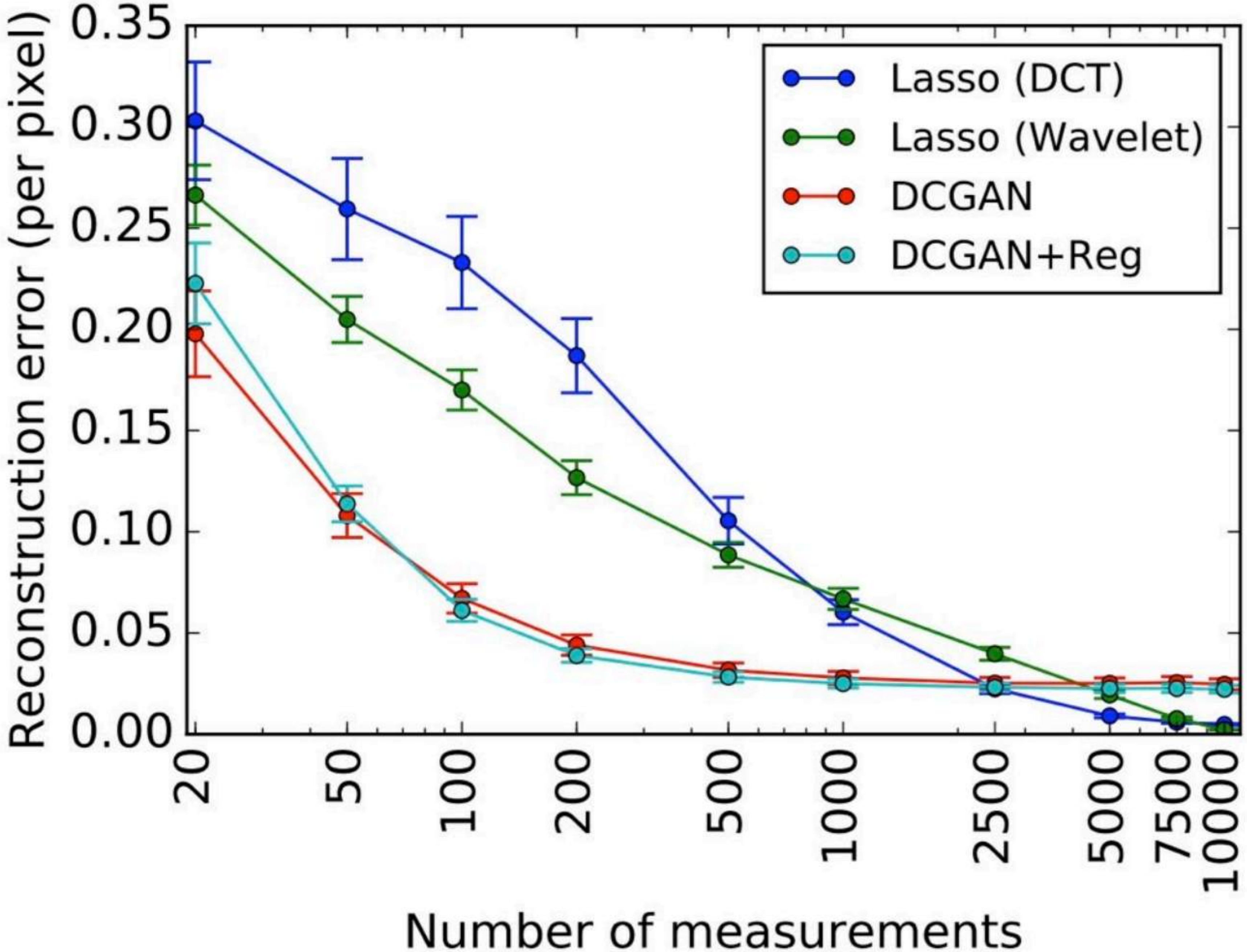
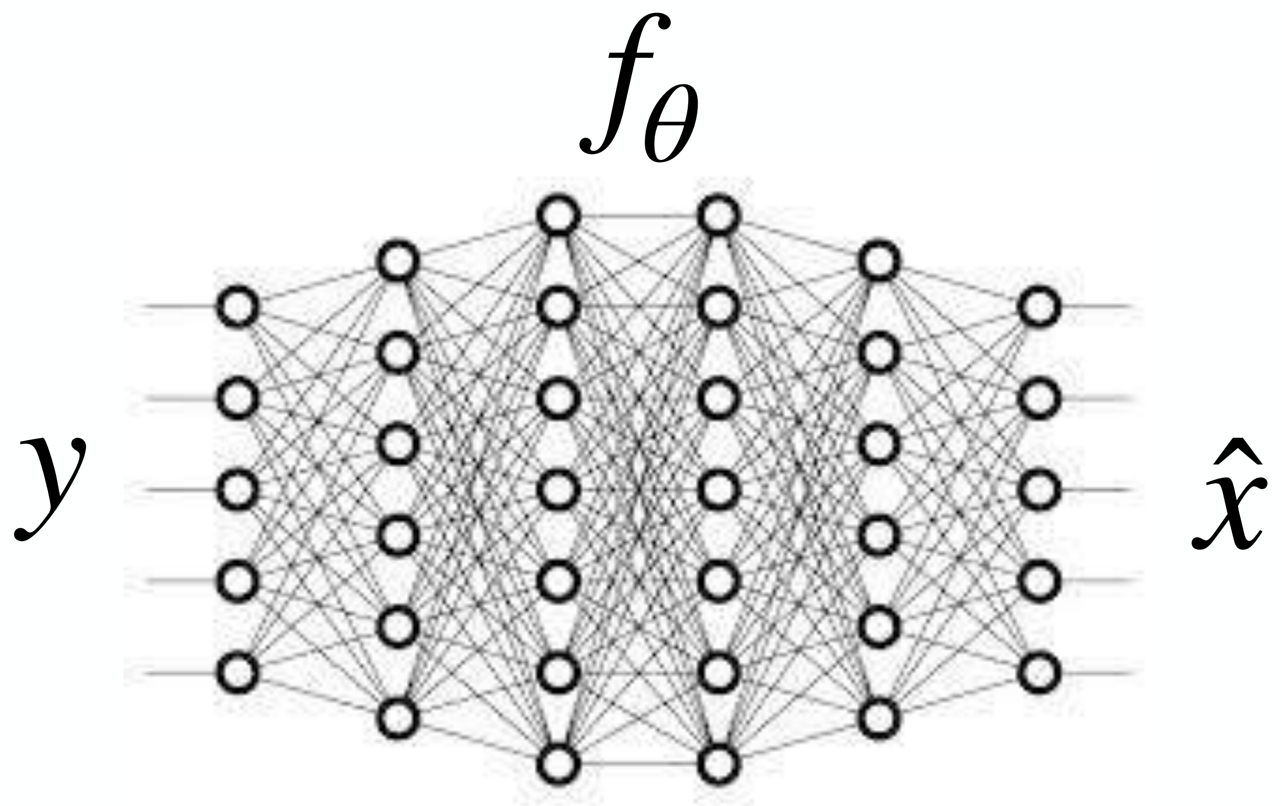


Compressed sensing using generative models, Bora et al. ICML 2017

End-to-end methods

End-to-end methods



End-to-end methods

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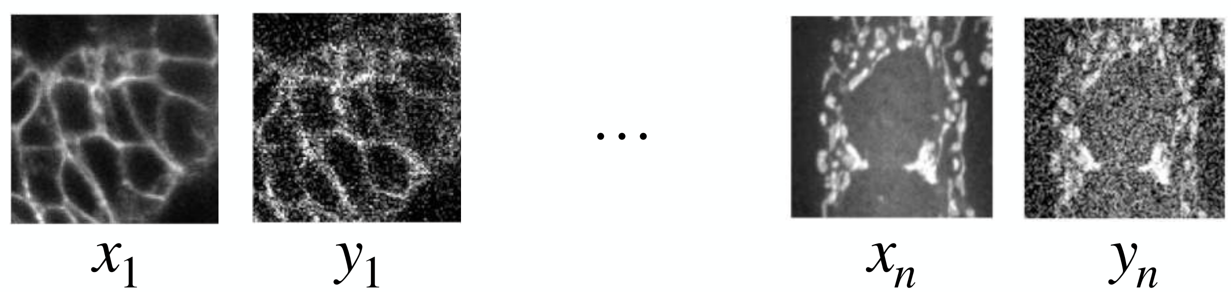

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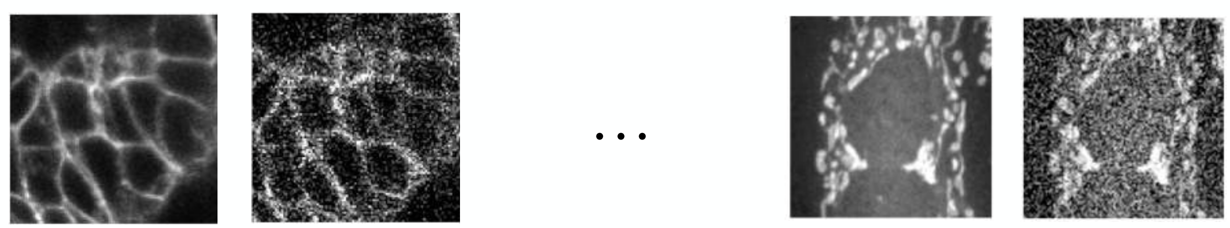
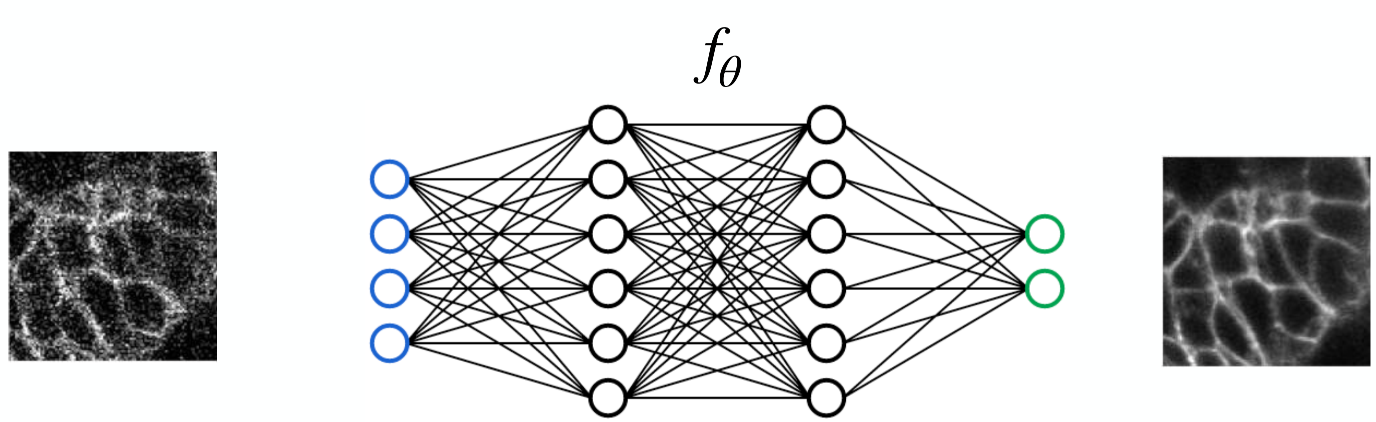


x_1 y_1 $\dots$ x_n y_n

- Directly learn the mapping from observations to reconstructions from data



$$\min_\theta \mathscr{L}(f_\theta(y), x)$$

End-to-end methods in MRI reconstruction

- fastMRI public leaderboard

AIRS-Net 11/5/2020	8x	0.0070	0.9022	38.1	✓
HUMUS-Net 3/3/2022	8x	0.0081	0.8945	37.3	✓
HUMUS-Net 3/4/2022	8x	0.0086	0.8936	37.0	✓
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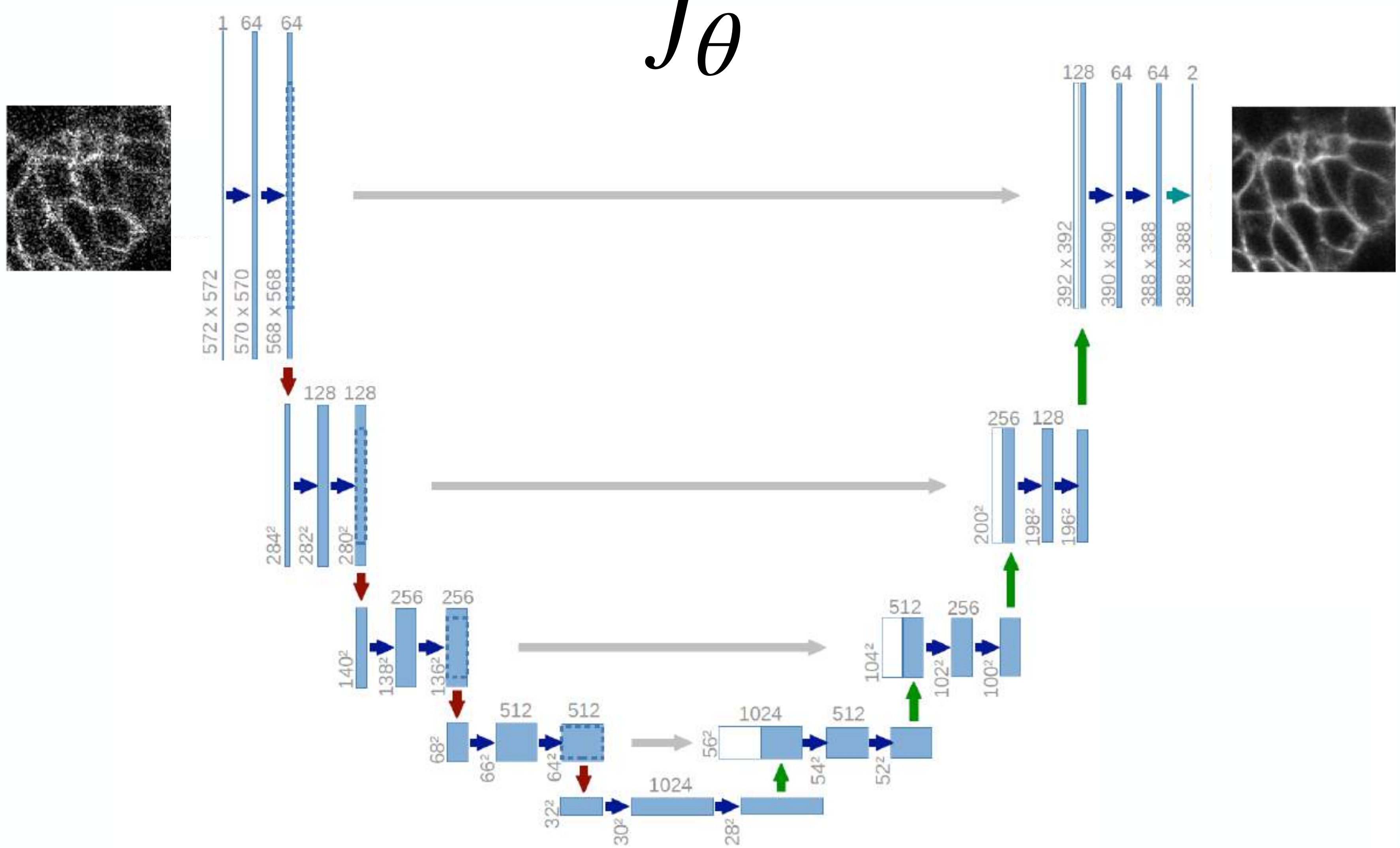
All end-to-end methods!

U-Net

f_θ



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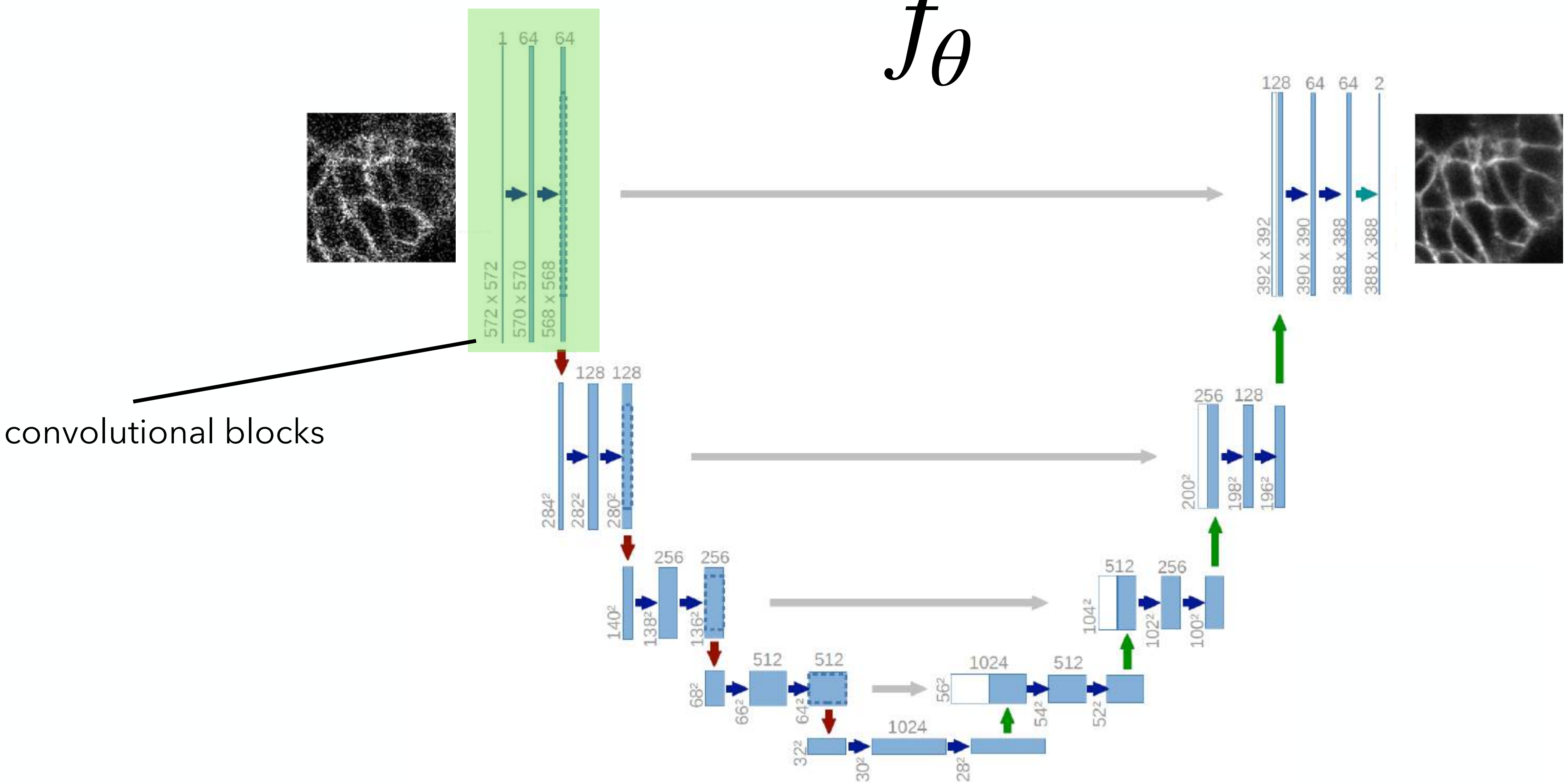

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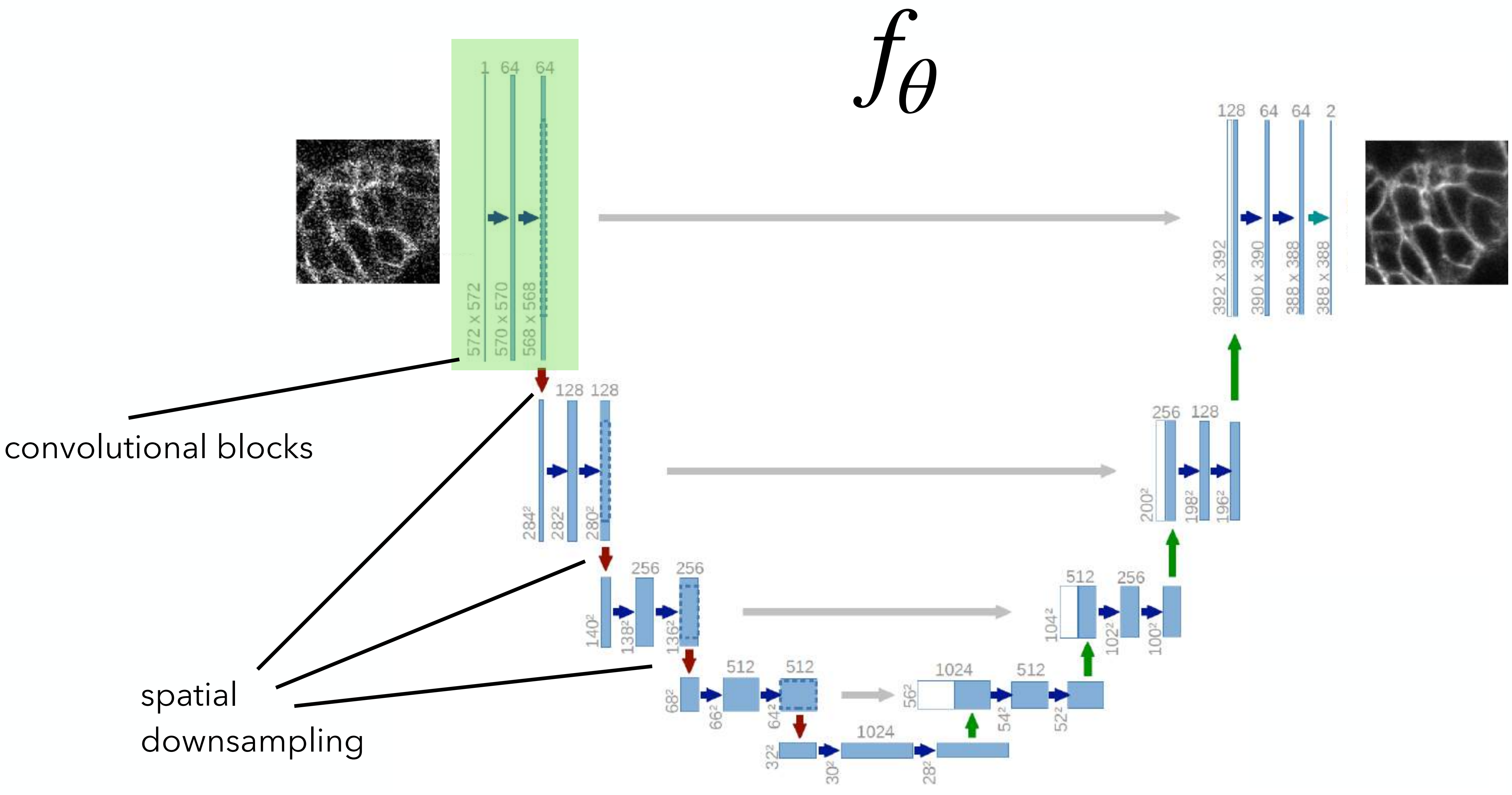

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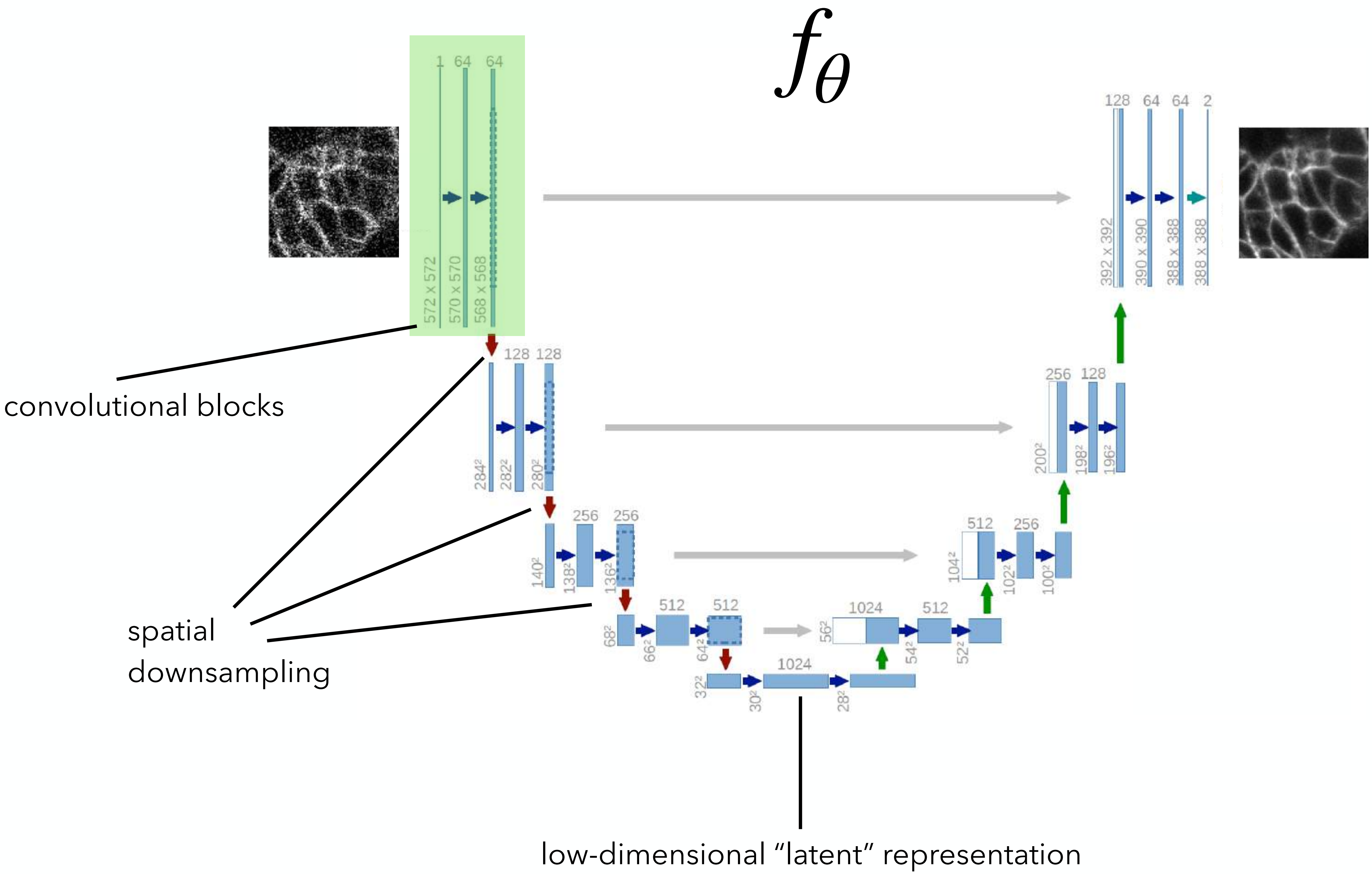

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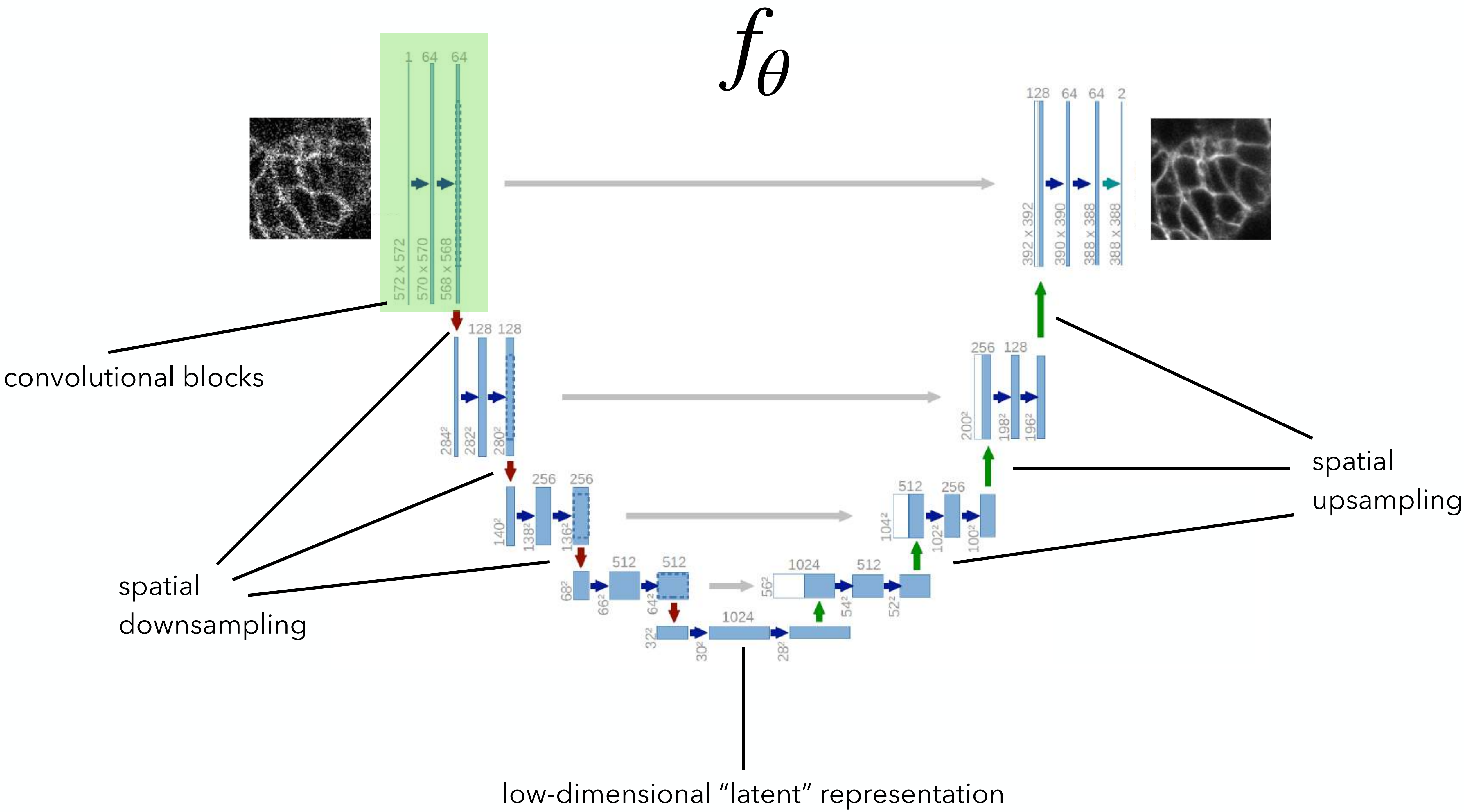

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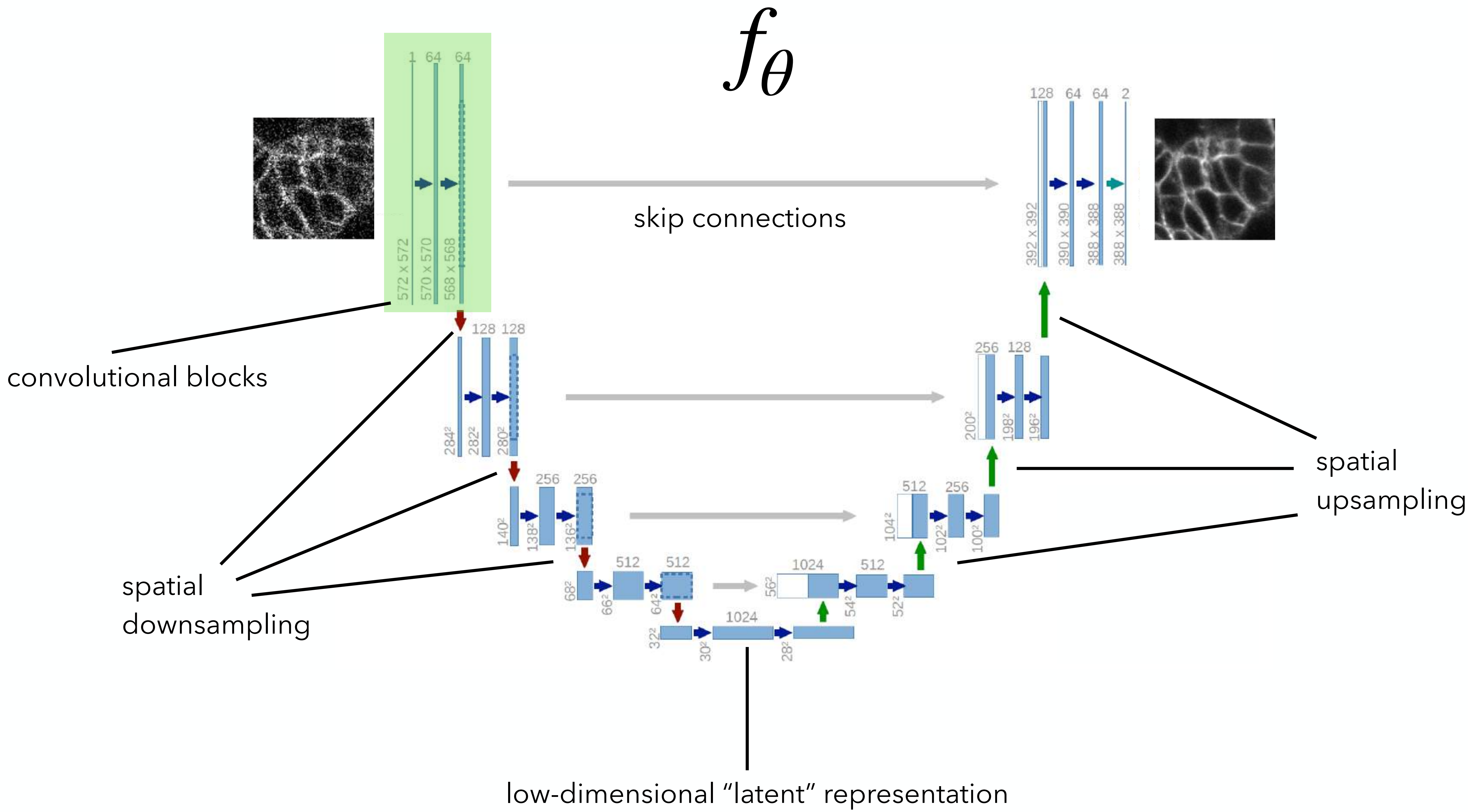

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Unrolled Networks

- Inverse problem formulation

$$\hat{x} = arg\,\min_{x} \|\mathscr{A}(x) - y\|^2 + \mathscr{R}(x)$$

- Iterative solution via GD

$$x^{t+1} = x^t - \mu^t \left[\mathscr{A}^* \left(\mathscr{A}(x^t) - y\right) + \nabla \mathscr{R}(x^t)\right]$$

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What is the best regularizer?

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Parameterize regularizer gradient as NN!

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$$\xrightarrow{\quad x_0 \quad}$$

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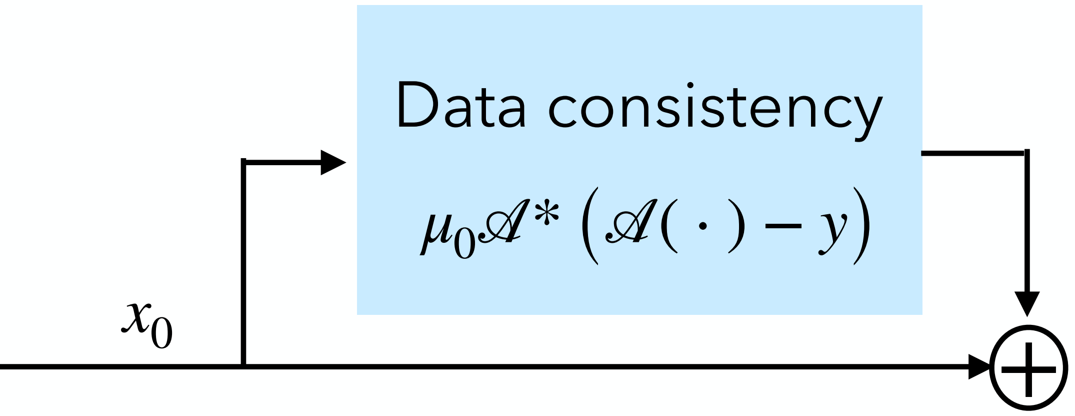

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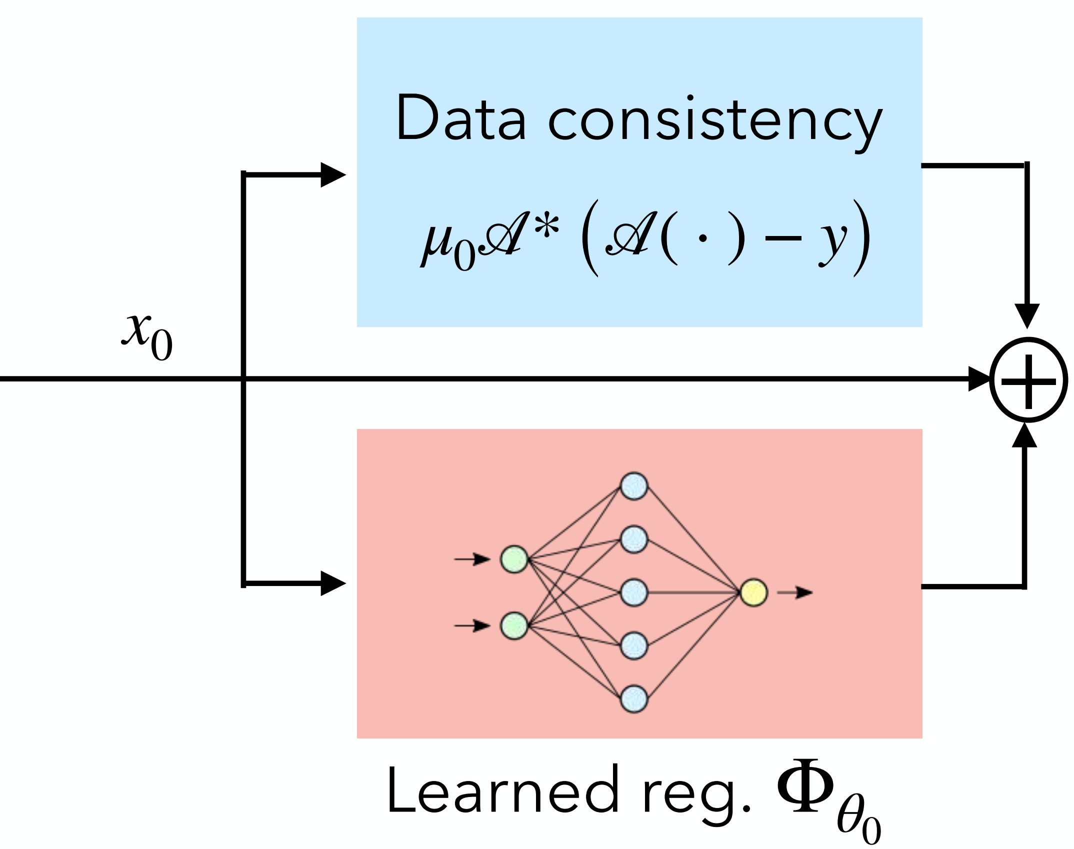

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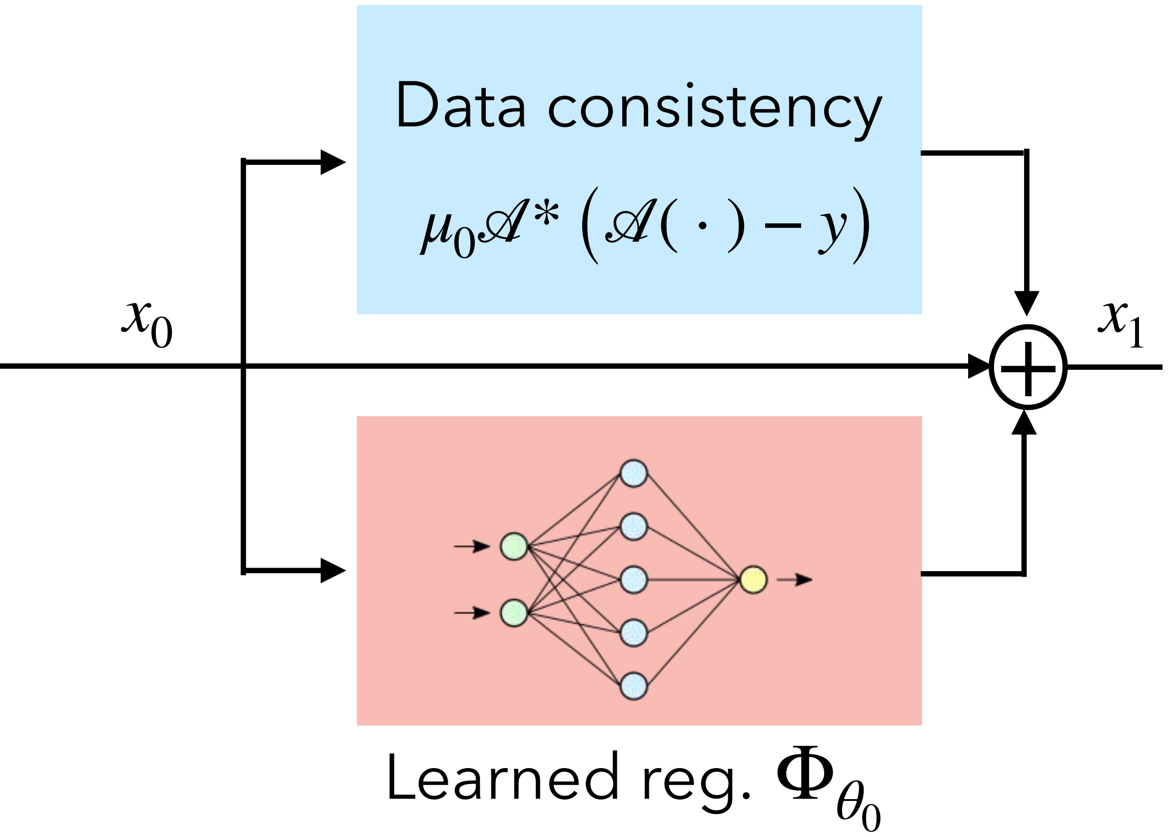

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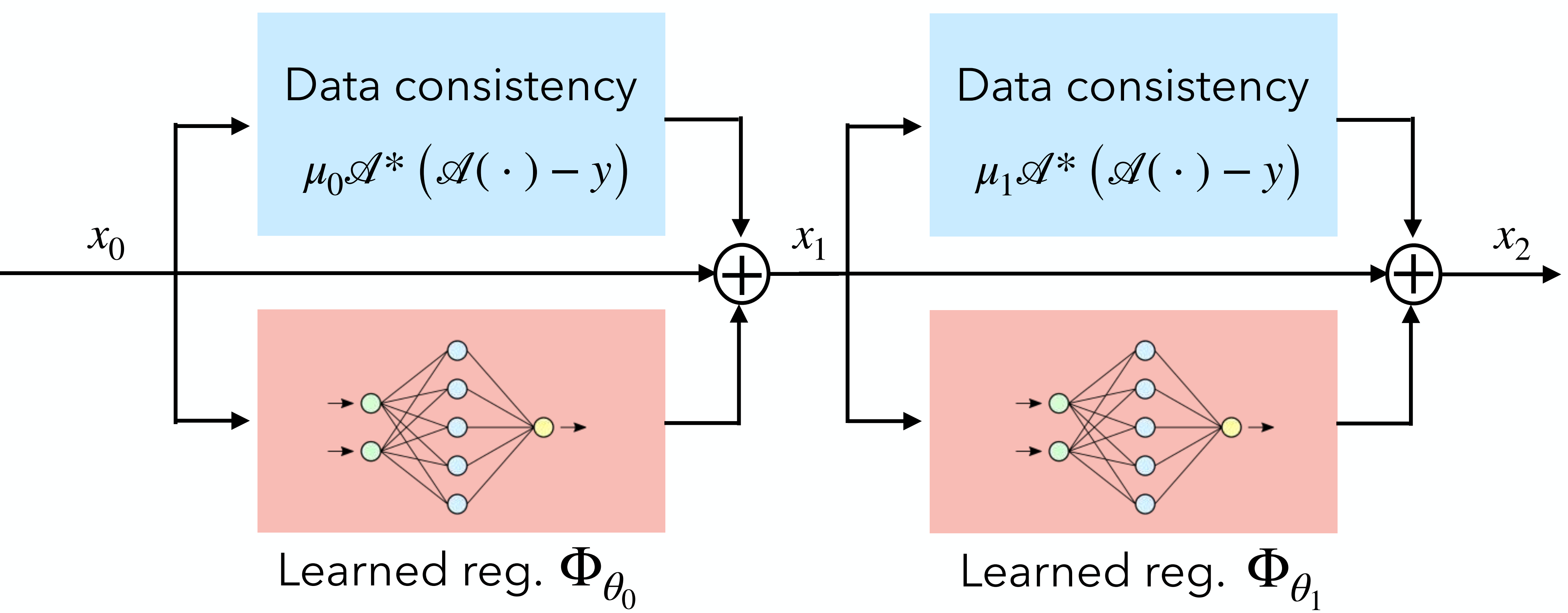

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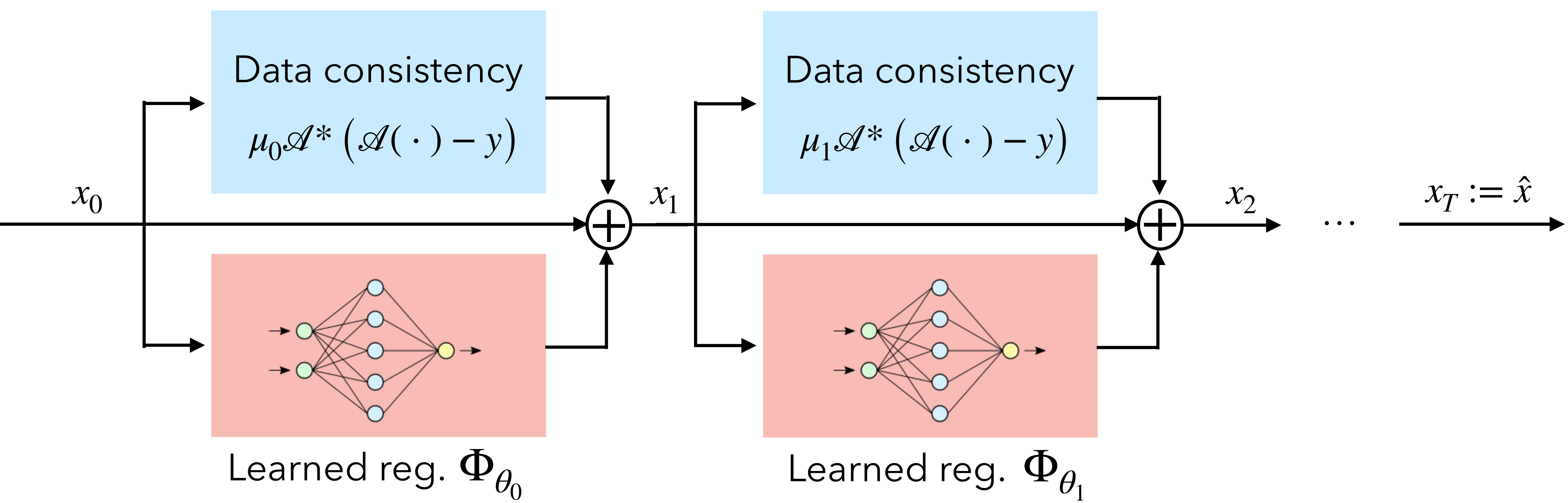

E2E VarNet

- Unroll GD iterations in k-space

Sriram, A., Zbontar, J., Murrell, T., Defazio, A., Zitnick, C. L., Yakubova, N., ... & Johnson, P. (2020). End-to-end variational networks for accelerated MRI reconstruction. In *International Conference on Medical Image Computing and Computer-Assisted Intervention* (pp. 64-73). Springer, Cham.

