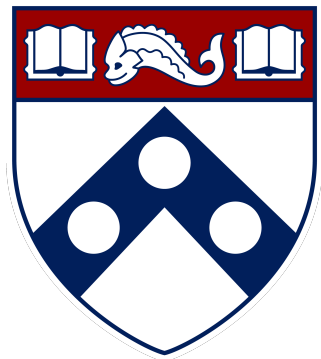
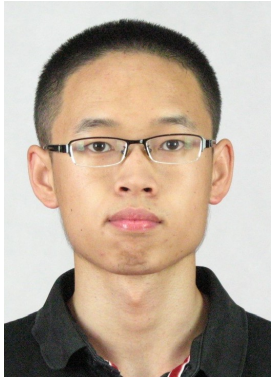
Non-asymptotic theory for diffusion models



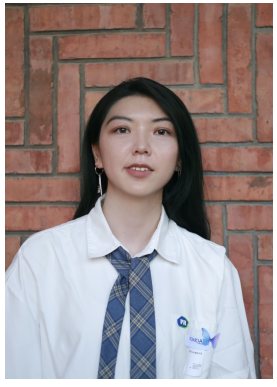
Yuxin Chen

Wharton Statistics & Data Science

*= equal contributions



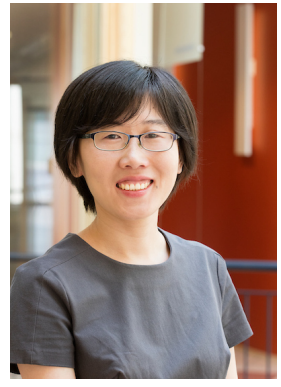
Gen Li* **CUHK**



Yu Huang* **UPenn**

Timofey Efimov CMU

Yuting Wei UPenn



Yuejie Chi CMU

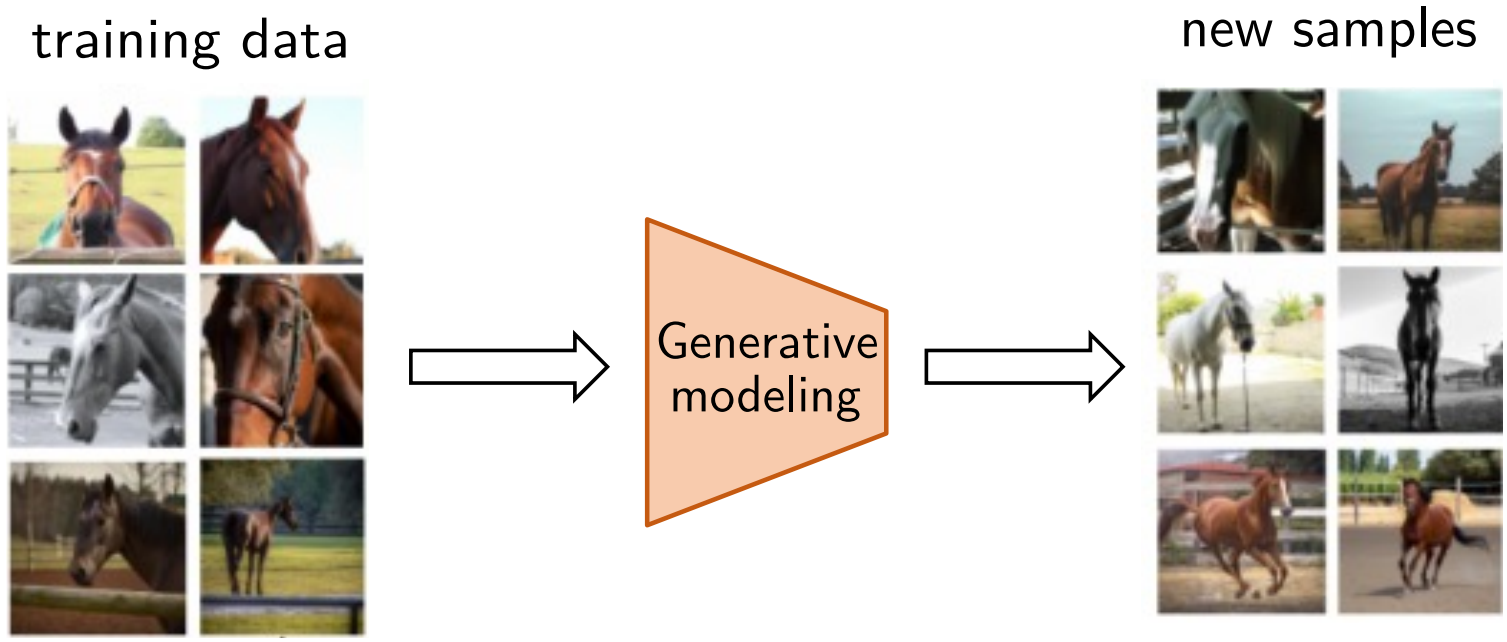
The era of generative AI

Generative models

training data

- Given training data $\underbrace{X^{\text{train},i} \sim p_{\text{data}}}_{\text{from a general distribution}}$ $(1 \leq i \leq N)$ in $\mathbb{R}^d$

Generative models



- Given training data $\underbrace{X^{\text{train},i} \sim p_{\text{data}}}_{\text{from a general distribution}}$ $(1 \leq i \leq N)$ in $\mathbb{R}^d$
- Generate new samples $Y \sim p_{\text{data}}$

Generative adversarial networks (GAN)

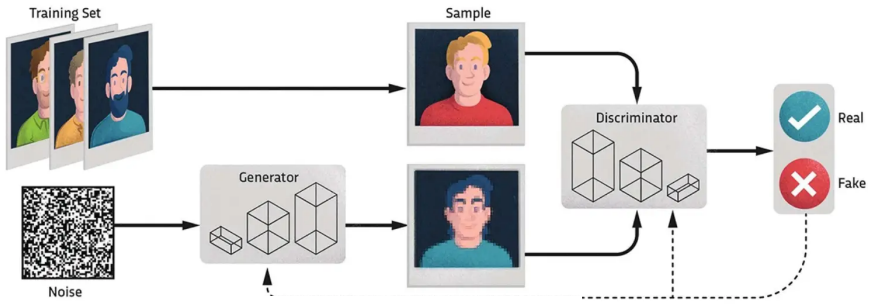


fig. credit: Science Focus

Variational autoencoder (VAE)

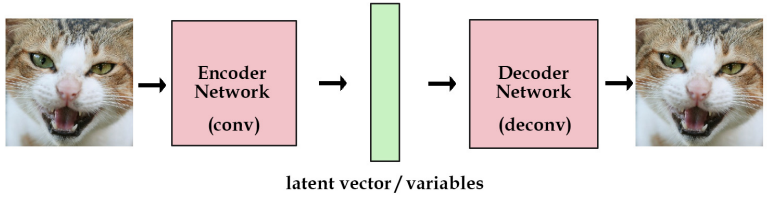


fig. credit: kevin frans blog

Diffusion models

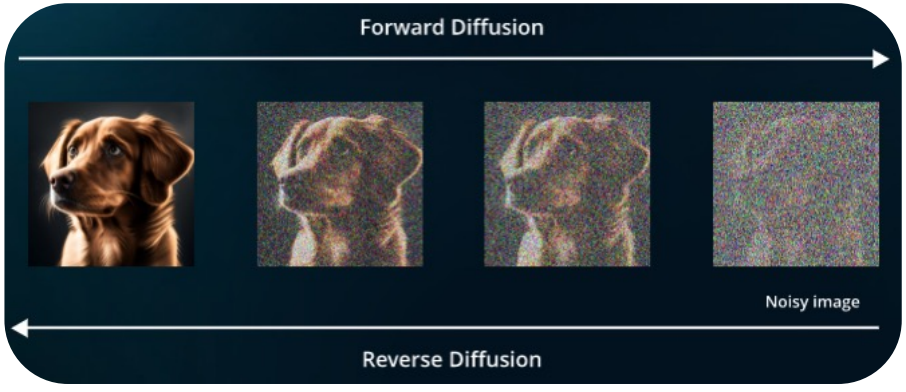


fig. credit: LeewayHertz

Inspired by nonequilibrium thermodynamics

— Sohl-Dickstein, Weiss, Maheswaranathan, Ganguli '15

Diffusion models

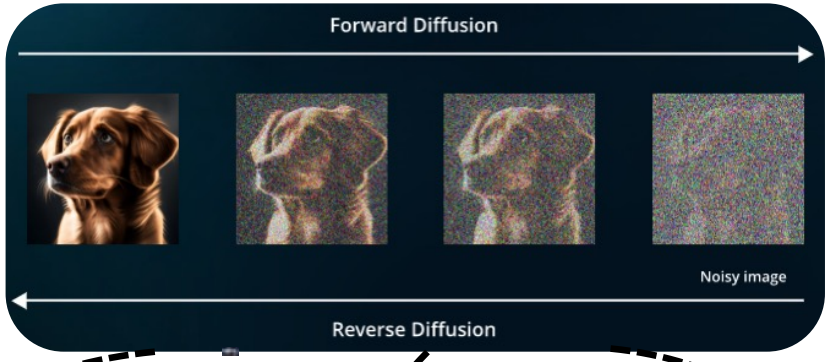
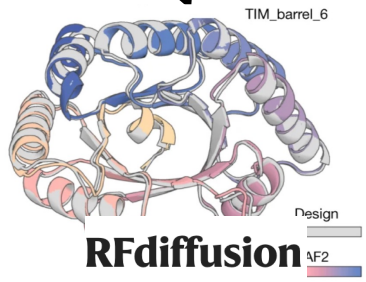