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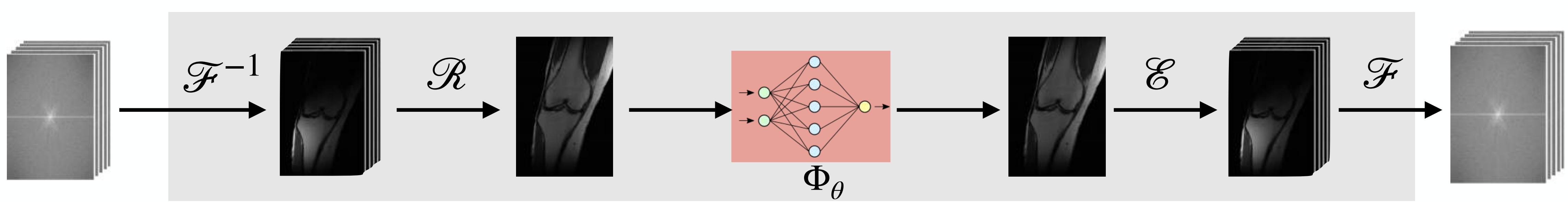

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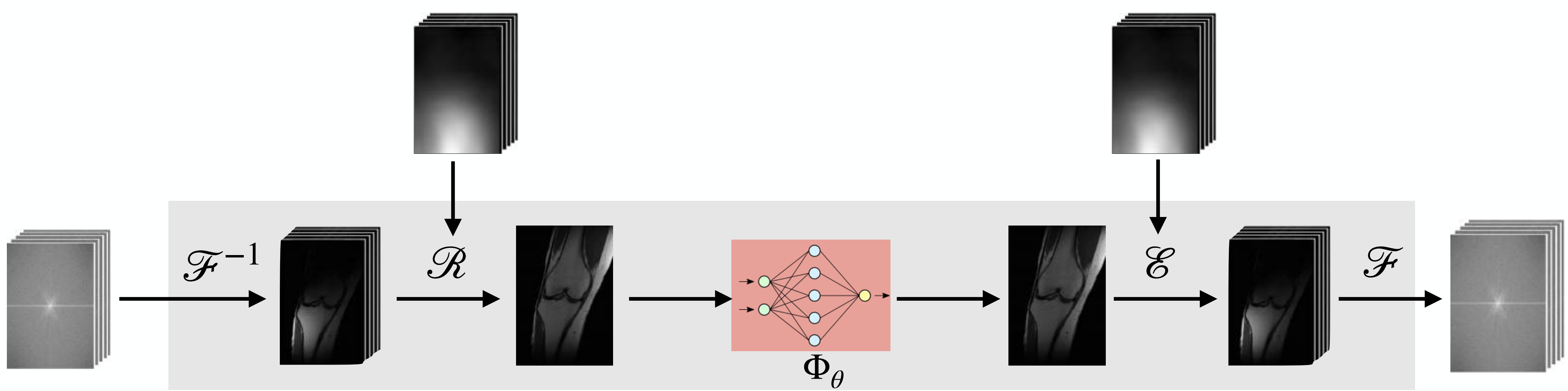

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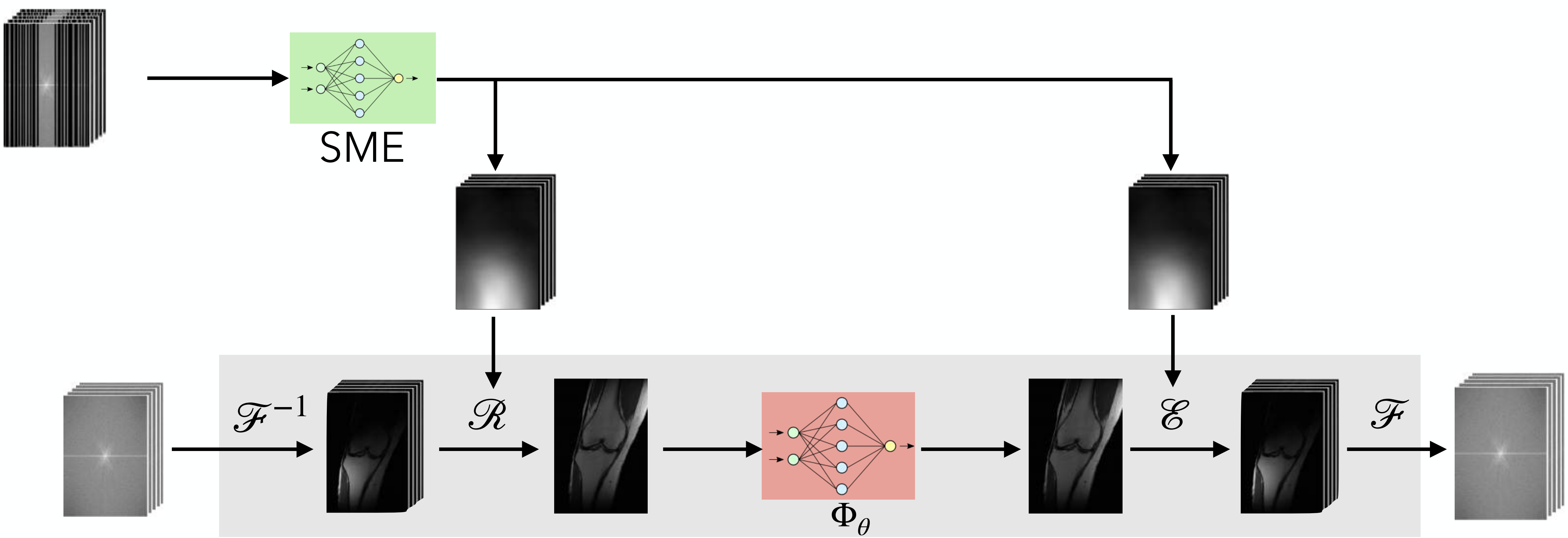

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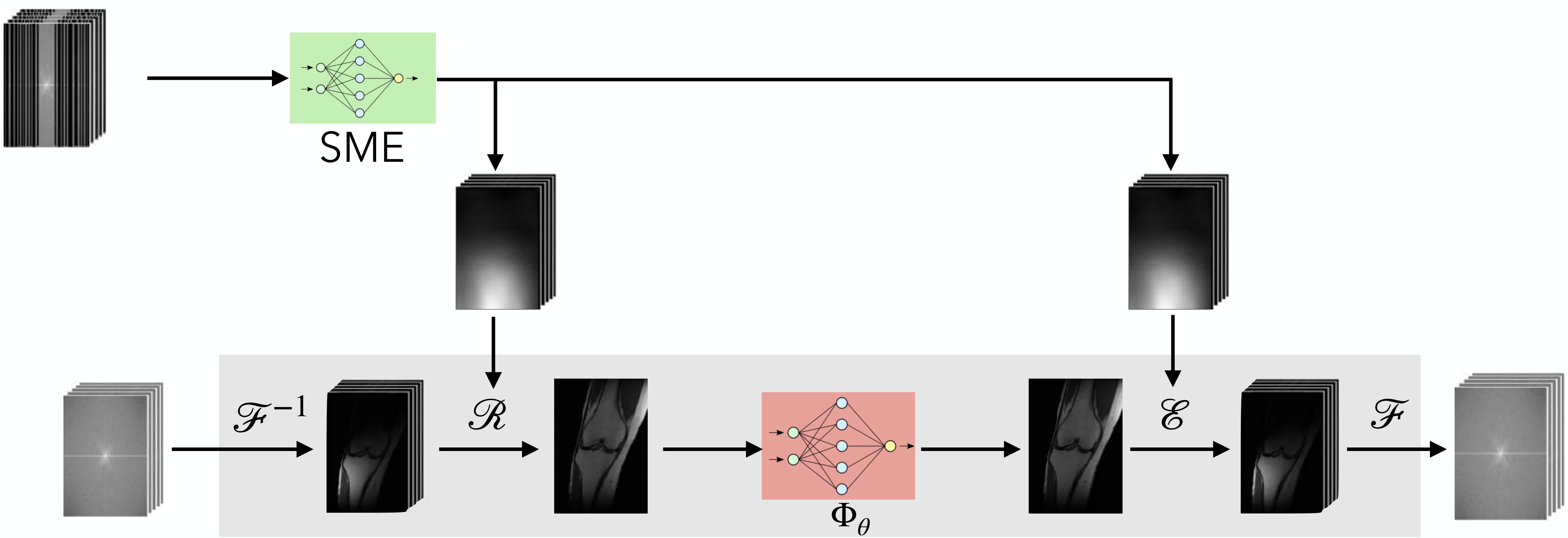

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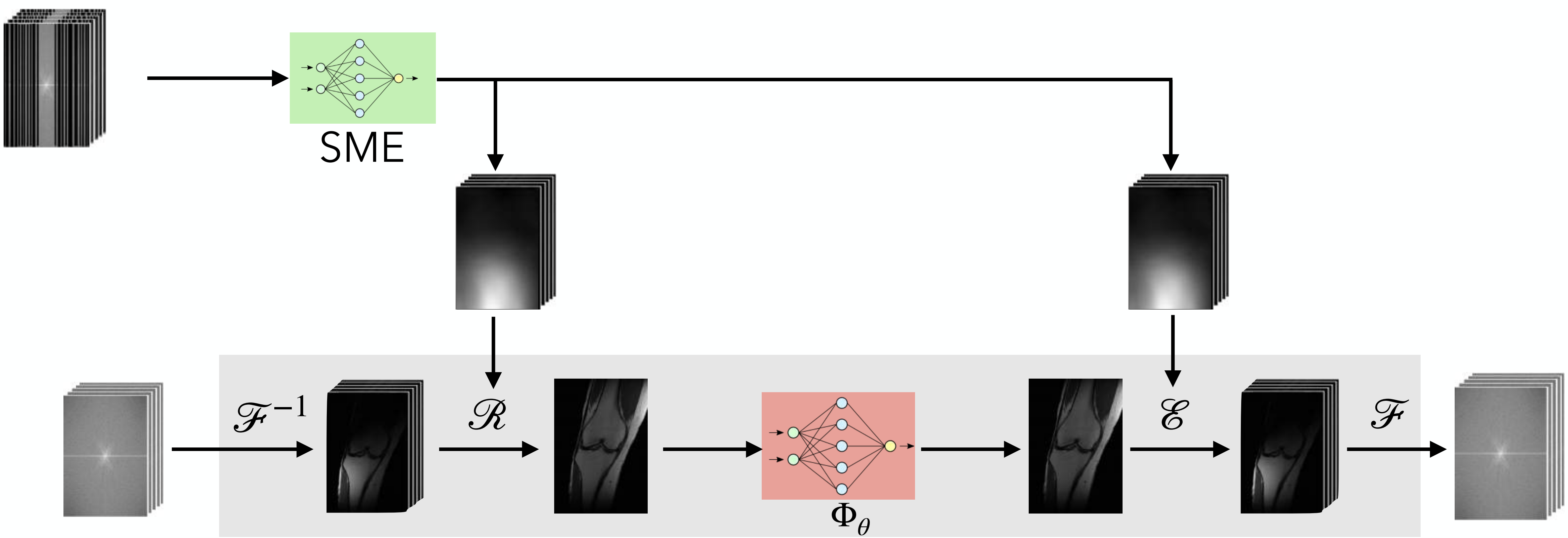

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Can we do better with modern architectures?

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Transformers?

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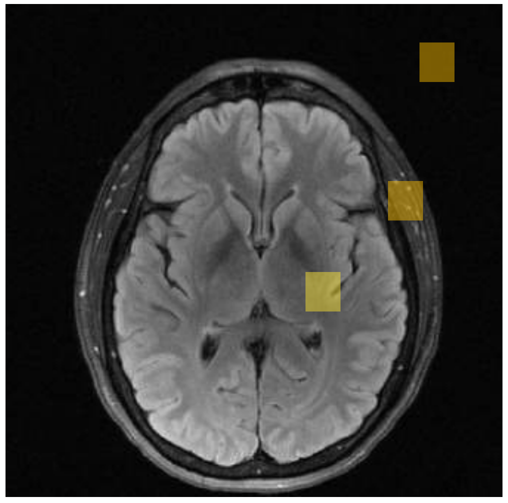
  - conv kernels are content-independent



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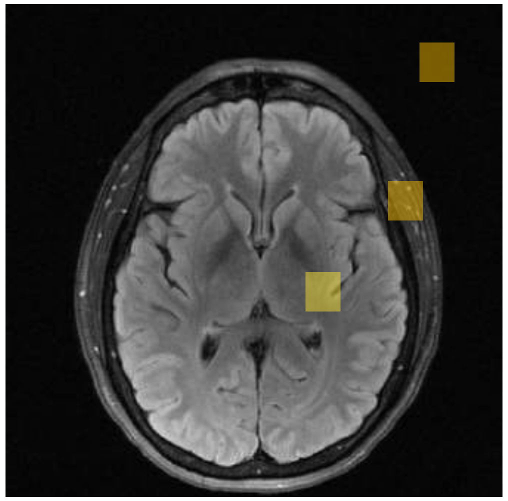

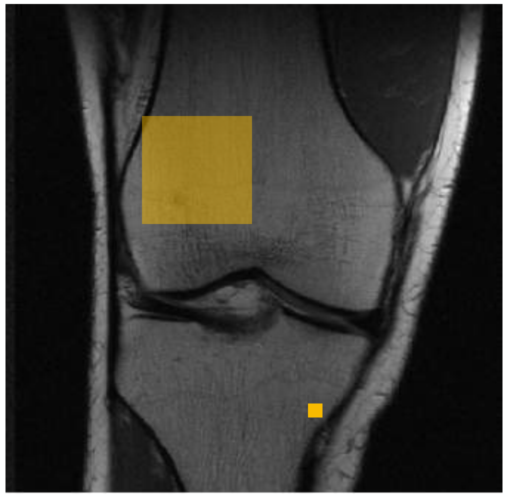

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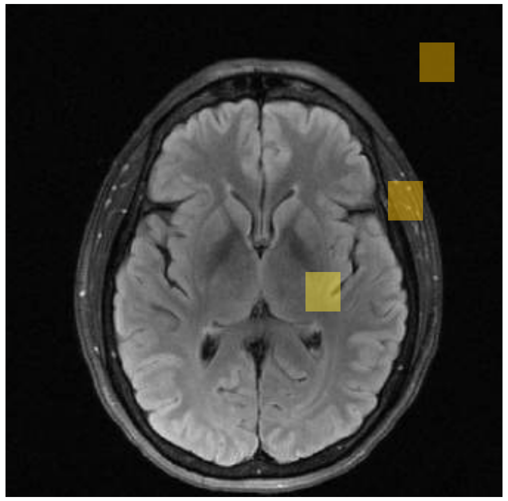

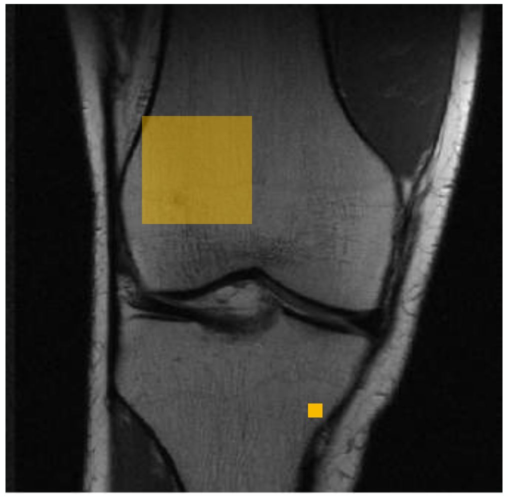

- Self-attention mechanism

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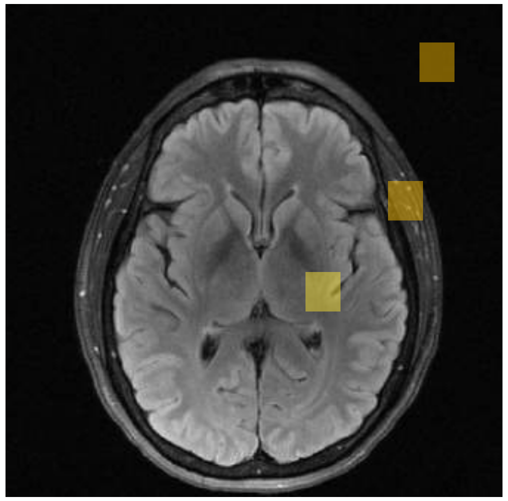
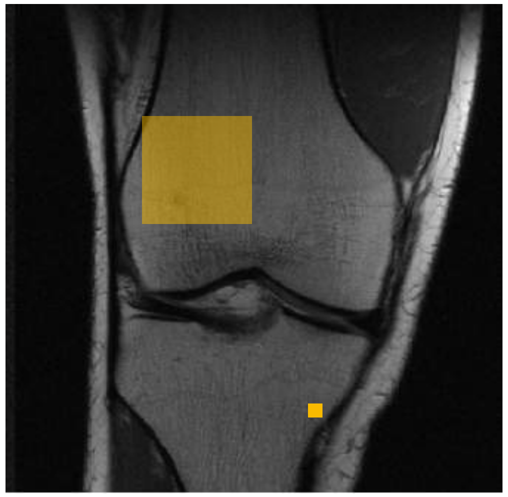
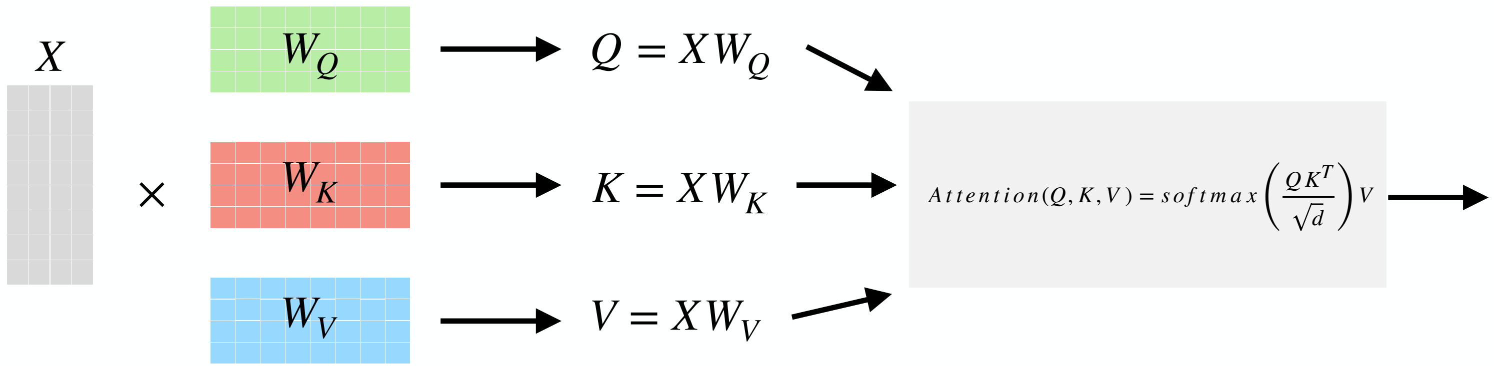


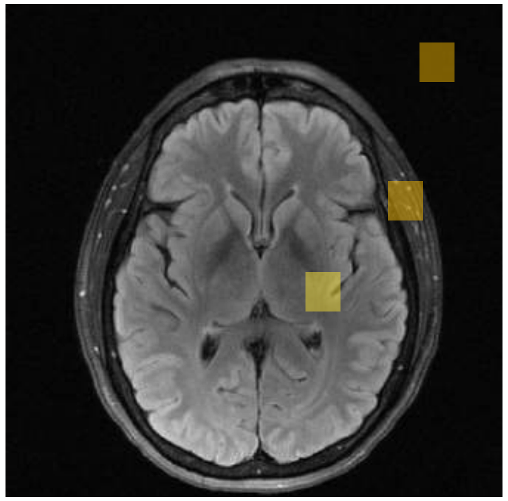


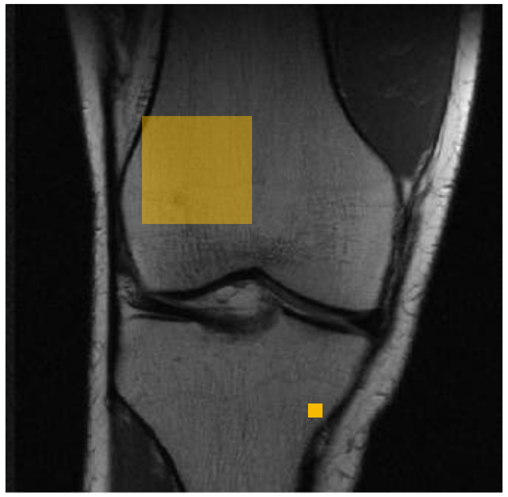
- Self-attention mechanism



Transformers?

- Benefits of Transformers
  - conv kernels are content-independent
  - conv is not efficient for long-range dependency modelling





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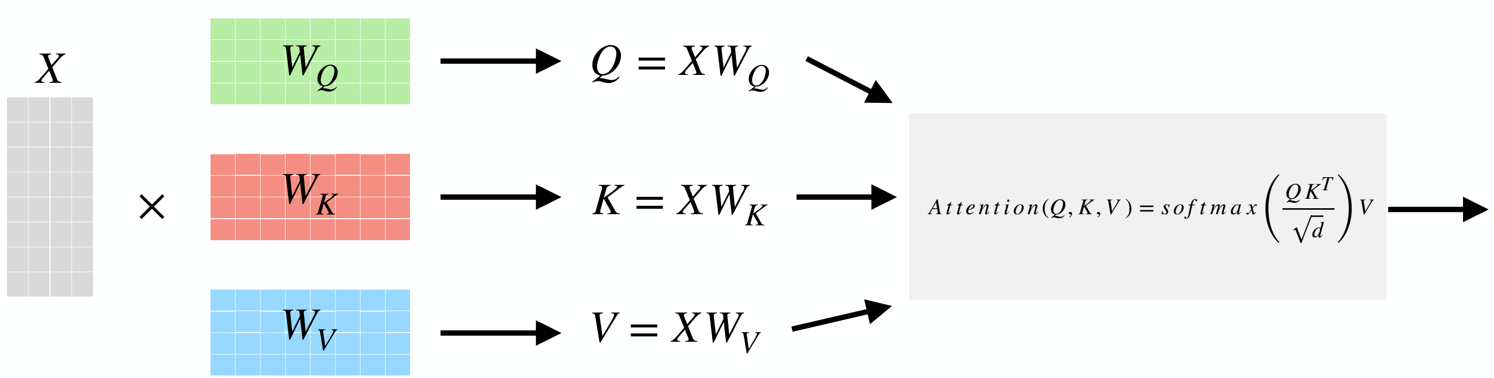

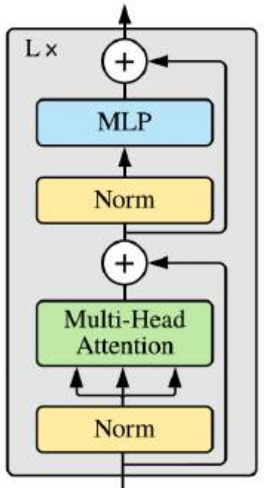

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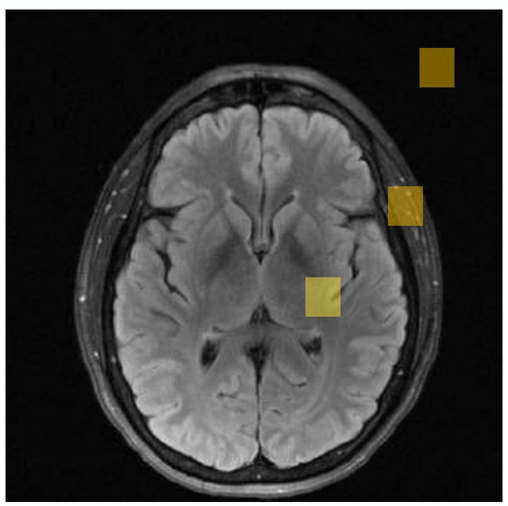

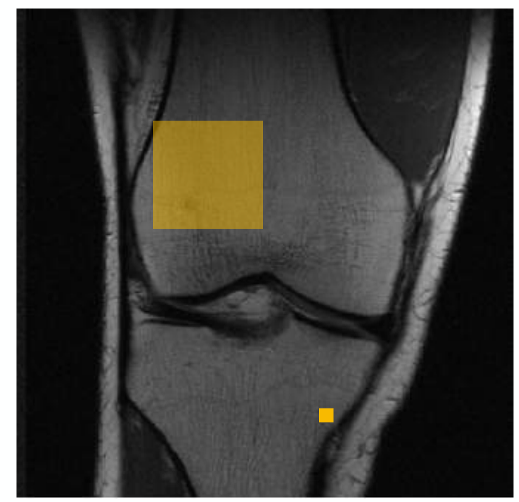

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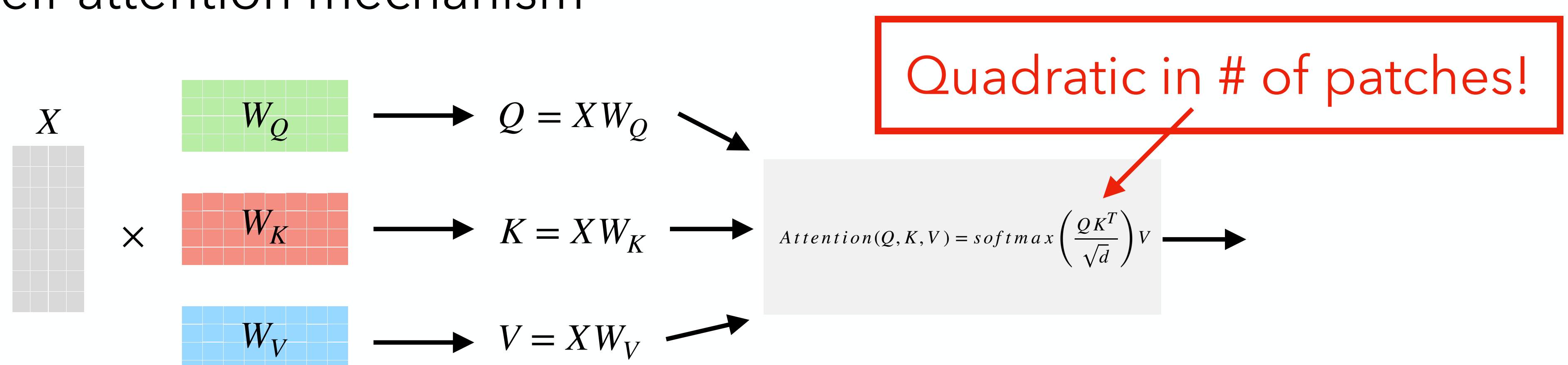
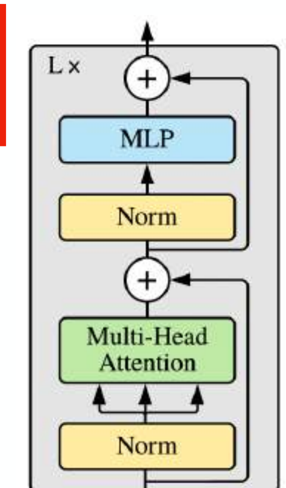
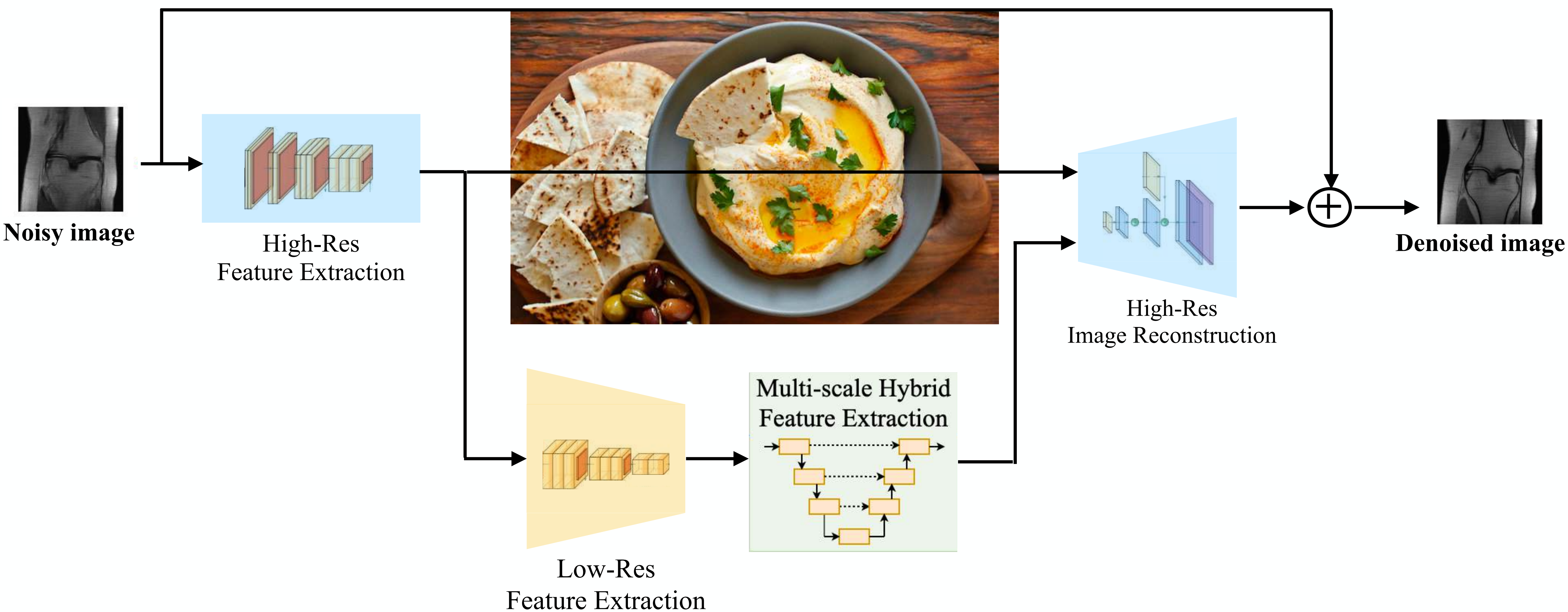




HUMUS-Net

Hybrid Unrolled Multi-scale Network Architecture for Accelerated MRI Reconstruction



HUMUS-Net Experiments

fastMRI multi-coil knee, 8x acceleration

Model	Test SSIM	Test PSNR

HUMUS-Net Experiments

fastMRI multi-coil knee, 8x acceleration

Model	Test SSIM	Test PSNR
E2E-VarNet	0.8920	37.1

HUMUS-Net Experiments

fastMRI multi-coil knee, 8x acceleration

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fastMRI multi-coil knee, 8x acceleration

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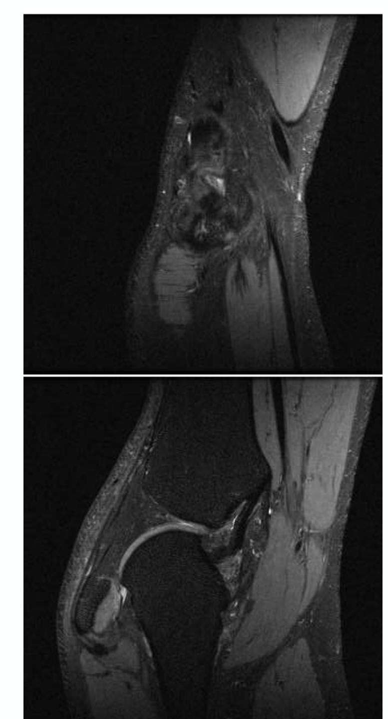
Stanford3D multi-coil knee, 8x acceleration

Model	Val. SSIM	Val. PSNR



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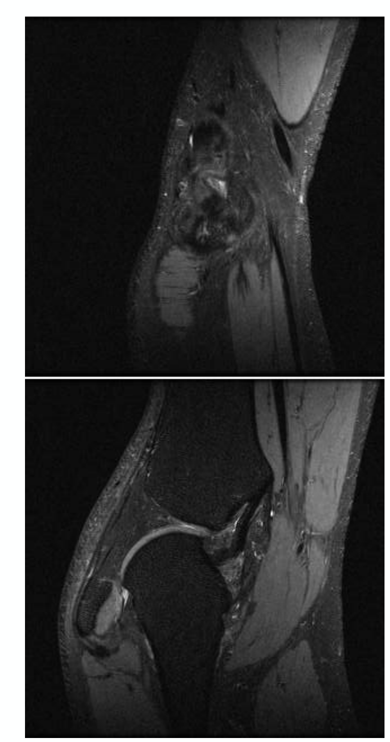
Stanford3D multi-coil knee, 8x acceleration

Model	Val. SSIM	Val. PSNR
E2E-VarNet	0.9432 (±0.0063)	39.99 (± 0.6144)



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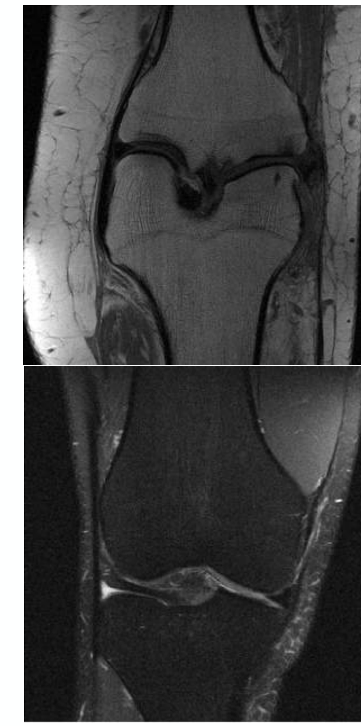

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Model	Val. SSIM	Val. PSNR
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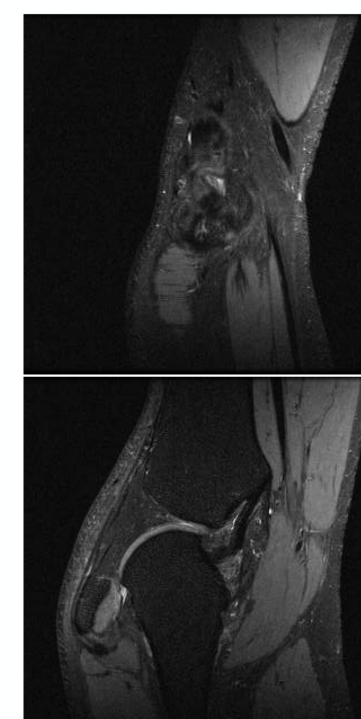

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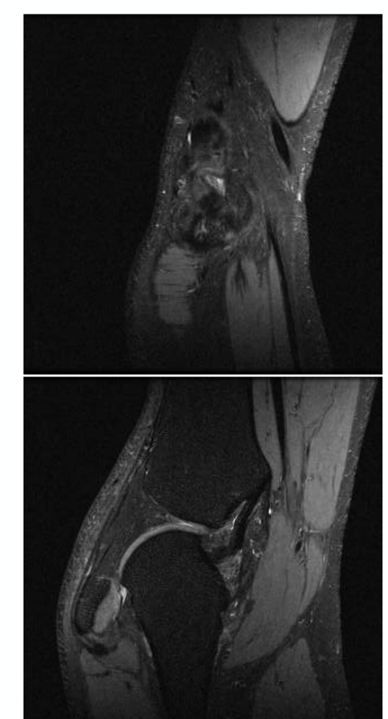
HUMUS-Net 2/23/2022	8x	0.0086	0.8936
fastMRI Repo End-to-End VarNet 11/11/2020	8x	0.0085	0.8920
SubtleMR 6/23/2020	8x	0.0085	0.8919
Deneme4 10/7/2021	8x	0.0085	0.8919



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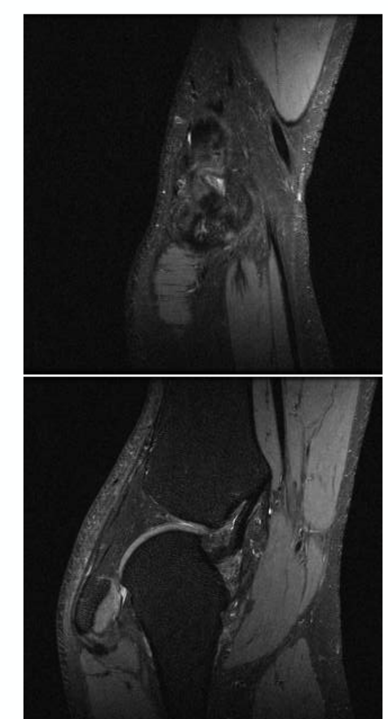
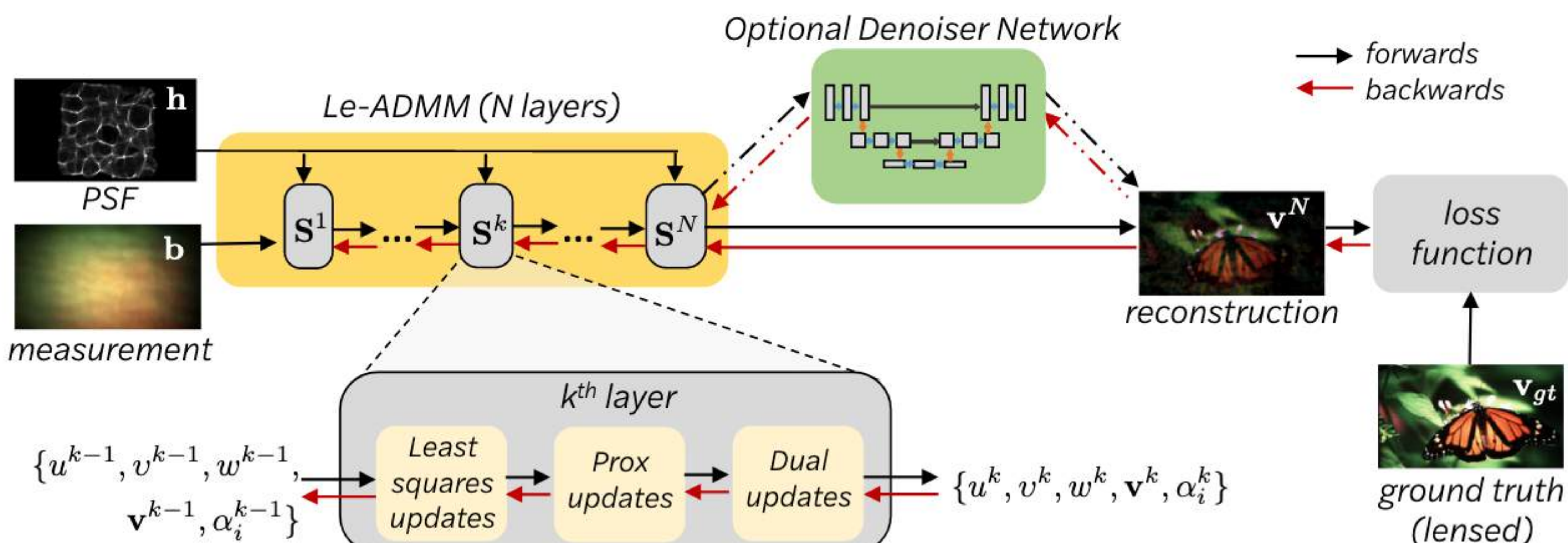


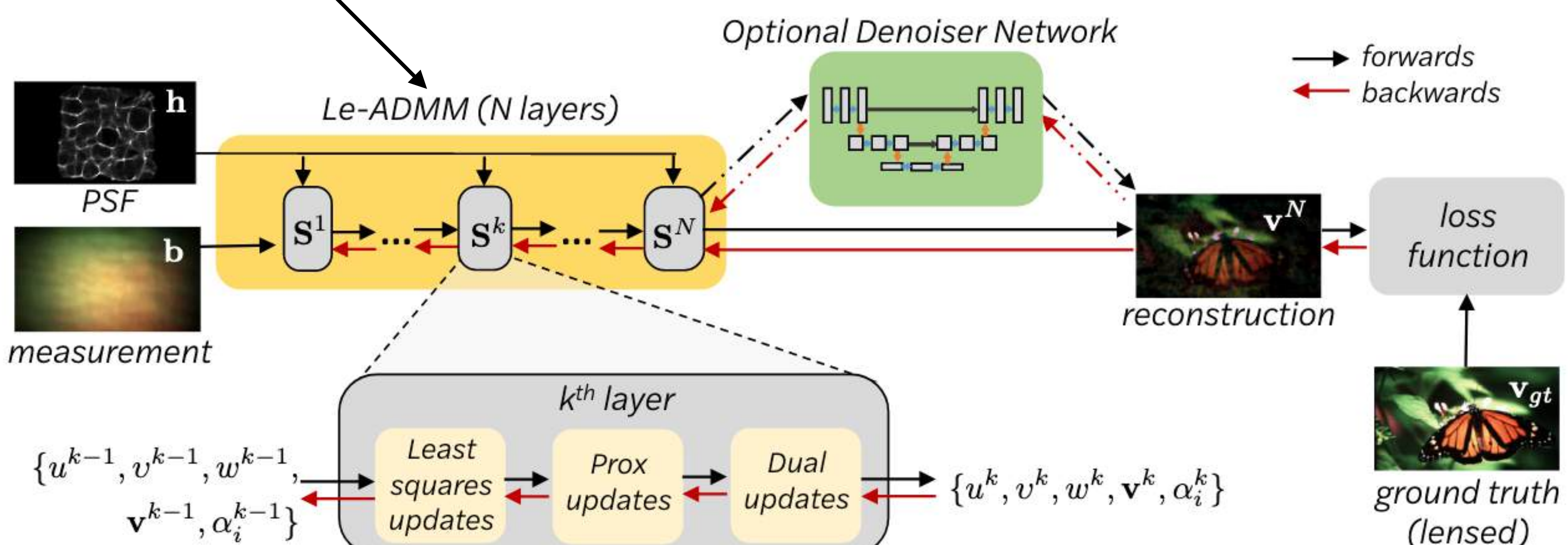
Deep Unrolling in lensless imaging



Monakhova, Kristina, et al. "Learned reconstructions for practical mask-based lensless imaging." *Optics express* 27.20 (2019): 28075-28090.

Deep Unrolling in lensless imaging

Learned (unrolled) ADMM



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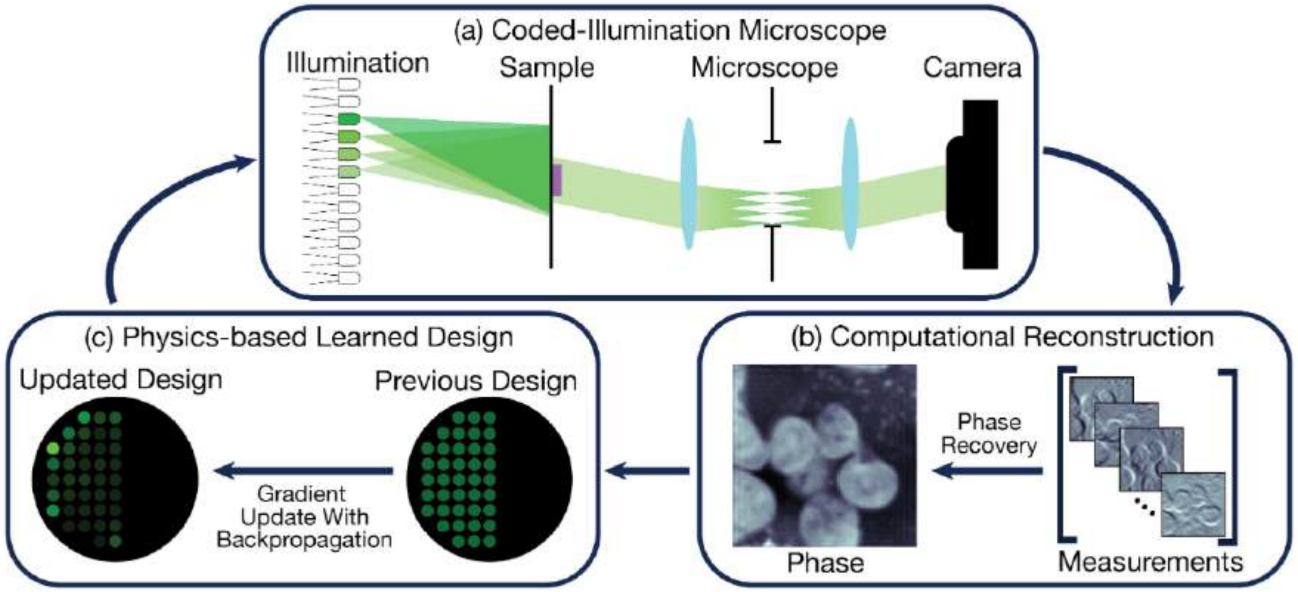
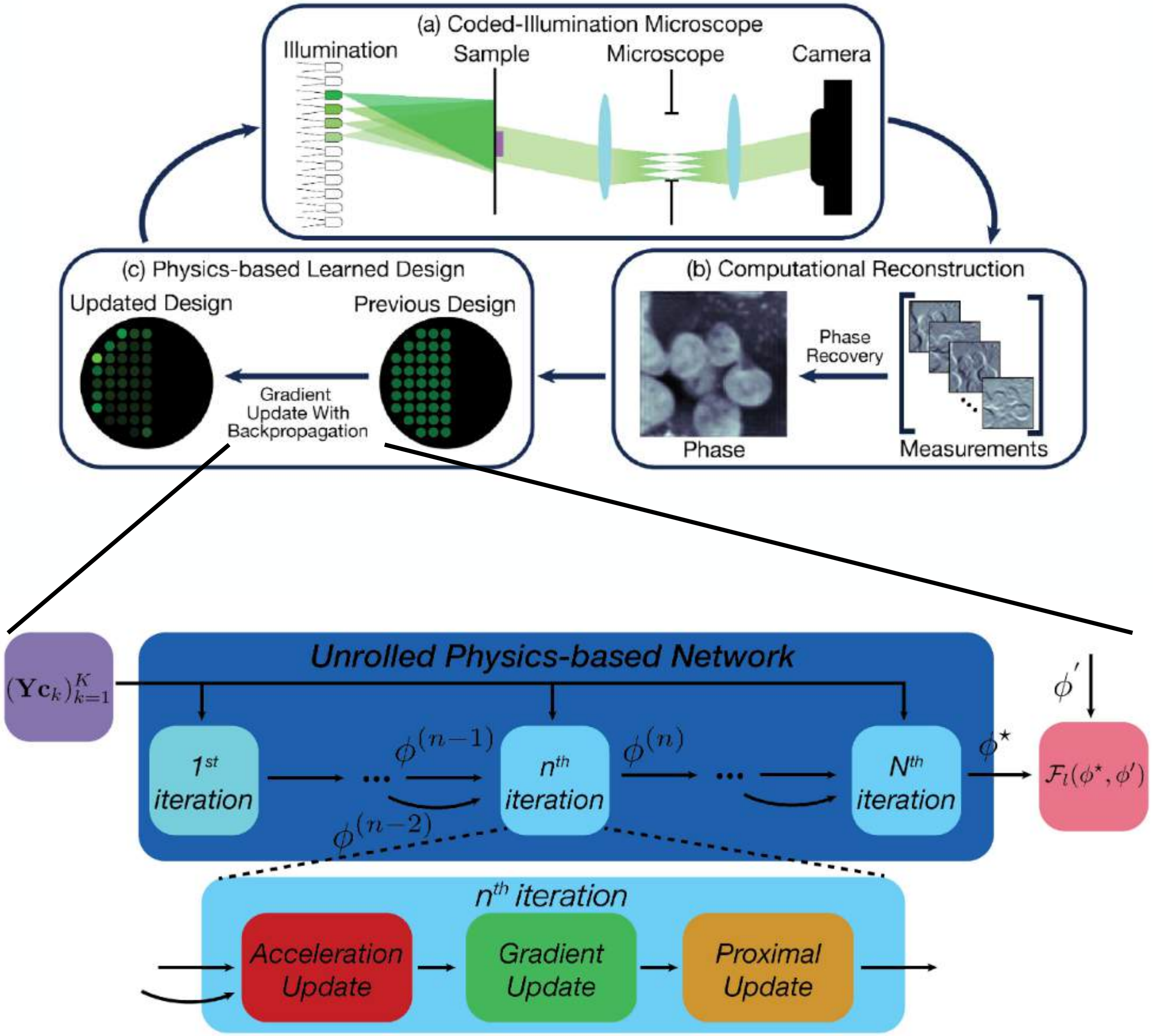
Deep unrolling in coded illumination pattern design



Kellman, M. R., Bostan, E., Repina, N. A., & Waller, L. (2019). Physics-based learned design: optimized coded-illumination for quantitative phase imaging. *IEEE Transactions on Computational Imaging*, *5*(3), 344-353.

Deep unrolling in coded illumination pattern design



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The Neumann Network

- Linear inverse problem formulation

$$\hat{x} = arg \min_x \|Ax - y\|^2 + \mathscr{R}(x)$$ and assume $$\mathscr{R}(x) = x^T R x$$

Gilton, D., Ongie, G. and Willett, R., 2019. Neumann networks for linear inverse problems in imaging. *IEEE Transactions on Computational Imaging*, *6*, pp.328-343.

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- Then the minimizer is

$$\hat{x} = (A^T A + R)^{-1} A^T y$$

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$$\boldsymbol{B}^{-1} = \eta \sum_{k=0}^{\infty} (\boldsymbol{I} - \eta \boldsymbol{B})^k$$

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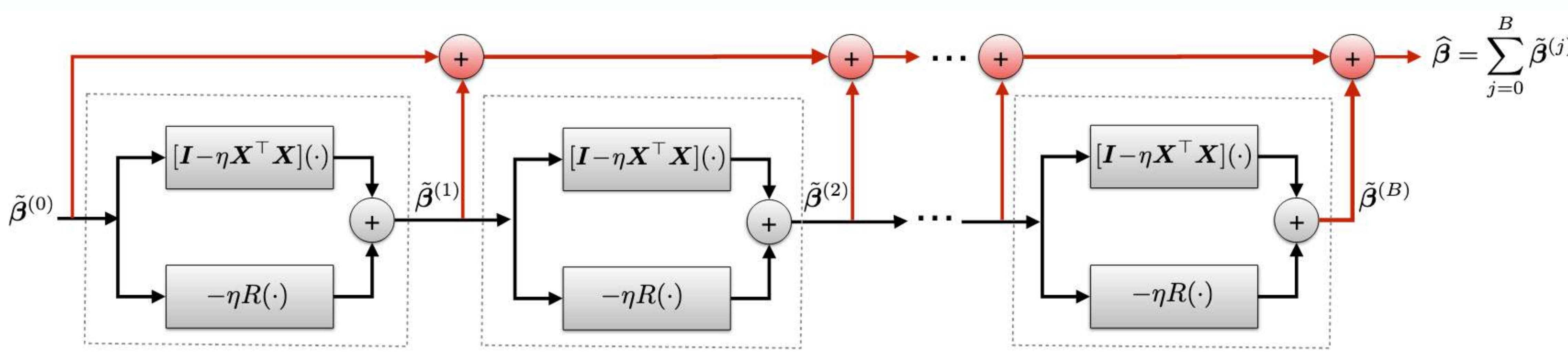

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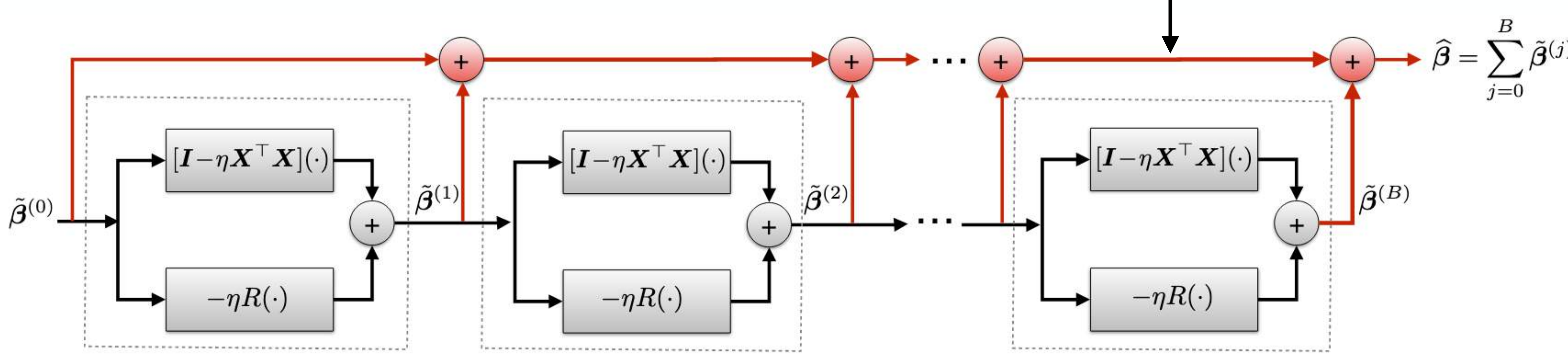
skip connections arise naturally!



Gilton, D., Ongie, G. and Willett, R., 2019. Neumann networks for linear inverse problems in imaging. *IEEE Transactions on Computational Imaging*, *6*, pp.328-343.

Diffusion Models

(Many slides stolen from Arash Vahdat and collaborators see refs at the end)

Text-to-Image Models

Text-to-Image Models

DALL·E 2

OpenAI

Text-to-Image Models

Text-to-Image Models

DALL·E 2

OpenAI

Midjourney

Google

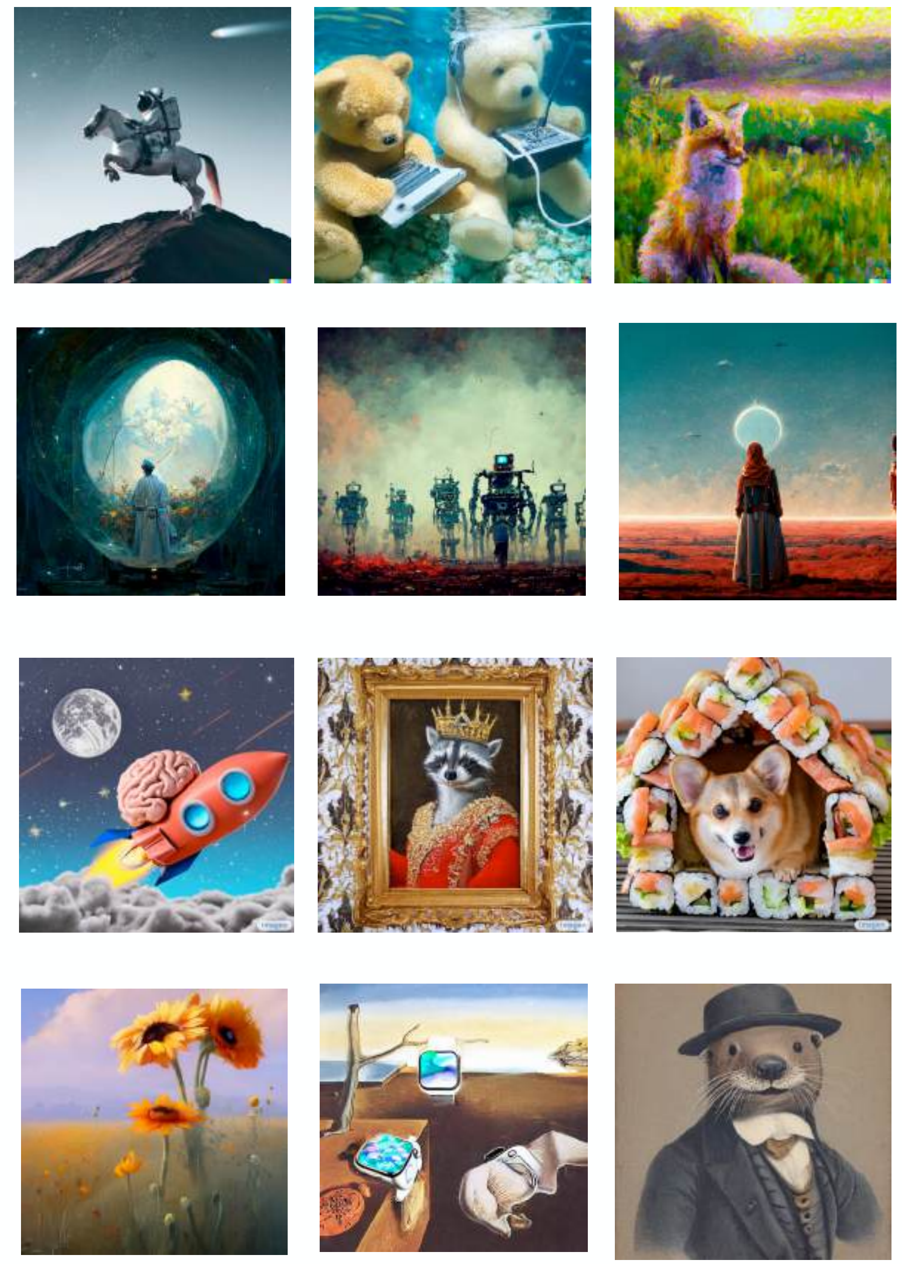
Text-to-Image Models

DALL·E 2

Midjourney

Imagen

Stable Diffusion



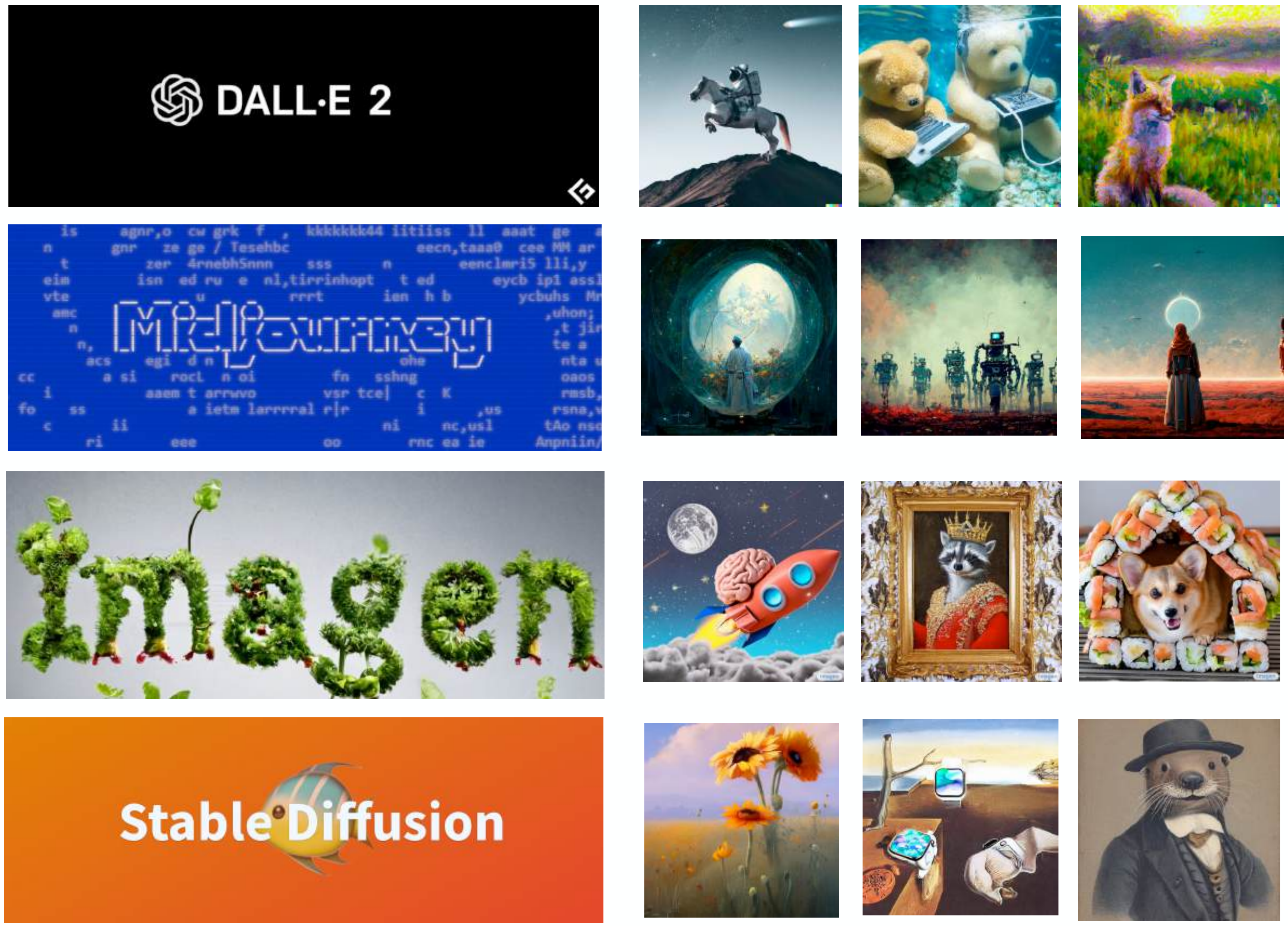
OpenAI

MIDJOURNEY AI

Google

stability.ai

Text-to-Image Models



OpenAI
MIDJOURNEY AI
Google
stability.ai

- What made this possible? Two key advances:
  - CLIP
  - Powerful generative models (diffusion)

Denoising Diffusion Probabilistic Models

$x_0 \sim q(x)$

real data distribution

Denoising Diffusion Probabilistic Models

$\cdots$

$x_0 \sim q(x)$

real data distribution

x_{t-1}

Denoising Diffusion Probabilistic Models

$x_0 \sim q(x)$

real data distribution

$\cdots$

x_{t-1}

x_t

Denoising Diffusion Probabilistic Models

$x_0 \sim q(x)$

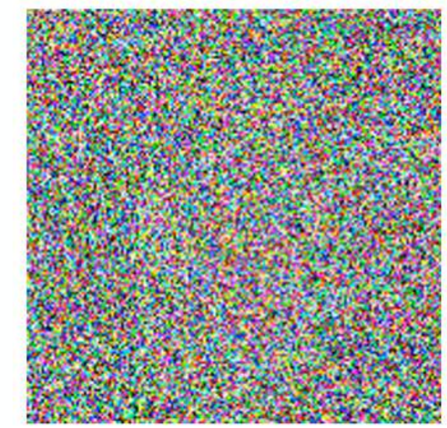
real data distribution

…

x_{t-1}

x_t

…



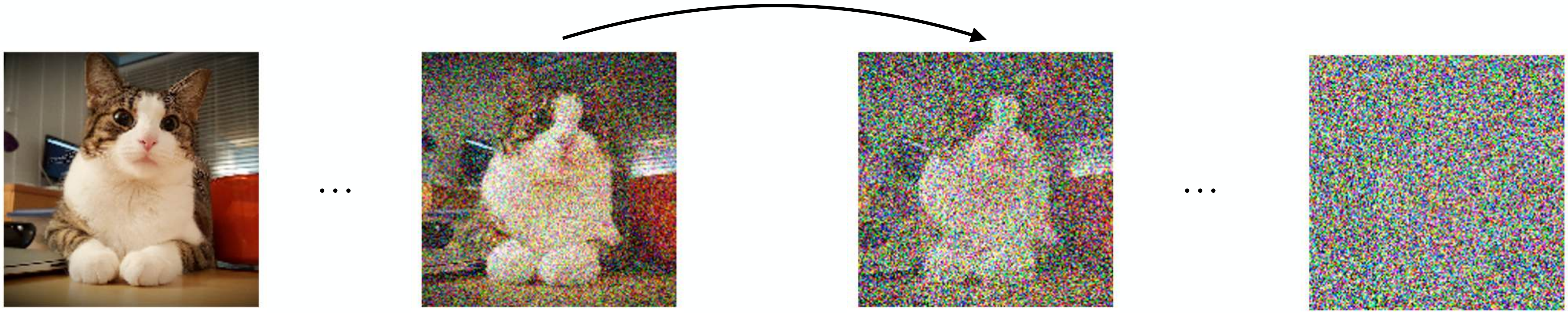
x_T

noise

Denoising Diffusion Probabilistic Models

forward diffusion process

$q(x_t | x_{t-1})$



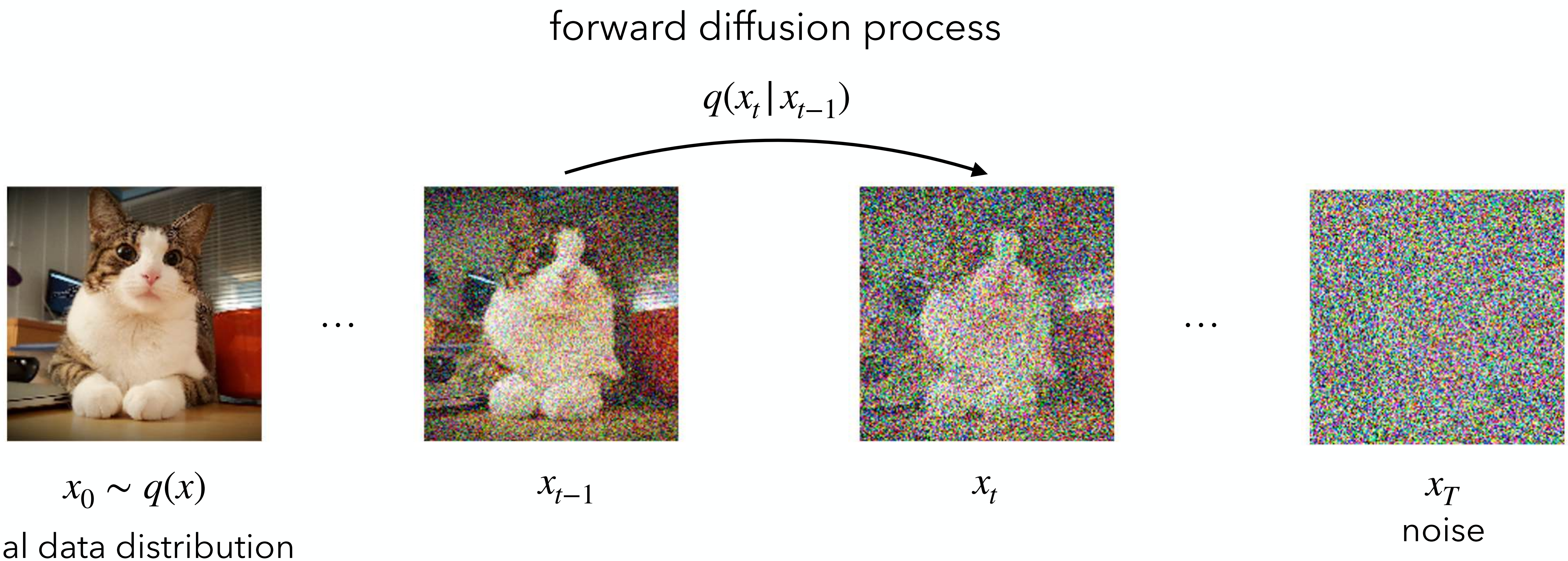
$x_0 \sim q(x)$
real data distribution

x_{t-1}

x_t

x_T
noise

Denoising Diffusion Probabilistic Models

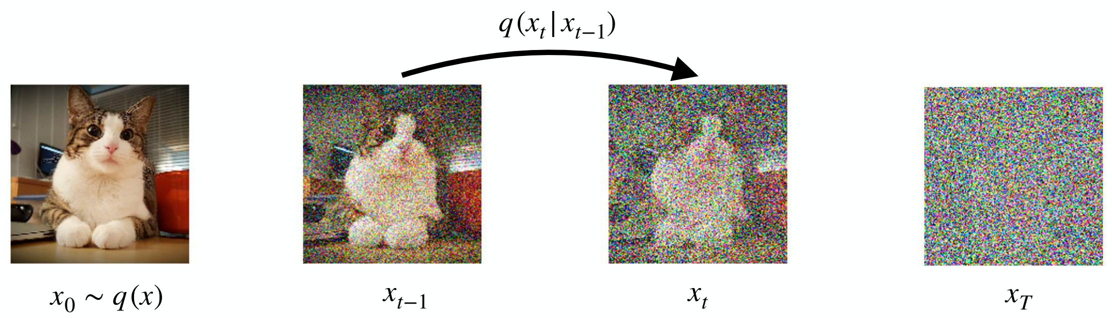


Forward diffusion process

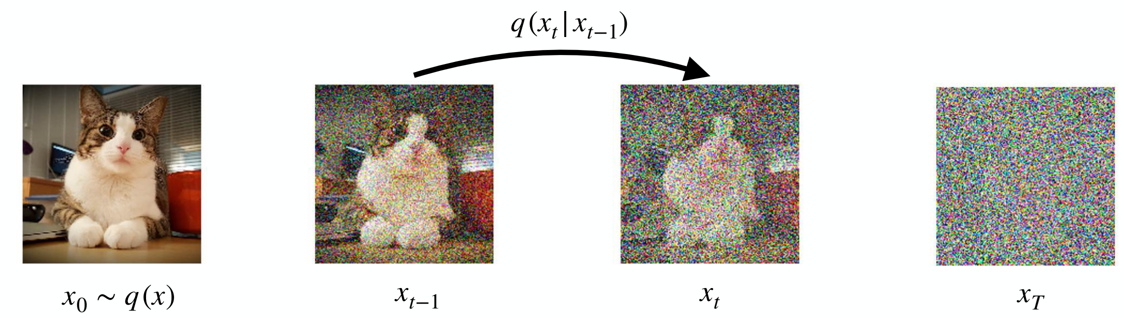
$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I) \qquad q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$

variance schedule: $\{\beta_t \in (0,1)\}_{t=1}^{T}$

Forward sampling



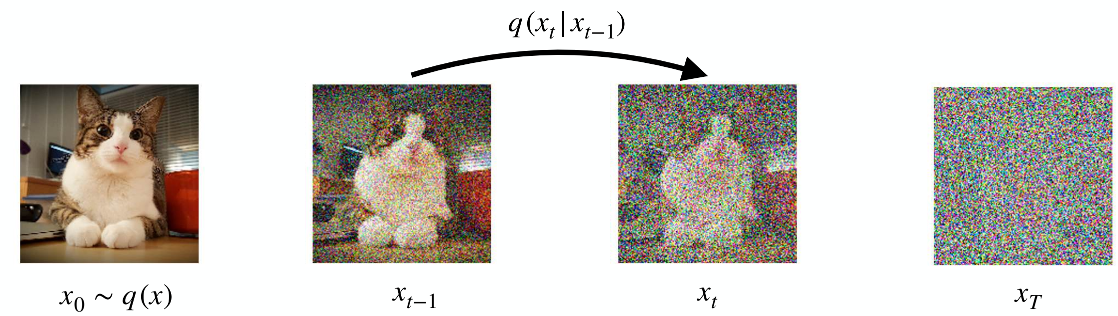
Forward sampling



- Reparametrization trick

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t\,; \sqrt{1-\beta_t}x_{t-1}, \beta_t I) \longrightarrow x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1}, \;\; \epsilon_{t-1} \sim \mathcal{N}(0,I)$$

Forward sampling



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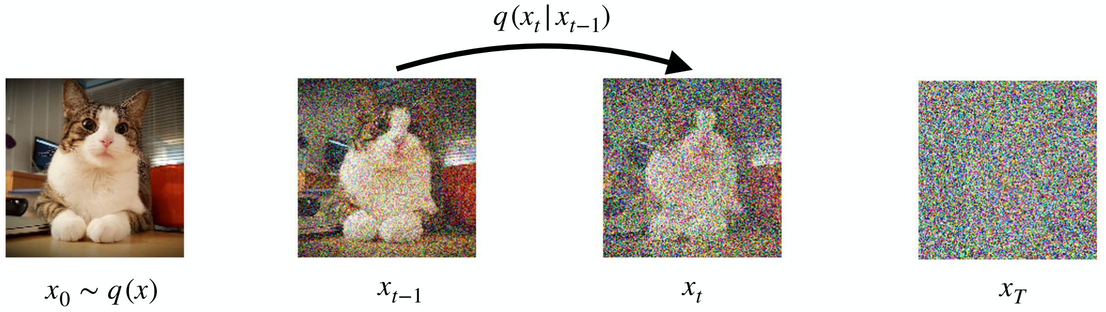
$$q(x_t|x_{t-1}) = \mathcal{N}(x_t\,; \sqrt{1-\beta_t}x_{t-1}, \beta_t I) \longrightarrow x_t = \underbrace{\sqrt{1-\beta_t}}_{\text{deterministic variable}}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1},\ \ \epsilon_{t-1} \sim \mathcal{N}(0,I)$$

Forward sampling

- Reparametrization trick



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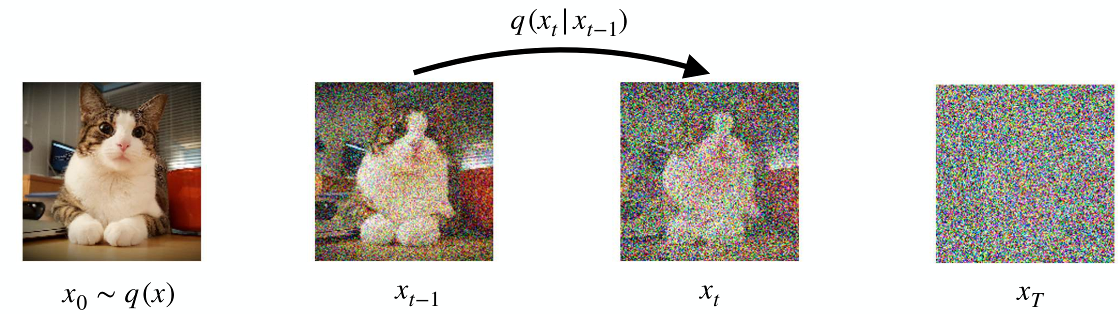
deterministic variable

aux. independent random variable

Forward sampling



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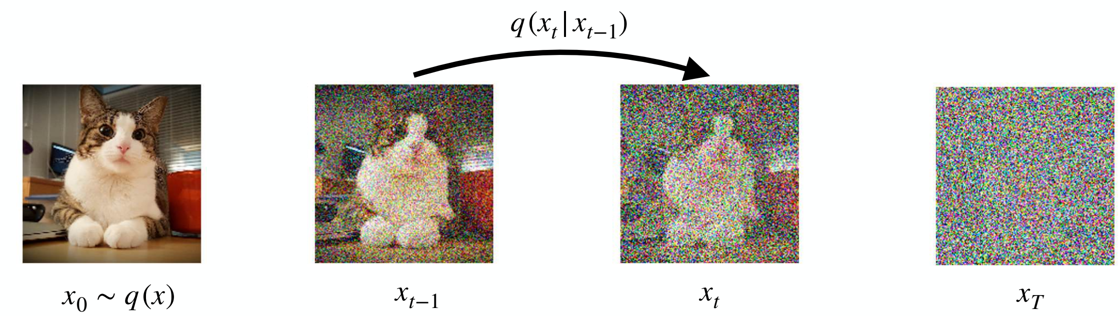
deterministic variable

aux. independent random variable

$$x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1} := \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1}$$

Forward sampling



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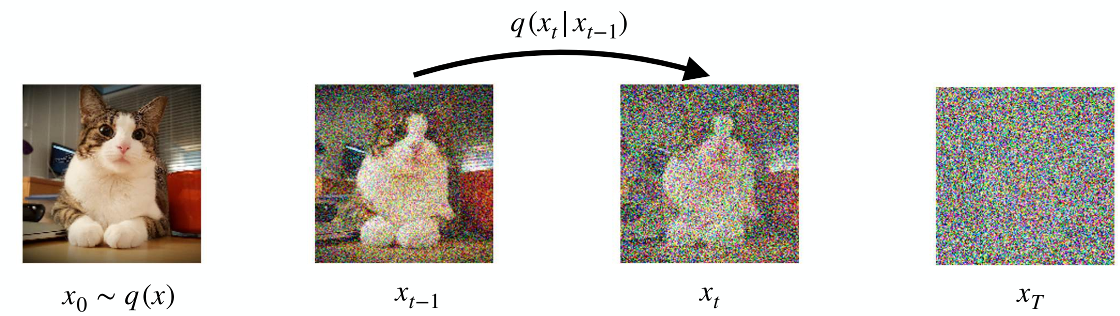
deterministic variable

aux. independent random variable

$$x_t = \sqrt{1-\beta_t} x_{t-1} + \sqrt{\beta_t} \epsilon_{t-1} := \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t} \epsilon_{t-1}$$
$$= \sqrt{\alpha_t} \sqrt{\alpha_{t-1}} x_{t-2} + \sqrt{\alpha_t} \sqrt{1-\alpha_{t-1}} \epsilon_{t-2} + \sqrt{1-\alpha_t} \epsilon_{t-1}$$

Forward sampling



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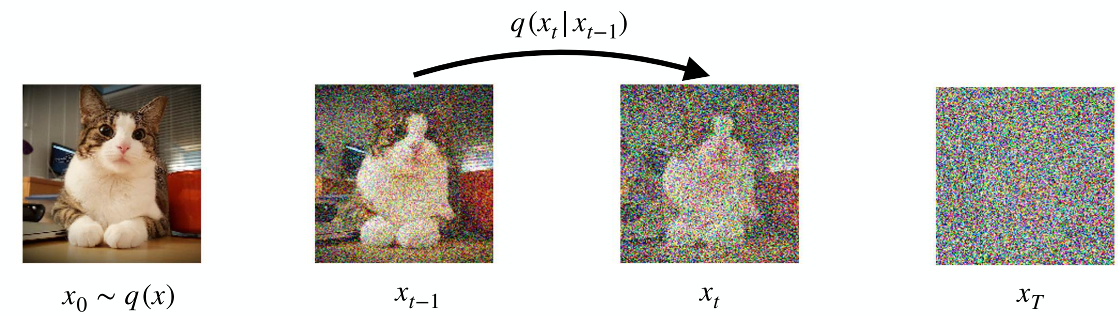
deterministic variable

aux. independent random variable

$$\begin{aligned} x_t &= \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1} := \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\epsilon_{t-2} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\epsilon}_{t-2} \end{aligned}$$

Forward sampling



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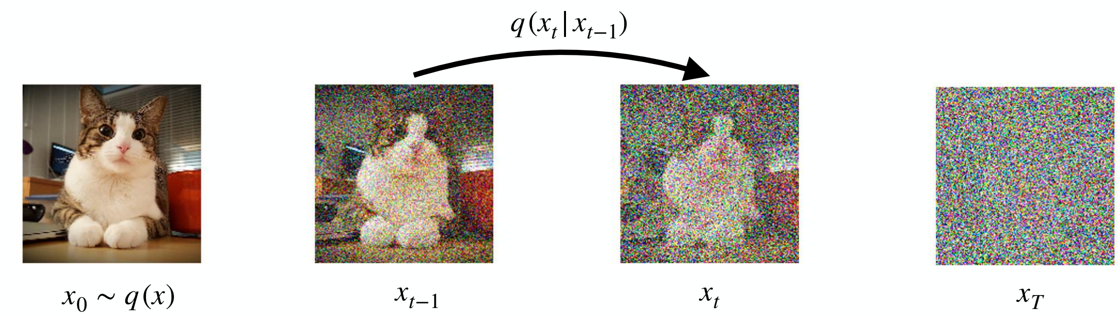
$$\begin{aligned} x_t &= \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1} := \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\epsilon_{t-2} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\epsilon}_{t-2} \quad = \ldots = \sqrt{\alpha_t\alpha_{t-1}\ldots\alpha_1}x_0 + \sqrt{1-\alpha_t\alpha_{t-1}\ldots\alpha_1}\bar{\epsilon} \end{aligned}$$

Forward sampling



- Reparametrization trick

$$q(x_t | x_{t-1}) = \mathcal{N}(x_t \,; \sqrt{1-\beta_t}x_{t-1}, \beta_t I) \longrightarrow x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1}, \;\; \epsilon_{t-1} \sim \mathcal{N}(0,I)$$

deterministic variable

aux. independent random variable

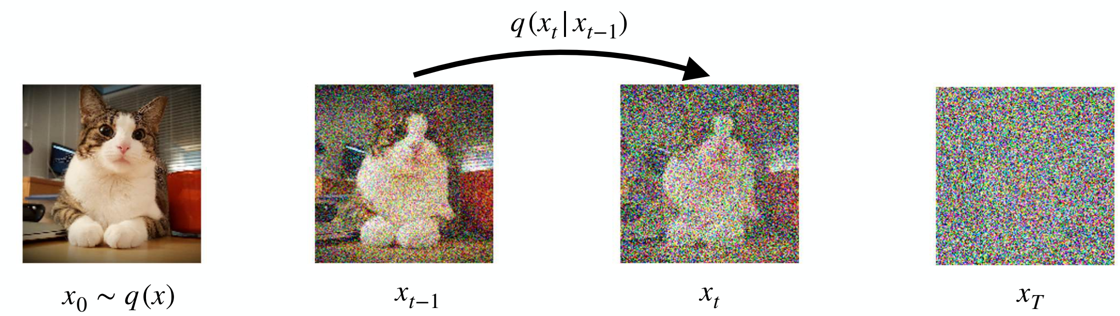
$$x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1} := \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1}$$

$$= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\epsilon_{t-2} + \sqrt{1-\alpha_t}\epsilon_{t-1}$$

$$= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\epsilon}_{t-2} \quad = \ldots = \sqrt{\alpha_t\alpha_{t-1}\ldots\alpha_1}x_0 + \sqrt{1-\alpha_t\alpha_{t-1}\ldots\alpha_1}\bar{\epsilon}$$

$$:= \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0,I)$$

Forward sampling



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$$\begin{aligned} x_t &= \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1} := \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\epsilon_{t-2} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\epsilon}_{t-2} \quad = \ldots = \sqrt{\alpha_t\alpha_{t-1}\ldots\alpha_1}x_0 + \sqrt{1-\alpha_t\alpha_{t-1}\ldots\alpha_1}\bar{\epsilon} \\ &:= \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0,I) \end{aligned}$$

Sampling from forward process at any t :

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0,I)$$

Reverse diffusion

"Creating noise from data is easy; creating data from noise is generative modeling."[1]

[1] Song, Y., Sohl-Dickstein, J., Kingma, D.P., Kumar, A., Ermon, S. and Poole, B., 2020. Score-based generative modeling through stochastic differential equations. *arXiv preprint arXiv:2011.13456*.

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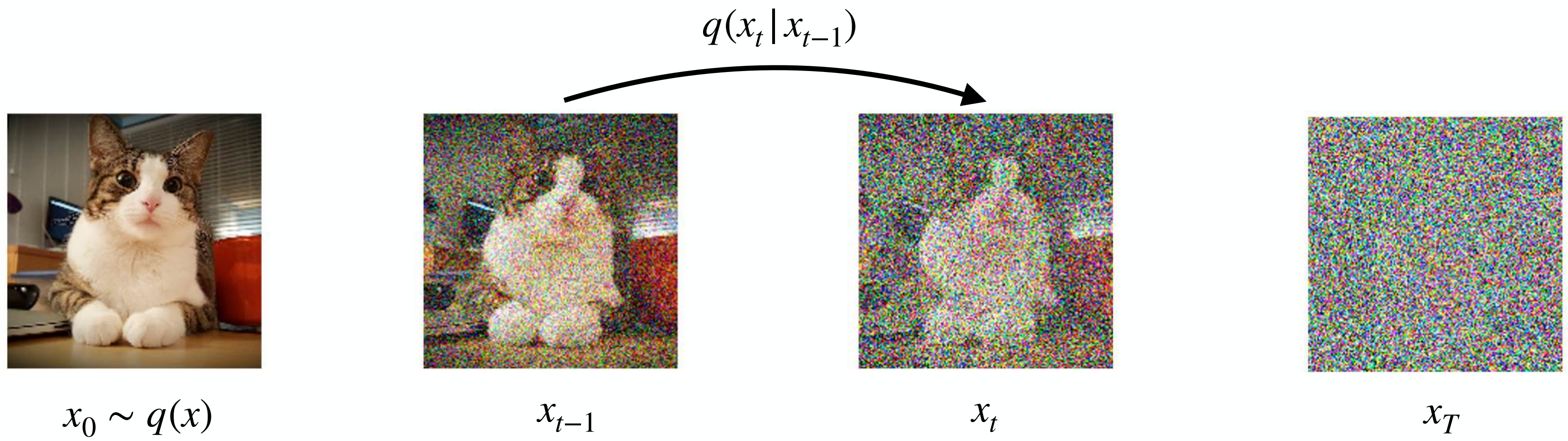

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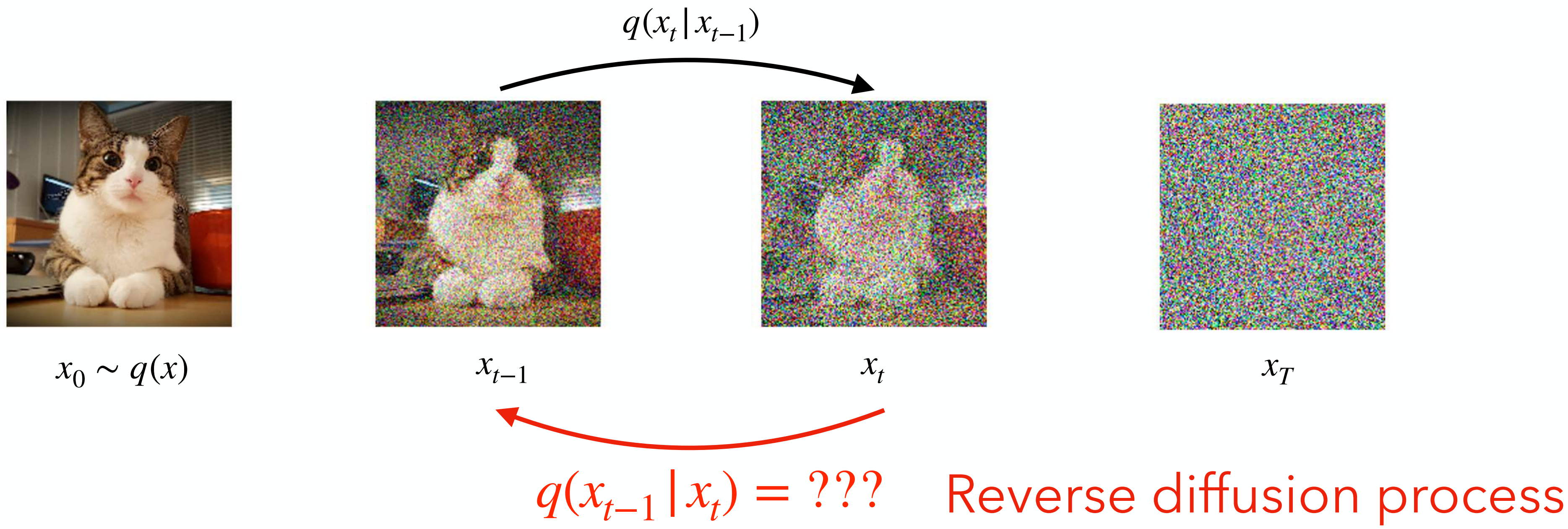

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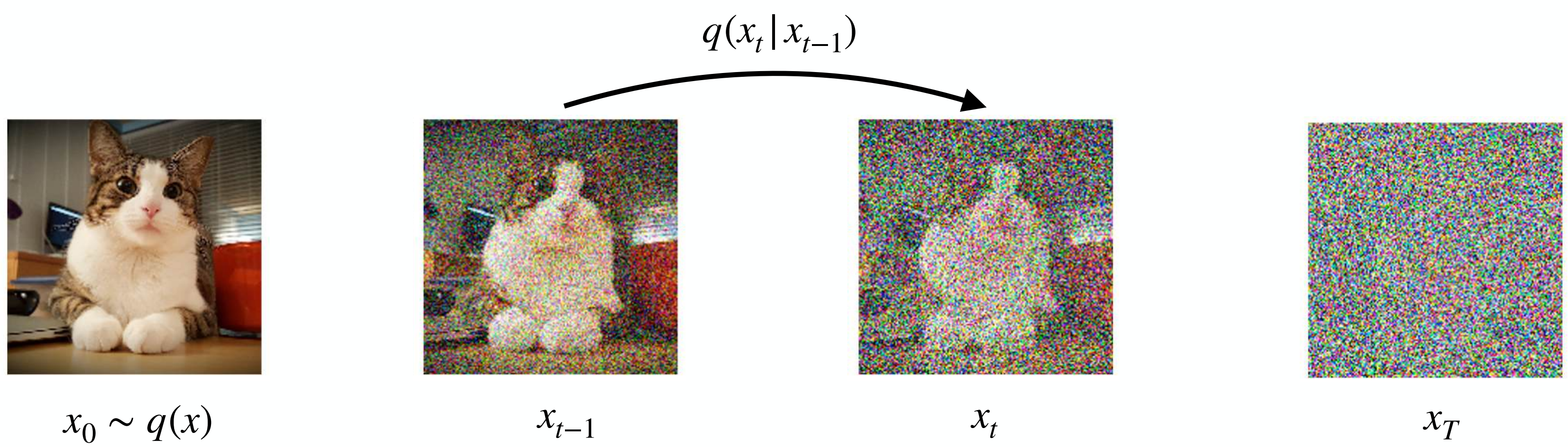

$q(x_{t-1}|x_t) = ???$ Reverse diffusion process

- If β_t is small, $q(x_{t-1}|x_t)$ is also Gaussian

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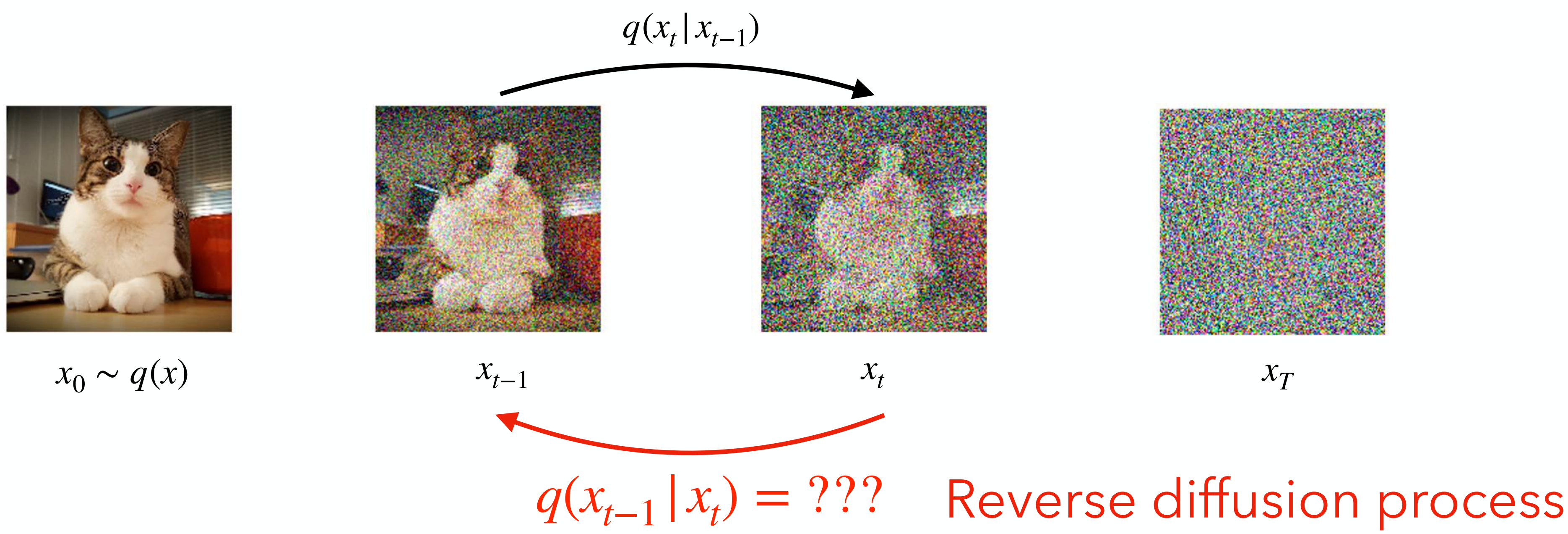

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- Estimating $q(x_{t-1} | x_t)$ is difficult, learn a model instead!