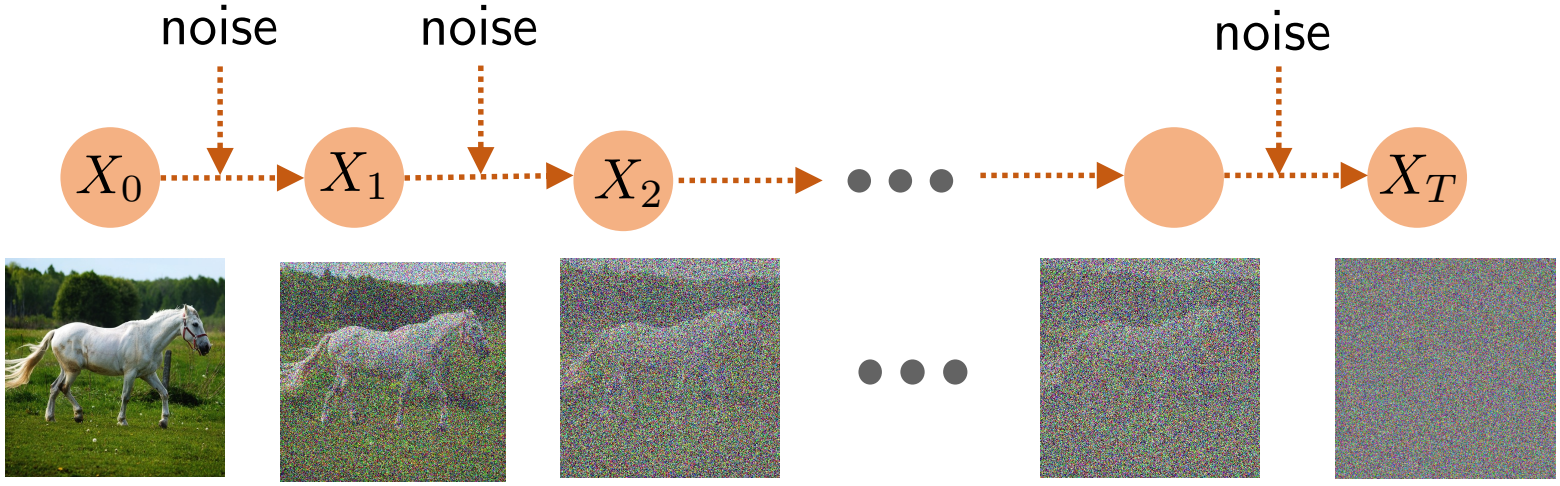
image generation

video generation

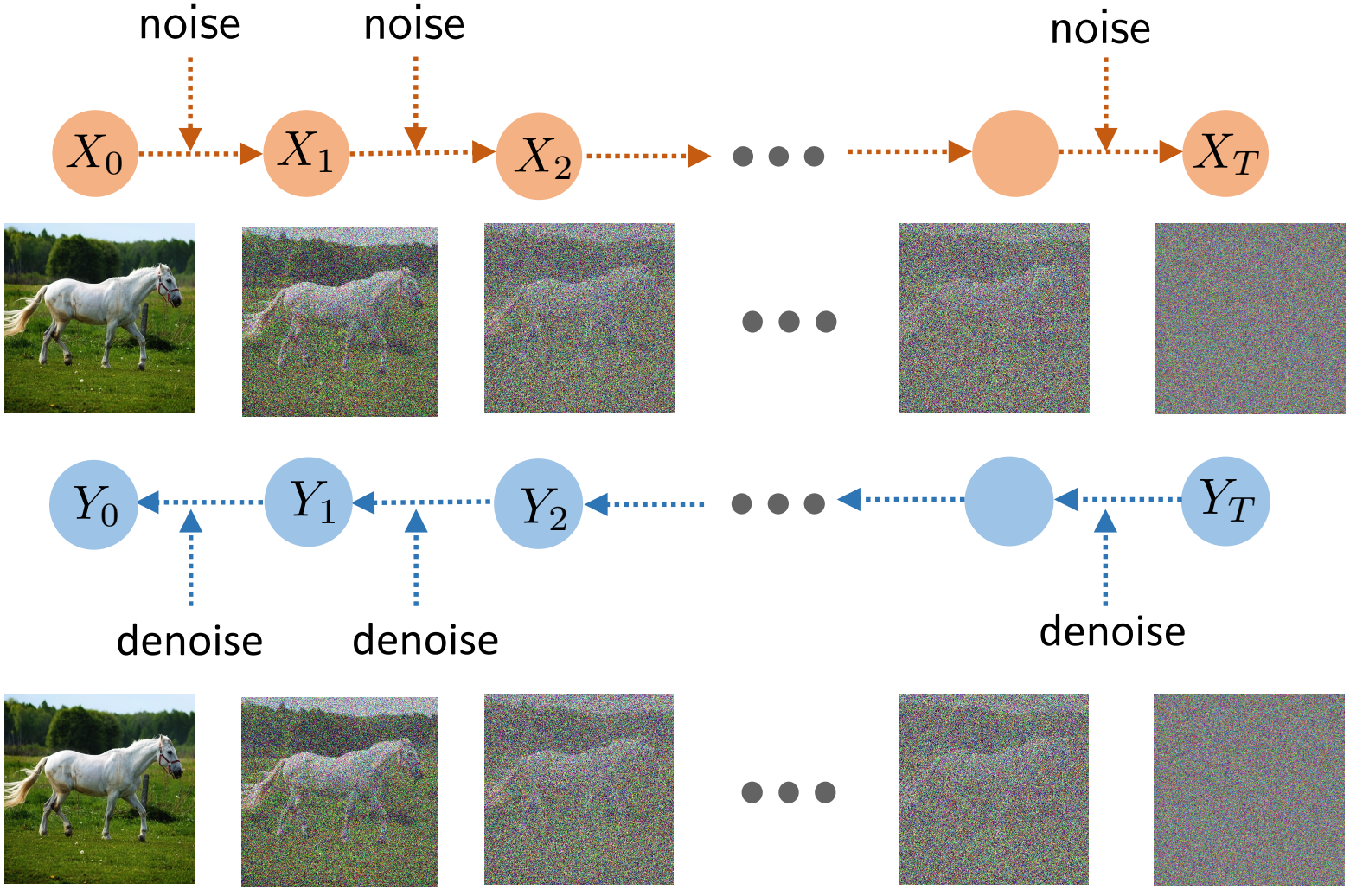


protein design

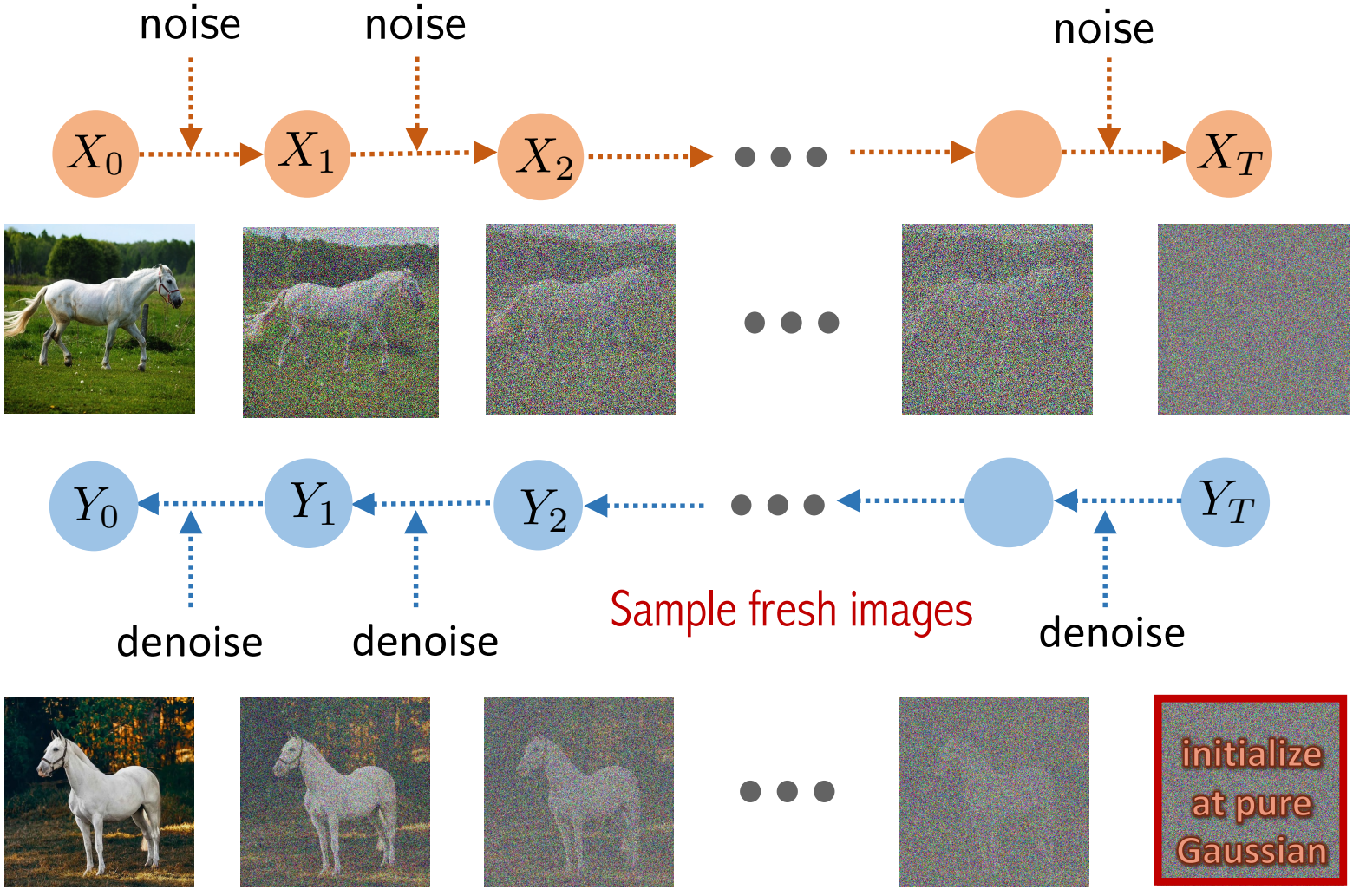
Preliminaries: score-based diffusion models



- **forward process:** (progressively) diffuse data into noise



- **forward process:** (progressively) diffuse data into noise
- **reverse process:** convert pure noise into data-like distributions