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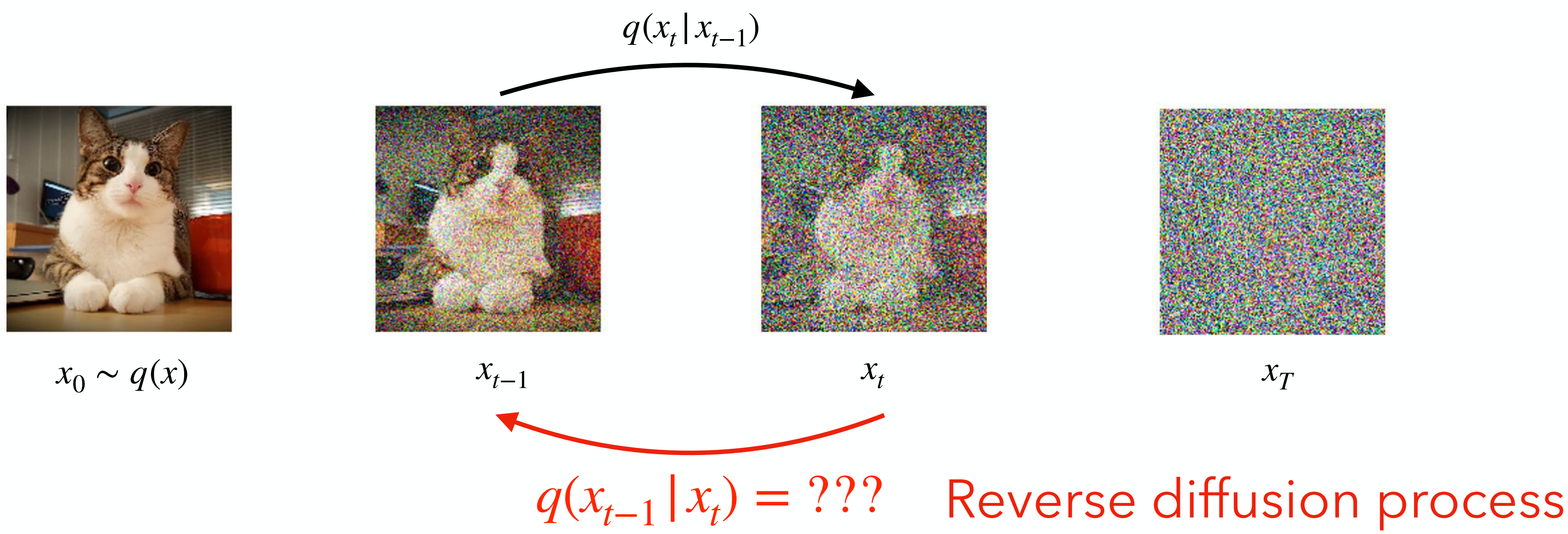

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Reverse diffusion process

$$p_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1};\ \mu_\theta(x_t, t),\ \Sigma_\theta(x_t, t)) \qquad p_\theta(x_{0:T}) = p_\theta(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} | x_t)$$

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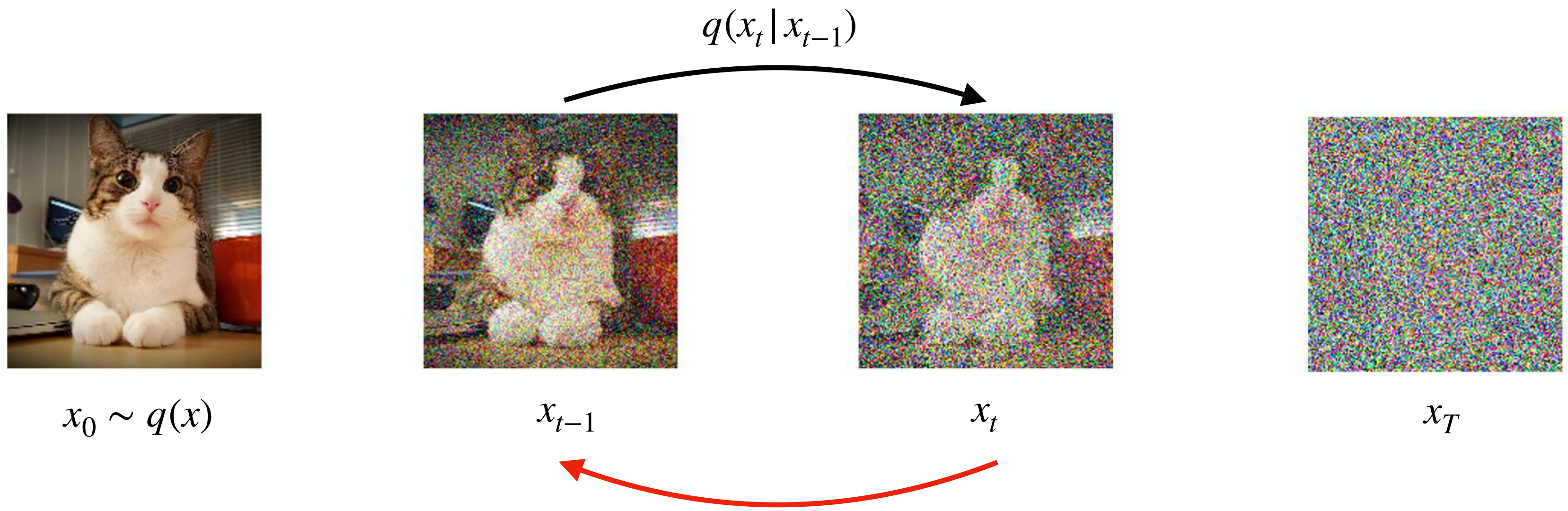

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How to learn p_θ ?

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Reverse conditional probability

- Reverse conditional probability is tractable

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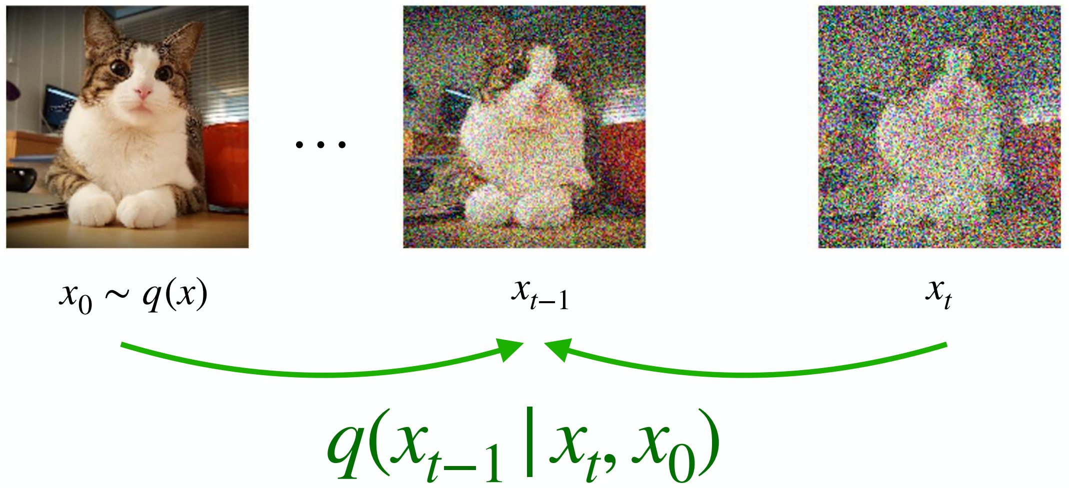

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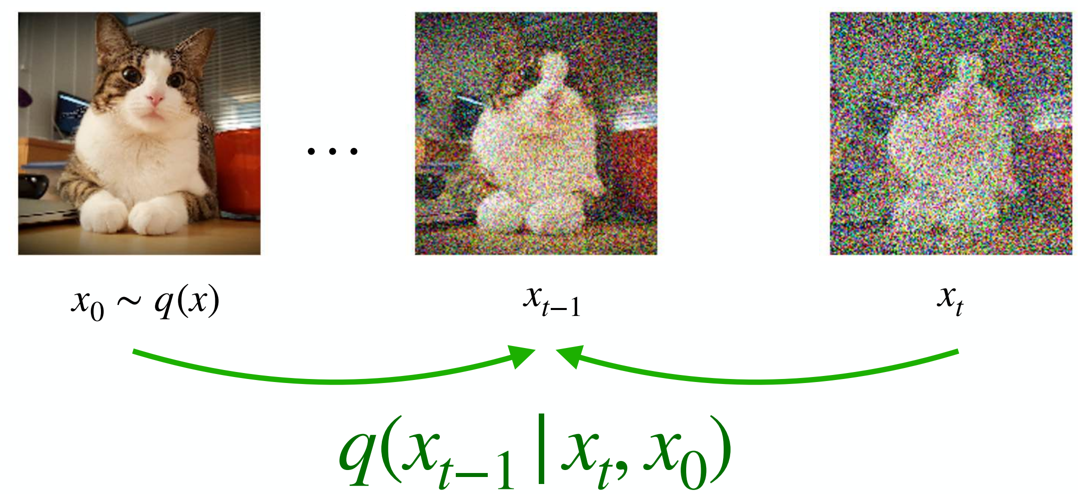
- Reverse conditional probability is tractable

$$q(x_{t-1} | x_t, x_0) = \frac{q(x_t | x_{t-1}, x_0)\ q(x_{t-1} | x_0)}{q(x_t | x_0)}$$



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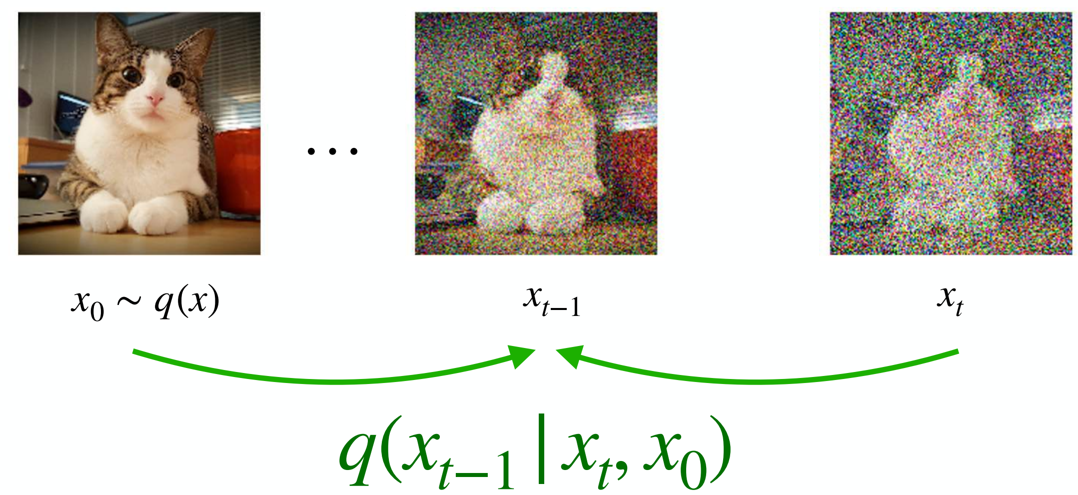

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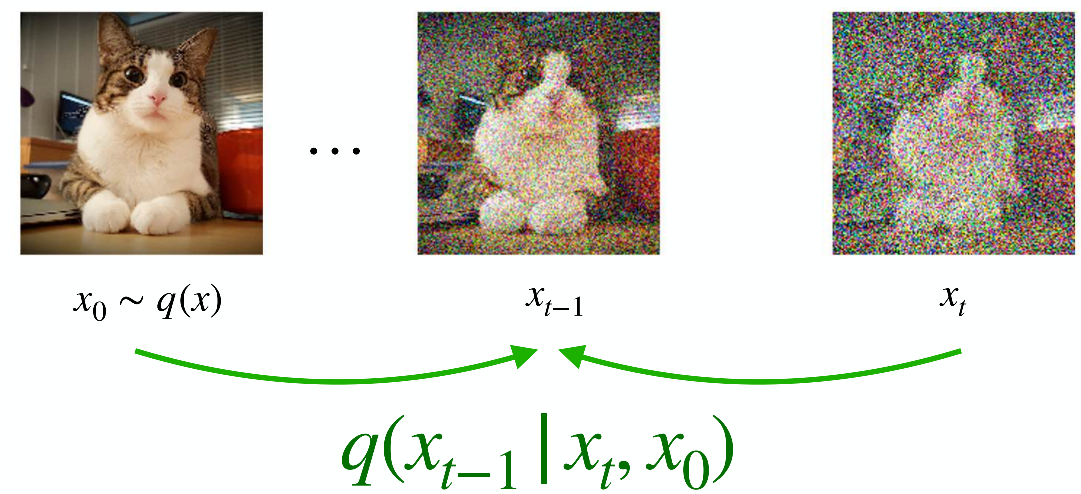

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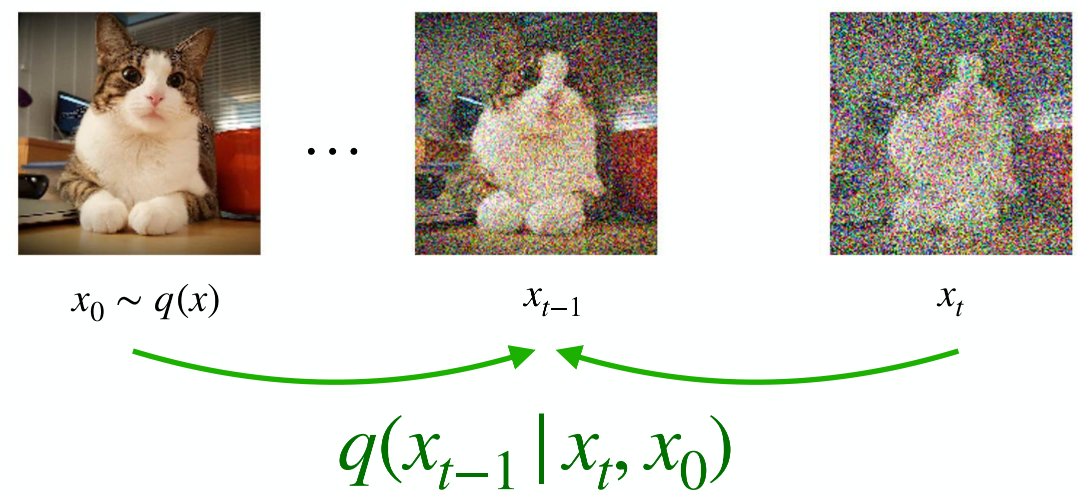

- Reverse process:

$$p_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1};\ \mu_\theta(x_t, t),\ \Sigma_\theta(x_t, t))$$

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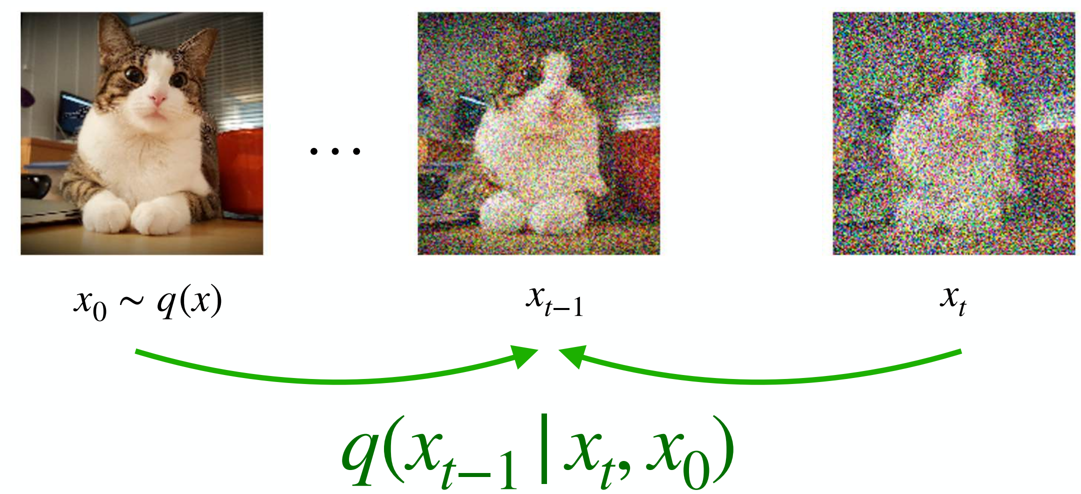

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Putting it all together

- Training

$$L_{simple} = \mathbb{E}_{t\sim[1,T],x_0,\epsilon_t}\left[\|\epsilon_t - \epsilon_\theta\left(\sqrt{\bar{\alpha}_t}x_o + \sqrt{1-\bar{\alpha}_t}\epsilon_t, t\right)\|^2\right]$$

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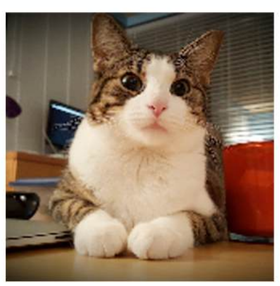
$x_0 \sim q(x)$ 

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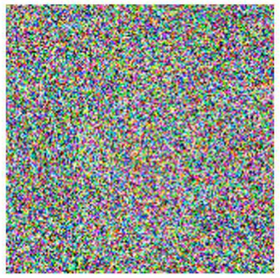

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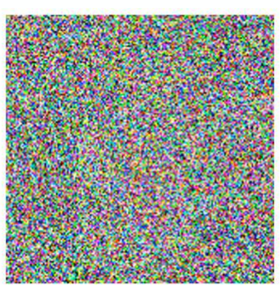

$t \sim \mathrm{U}[1,T]$

t

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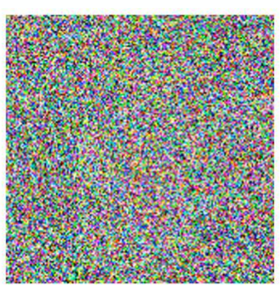
$\epsilon \sim \mathcal{N}(0,I)$ 

$t \sim \mathrm{U}[1,T]$ t

forward diffusion

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$$

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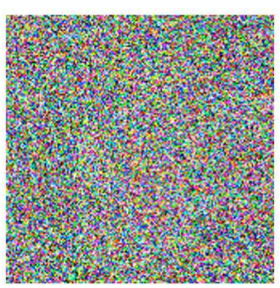

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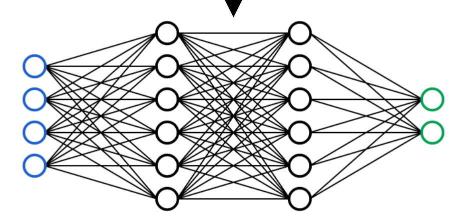

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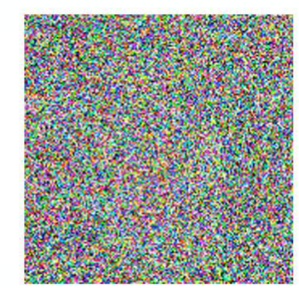

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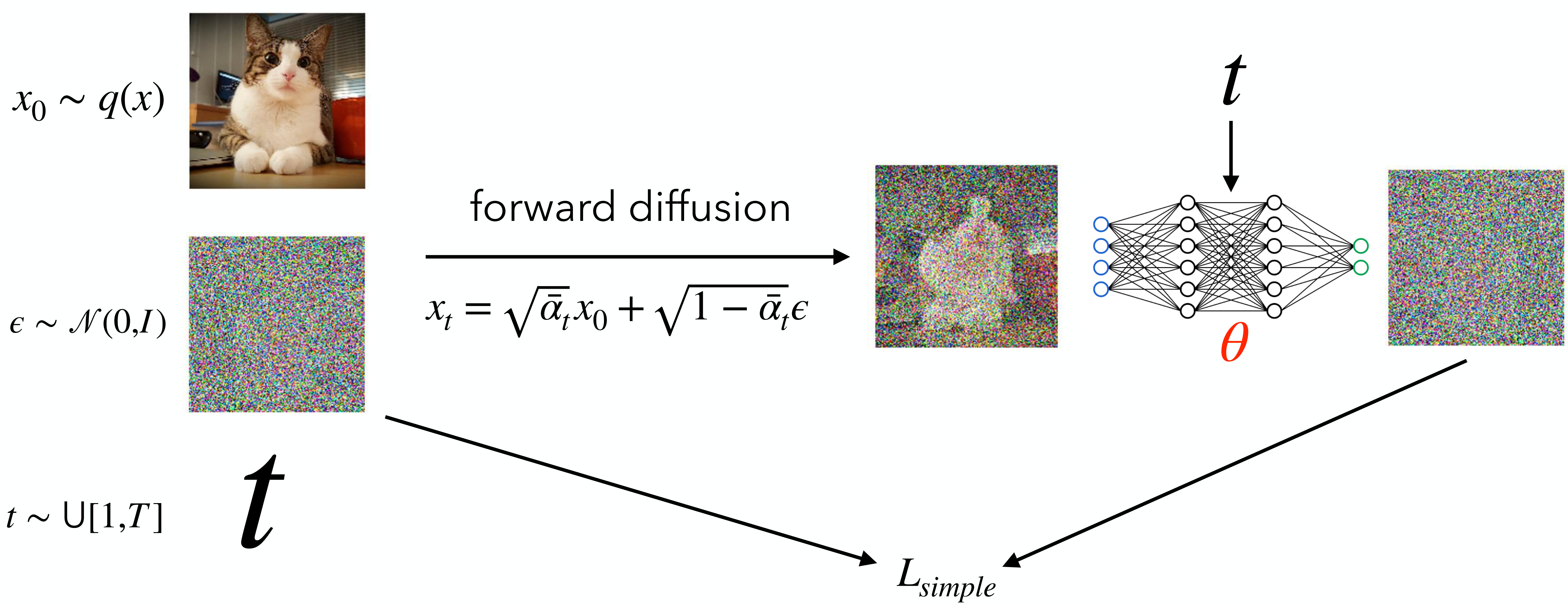
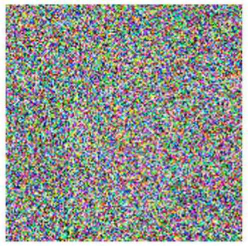


Putting it all together

- Sampling (naive)

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

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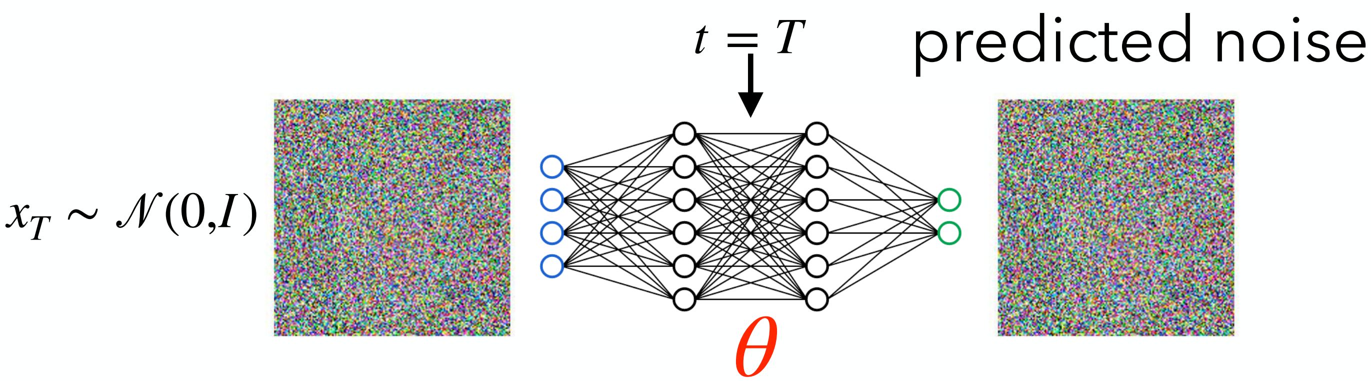

Putting it all together

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Reverse diffusion process parameterization

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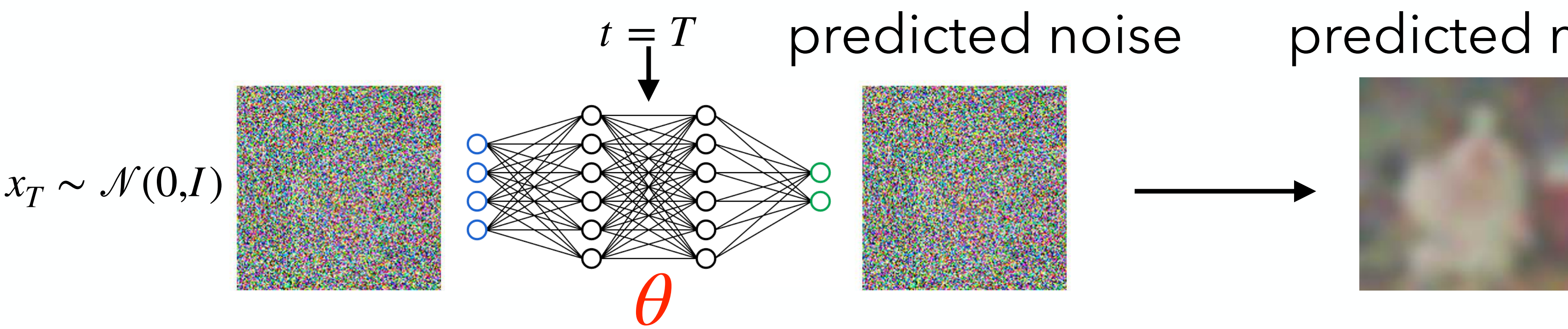

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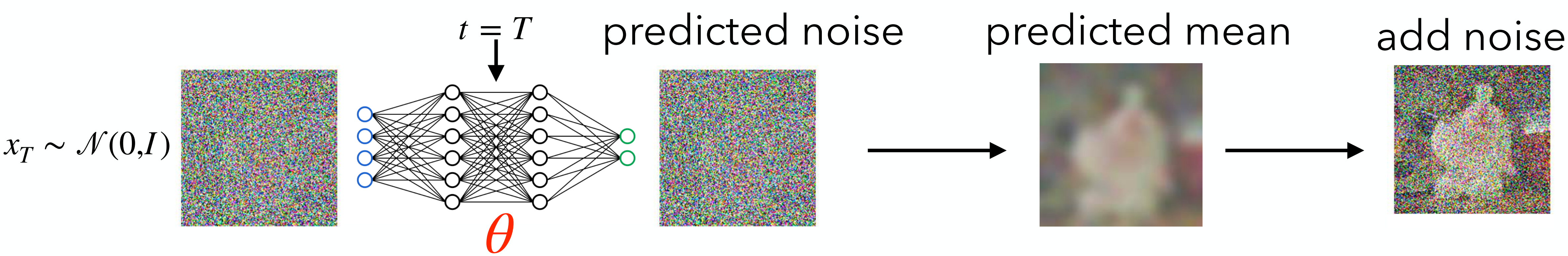

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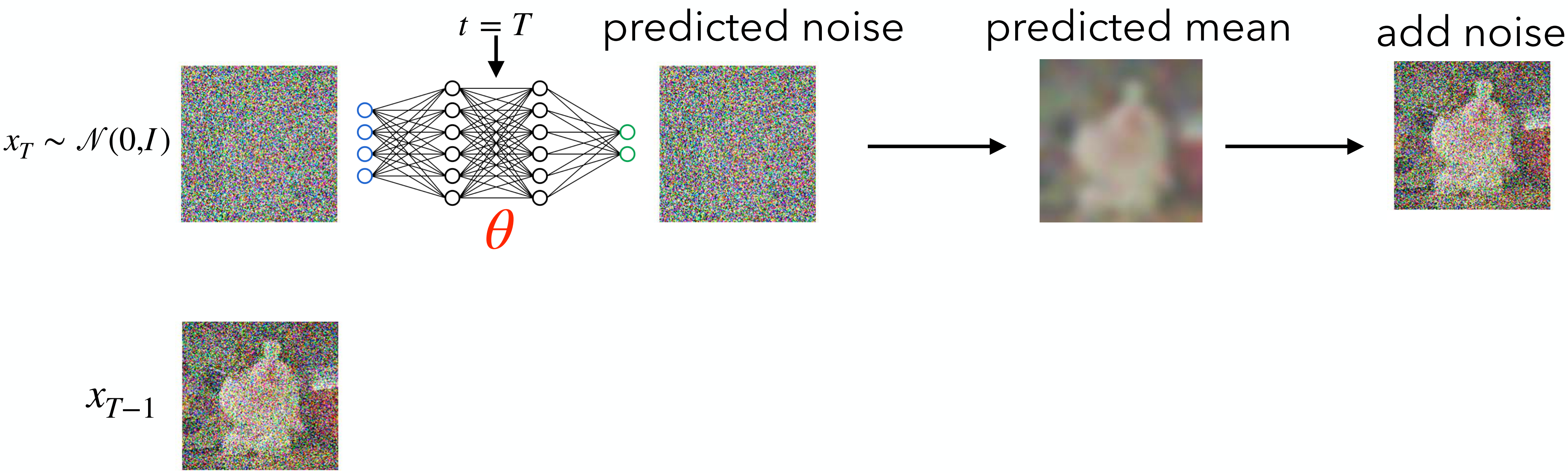

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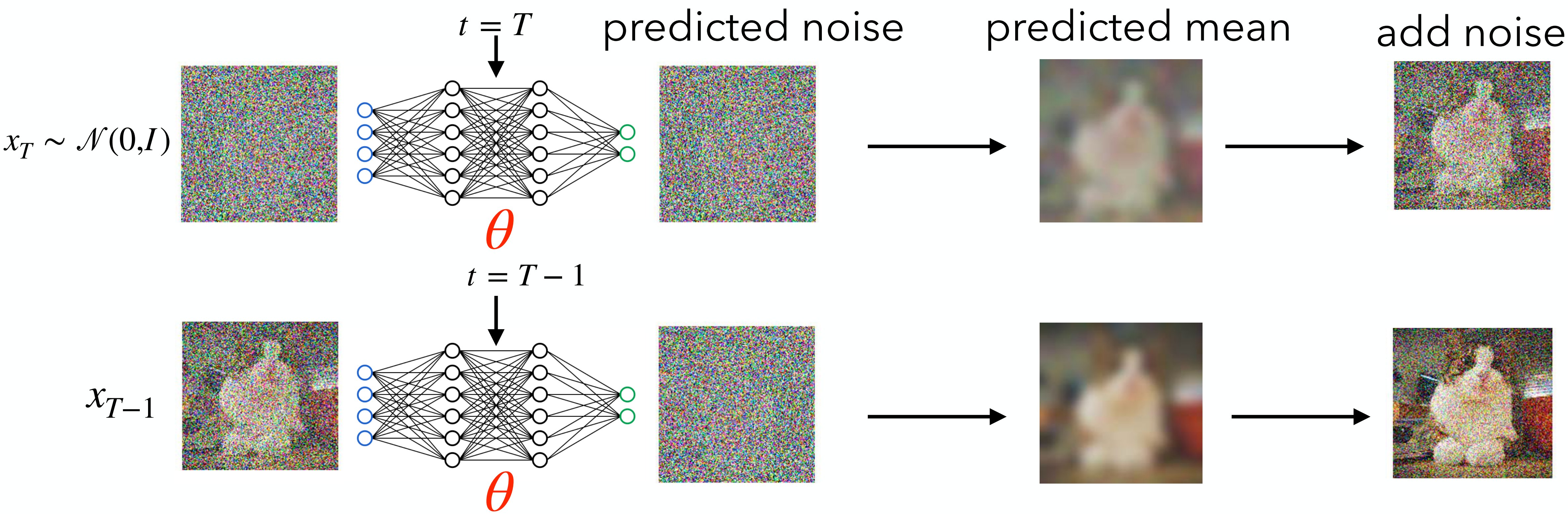

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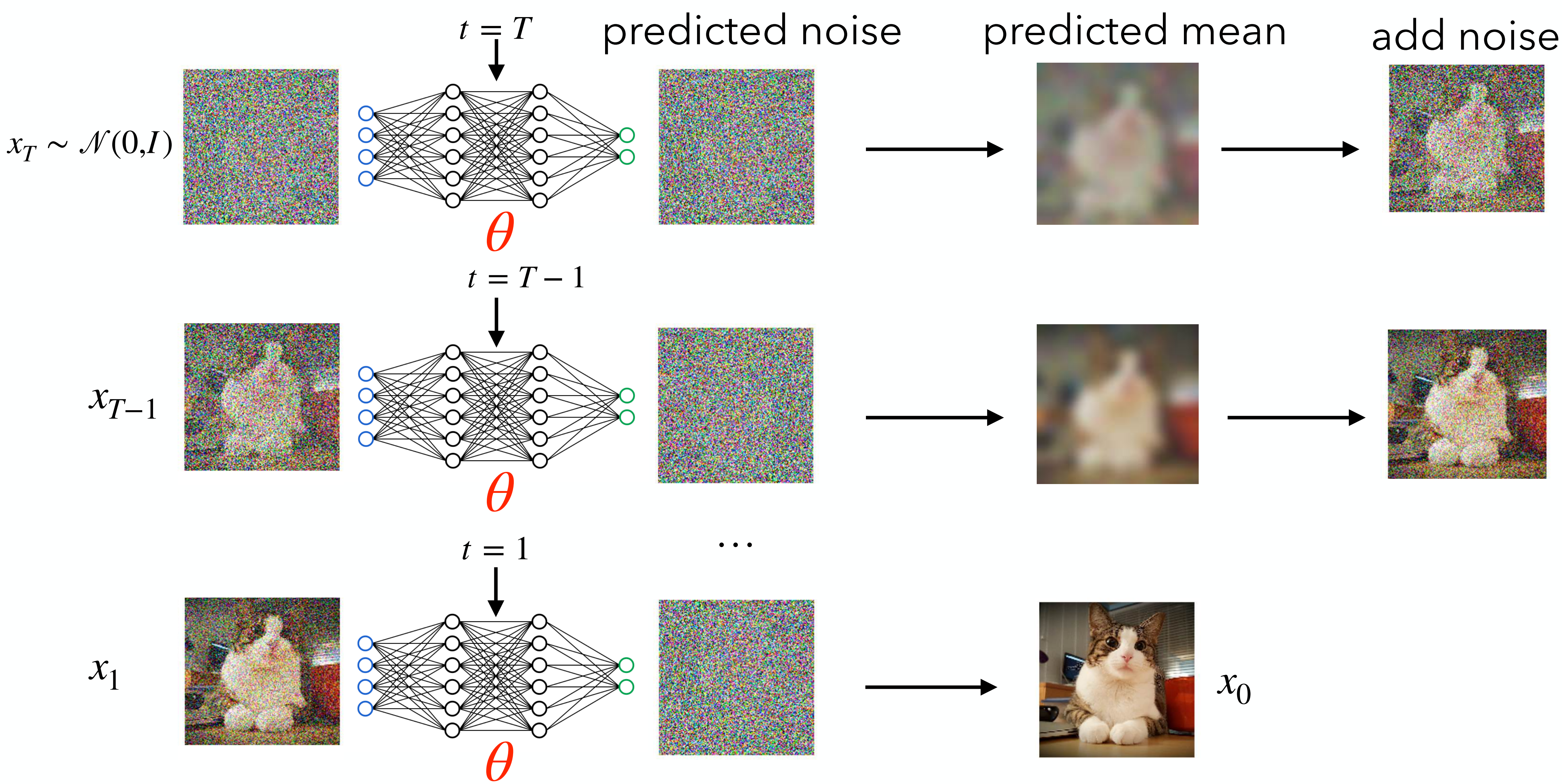
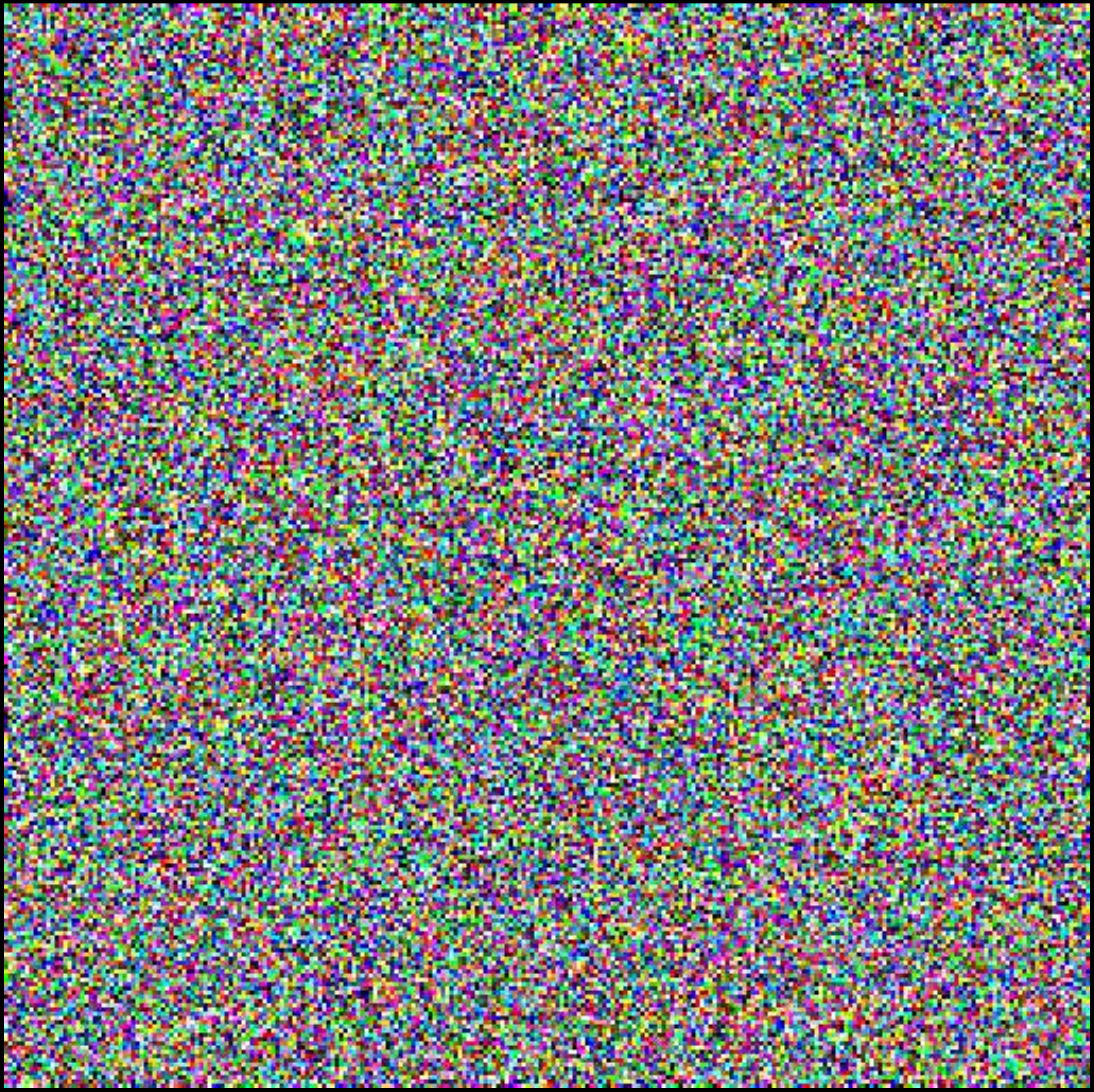
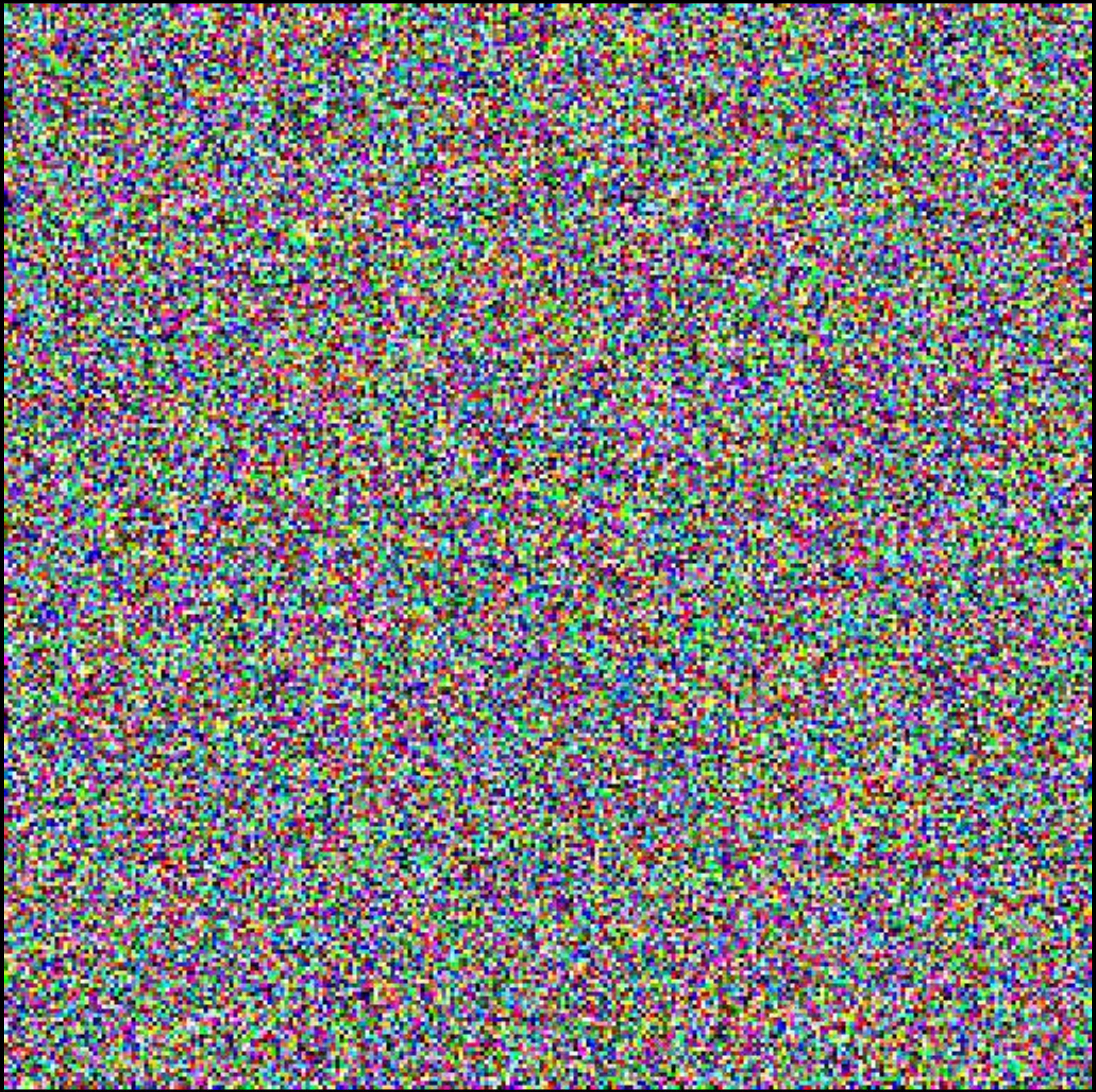




credit: Alex Nichol



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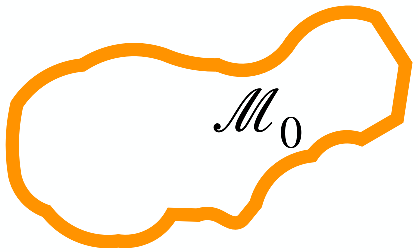
Geometric interpretation



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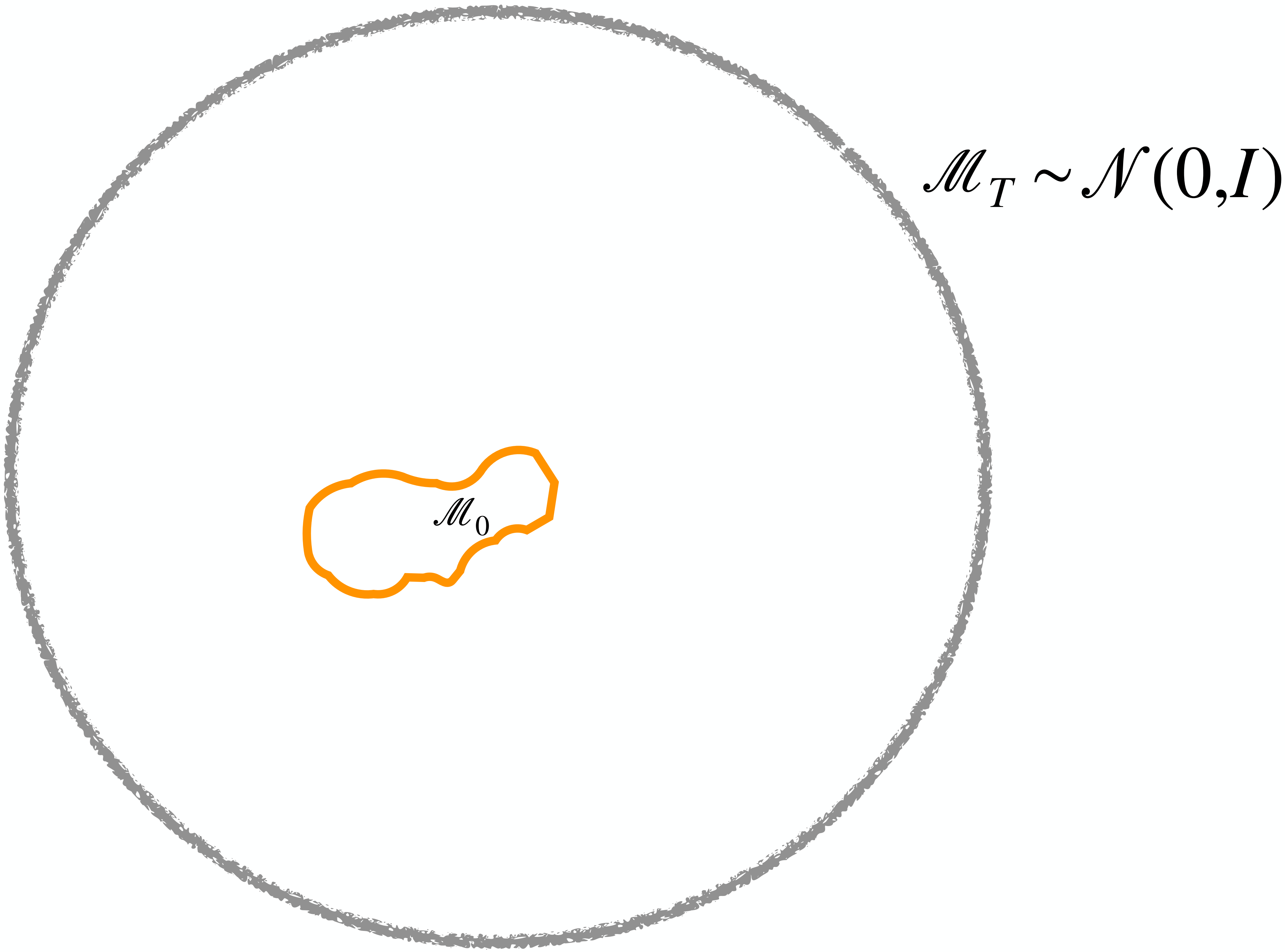

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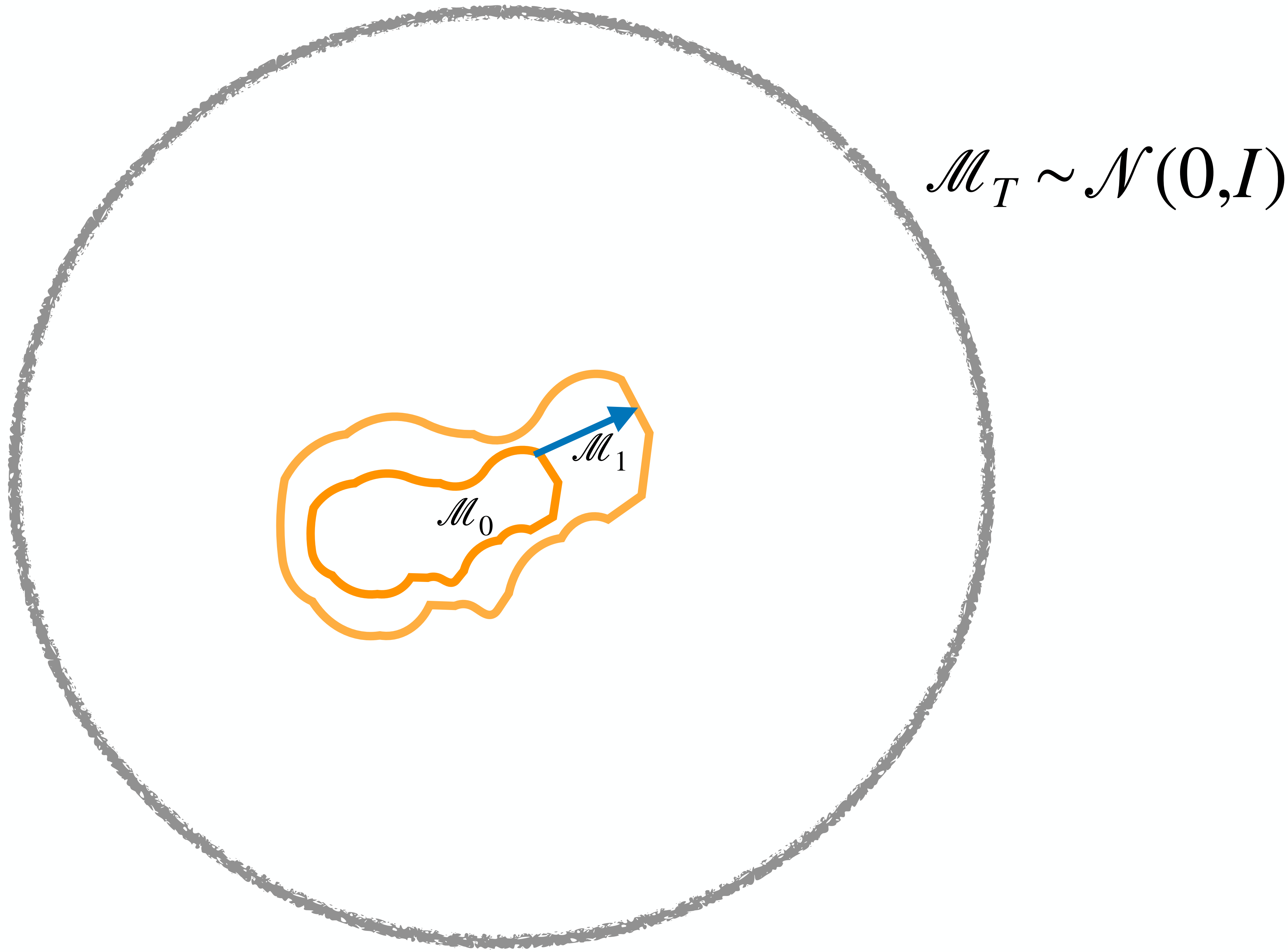
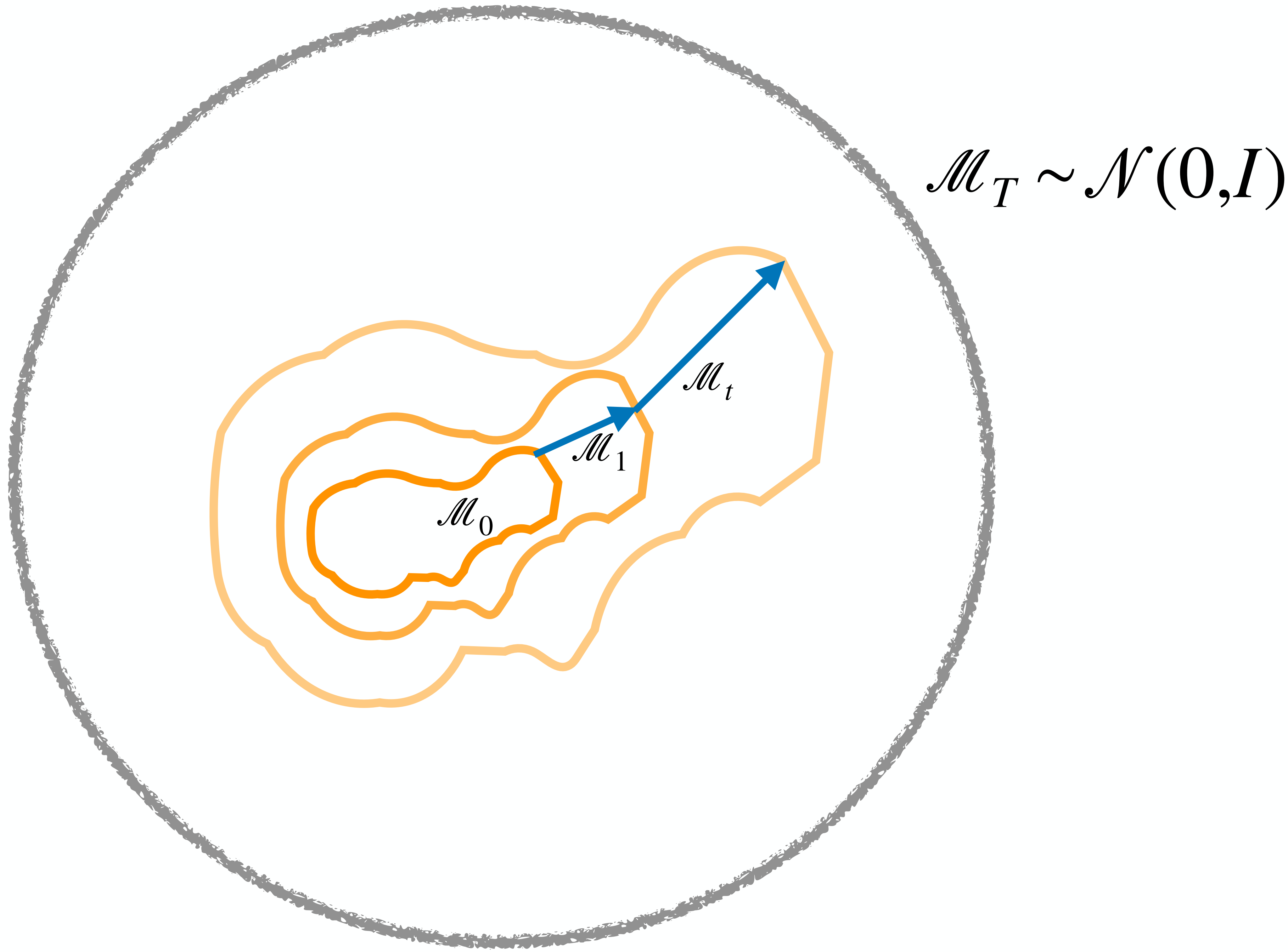
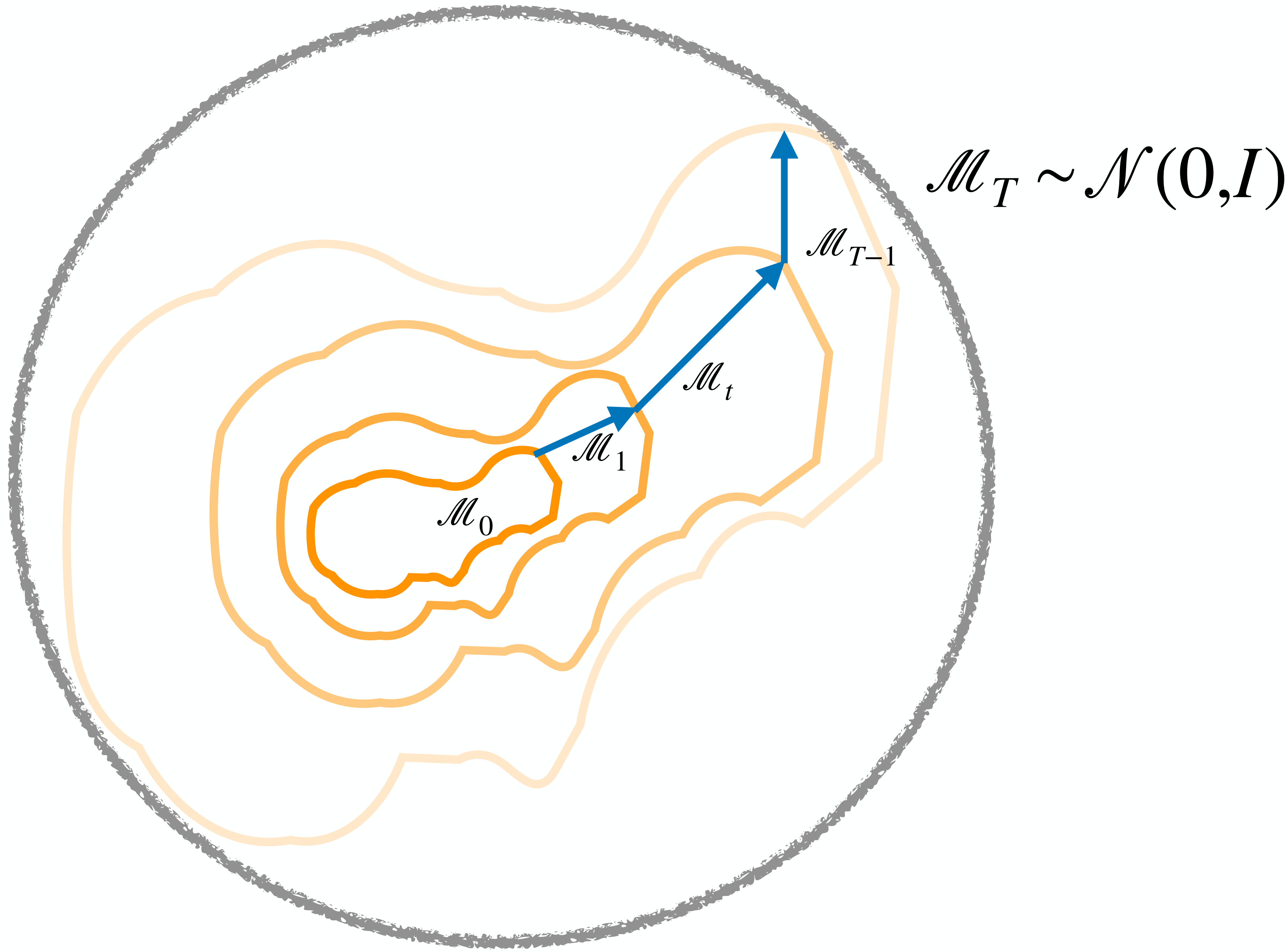


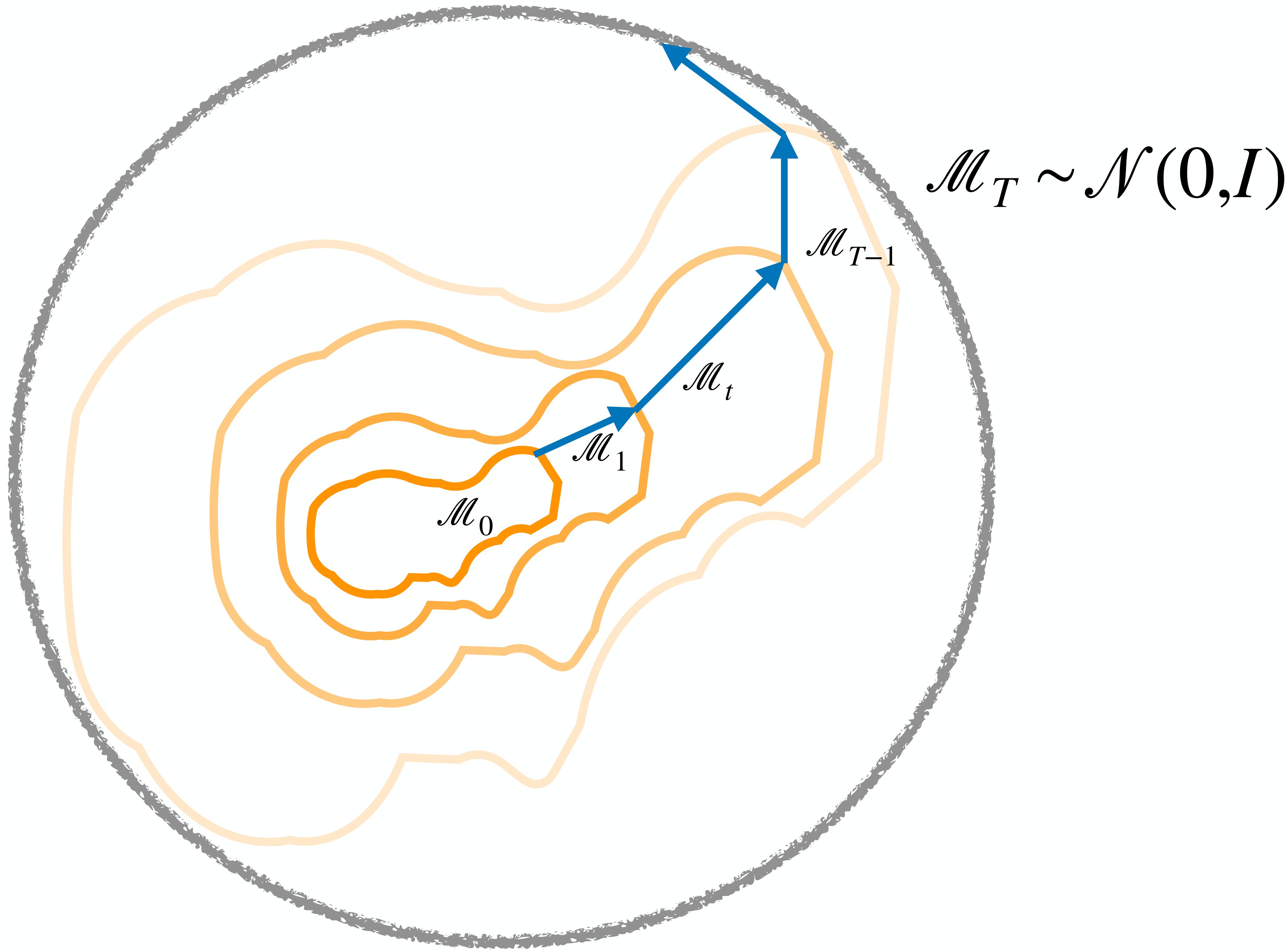
Geometric interpretation



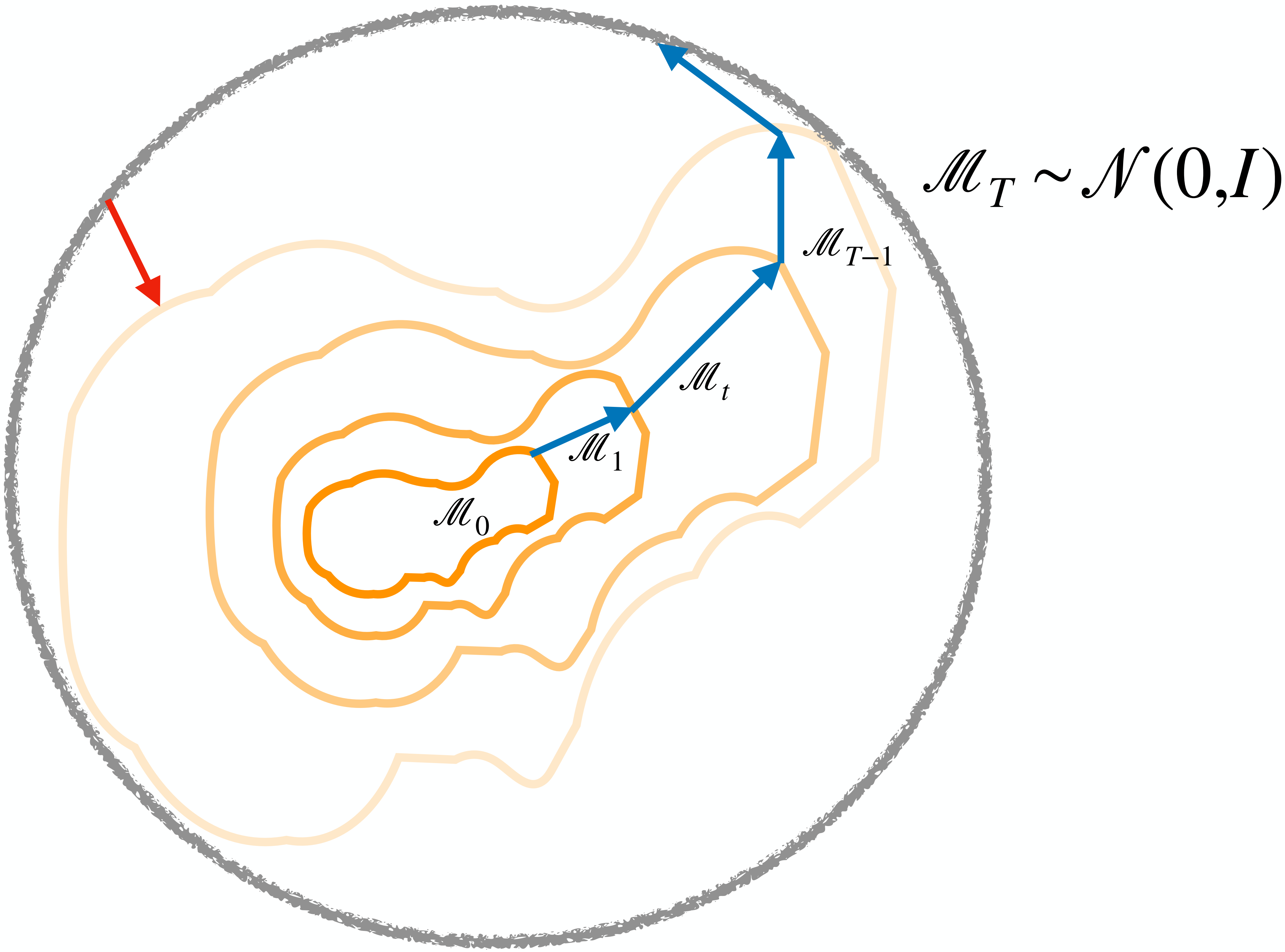
Geometric interpretation



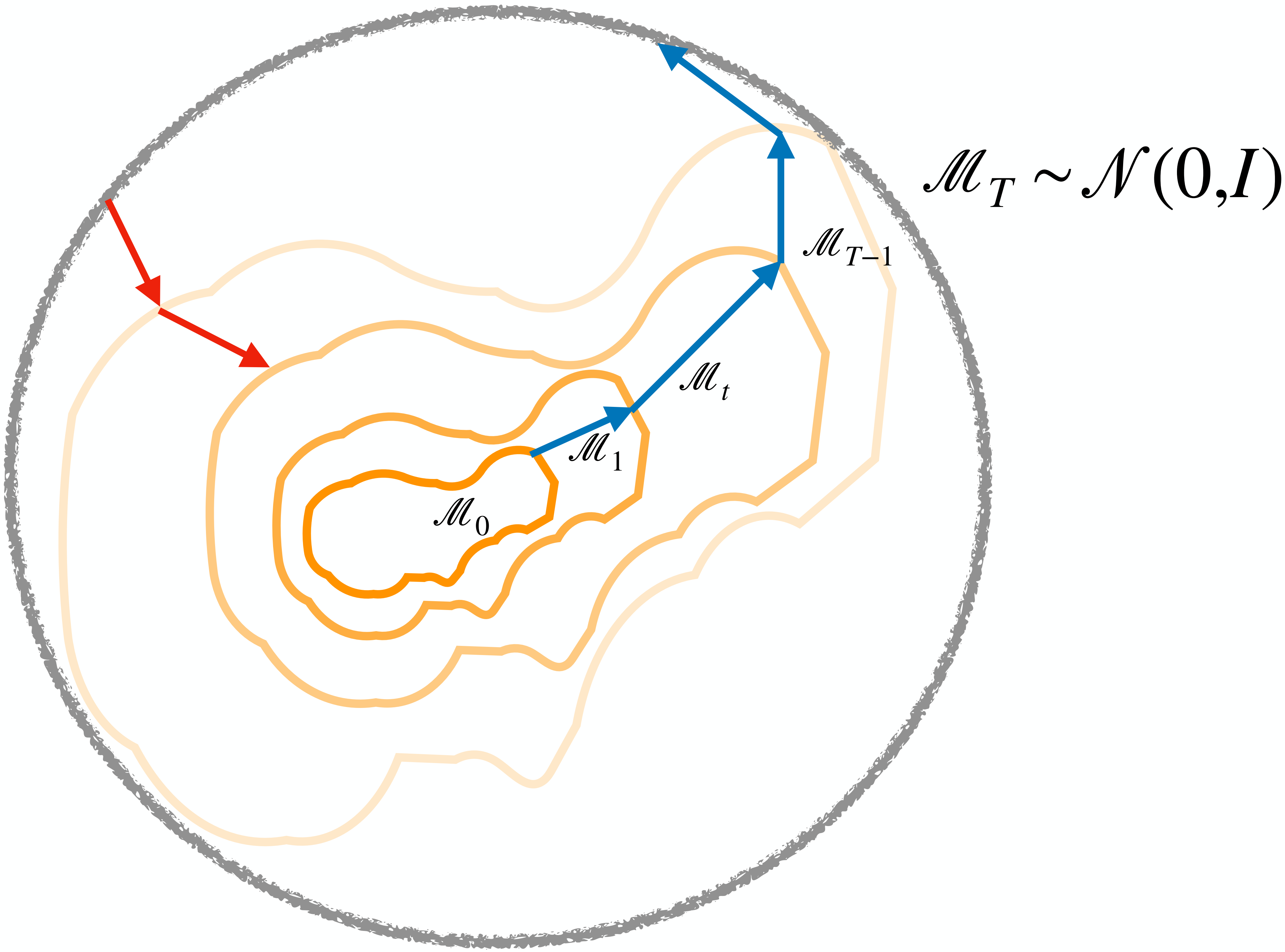
Geometric interpretation



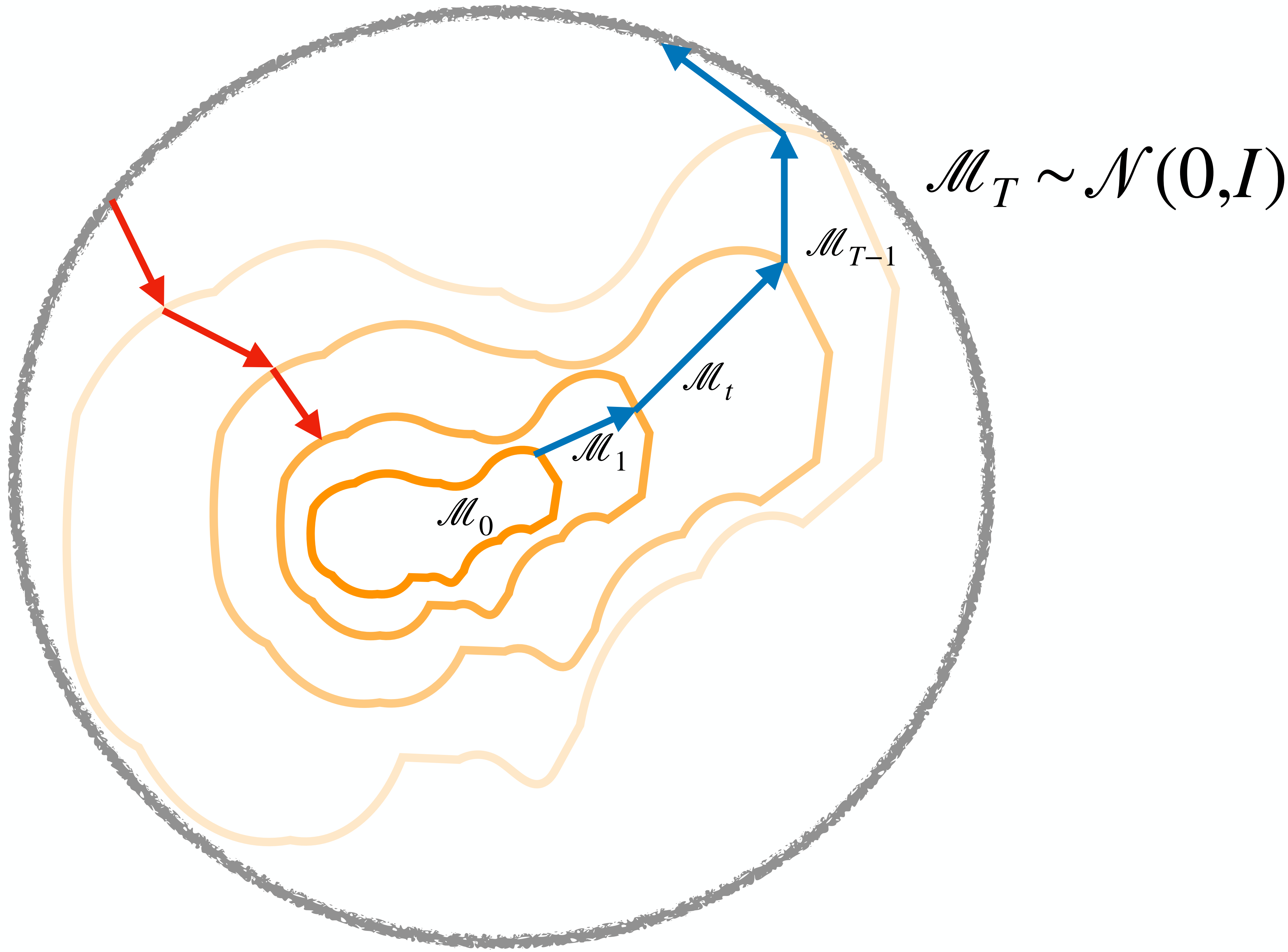
Geometric interpretation



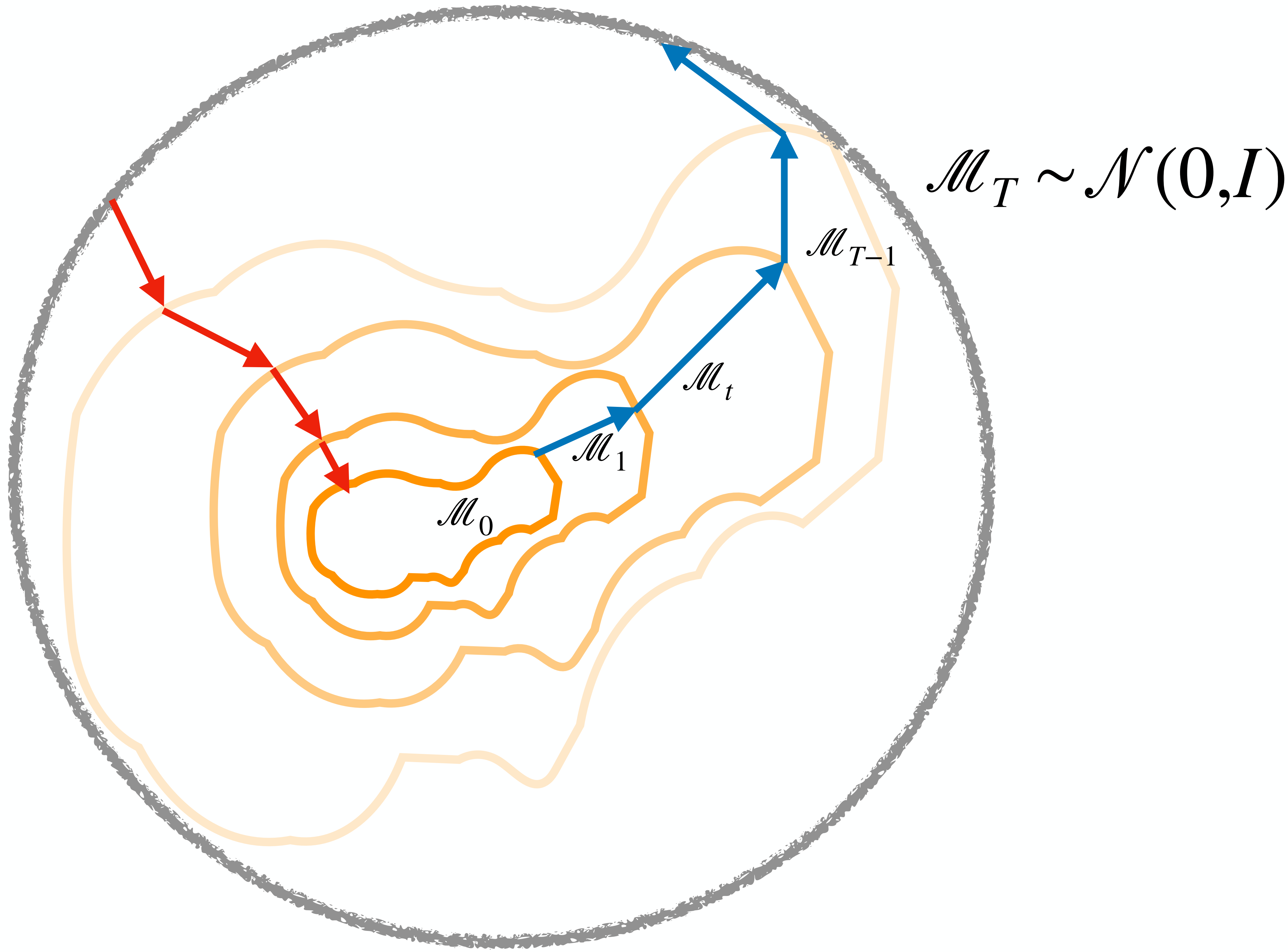
Geometric interpretation



Geometric interpretation



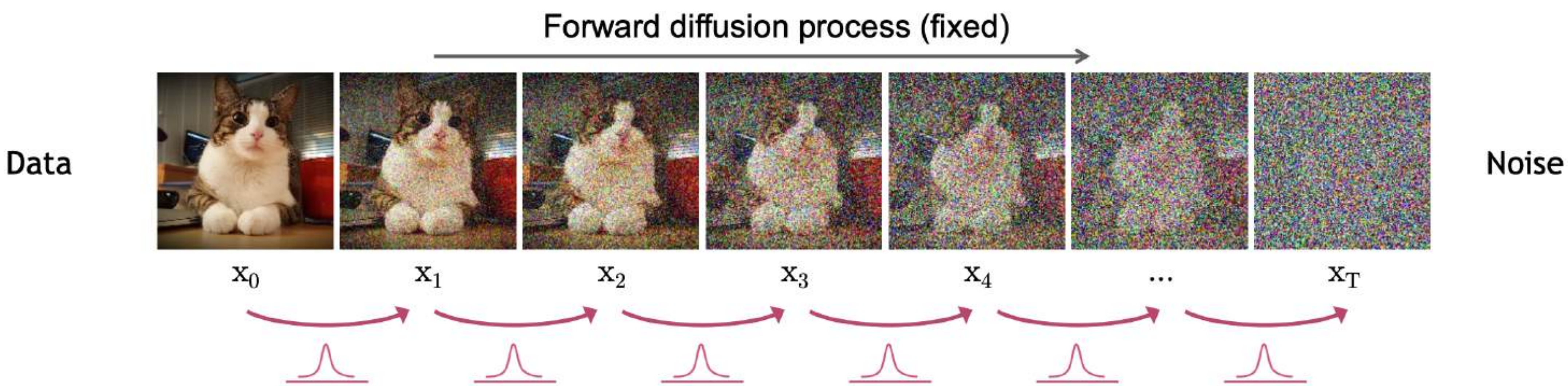
Geometric interpretation



Diffusion Models as Score Matching

Forward Diffusion

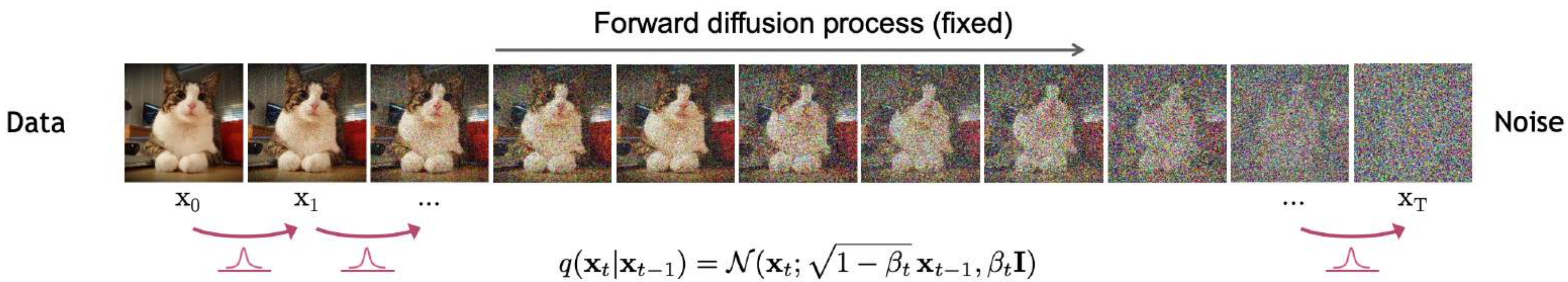
Consider the forward diffusion process again:



$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\,\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

Forward Diffusion

Consider the limit of **many small steps:**



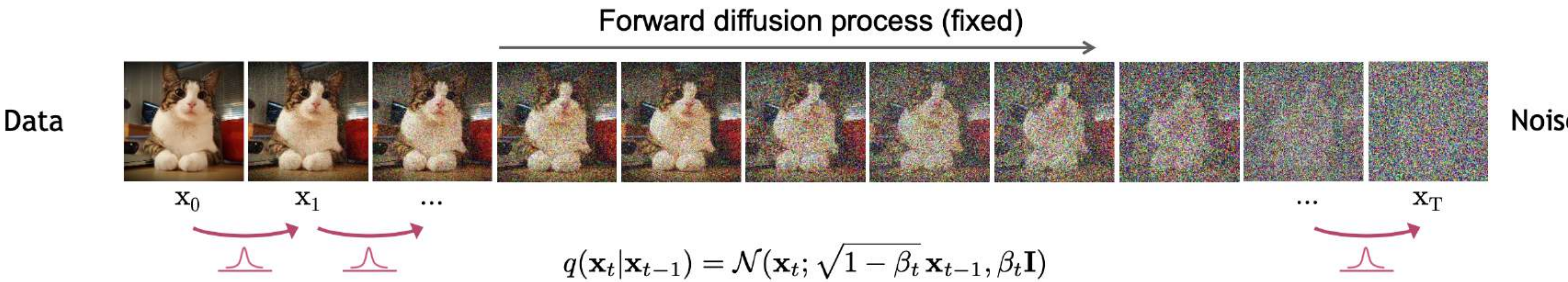
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\,\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

➡ $$\mathbf{x}_t = \sqrt{1-\beta_t}\,\mathbf{x}_{t-1} + \sqrt{\beta_t}\,\mathcal{N}(\mathbf{0},\mathbf{I})$$

Song et al., "Score-Based Generative Modeling through Stochastic Differential Equations", *ICLR*, 2021

Forward Diffusion

Consider the limit of **many small steps:**



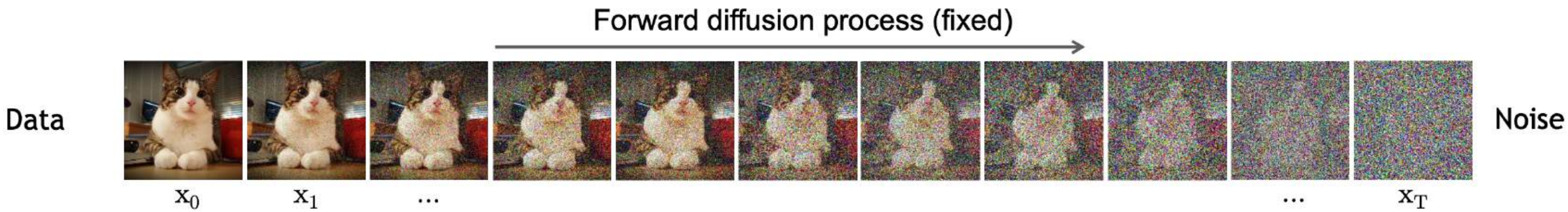
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\,\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

$$\begin{aligned} \mathbf{x}_t &= \sqrt{1-\beta_t}\,\mathbf{x}_{t-1} + \sqrt{\beta_t}\,\mathcal{N}(\mathbf{0},\mathbf{I}) \\ \Rightarrow \quad &= \sqrt{1-\beta(t)\Delta t}\,\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t}\,\mathcal{N}(\mathbf{0},\mathbf{I}) \qquad (\beta_t := \beta(t)\Delta t) \end{aligned}$$

Song et al., “Score-Based Generative Modeling through Stochastic Differential Equations”, *ICLR*, 2021

Forward Diffusion

Consider the limit of **many small steps:**



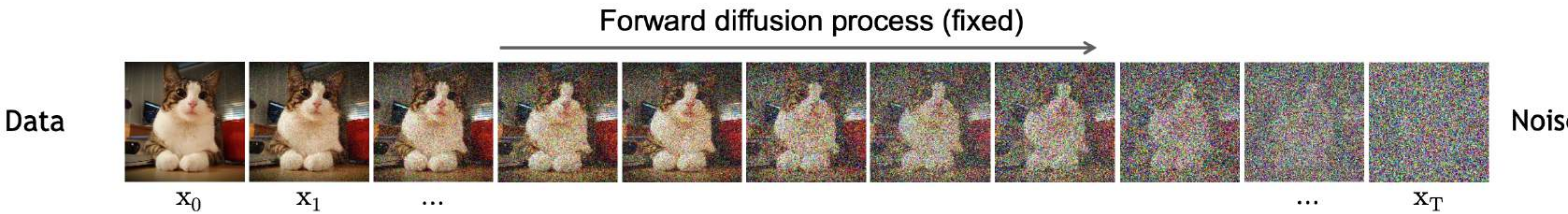
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\,\mathbf{x}_{t-1}, \beta_t\mathbf{I})$$

$$\begin{aligned}
\mathbf{x}_t &= \sqrt{1-\beta_t}\,\mathbf{x}_{t-1} + \sqrt{\beta_t}\,\mathcal{N}(\mathbf{0},\mathbf{I}) \\
&= \sqrt{1-\beta(t)\Delta t}\,\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t}\,\mathcal{N}(\mathbf{0},\mathbf{I}) && (\beta_t := \beta(t)\Delta t) \\
&\approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2}\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t}\,\mathcal{N}(\mathbf{0},\mathbf{I}) && \text{(Taylor expansion)}
\end{aligned}$$