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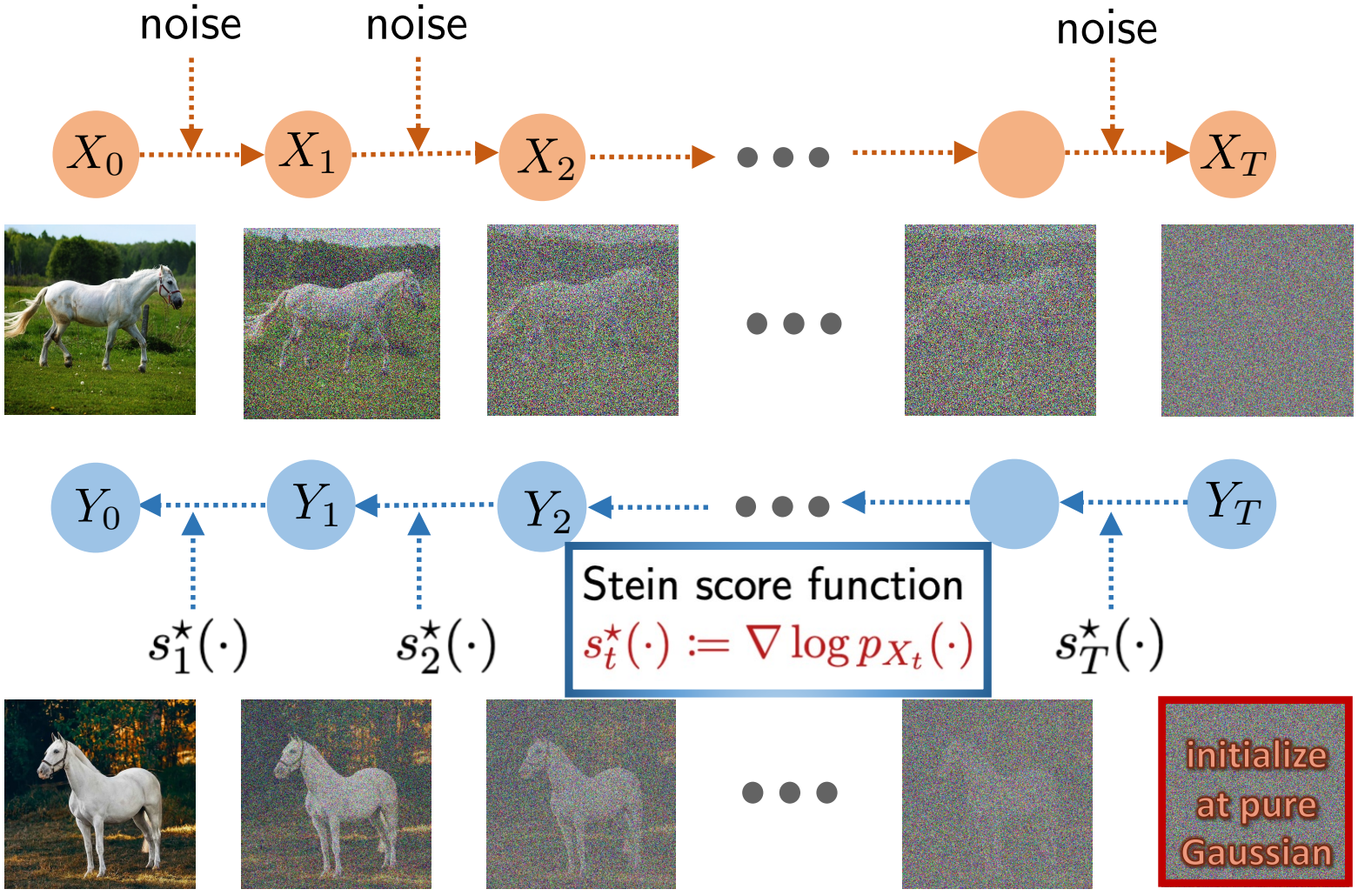

- **forward process:** (progressively) diffuse data into noise
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Goal: $Y_t \overset{\mathrm{d}}{\approx} X_t, \quad t = T, \cdots, 1$

key component: score functions of forward process: $\underbrace{\nabla \log p_{X_t}(X)}_{\text{w.r.t. } X}$

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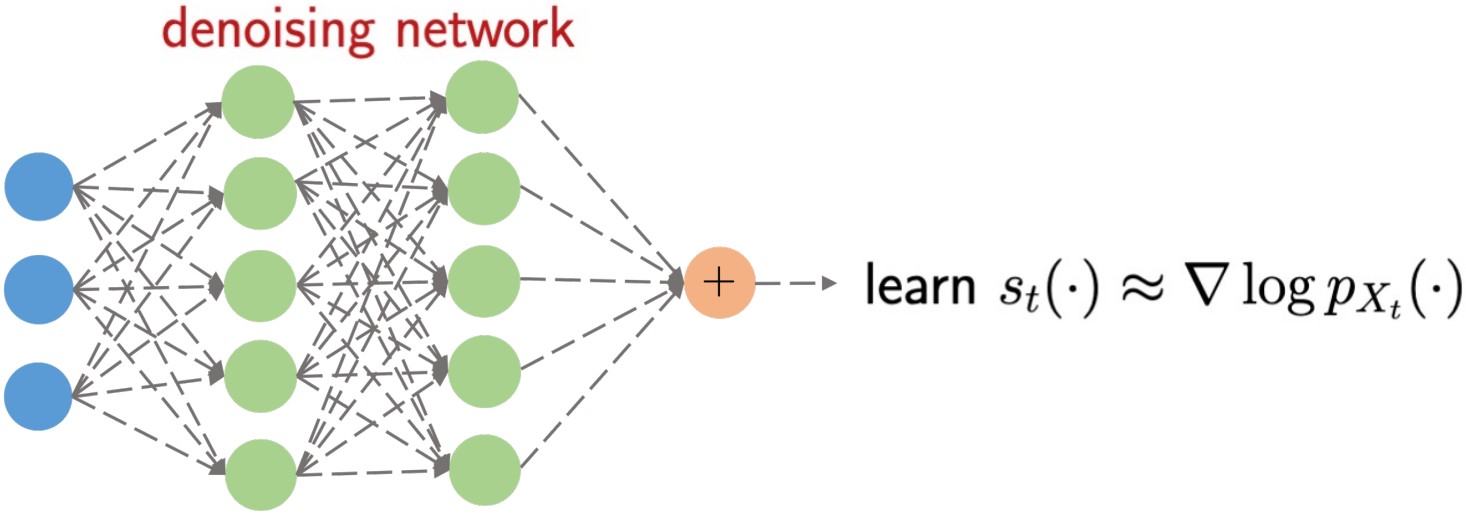