[Song et al., "Score-Based Generative Modeling through Stochastic Differential Equations", *ICLR*, 2021](#)

Forward Diffusion

Consider the limit of **many small steps:**



$$\mathbf{x}_t \approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2}\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t}\,\mathcal{N}(\mathbf{0},\mathbf{I})$$

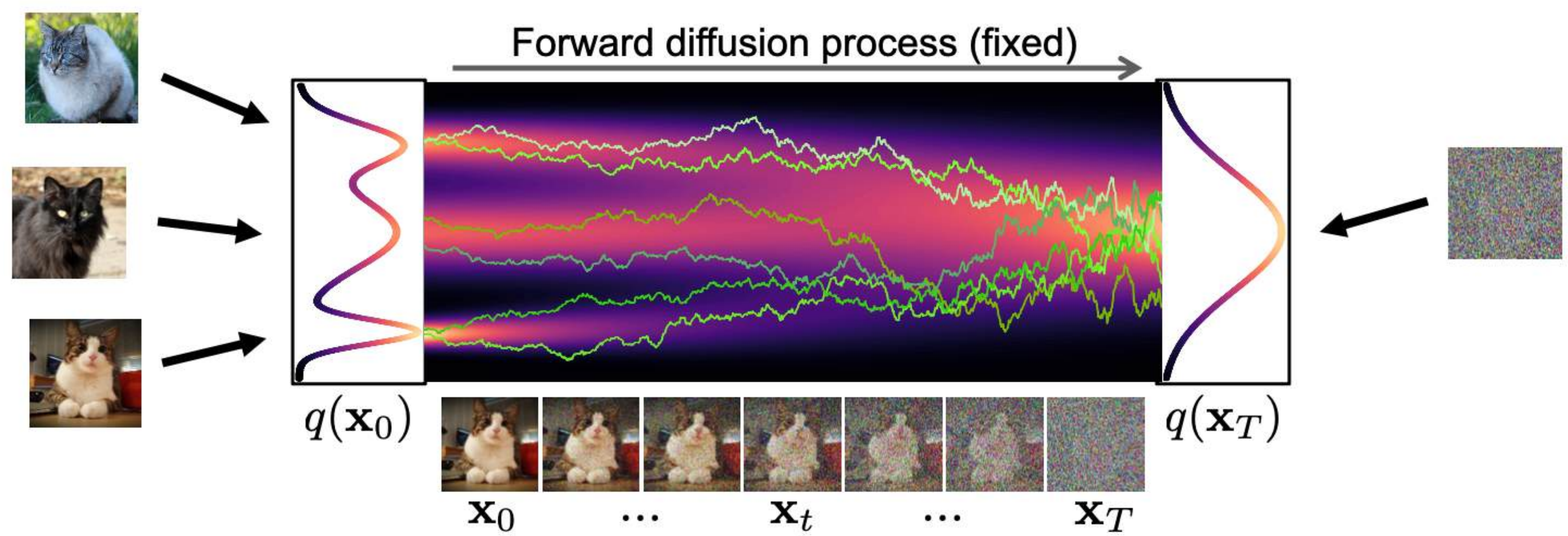
$$\Downarrow$$

$$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\boldsymbol{\omega}_t$$

Stochastic Differential Equation (SDE)
describing the diffusion in infinitesimal limit

Song et al., "Score-Based Generative Modeling through Stochastic Differential Equations", *ICLR*, 2021

The Generative Reverse Stochastic Differential Equation



Forward Diffusion SDE: $$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\boldsymbol{\omega}_t$$

Reverse Generative Diffusion SDE: $$\mathrm{d}\mathbf{x}_t = \overbrace{\left[-\frac{1}{2}\beta(t)\mathbf{x}_t - \beta(t)\underbrace{\nabla_{\mathbf{x}_t}\log q_t(\mathbf{x}_t)}_{\text{“Score Function”}}\right]}^{\text{drift term}}\mathrm{d}t + \overbrace{\sqrt{\beta(t)}\,\mathrm{d}\bar{\boldsymbol{\omega}}_t}^{\text{diffusion term}}$$

➡ **Simulate reverse diffusion process: Data generation from random noise!**

[Song et al., “Score-Based Generative Modeling through Stochastic Differential Equations”, *ICLR*, 2021]

Diffusion Models in Inverse Problems

General framework

$$y = \mathscr{A}(x_0) + z$$

Unconditional sampling

$$\hat{\mathbf{x}}_{t_{i-1}} = \boldsymbol{h}(\hat{\mathbf{x}}_{t_i}, \mathbf{z}_i, \boldsymbol{s}_{\boldsymbol{\theta}*}(\hat{\mathbf{x}}_{t_i}, t_i))$$

Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

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Measurement conditioned sampling

1) Data consistency step

$$\hat{\mathbf{x}}'_{t_i} = \boldsymbol{k}(\hat{\mathbf{x}}_{t_i}, \hat{\mathbf{y}}_{t_i}, \lambda)$$

2) Unconditional diffusion step

$$\hat{\mathbf{x}}_{t_{i-1}} = \boldsymbol{h}(\hat{\mathbf{x}}'_{t_i}, \mathbf{z}_i, \boldsymbol{s}_{\boldsymbol{\theta}*}(\hat{\mathbf{x}}_{t_i}, t_i)), \quad i = N, N-1, \cdots, 1$$

Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

General framework

$$y = \mathscr{A}(x_0) + z$$

Unconditional sampling

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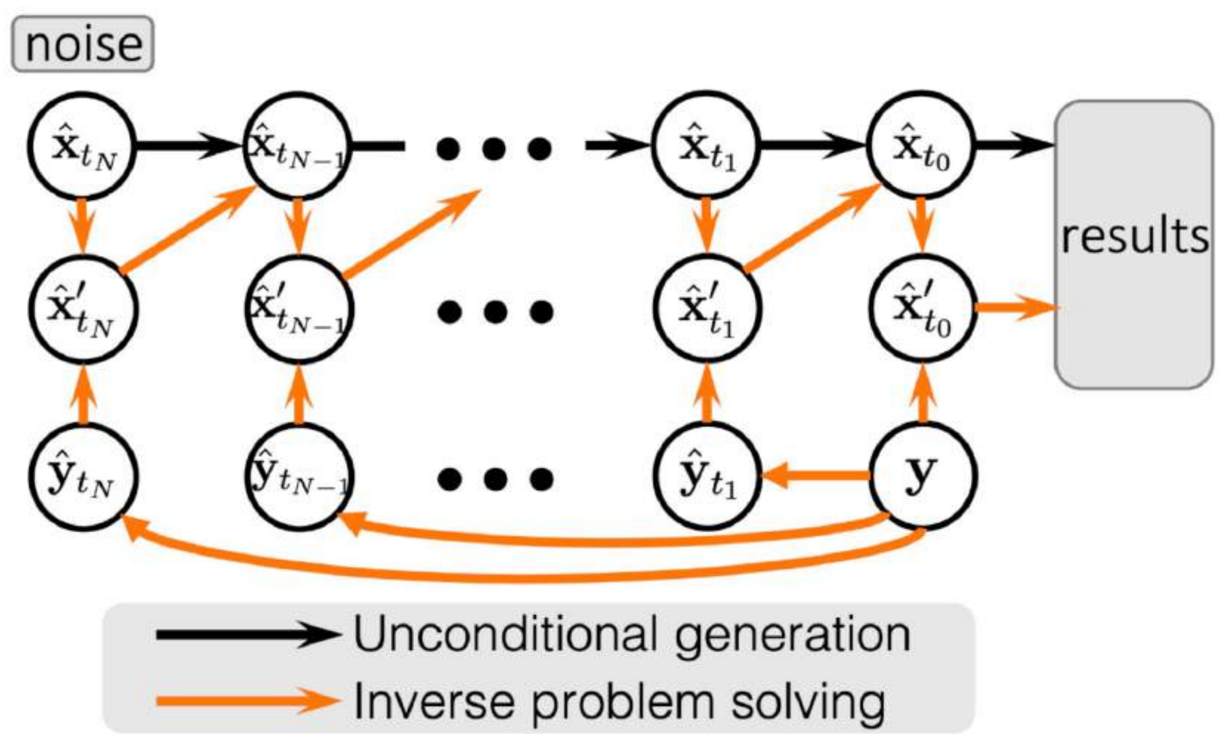


Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

Medical imaging example

Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

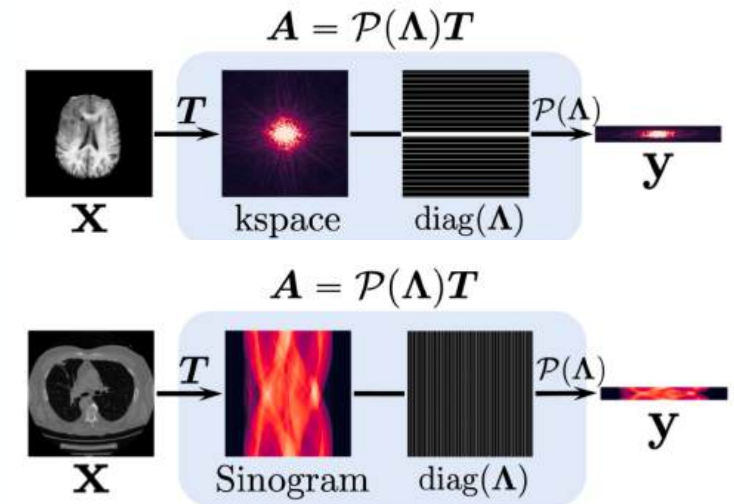
Medical imaging example

Assume that the forward model has the form:

$$\mathscr{A}(x_0) = \mathscr{P}(\Lambda)Tx_0$$

subsampling

invertible



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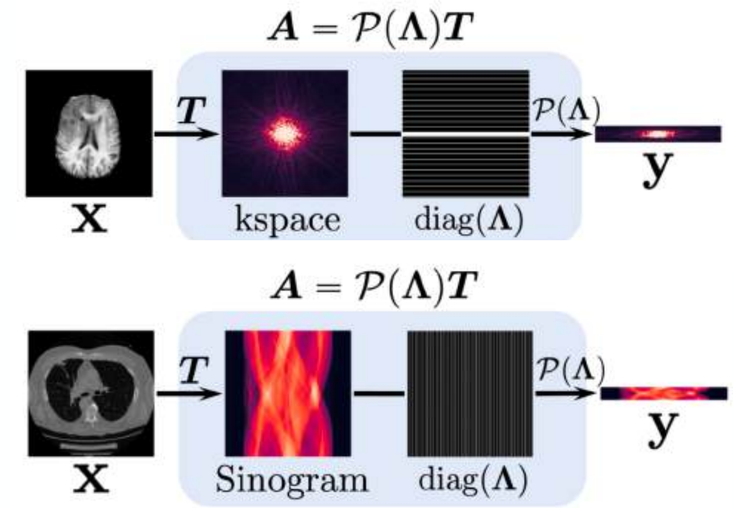


Measurement conditioned sampling

1) Data consistency

$$\hat{\mathbf{x}}'_{t_i} = \boldsymbol{k}(\hat{\mathbf{x}}_{t_i}, \hat{\mathbf{y}}_{t_i}, \lambda)$$

2) Unconditional diffusion

$$\hat{\mathbf{x}}_{t_{i-1}} = \boldsymbol{h}(\hat{\mathbf{x}}'_{t_i}, \mathbf{z}_i, \boldsymbol{s}_{\boldsymbol{\theta}*}(\hat{\mathbf{x}}_{t_i}, t_i)), \quad i = N, N-1, \cdots, 1$$

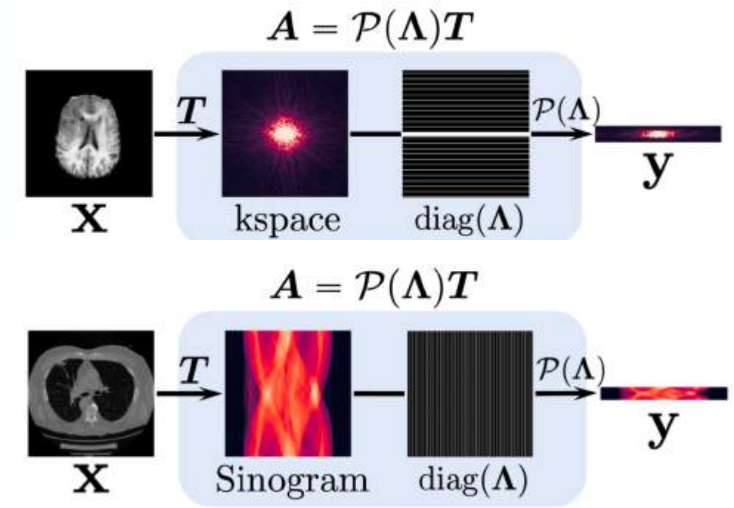
Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

Medical imaging example

Assume that the forward model has the form:

$$\mathscr{A}(x_0) = \mathscr{P}(\Lambda) T x_0$$

subsampling invertible



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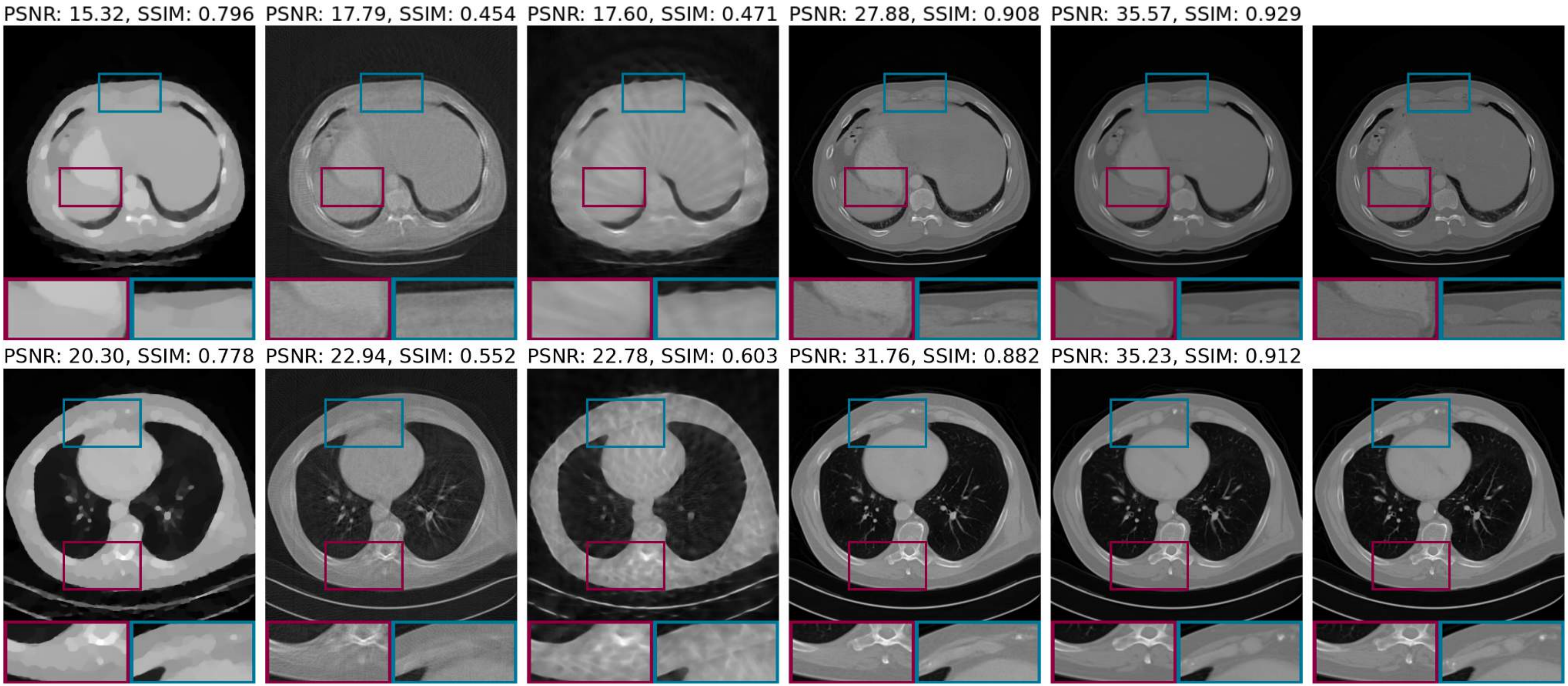
$$\hat{\mathbf{x}}_{t_{i-1}} = \boldsymbol{h}(\hat{\mathbf{x}}'_{t_i}, \mathbf{z}_i, \boldsymbol{s}_{\boldsymbol{\theta}*}(\hat{\mathbf{x}}_{t_i}, t_i)), \quad i = N, N-1, \cdots, 1$$

Data consistency:

$$\hat{\mathbf{x}}'_{t_i} = \underset{\boldsymbol{z}\in\mathbb{R}^n}{\arg\min}\{(1-\lambda)\,\|\boldsymbol{z} - \hat{\mathbf{x}}_{t_i}\|^2_{\boldsymbol{T}} + \min_{\boldsymbol{u}\in\mathbb{R}^n} \lambda\,\|\boldsymbol{z} - \boldsymbol{u}\|^2_{\boldsymbol{T}}\} \quad s.t. \quad \boldsymbol{A}\boldsymbol{u} = \hat{\mathbf{y}}_{t_i}$$

Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

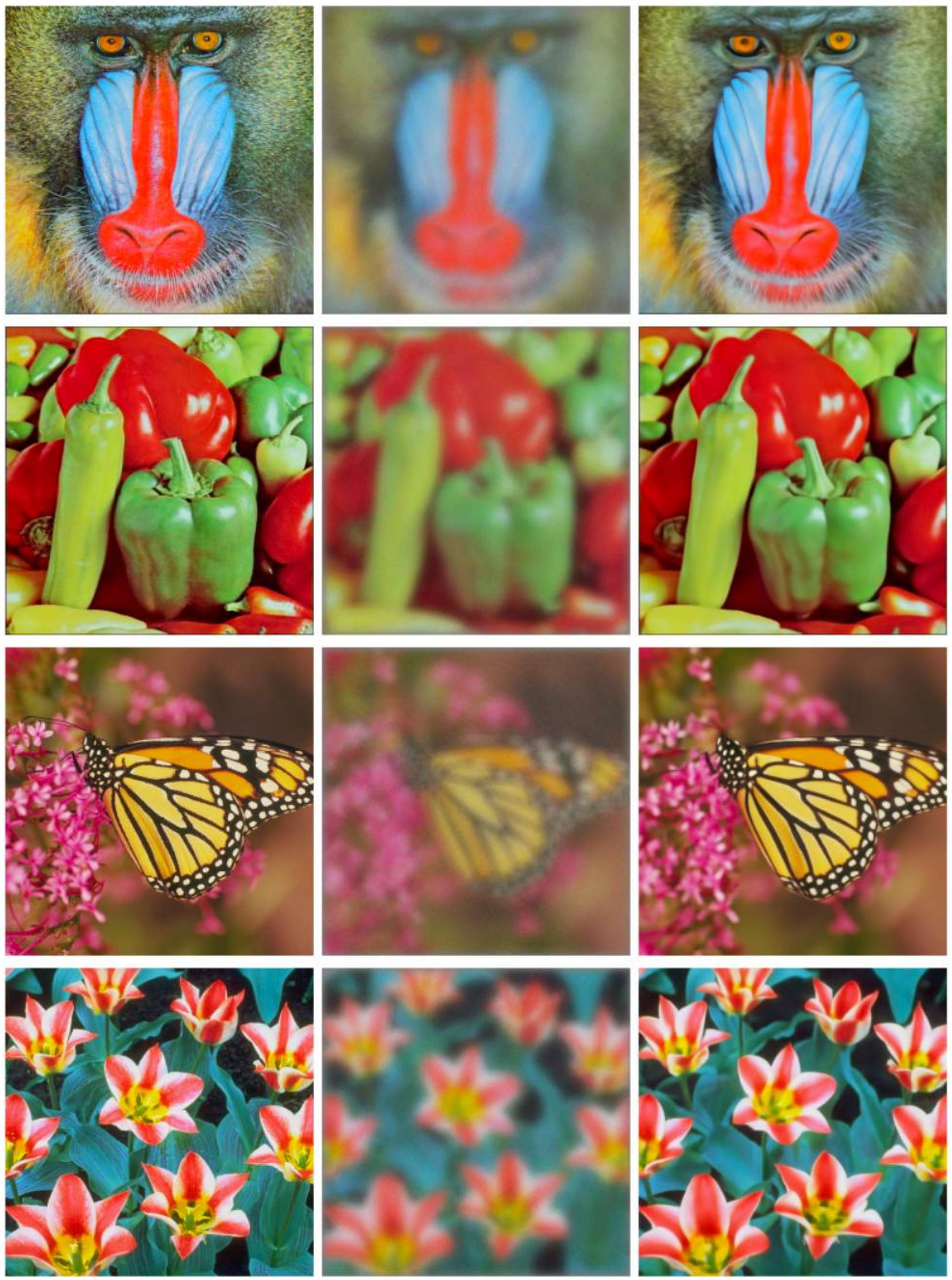
Reconstruction results



(a) FISTA-TV (b) cGAN (c) Neumann (d) SIN-4c-PRN (e) Ours (f) Ground truth

Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

Deblurring and inpainting results

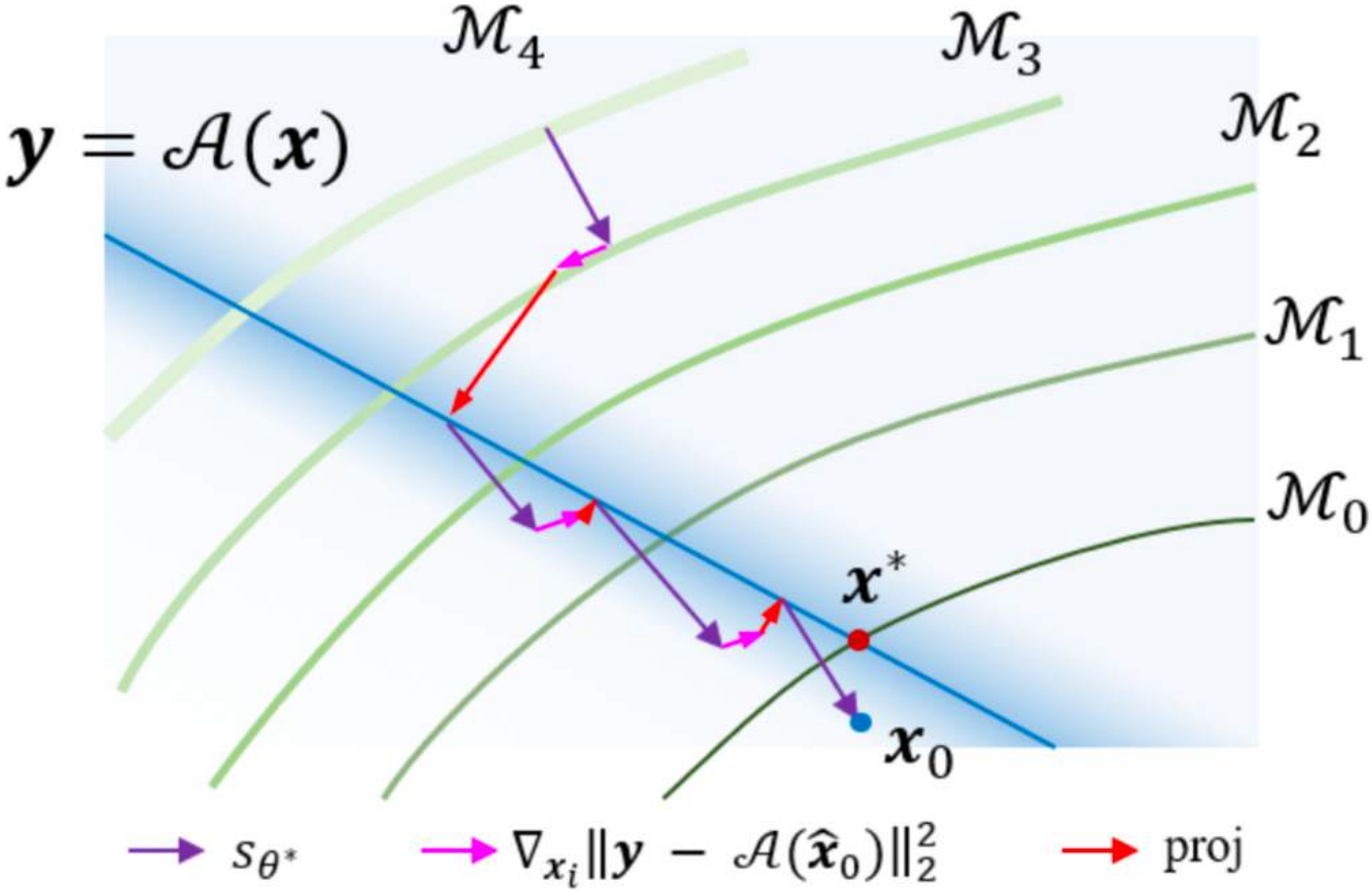


Original Blurred DDRM (20)

Original Occluded DDRM (20)

Kawar, Bahjat, et al. "Denoising diffusion restoration models." *arXiv preprint arXiv:2201.11793* (2022).

Intuition



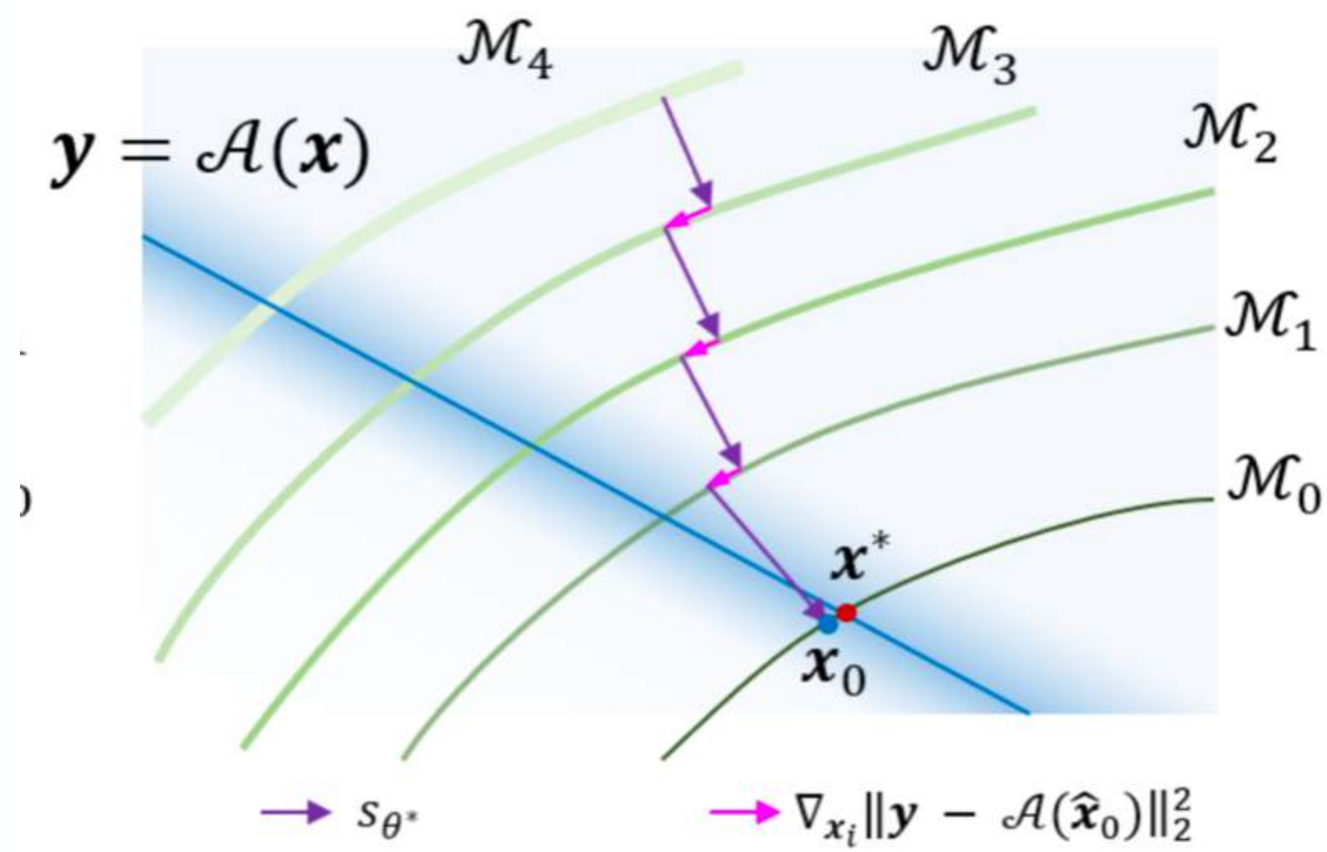
Song, Yang, et al. "Solving inverse problems in medical imaging with score-based generative models." *arXiv preprint arXiv:2111.08005* (2021).

Diffusion Posterior Sampling

- **Bayesian framework**

$$\boldsymbol{y} = \mathcal{A}(\boldsymbol{x}) + \boldsymbol{n} \qquad\qquad p_\theta(\boldsymbol{x}|\boldsymbol{y}) \propto p_\theta(\boldsymbol{x})p(\boldsymbol{y}|\boldsymbol{x})$$

solve inverse problem = sample from posterior



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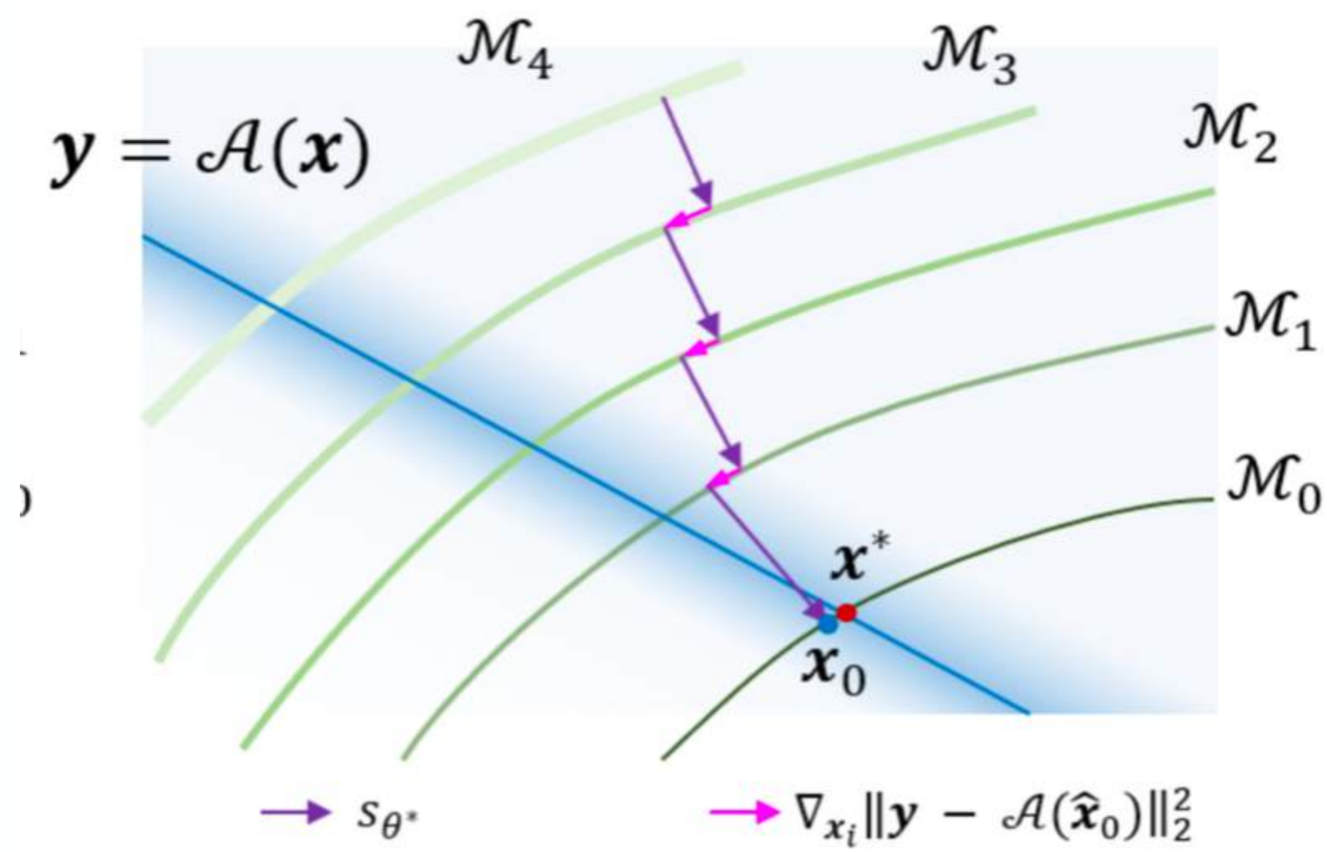
- **Bayesian framework**

$$\boldsymbol{y} = \mathcal{A}(\boldsymbol{x}) + \boldsymbol{n} \qquad\qquad p_\theta(\boldsymbol{x}|\boldsymbol{y}) \propto p_\theta(\boldsymbol{x})p(\boldsymbol{y}|\boldsymbol{x})$$

solve inverse problem = sample from posterior

- **Hijacking the diffusion process**

$$\nabla_{\boldsymbol{x}} \log p_\theta(\boldsymbol{x}|\boldsymbol{y}) = \nabla_{\boldsymbol{x}} \log p_\theta(\boldsymbol{x}) + \nabla_{\boldsymbol{x}} \log p(\boldsymbol{y}|\boldsymbol{x})$$



Diffusion Posterior Sampling

- **Bayesian framework**

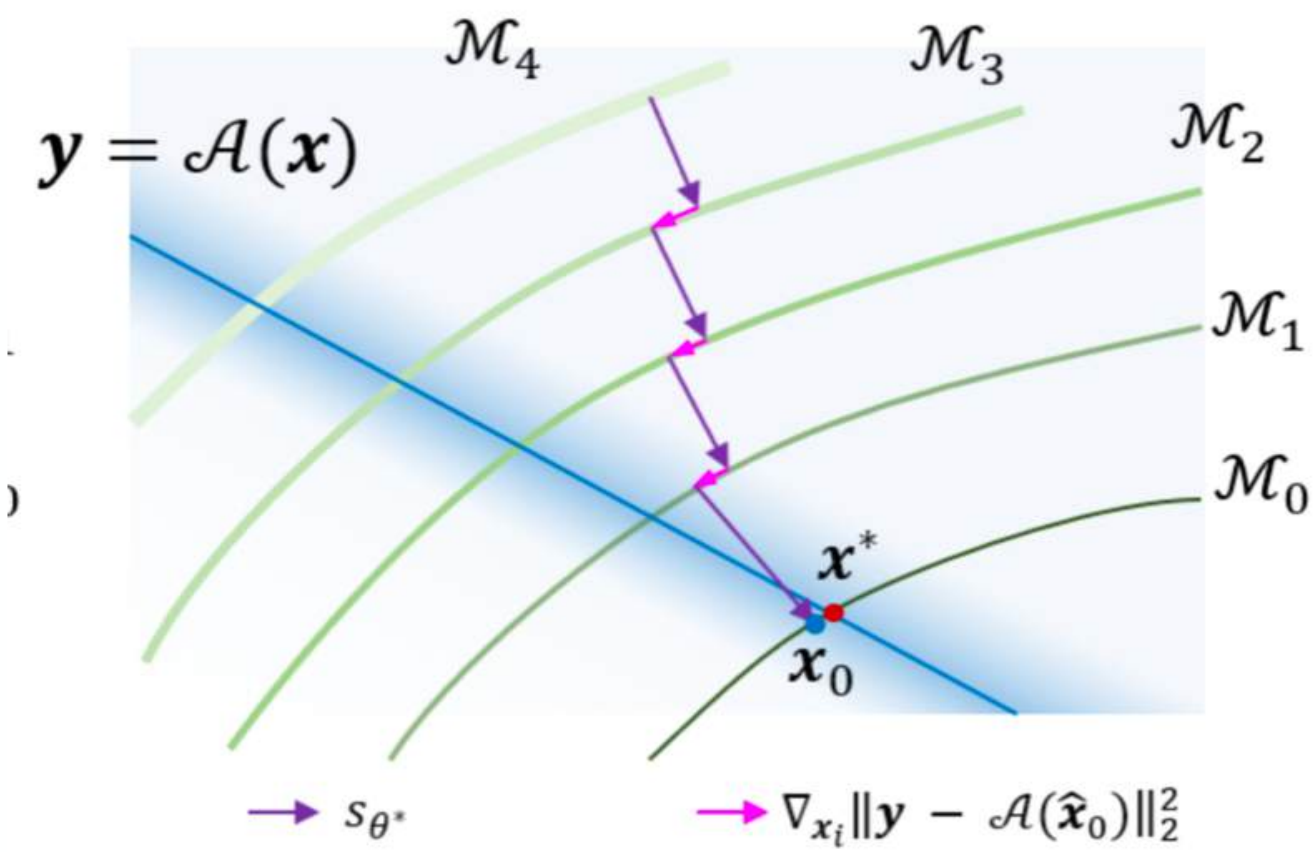
$$y = \mathcal{A}(x) + n \qquad\qquad p_\theta(x|y) \propto p_\theta(x)p(y|x)$$

solve inverse problem = sample from posterior

- **Hijacking the diffusion process**

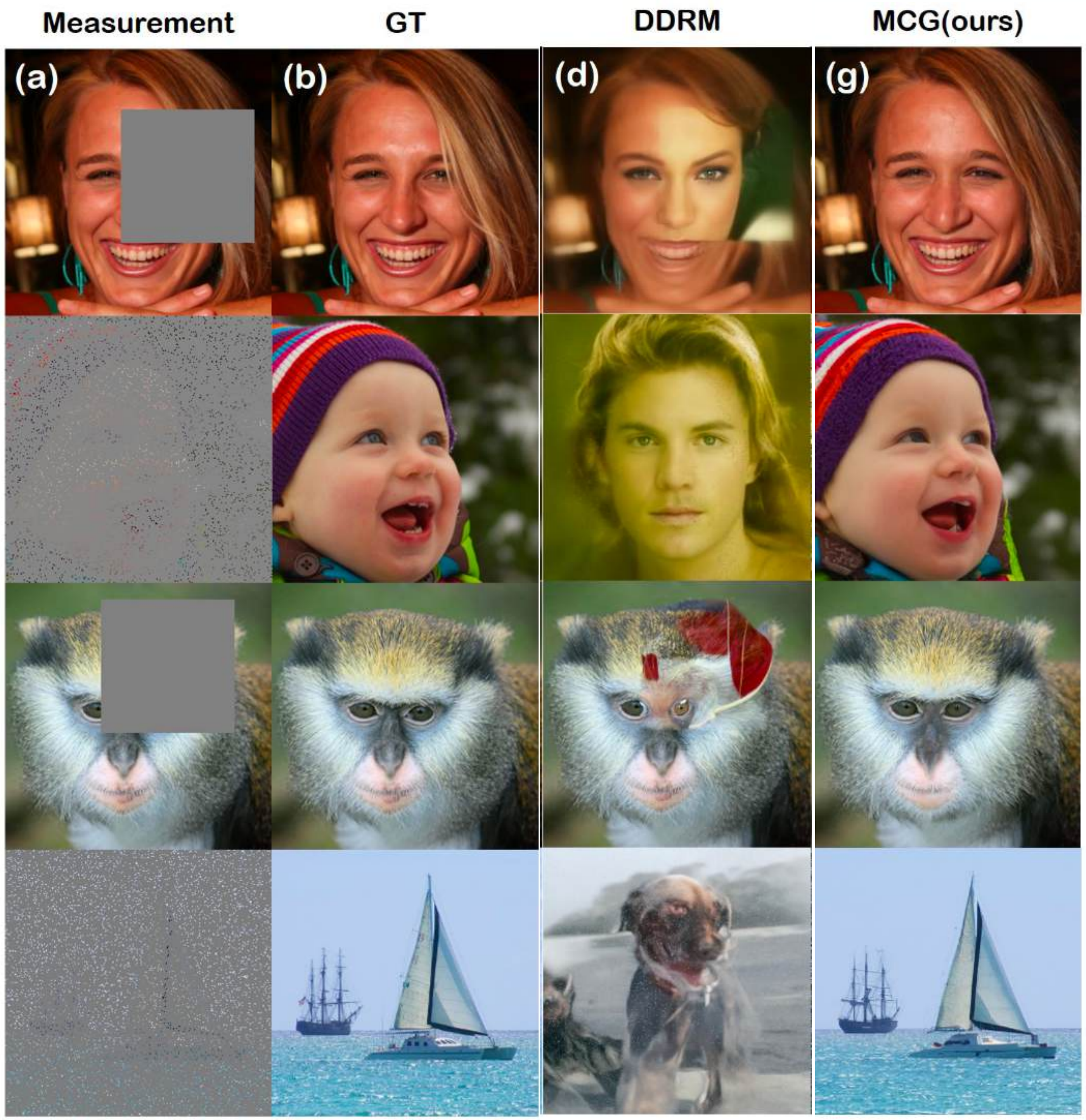
$$\nabla_x \log p_\theta(x|y) = \nabla_x \log p_\theta(x) + \nabla_x \log p(y|x)$$

prior = pre-trained diffusion model



Chung, Hyungjin, et al. "Diffusion posterior sampling for general noisy inverse problems." *arXiv preprint arXiv:2209.14687* (2022).

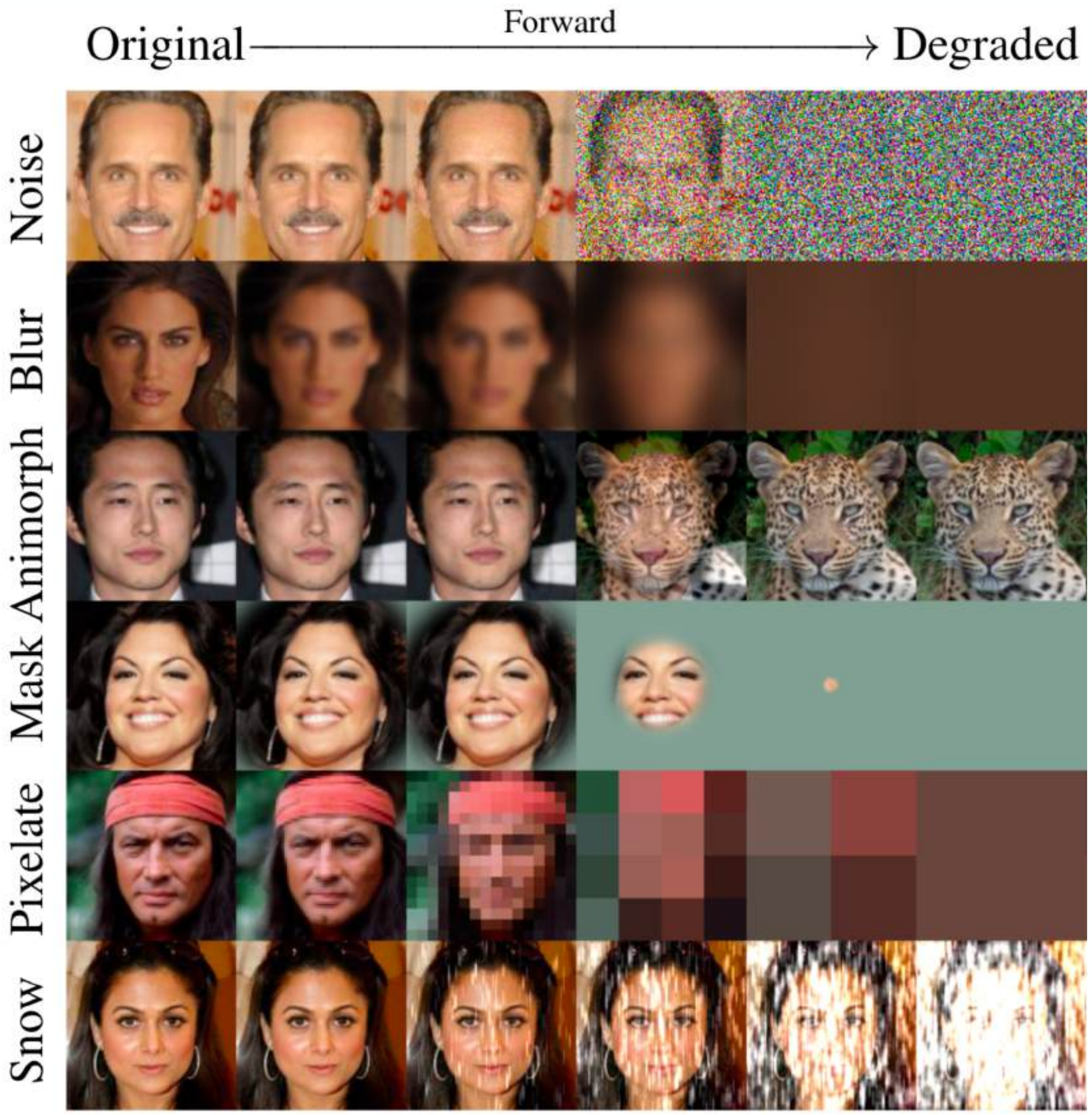
Diffusion posterior sampling



Chung, H., Sim, B., Ryu, D. and Ye, J.C., 2022. Improving Diffusion Models for Inverse Problems using Manifold Constraints. *arXiv preprint arXiv:2206.00941*.

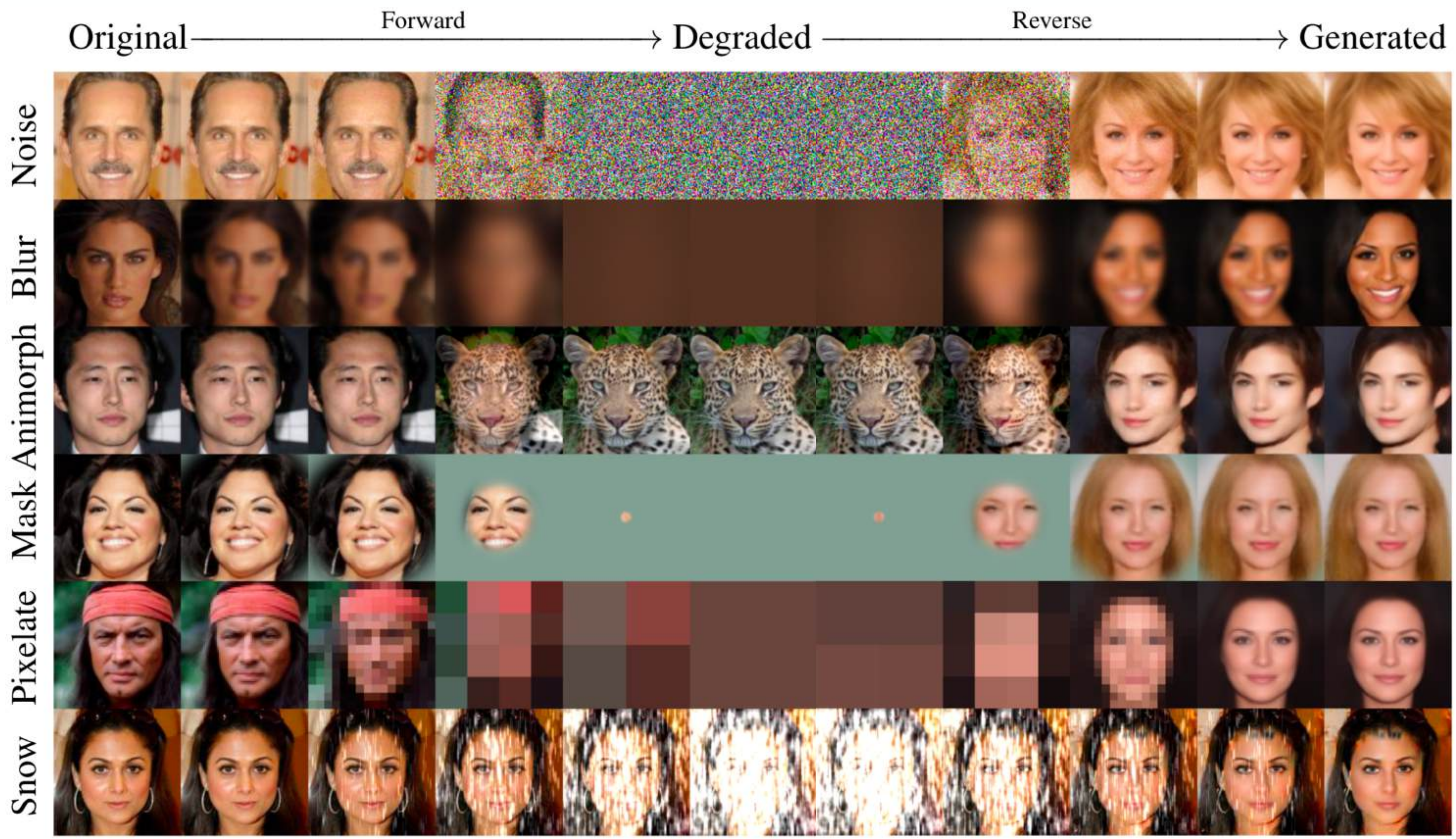
Dirac Diffusion

Cold diffusion



Bansal, Arpit, et al. "Cold diffusion: Inverting arbitrary image transforms without noise." *arXiv preprint arXiv:2208.09392* (2022).

Cold diffusion



Bansal, Arpit, et al. "Cold diffusion: Inverting arbitrary image transforms without noise." *arXiv preprint arXiv:2208.09392* (2022).

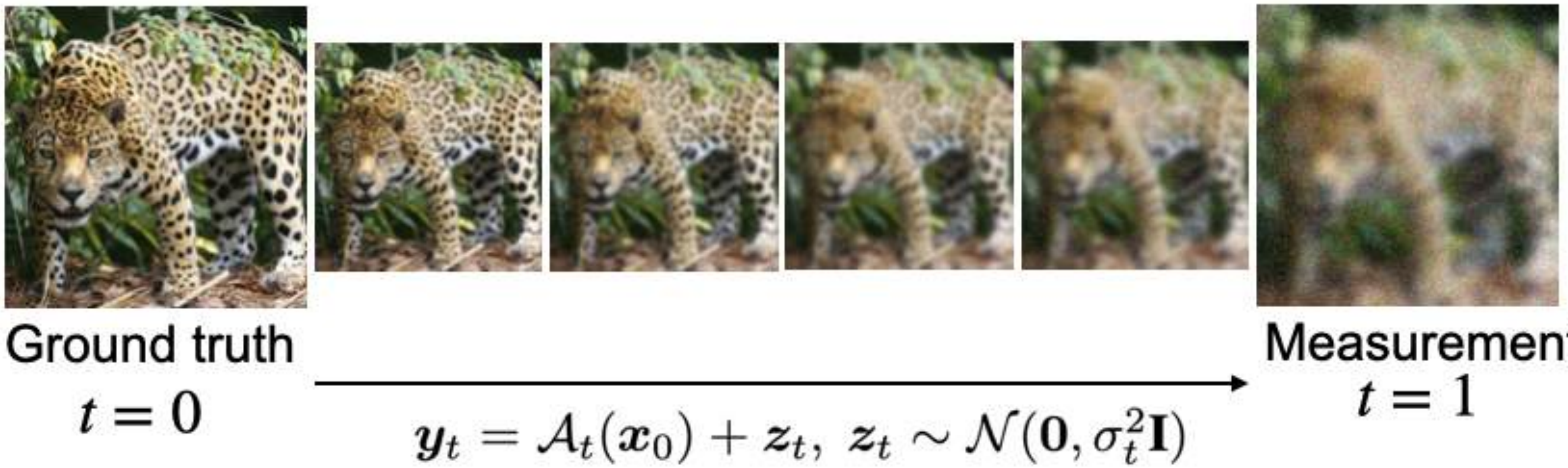
Stochastic Degradation Process (SDP)

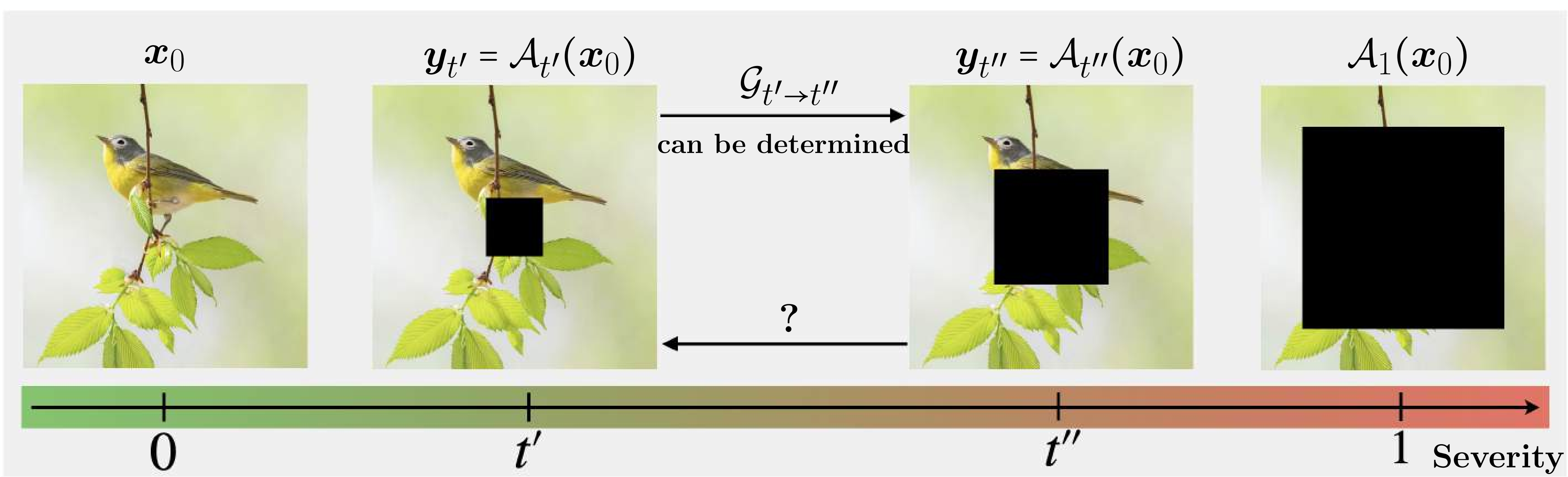
Ground truth $t = 0$

Measurement $t = 1$

$$\boldsymbol{y}_t = \mathcal{A}_t(\boldsymbol{x}_0) + \boldsymbol{z}_t,\ \boldsymbol{z}_t \sim \mathcal{N}(\mathbf{0}, \sigma_t^2 \mathbf{I})$$

Degradation Severity



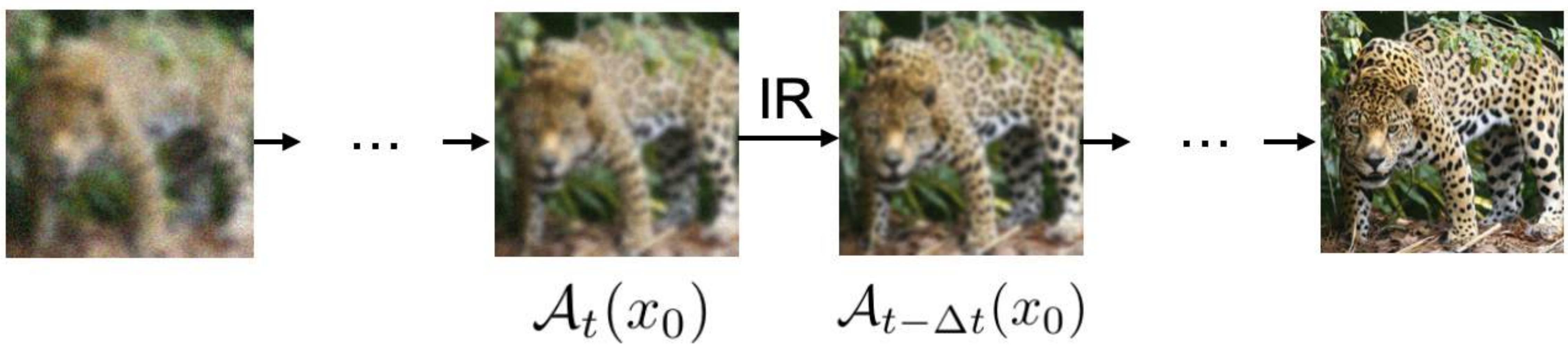


<u>Property 1</u>: $\mathcal{A}_t$ is more severe than $\mathcal{A}_{t'}$, $\forall t > t'$

<u>Property 2</u>: $\mathcal{A}_0(\mathbf{x_0}) = \mathbf{x_0}$

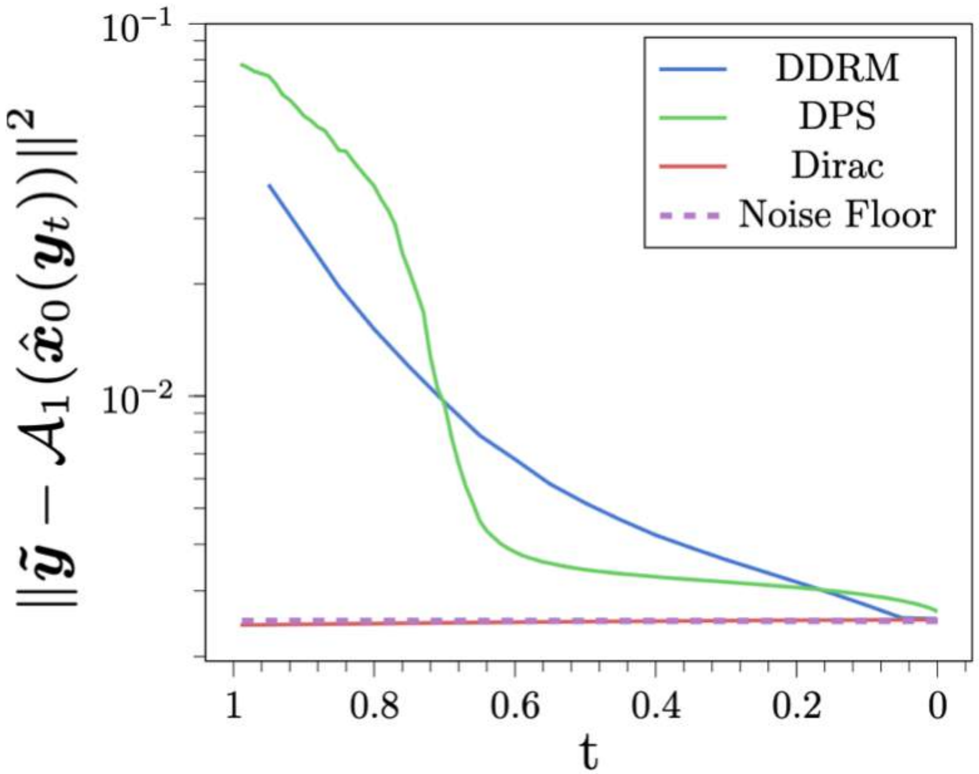
DiracDiffusion
(Denoising and Incremental Reconstruction with Assured Data-Consistency)

We learn to iteratively reverse small steps of degradation, which we call **incremental reconstruction** (IR).

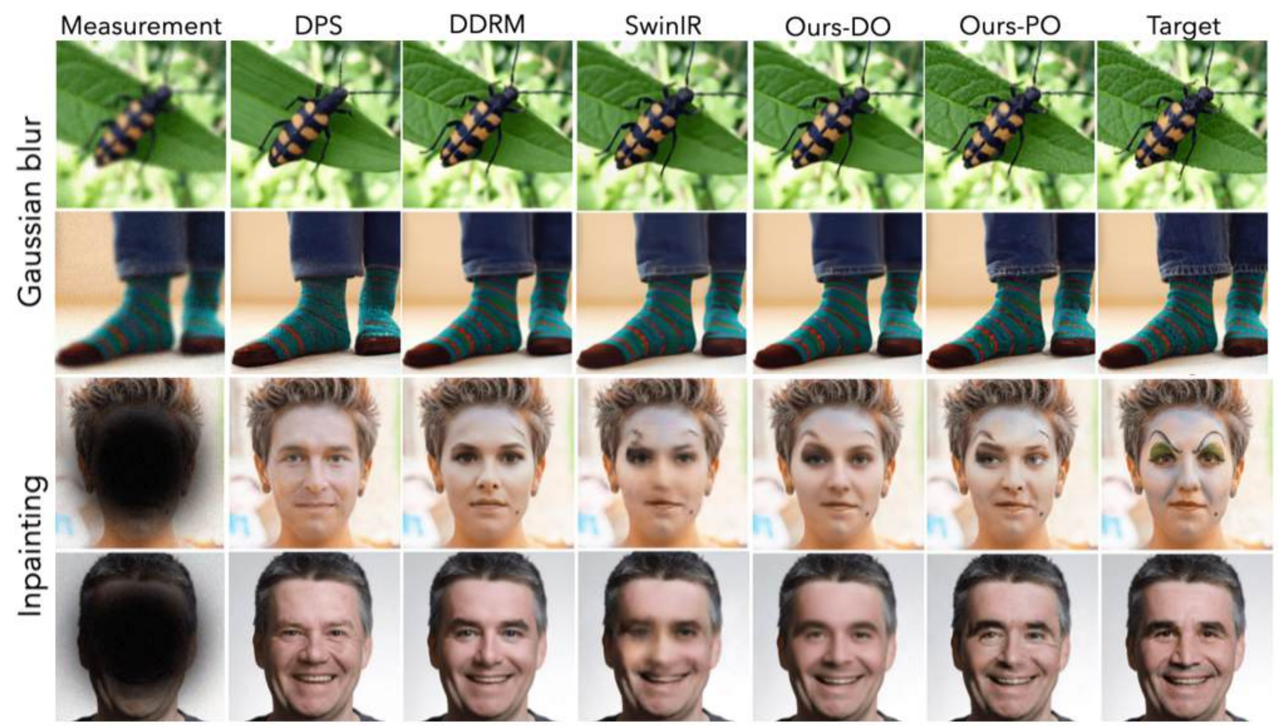


Experimental Results

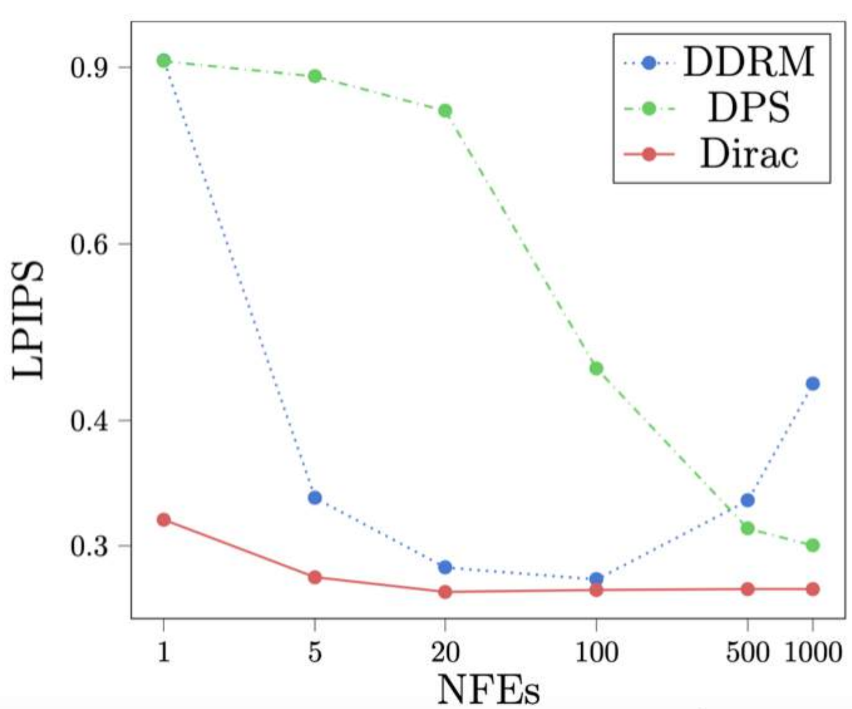
Data-consistency



Excellent reconstruction quality



Fast sampling



Method	Deblurring PSNR(↑)	SSIM(↑)	LPIPS(↓)	FID(↓)	Inpainting PSNR(↑)	SSIM(↑)	LPIPS(↓)	FID(↓)
Dirac-PO (ours)	26.67	0.7418	**0.2716**	**53.36**	25.41	0.7595	0.2611	**39.43**
Dirac-DO (ours)	28.47	0.8054	0.2972	69.15	**26.98**	**0.8435**	**0.2234**	51.87
DPS (Chung et al., 2022a)	25.56	0.6878	0.3008	65.68	21.06	0.7238	0.2899	57.92
DDRM (Kawar et al., 2022a)	27.21	0.7671	0.2849	65.84	25.62	0.8132	0.2313	54.37
SwinIR (Liang et al., 2021)	**28.53**	**0.8070**	0.3048	72.93	24.46	0.8134	0.2660	59.94
PnP-ADMM (Chan et al., 2016)	27.02	0.7596	0.3973	74.17	12.27	0.6205	0.4471	192.36
ADMM-TV	26.03	0.7323	0.4126	89.93	11.73	0.5618	0.5042	264.62

Method	Deblurring PSNR(↑)	SSIM(↑)	LPIPS(↓)	FID(↓)	Inpainting PSNR(↑)	SSIM(↑)	LPIPS(↓)	FID(↓)
Dirac-PO (ours)	24.68	0.6582	**0.3302**	53.91	26.36	0.8087	0.2079	34.33
Dirac-DO (ours)	**25.76**	**0.7085**	0.3705	83.23	**28.92**	**0.8958**	**0.1676**	38.25
DPS (Chung et al., 2022a)	21.51	0.5163	0.4235	**52.60**	22.71	0.8026	0.1986	34.55
DDRM (Kawar et al., 2022a)	24.53	0.6676	0.3917	61.06	25.92	0.8347	0.2138	**33.71**
SwinIR (Liang et al., 2021)	25.07	0.6801	0.4159	84.80	26.87	0.8490	0.2161	45.69
PnP-ADMM (Chan et al., 2016)	25.02	0.6722	0.4565	98.72	18.14	0.7901	0.2709	101.25
ADMM-TV	24.31	0.6441	0.4578	88.26	17.60	0.7229	0.3157	120.22

Table 1. Experimental results on the FFHQ (top) and ImageNet (bottom) test splits.

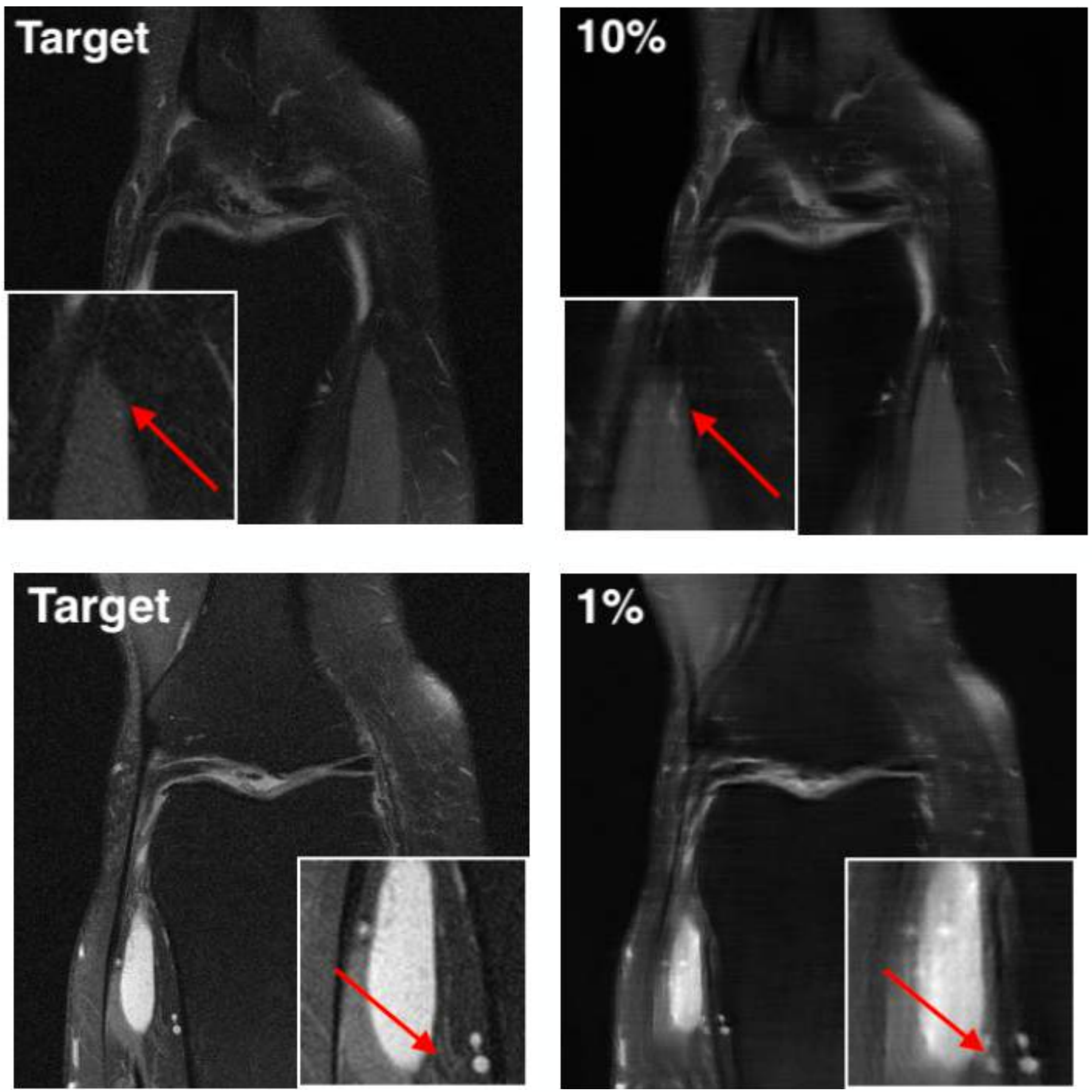
Untrained methods


TIME IS
RUNNING
OUT
0:53 47
0:27 08

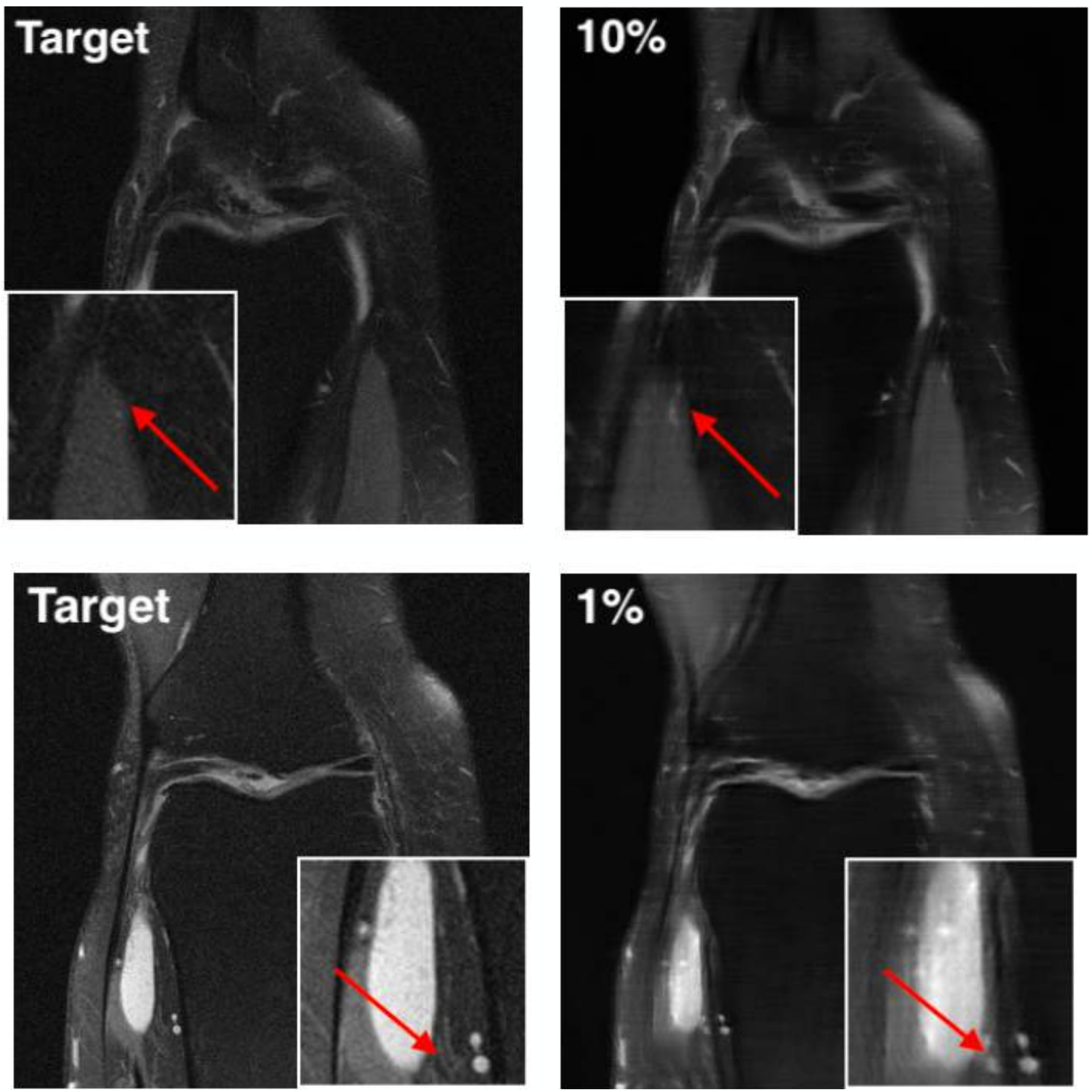
Future Directions

Reliability Challenge

Hallucinations

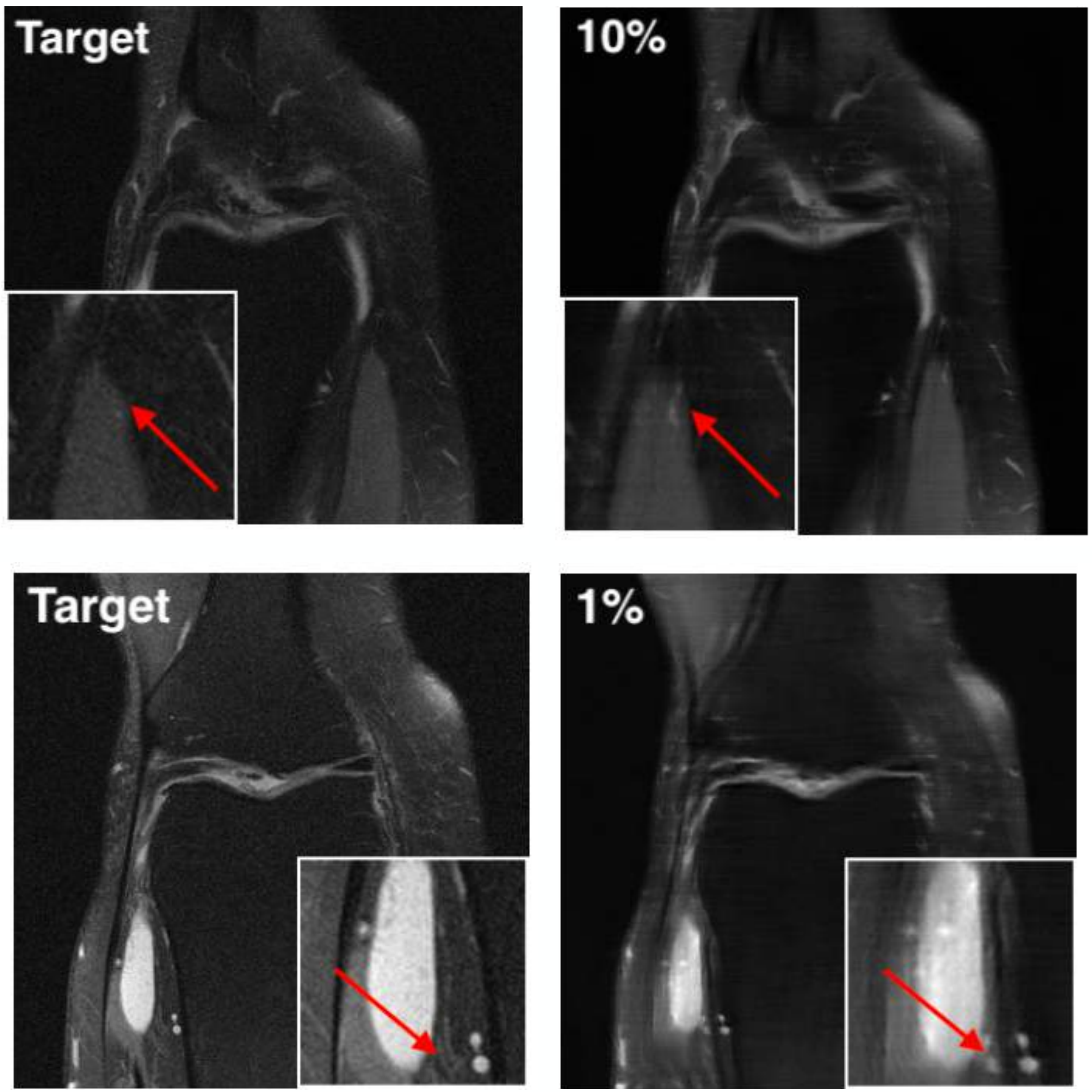


Hallucinations



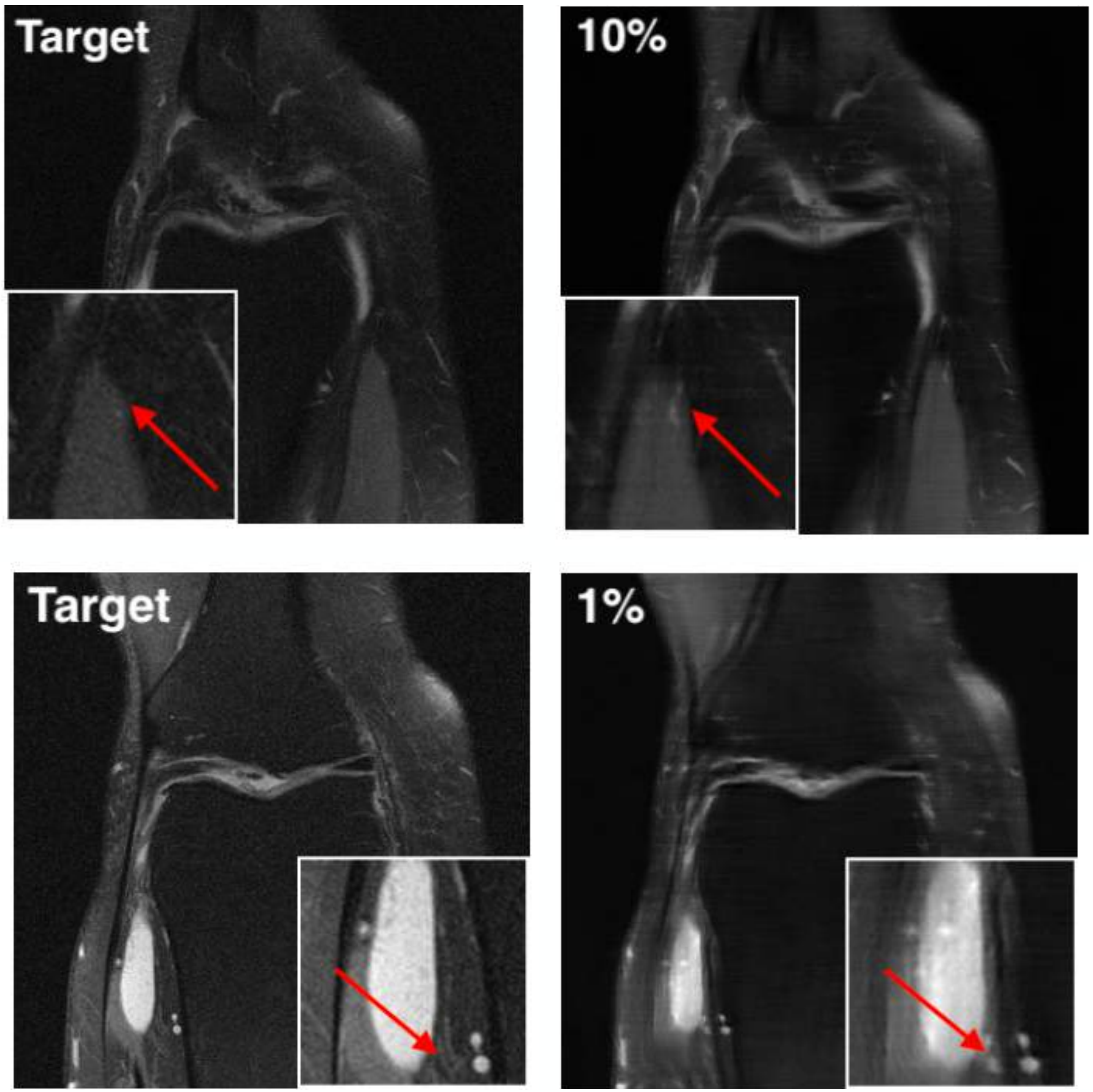
- DL model “sees” features on reconstructions that shouldn’t be present

Hallucinations



- DL model "sees" features on reconstructions that shouldn't be present
- Hallucinated features appear real as opposed to reconstruction artifacts

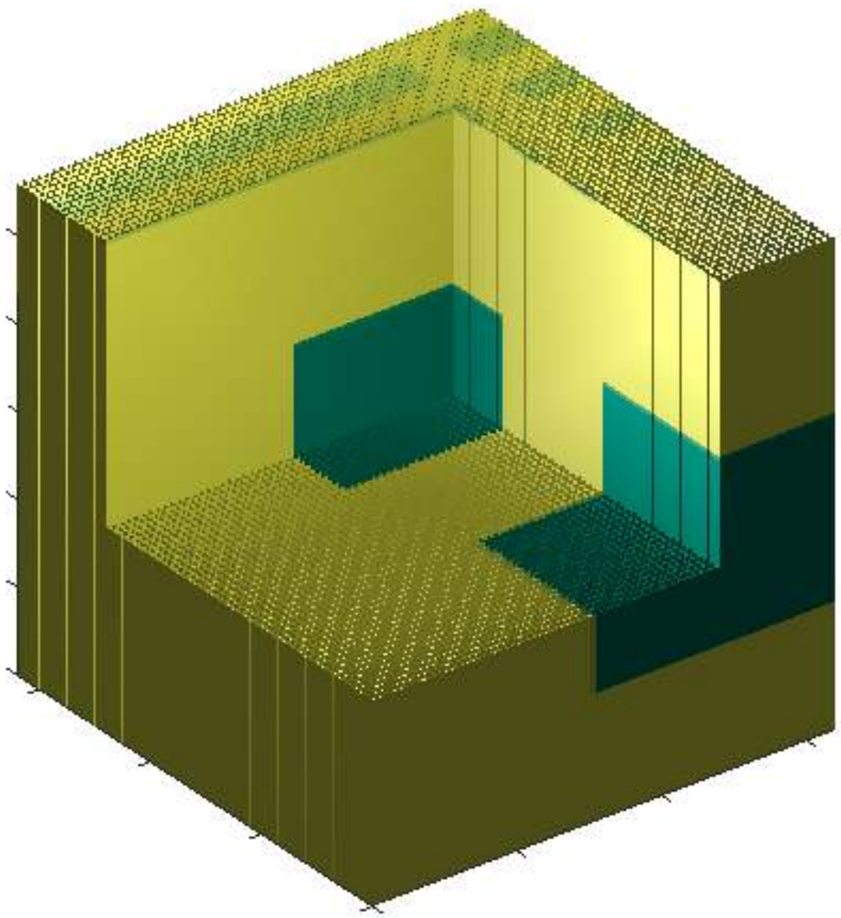
Hallucinations



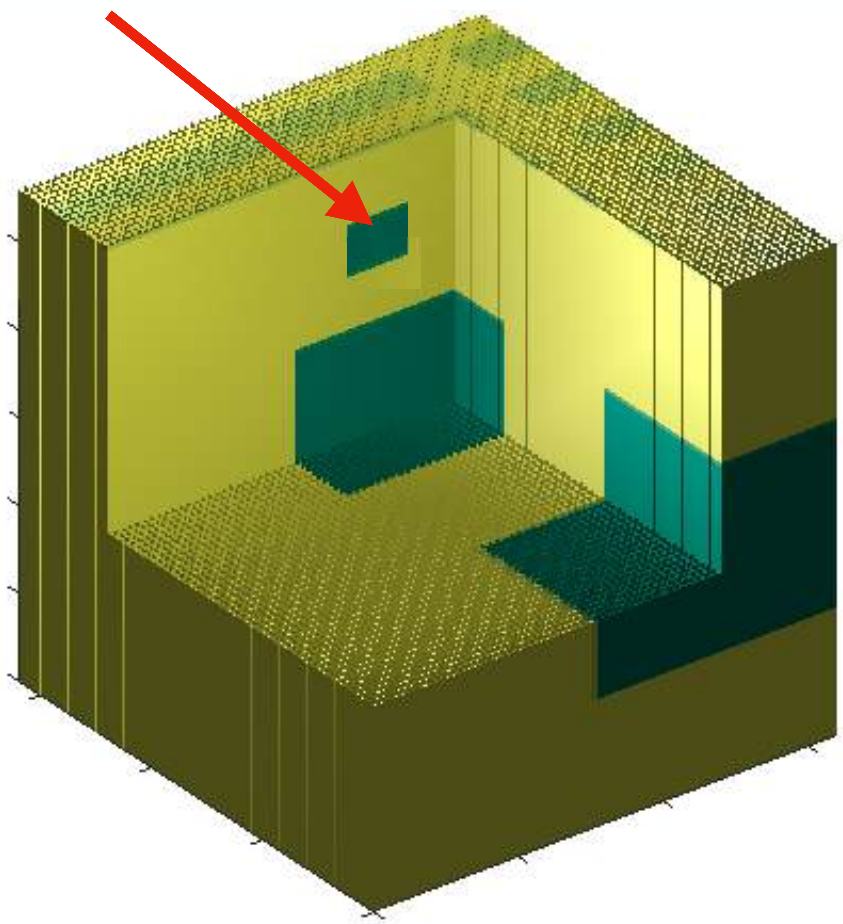
- DL model "sees" features on reconstructions that shouldn't be present
- Hallucinated features appear real as opposed to reconstruction artifacts
- Can lead to critical mistakes (misdiagnosis)