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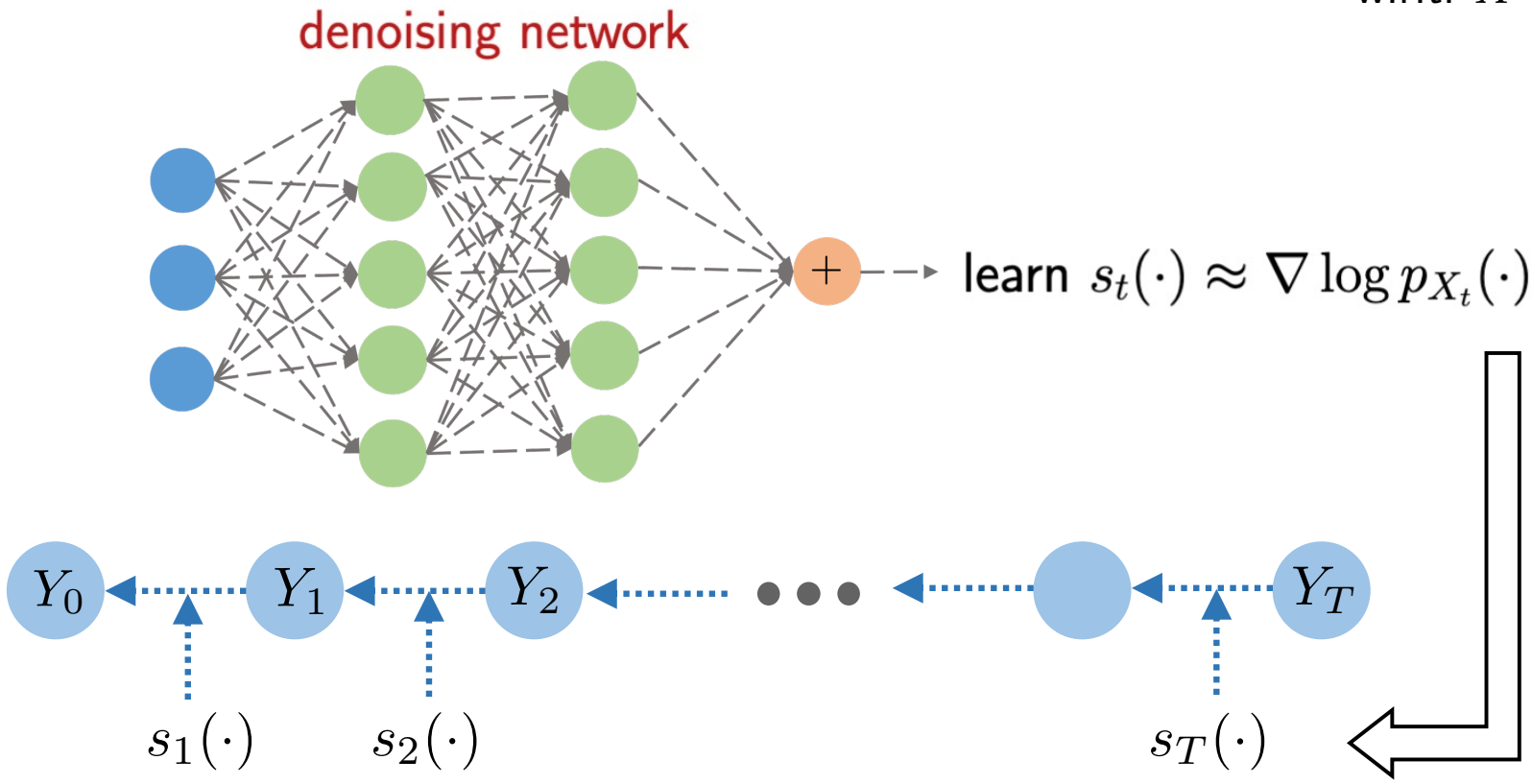

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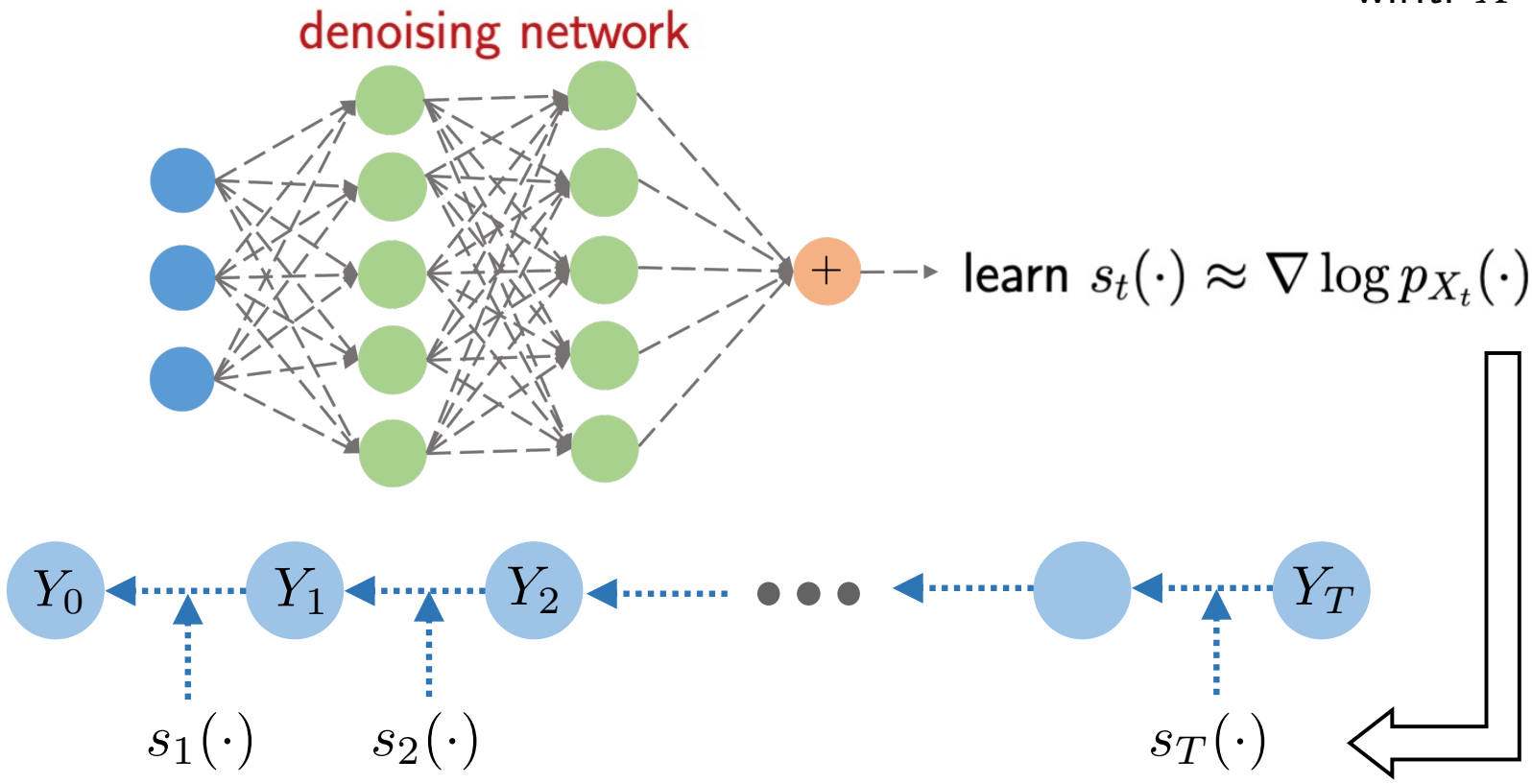

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Two mainstream approaches

— Ho, Jain, Abbeel '20

$$X_0 \sim p_{\text{data}}, \quad X_t = \sqrt{1-\beta_t} X_{t-1} + \sqrt{\beta_t}\mathcal{N}(0, I_d), \quad 1 \le t \le T$$

1. A stochastic sampler: **denoising diffusion probabilistic models**

   DDPM

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$$Y_T \sim \mathcal{N}(0, I_d)$$

$$Y_{t-1} = \Psi_t(Y_t, \mathsf{noise}), \quad t = T, \cdots, 1$$

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$$Y_{t-1} = \underbrace{\frac{1}{\sqrt{1-\beta_t}}\Big(Y_t + \beta_t s_t(Y_t)\Big)}_{\text{deterministic component}} + \underbrace{\sqrt{\frac{\beta_t}{1-\beta_t}}\mathcal{N}(0, I_d)}_{\text{random component}}, \quad t = T, \cdots, 1$$

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— Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole '20
— Song, Meng, Ermon '20

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$$Y_{t-1} = \underbrace{\frac{1}{\sqrt{1-\beta_t}}\left(Y_t + \frac{\beta_t}{2} s_t(Y_t)\right)}_{\text{purely deterministic}}, \qquad t = T, \cdots, 1$$

Interpretations: continuous-time limits

forward process
(marginal: $q_t := p_{X_t}$)

$$X_t = \sqrt{1-\beta_t} X_{t-1} + \sqrt{\beta_t}\mathcal{N}(0, I_d)$$

$$\implies \quad \mathrm{d}X_t = -\frac{1}{2}\beta(t) X_t \mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}W_t \quad \text{(SDE)}$$

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$\Big\|$ marginals

DDPM-type
stochastic sampler
(time-reversed SDE, Anderson '82)

$$Y_{t-1} = \frac{1}{\sqrt{1-\beta_t}}\Big(Y_t + \beta_t \nabla \log q_t(Y_t)\Big) + \sqrt{\frac{\beta_t}{1-\beta_t}}\mathcal{N}(0, I_d)$$
$$\Longrightarrow \quad \mathrm{d}Y_t = \Big(-\frac{1}{2}\beta(t) Y_t - \beta(t)\nabla \log q_t(Y_t)\Big)\mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}\widetilde{W}_t \quad \text{(reversed)}$$

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deterministic sampler
(probability flow ODE)

$$Y_{t-1} = \frac{1}{\sqrt{1-\beta_t}}\left(Y_t + \frac{\beta_t}{2}\nabla \log q_t(Y_t)\right)$$
$$\Longrightarrow \quad \mathrm{d}Y_t = \left(-\frac{1}{2}\beta(t) Y_t - \frac{1}{2}\beta(t)\nabla \log q_t(Y_t)\right)\mathrm{d}t \quad \text{(reversed)}$$

Key takeaway: in continuous-time limits, sampling is feasible once perfect score functions are available

— *almost no restriction on target data distributions*

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Questions:

- what happens in discrete time? — effect of discretization error
- what if we only have imperfect scores? — effect of score error

Towards mathematical theory for diffusion models

- hard to develop full-fledged **end-to-end** theory

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This talk:

1. non-asymptotic convergence theory in discrete time
2. acceleration?

Part 1: sharp convergence theory for probability flow ODE

"A sharp convergence theory for the probability flow ODEs of diffusion models,"
G. Li, Y. Wei, Y. Chi, Y. Chen, `arXiv:2408.02320`, 2024

"Towards non-asymptotic convergence for diffusion-based generative models,"
G. Li, Y. Wei, Y. Chen, Y. Chi, `arXiv:2306.09251`, ICLR 2024

Prior analyses for DDIM & DDPM

— *Li, Lu, Tan '22*
— *Chen, Lee, Lu '22*
— *Chen, Chewi, Li, Li, Salim, Zhang '22*
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discrete-time diffusion process

continuous-time limits via SDE/ODE toolbox (e.g., Girsanov thm)

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control discretization error

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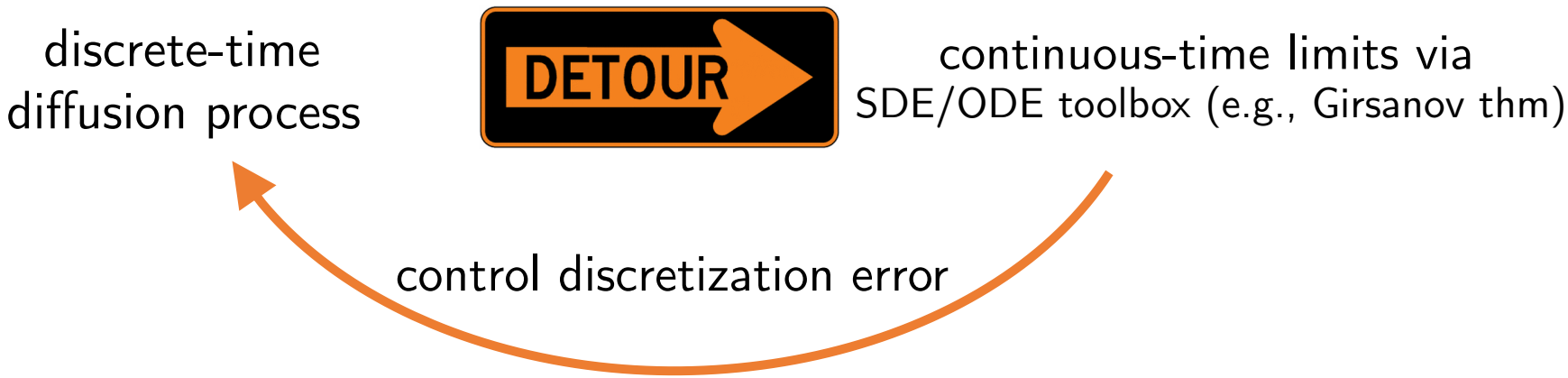

Analogy: (stochastic) gradient descent vs. gradient flow, TD learning via ODE

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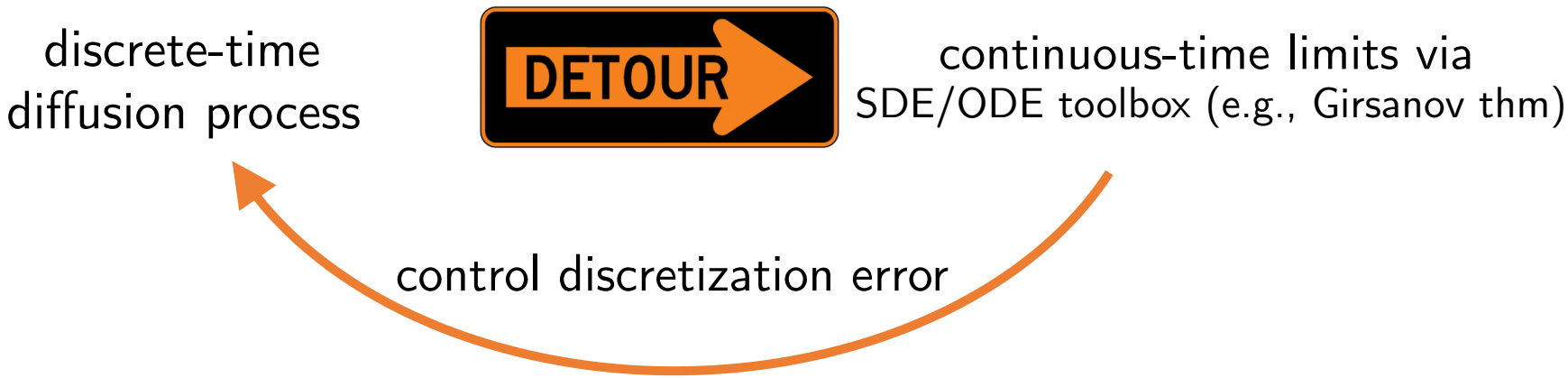

- Built upon toolboxes from SDE/ODE
- Existing analyses **highly inadequate** for deterministic samplers

Can we develop a versatile non-asymptotic framework that

- *analyzes discrete-time processes directly*
- *accommodates both deterministic & stochastic samplers?*

Assumptions: target data distribution

$\mathbb{P}(\|X_0\|_2 \leq T^{c_R}) = 1$ for arbitrarily large const $c_R > 0$

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- support size can be very large
- very general: *no need of assumptions like log-concavity, smoothness, etc*

Assumptions: score estimates $\{s_t(\cdot)\}$

- ℓ_2 *score estimation error:* $s_t^\star(X) := \nabla \log p_{X_t}(X)$,

$$\frac{1}{T}\sum_{t=1}^{T} \mathop{\mathbb{E}}_{X\sim p_{X_t}} \left[\|s_t(X) - s_t^\star(X)\|_2^2\right] \le \varepsilon_{\mathsf{score}}^2$$

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- *Jacobian estimation error:*

$$\frac{1}{T}\sum_{t=1}^{T} \mathop{\mathbb{E}}_{X\sim p_{X_t}} \left[\left\|\frac{\partial s_t}{\partial X}(X) - \frac{\partial s_t^\star}{\partial X}(X)\right\|\right] \le \varepsilon_{\text{Jacobi}}$$

Learning rates

$$X_0 \sim p_{\mathsf{data}}, \quad X_t = \sqrt{1-\beta_t} X_{t-1} + \sqrt{\beta_t} \mathcal{N}(0, I_d)$$

For some large constants $c_0, c_1 > 0$,

$$\beta_1 = \frac{1}{T^{c_0}}$$
$$\beta_t = \frac{c_1 \log T}{T} \min\left\{ \beta_1 \Big(1 + \frac{c_1 \log T}{T}\Big)^t, 1 \right\}$$