Critical reconstruction errors

- 3D nano-scale imaging example



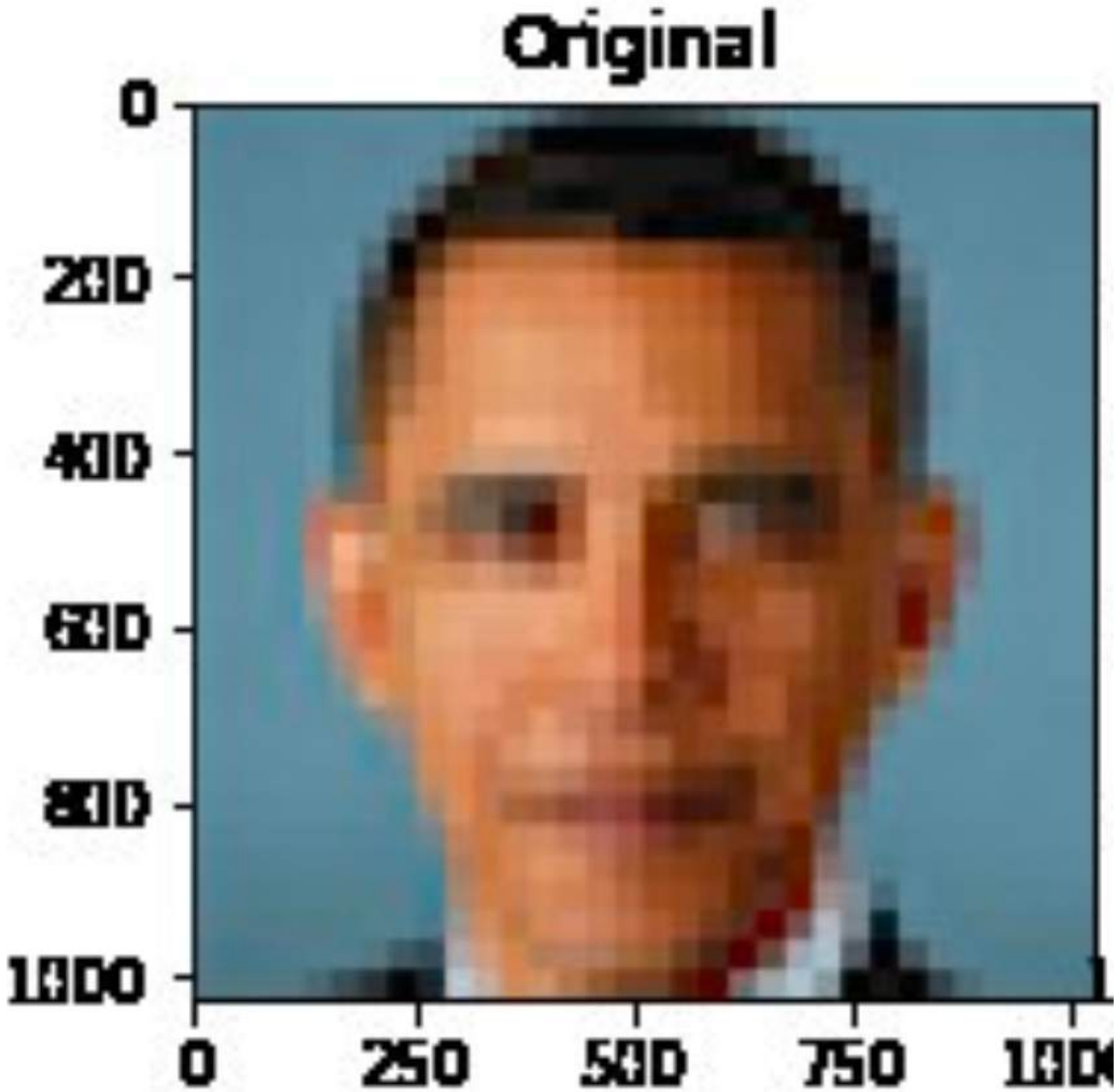
Target nano-structure



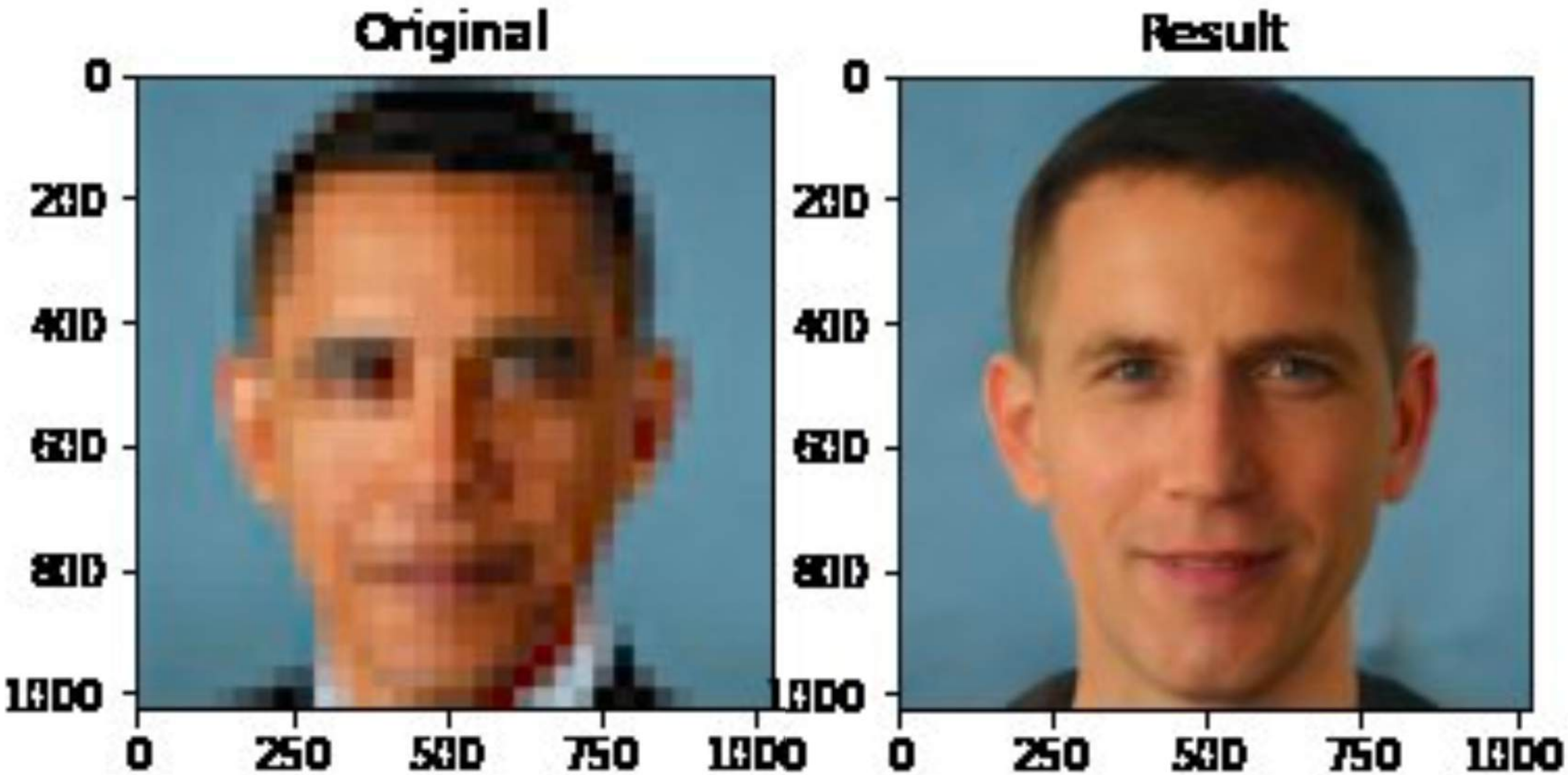
DL reconstruction

Bias

Bias

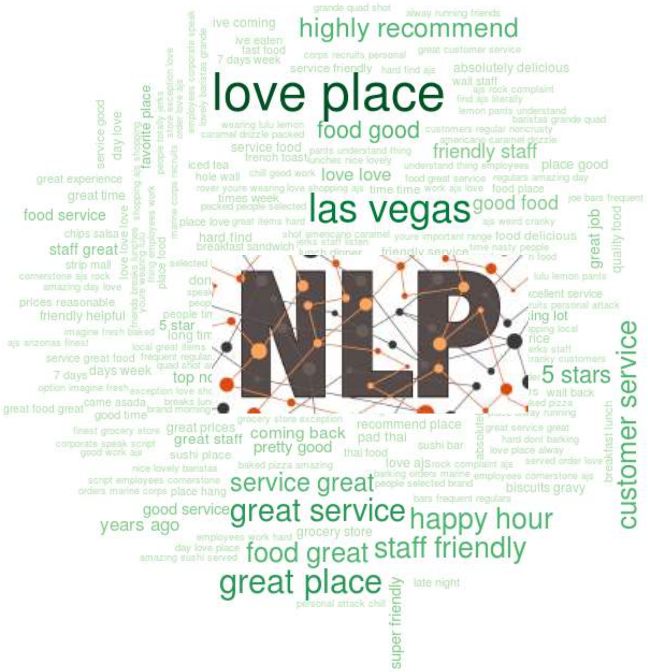


Bias

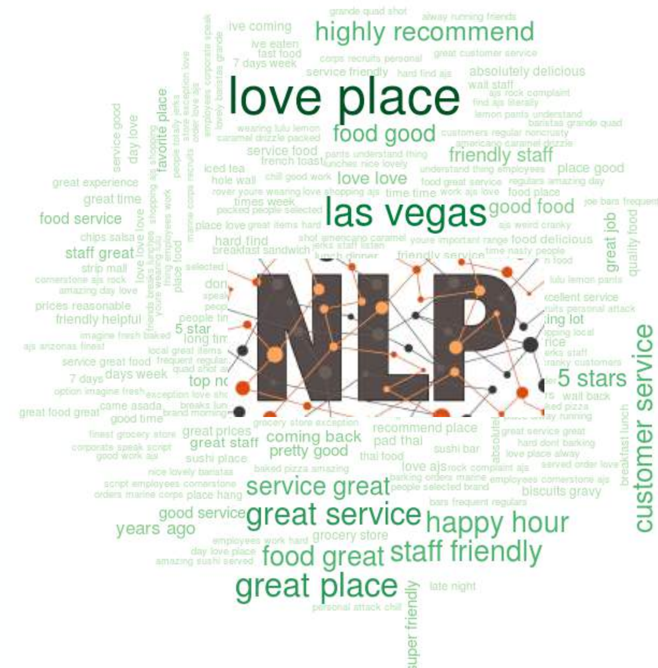


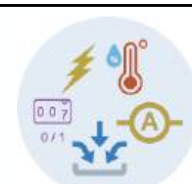
Data Scarcity Challenge

Deep learning is data-hungry

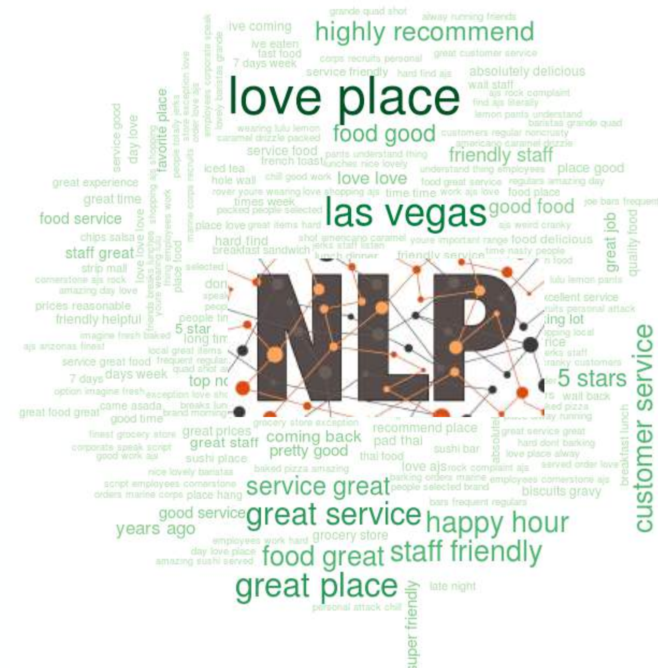


Deep learning is data-hungry



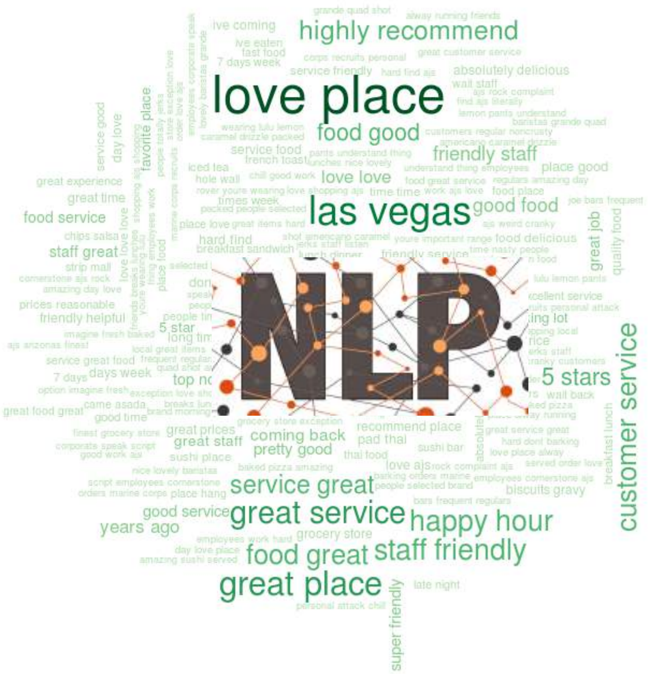
	'Internet data'
Data acquisition 	readily available

Deep learning is data-hungry



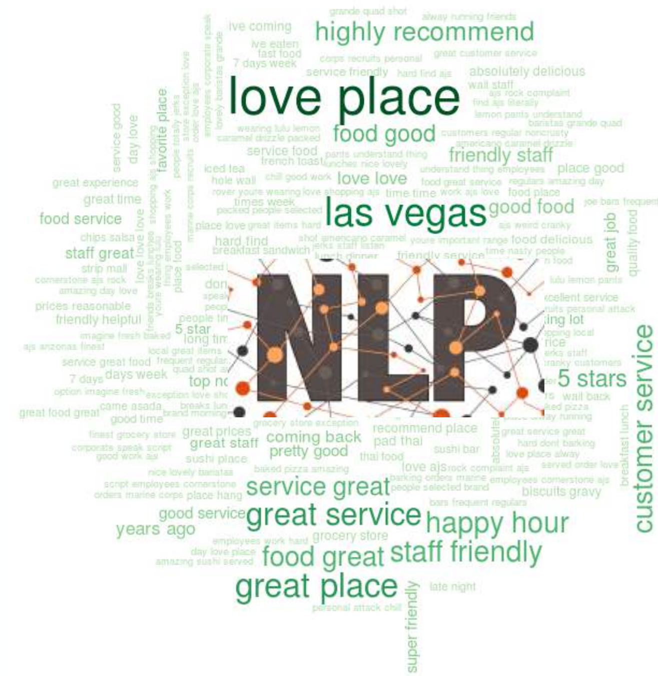
	'Internet data'
Data acquisition	readily available
Cost	very low

Deep learning is data-hungry



	'Internet data'
Data acquisition	readily available
Cost	very low
Amount of data	huge

Deep learning is data-hungry



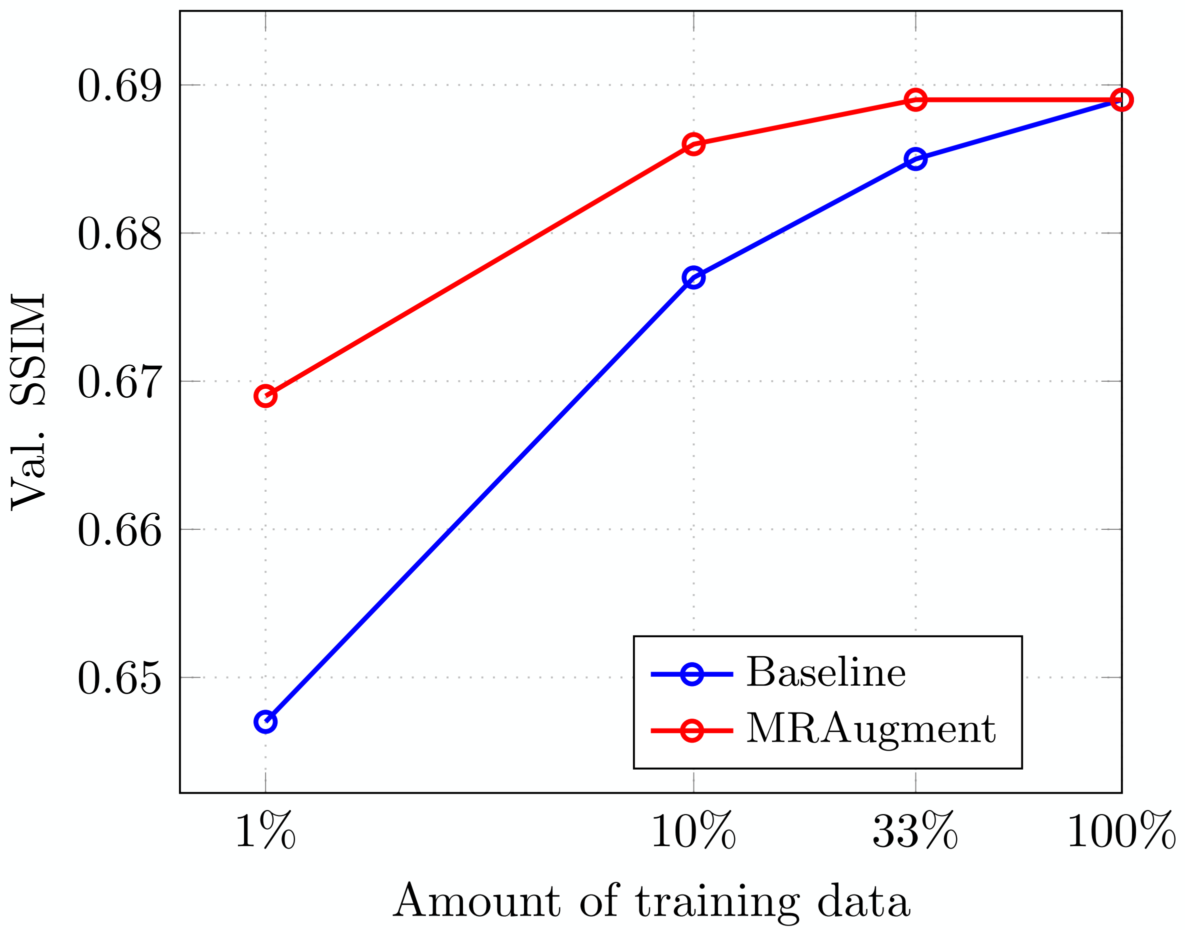
	'Internet data'
Data acquisition	readily available
Cost	very low
Amount of data	huge

How about scientific data?

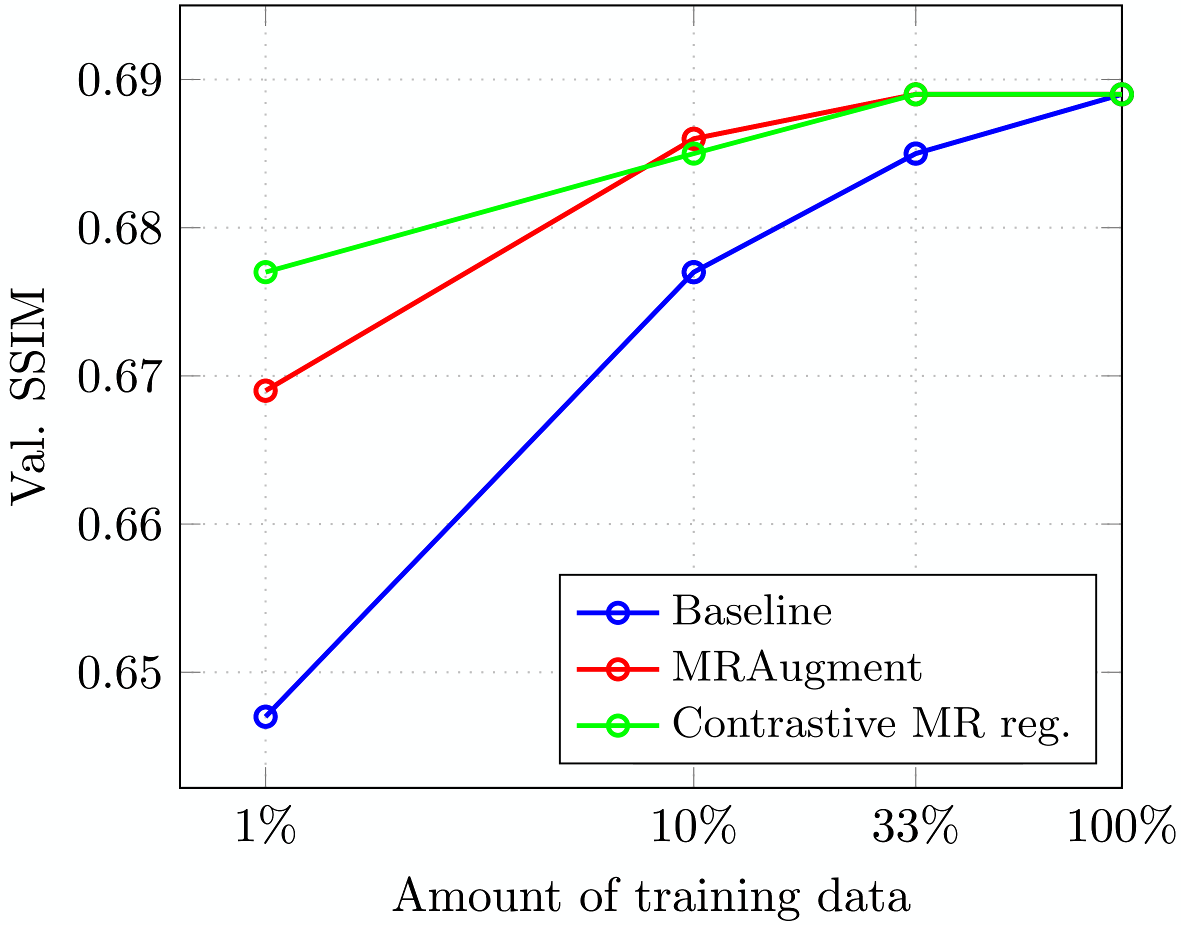
Create a Phase Retrieval DataSet

Reduce reliance on training data

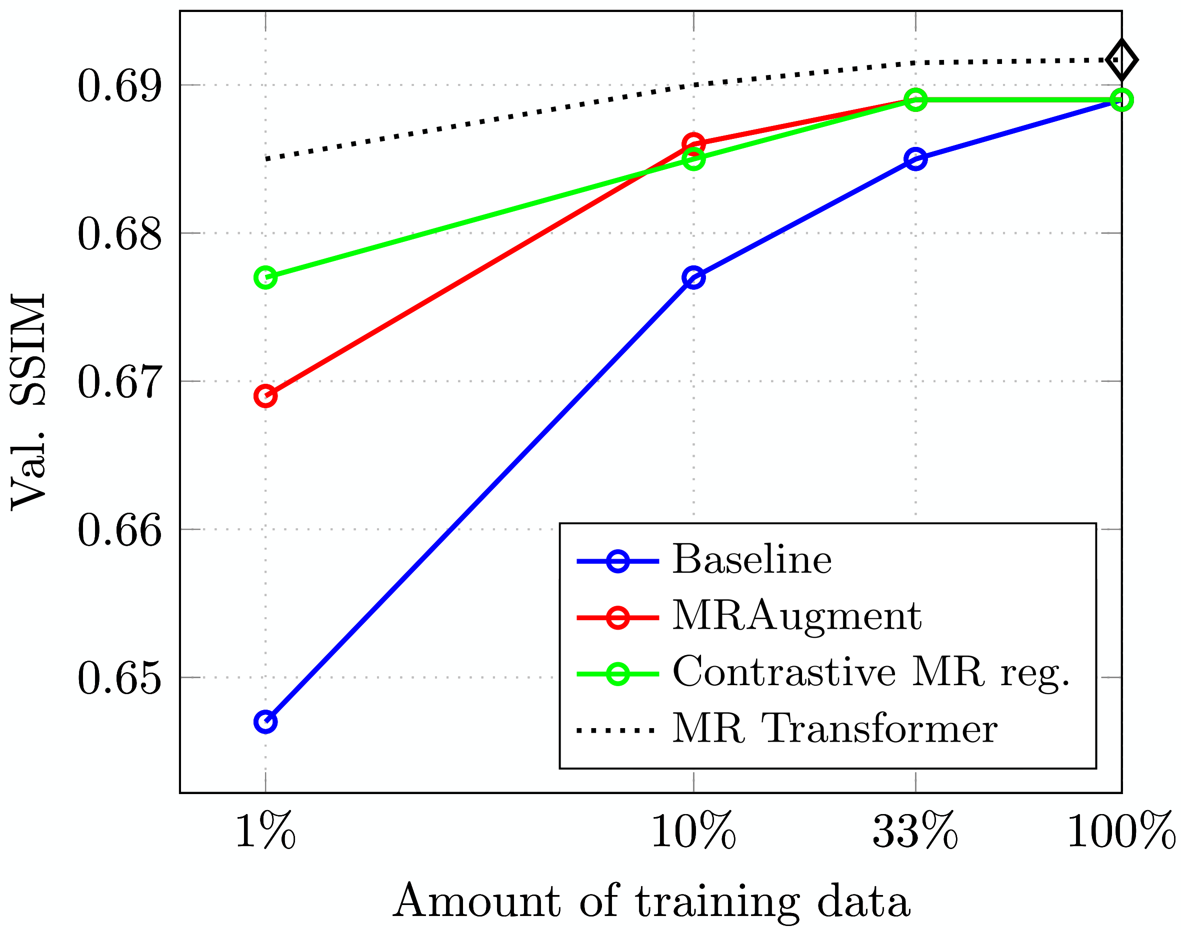
Reduce reliance on training data



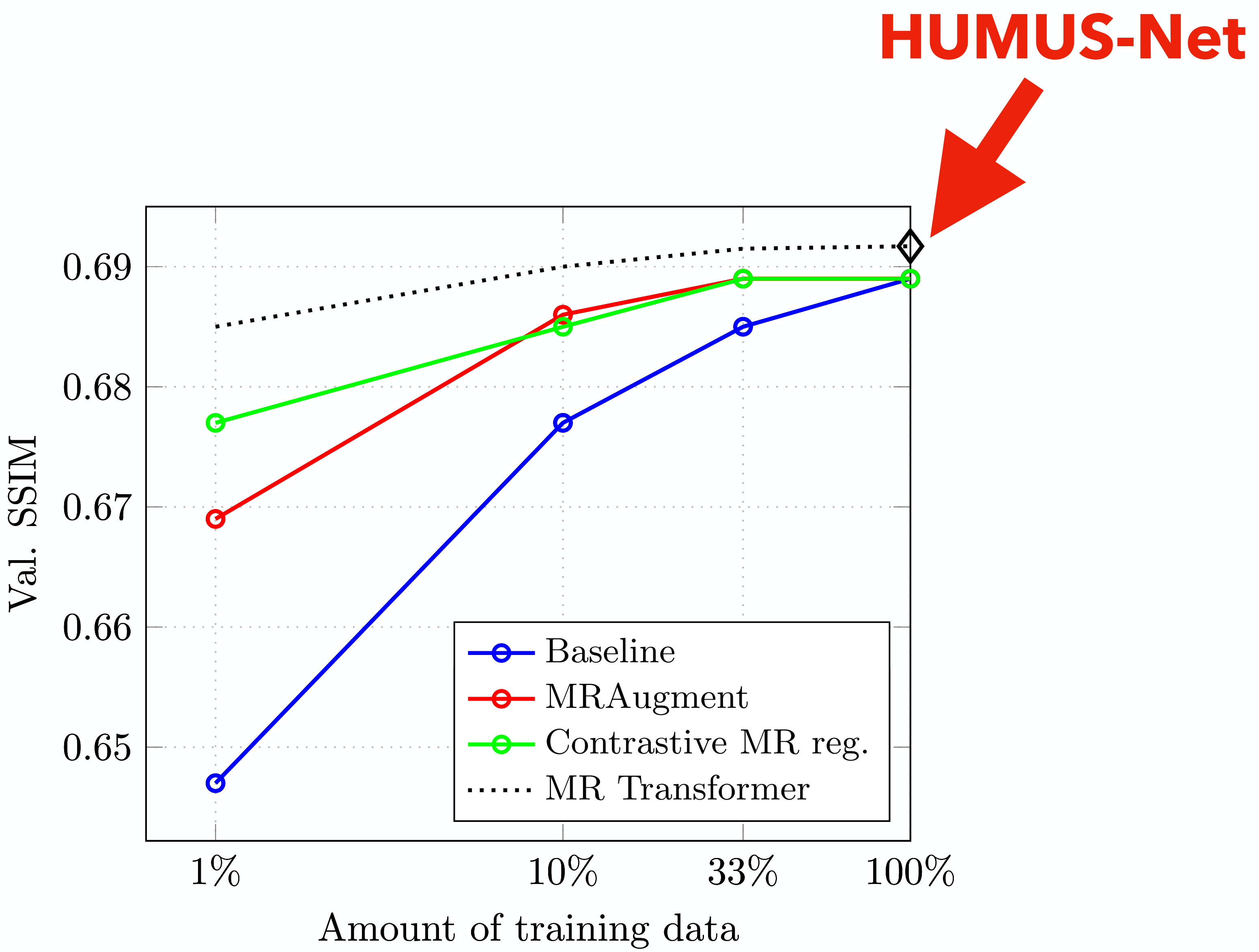
Reduce reliance on training data



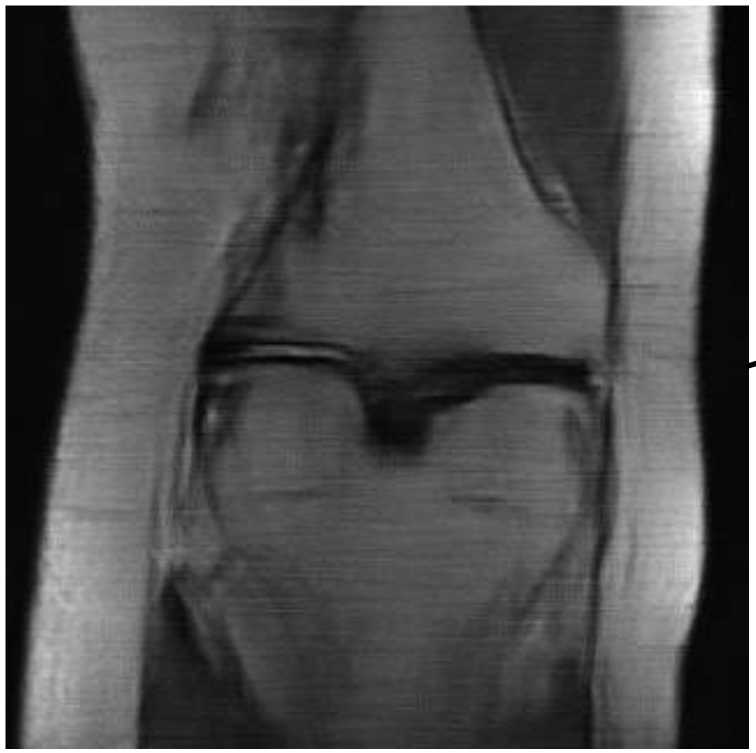
Reduce reliance on training data

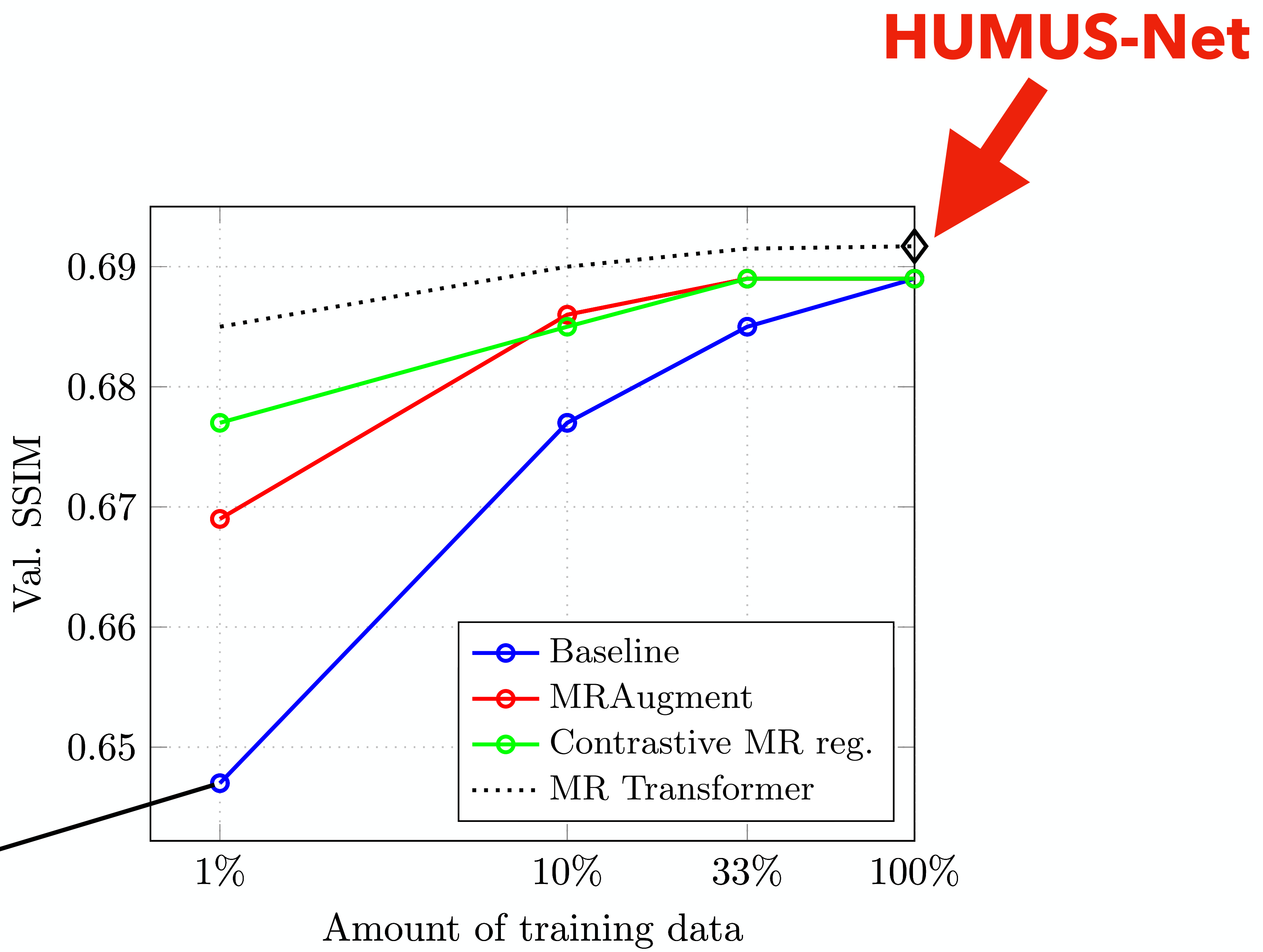


Reduce reliance on training data

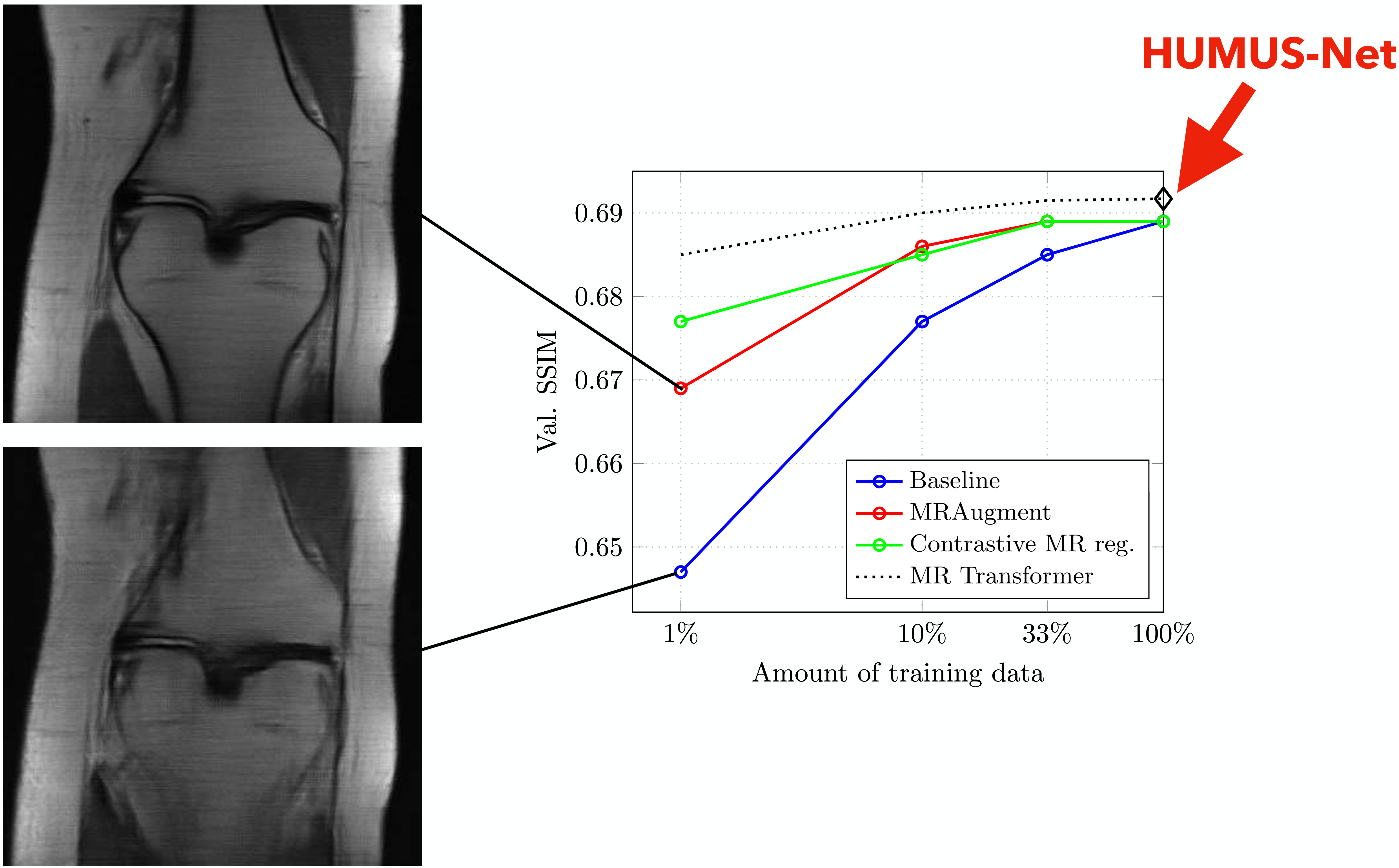


Reduce reliance on training data





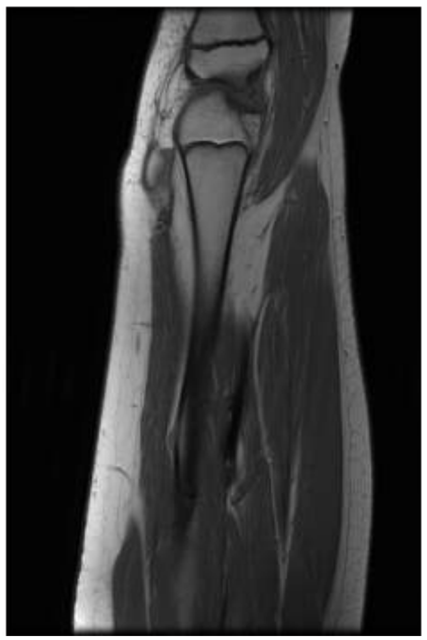
Reduce reliance on training data



Computational/complexity Challenge

Complexity of scientific data

High spatial resolution

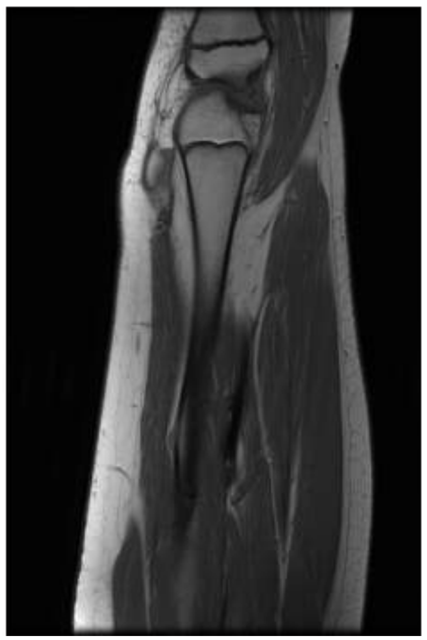


640×368

32×32

Complexity of scientific data

High spatial resolution



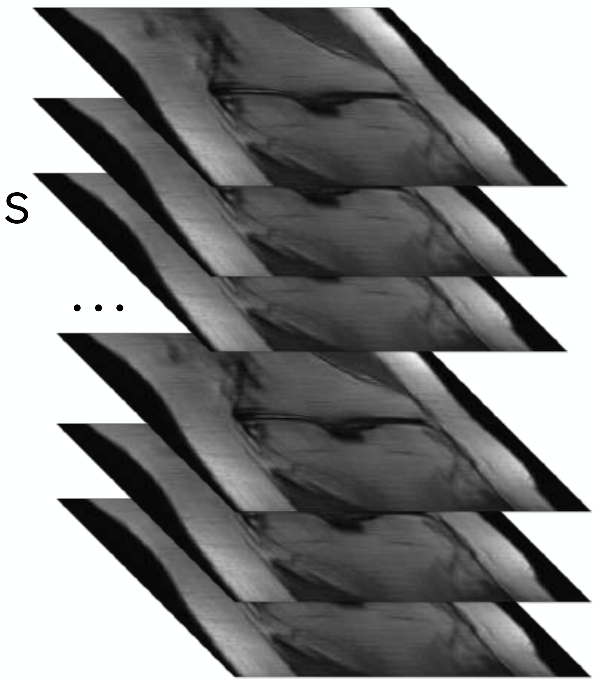
640×368

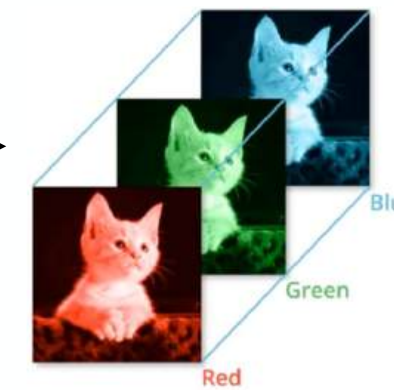
32×32

Large number of image channels

15+ coils

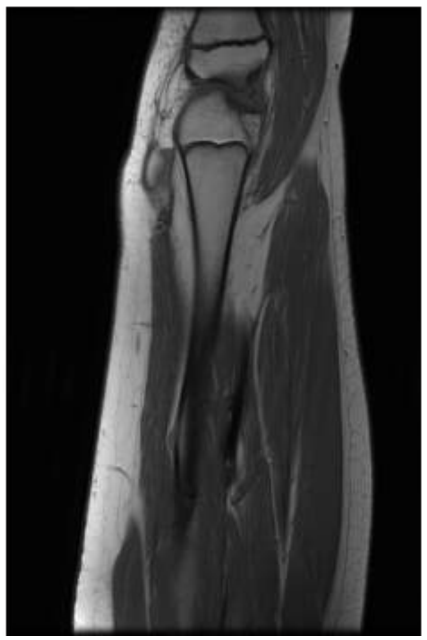
…





Complexity of scientific data

High spatial resolution



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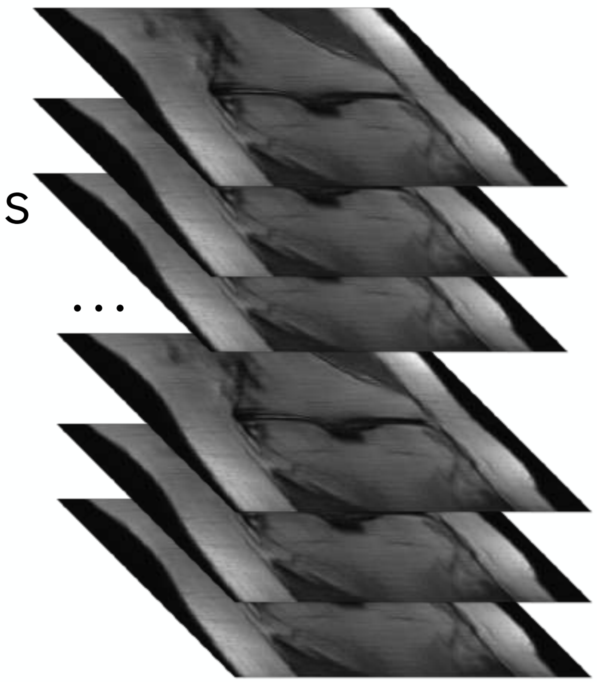

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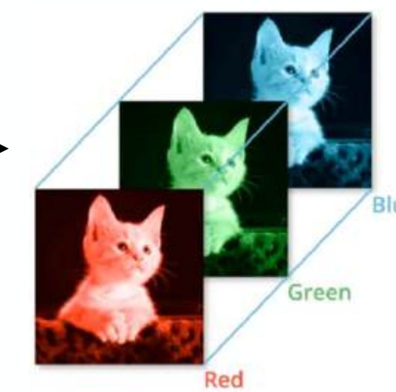
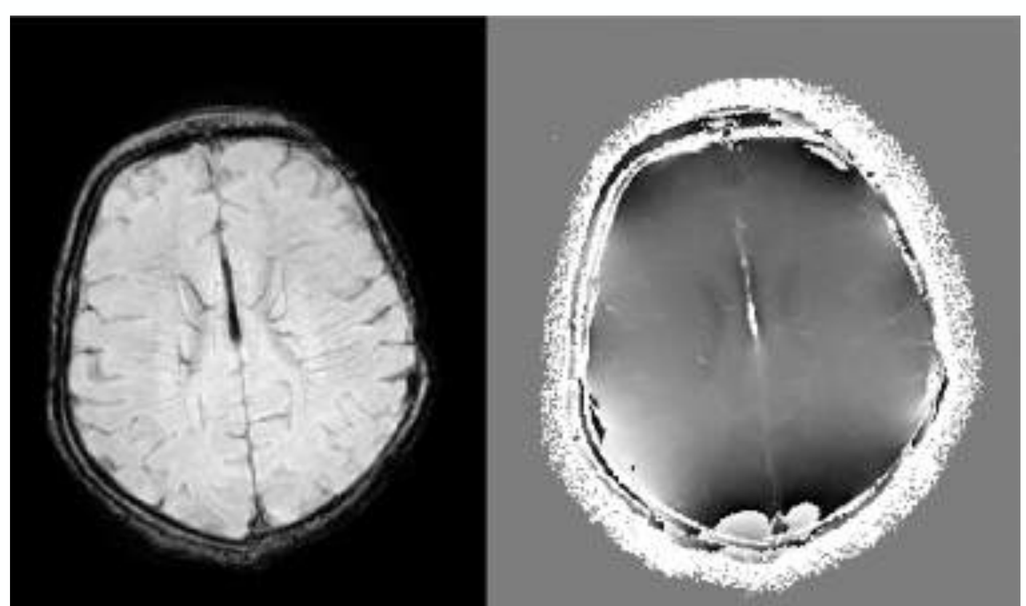


Complex valued images



magnitude *phase*

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Great Talk by Alex Dimakis on Generative models

https://simons.berkeley.edu/sites/default/files/docs/18458/simons-dimakis.pdf

Great Tutorial By Arash Vahdat and Collaborators on Diffusion Models

https://www.youtube.com/watch?v=cS6JQpEY9cs

https://www.youtube.com/watch?v=1d4r19GEVos

- Additional References: https://docs.google.com/spreadsheets/d/1e36mDqj8SY9ODT3Kz8frqSchK2QDWZdHuzVy-EKjhFo/edit?usp=sharing