- 2 phases: (i) exponentially growing; (ii) flat
- common choice in diffusion model theory (e.g., Benton et al. '23)

Main result: probability flow ODE sampler

$$X_t = \sqrt{1-\beta_t} X_{t-1} + \sqrt{\beta_t}\mathcal{N}(0, I_d), \qquad t = 1, \cdots, T$$
$$Y_{t-1} = \frac{1}{\sqrt{1-\beta_t}} \left(Y_t + \frac{\beta_t}{2} s_t(Y_t) \right), \qquad t = T, \cdots, 1 \tag{1}$$

Theorem 1 (Li, Wei, Chi, Chen '24)

The probability flow ODE sampler (1) *obeys (up to log factor)*

$$\mathsf{TV}(p_{X_1}, p_{Y_1}) \lesssim \frac{d}{T} + \sqrt{d}\varepsilon_{\mathsf{score}} + d\varepsilon_{\mathsf{Jacobi}}$$

provided that $T \gtrsim d^2 \mathrm{polylog}(T)$

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- **iteration complexity:** d/ε for small enough ε
  (to yield TV dist $\leq \varepsilon$)
- **stability:** $\mathsf{TV}(p_{X_1}, p_{Y_1}) \propto$ error measures $\varepsilon_{\text{score}}$ and $\varepsilon_{\text{Jacobi}}$

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$$\mathsf{TV}(p_{X_1}, p_{Y_1}) \lesssim \frac{d}{T} + \sqrt{d}\varepsilon_{\mathsf{score}} + d\varepsilon_{\mathsf{Jacobi}}$$

provided that $T \gtrsim d^2 \mathrm{polylog}(T)$

- **general data distribution:** no need of smoothness, log-concavity

Main result: probability flow ODE sampler

$$
\begin{aligned}
X_t &= \sqrt{1-\beta_t} X_{t-1} + \sqrt{\beta_t}\mathcal{N}(0, I_d), \qquad && t = 1, \cdots, T \\
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\end{aligned} \tag{1}
$$

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Comparison w/ prior probability flow ODE theory

$$\text{(our theory)} \quad \mathsf{TV}\big(p_{X_1}, p_{Y_1}\big) \lesssim \frac{d}{T} + \sqrt{d}\varepsilon_{\text{score}} + d\varepsilon_{\text{Jacobi}}$$

- *Chen, Daras, Dimakis '23:* no concrete poly dependency
  ours: d/ε
  exponential in smoothness parameter
  ours: independent of smoothness pars
  needs exact score functions
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- *Chen, Chewi, Lee, Li, Lu, Salim '23:* requires additional stochastic correction steps & smoothness
  (different from probability flow ODE)
- *Huang, Huang, Lin '24:* suboptimal d-dependency (i.e., d^2/ε)
  (ours: d/ε)

Proof strategy

$$X_t = \sqrt{1-\beta_t} X_{t-1} + \sqrt{\beta_t}\mathcal{N}(0, I), \quad Y_{t-1} = \underbrace{\frac{1}{\sqrt{1-\beta_t}} Y_t + \frac{\beta_t}{2\sqrt{1-\beta_t}} s_t(Y_t)}_{=: \Phi_t(Y_t)}$$

$\mathsf{TV}\left(p_{X_t}, p_{Y_t}\right) \approx 0$

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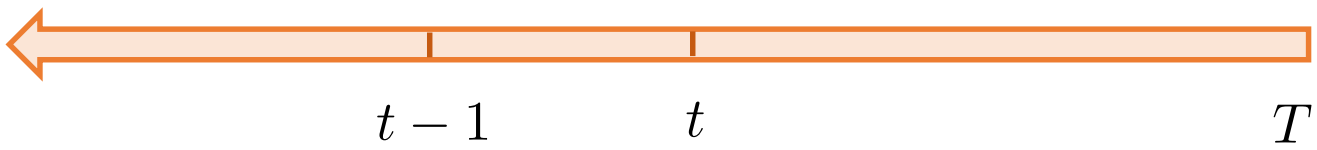

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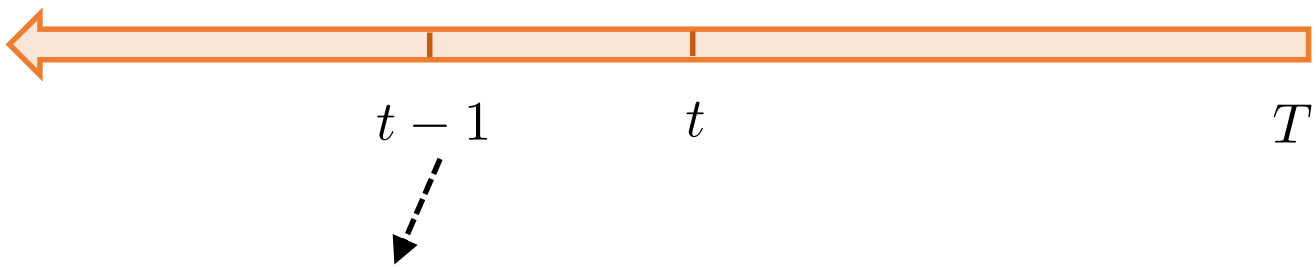

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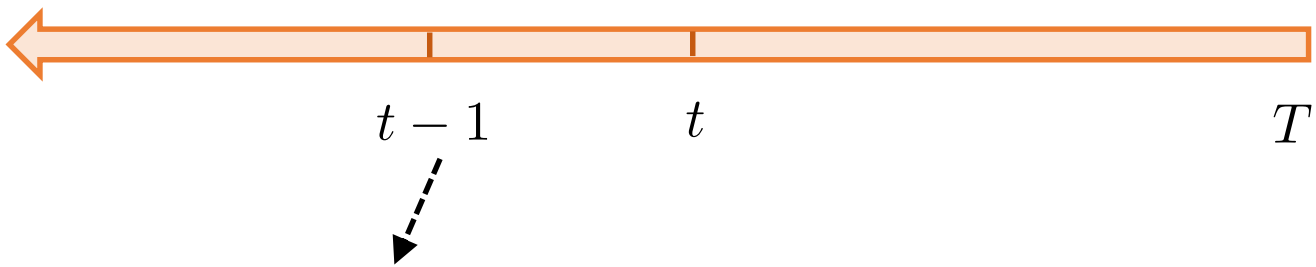

$$\frac{p_{Y_{t-1}}(\Phi_t(y_t))}{p_{X_{t-1}}(\Phi_t(y_t))} = \underbrace{\frac{p_{Y_{t-1}}(\Phi_t(y_t))}{p_{Y_t}(y_t)}}_{\text{relation btw } Y_t \ \& \ Y_{t-1}} \left(\underbrace{\frac{p_{X_{t-1}}(\Phi_t(y_t))}{p_{X_t}(y_t)}}_{\text{relation btw } X_t \ \& \ X_{t-1}} \right)^{-1} \frac{p_{Y_t}(y_t)}{p_{X_t}(y_t)}$$

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$t-1$ $\qquad$ t $\qquad$ T

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some concentration bounds

Part 2: acceleration

"Accelerating convergence of score-based diffusion models, provably," G. Li*, Y. Huang*, T. Efimov, Y. Wei, Y. Chi, Y. Chen, `arXiv:2403.03852`, 2024

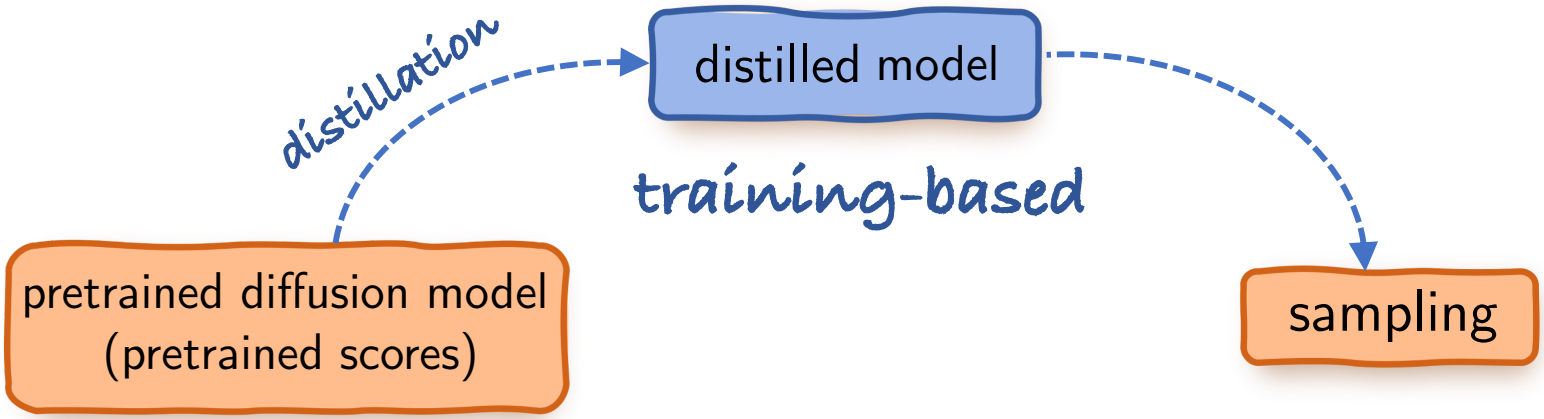
Diffusion-based sampling is often slow

— *Song, Meng, Ermon '20*

Diffusion-based sampling is often slow

50K 32×32 images: DDPM (20h) *vs.* single-step GANs ($<$ 1min)

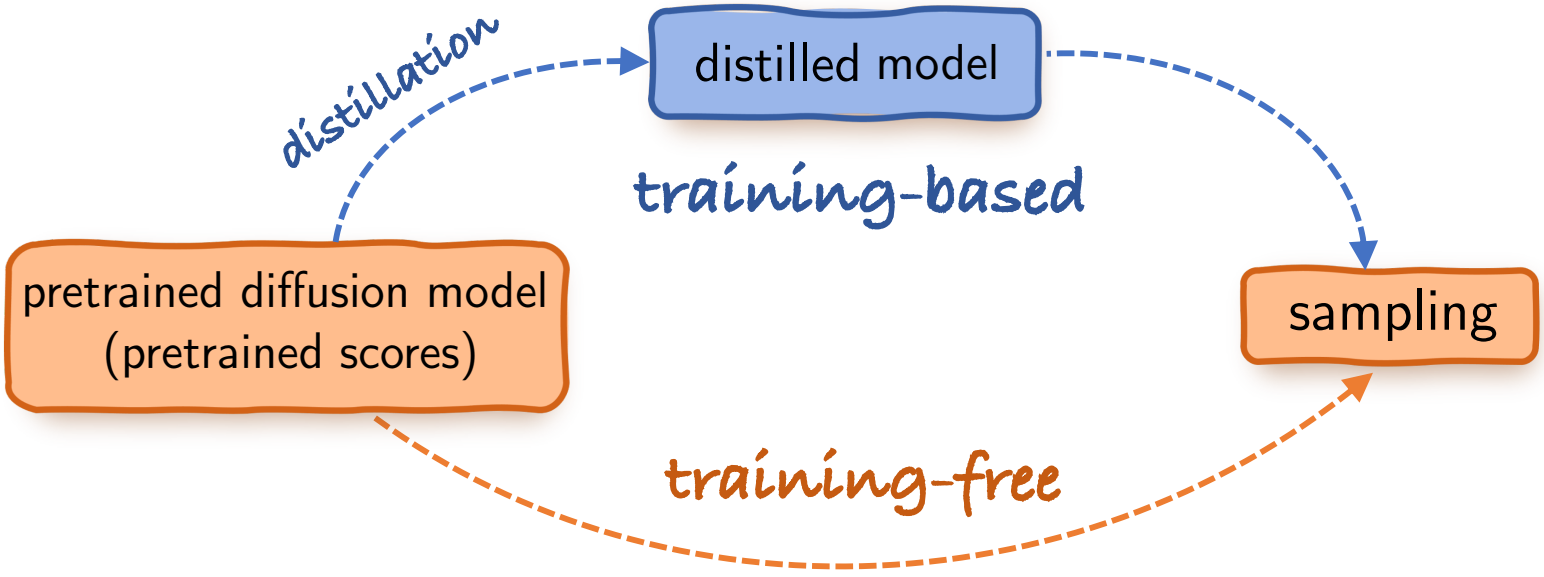
— *Song, Meng, Ermon '20*



- **Training-based:** distill pre-trained diffusion model into another model that can be executed rapidly

  requires additional training

  - e.g., progressive distillation (Salimans et al. '22), consistency model (Song et al. '23), ...



- **Training-free:** directly invoke pre-trained diffusion models (particularly score estimates) for sampling w/o additional training
  - e.g., DPM-Solver/++ (Lu et al. '22), UniPC (Zhao et al. '23), ...

Can we design a training-free deterministic sampler that converges provably faster than probability flow ODE?

Proposed accelerated deterministic sampler

$$Y_t^- = \Phi_t(Y_t), \qquad Y_{t-1} = \Psi_t(Y_t, Y_t^-) \qquad \text{for } t = T, \cdots, 1 \qquad (2)$$

- compute $\underbrace{\text{a midpoint } Y_t^-}_{\text{estimate of } Y_{t+1} \text{ using } Y_t}$; update based on $\underbrace{\text{both } Y_t \text{ and } Y_t^-}_{\text{provide 2nd-order info}}$

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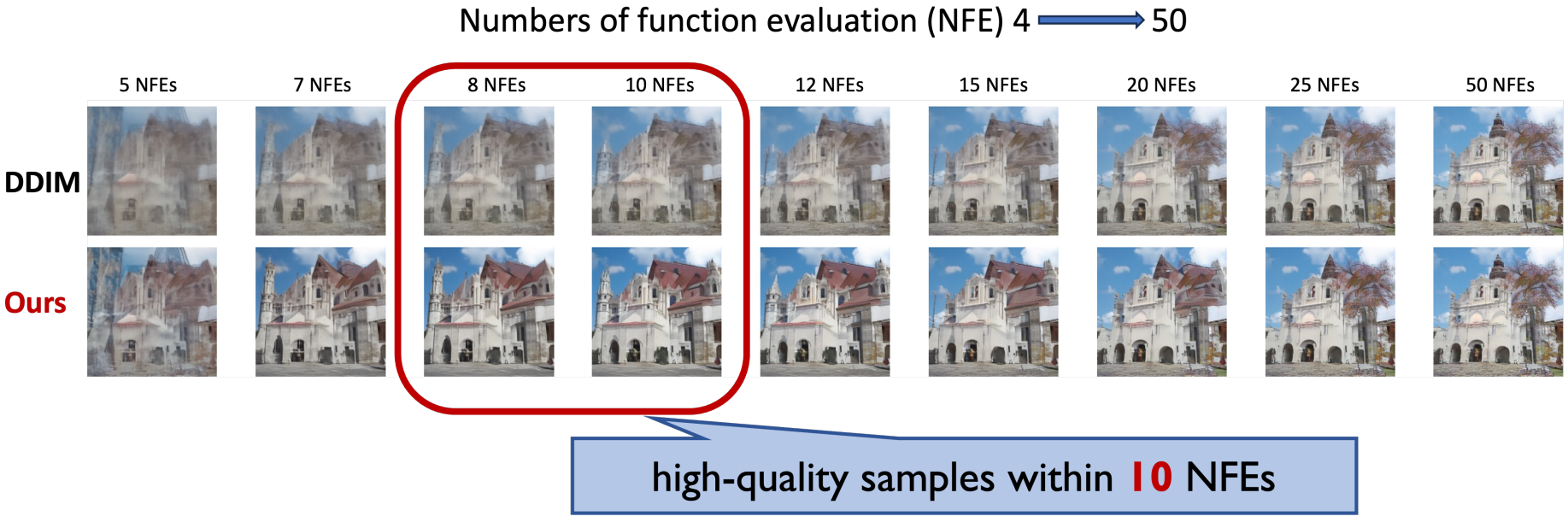
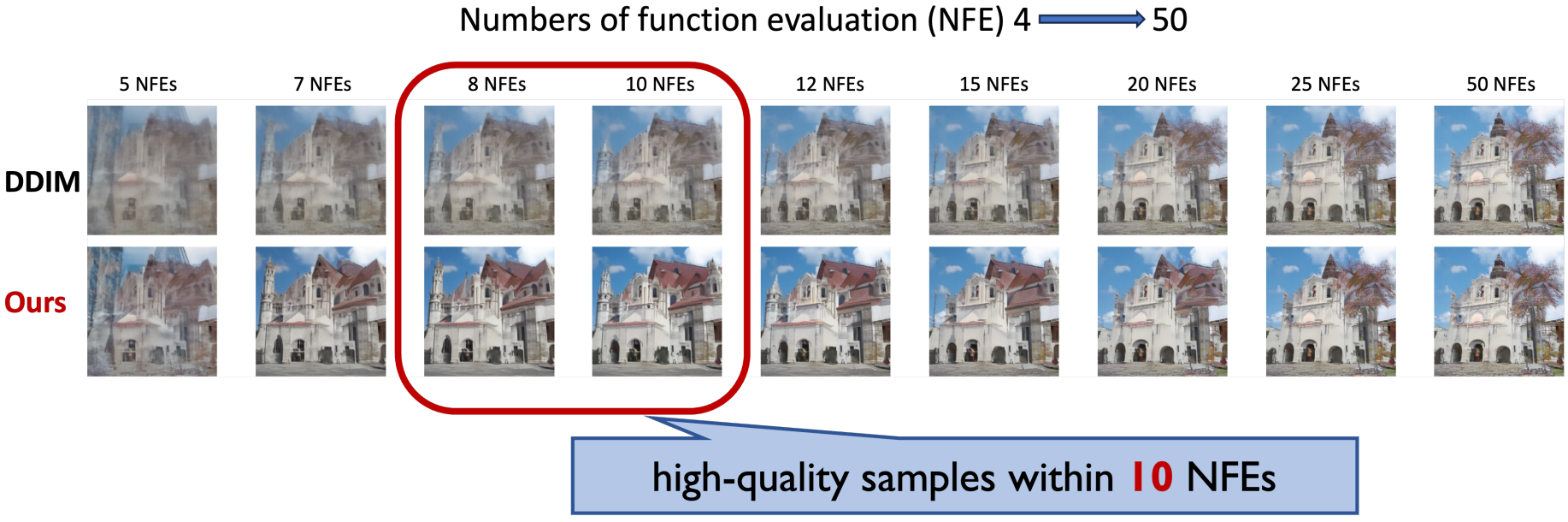
- 2 score function evaluations per iteration


Numbers of function evaluation (NFE) 4 50
5 NFEs
7 NFEs
8 NFEs
10 NFEs
12 NFEs
15 NFEs
20 NFEs
25 NFEs
50 NFEs
DDIM
Ours
high-quality samples within 10 NFEs



sampled images with 5 NFEs: crisper and less noisy

Recap: our assumptions

- ℓ_2 **score estimation error:**

$$\frac{1}{T}\sum_{t=1}^{T} \mathop{\mathbb{E}}_{X\sim p_{X_t}} \left[\|s_t(X) - s_t^\star(X)\|_2^2\right] \leq \varepsilon_{\text{score}}^2$$

- **Jacobian estimation error:**

$$\frac{1}{T}\sum_{t=1}^{T} \mathop{\mathbb{E}}_{X\sim p_{X_t}} \left[\left\|\frac{\partial s_t}{\partial X}(X) - \frac{\partial s_t^\star}{\partial X}(X)\right\|\right] \leq \varepsilon_{\text{Jacobi}}$$

- $\mathbb{P}(\|X_0\|_2 \leq T^{c_R}) = 1$ for arbitrarily large const $c_R > 0$

Main result: accelerated deterministic sampler

Theorem 2 (Li, Huang, Efimov, Wei, Chi, Chen '24)

Our accelerated deterministic sampler (2) *obeys (up to log factor)*

$$\mathsf{TV}(p_{X_1}, p_{Y_1}) \lesssim \frac{d^6}{T^2} + \sqrt{d}\varepsilon_{\mathsf{score}} + d\varepsilon_{\mathsf{Jacobi}}$$

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- **stability:** TV distance propotional to $\varepsilon_{\mathsf{score}} + \varepsilon_{\mathsf{Jacobi}}$
- **minimal assumptions** on data distributions
- d-**dependency:** might be improvable to $\frac{d^4}{T^2}$ (ongoing work)

Interpretation via high-order discretization

$$X_t \overset{\mathrm{d}}{=} \sqrt{\overline{\alpha}_t} X_0 + \sqrt{1-\overline{\alpha}_t}\,\mathcal{N}(0, I_d) \qquad \text{with } \overline{\alpha}_t := \prod_{k=1}^{t} (1-\beta_k)$$

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General form for $0 < \gamma < 1$:

$$X(\gamma) := \sqrt{\gamma} X_0 + \sqrt{1-\gamma}\mathcal{N}(0, I_d)$$
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"solution" to probability flow ODE

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refined approximation?

$$\begin{aligned} s^\star_\gamma\big(X(\gamma)\big) &\approx s^\star_{\overline{\alpha}_t}\big(X(\overline{\alpha}_t)\big) + \frac{\mathrm{d}s^\star_\gamma\big(X(\gamma)\big)}{\mathrm{d}\gamma} (\gamma - \overline{\alpha}_t) \\ &\approx s_t(X_t) + \frac{\gamma - \overline{\alpha}_t}{\overline{\alpha}_t - \overline{\alpha}_{t+1}} \Big(s_t\big(X_t\big) - s_{t+1}\big(X_{t+1}\big) \Big) \end{aligned}$$

Interpretation via high-order discretization

$$X(\overline{\alpha}_{t-1}) = \frac{1}{\sqrt{\alpha_t}} X(\overline{\alpha}_t) + \frac{\sqrt{\overline{\alpha}_{t-1}}}{2} \int_{\overline{\alpha}_t}^{\overline{\alpha}_{t-1}} \frac{1}{\sqrt{\gamma^3}} \underbrace{s^\star_\gamma\big(X(\gamma)\big)}_{\text{approximated by?}} \mathrm{d}\gamma$$

Scheme 1: $s^\star_\gamma\big(X(\gamma)\big) \approx s^\star_{\overline{\alpha}_t}\big(X(\overline{\alpha}_t)\big) \approx s_t(X_t)$

$$\Longrightarrow \quad X(\overline{\alpha}_{t-1}) \approx \frac{1}{\sqrt{\alpha_t}} \left(X(\overline{\alpha}_t) + \frac{1-\alpha_t}{2} s_t(X_t) \right) \qquad \text{original DDIM}$$

Scheme 2: $s^\star_\gamma\big(X(\gamma)\big) \approx s_t(X_t) + \frac{\gamma - \overline{\alpha}_t}{\overline{\alpha}_t - \overline{\alpha}_{t+1}} \big(s_t(X_t) - s_{t+1}(X_{t+1})\big)$

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— *similar in spirit to DPM-Solver-2 (Lu et al '22)*

Can we design a training-free stochastic sampler that converges provably faster than DDPM?

Proposed accelerated stochastic sampler

$$Y_t^+ = \Phi_t(Y_t, Z_t), \quad Y_{t-1} = \Psi_t(Y_t^+, Z_t^+) \quad \text{with } Z_t, Z_t^+ \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, I_d) \quad (3)$$

- compute a midpoint Y_t^+; then compute Y_{t-1} using Y_t^+ (similar to extragradient method)

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$$\Phi_t(x, z) = x + \sqrt{\frac{1-\alpha_t}{2}} z \quad \text{injecting additional noise}$$

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- compute a midpoint Y_t^+; then compute Y_{t-1} using Y_t^+ (similar to extragradient method)
- 1 score function evaluation per iteration

Main result: accelerated stochastic sampler

Theorem 3 (Li, Huang, Efimov, Wei, Chi, Chen '24)

The accelerated stochastic sampler (3) *obeys (up to log factor)*

$$\mathsf{TV}(p_{X_1}, p_{Y_1}) \lesssim \sqrt{\mathsf{KL}(p_{X_1} \,\|\, p_{Y_1})} \lesssim \frac{d^3}{T} + \sqrt{d}\varepsilon_{\mathsf{score}}$$

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- **iteration complexity**: $\frac{\mathrm{poly}(d)}{\varepsilon}$
  - outperforms vanilla DDPM (iteration complexity: d/ε^2)
    — *Chen et al. '23, Li et el. 23, Benton et al. '23*
- **general data distributions**
- ℓ_2 score error assumption suffices (no need of Jacobians)

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- **intuition:** higher-order approx. of $p_{X_{t-1}|X_t}$ via simply adding noise

Interpretation via higher-order approximation

characterizing $p_{X_{t-1}|X_t=x_t} \approx \mathcal{N}\big(\mu_t^\star(x_t), \Sigma_t^\star(x_t)\big)$

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&\approx \Psi_t\left(\Phi_t(Y_t, Z_t), Z_t^+\right) \qquad \text{(Ours)}
\end{aligned}
$$

Concluding remarks

- Sharp convergence theory for probability flow ODE
- New schemes via higher-order approximation to achieve provable acceleration in score-based diffusion models

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Future directions:

- better dimension-dependency for accelerated samplers?
- acceleration via higher-order ODE/SDE?
  e.g., DPM-Solver-3 (third-order ODE)
- end-to-end theory to account for score learning + sampling?

Papers:

"A sharp convergence theory for the probability flow ODEs of diffusion models," G. Li, Y. Wei, Y. Chi, Y. Chen, arXiv:2408.02320, 2024

"Towards non-asymptotic convergence for diffusion-based generative models," G. Li, Y. Wei, Y. Chen, Y. Chi, arXiv:2306.09251, ICLR 2024

"Accelerating convergence of score-based diffusion models, provably," G. Li*, Y. Huang*, T. Efimov, Y. Wei, Y. Chi, Y. Chen, arXiv:2403.03852, 2024 (*=equal contributions)