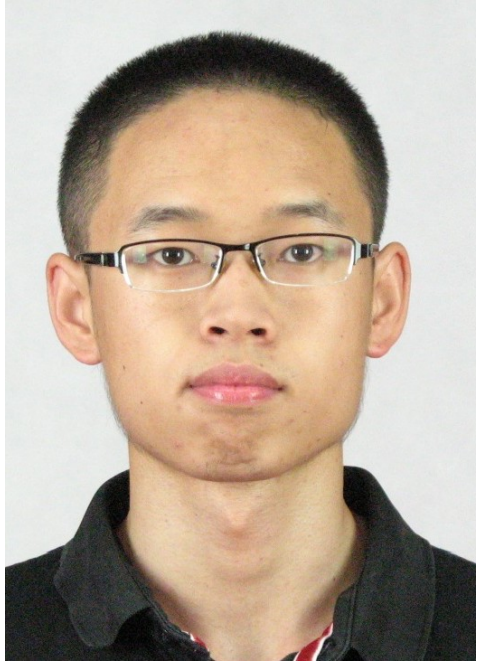
Faster Diffusion Models via Higher-Order Approximation

Yuchen Zhou

UIUC Statistics

Part 3: acceleration via higher-order approximation



Gen Li[*]
CUHK

Yuting Wei
UPenn

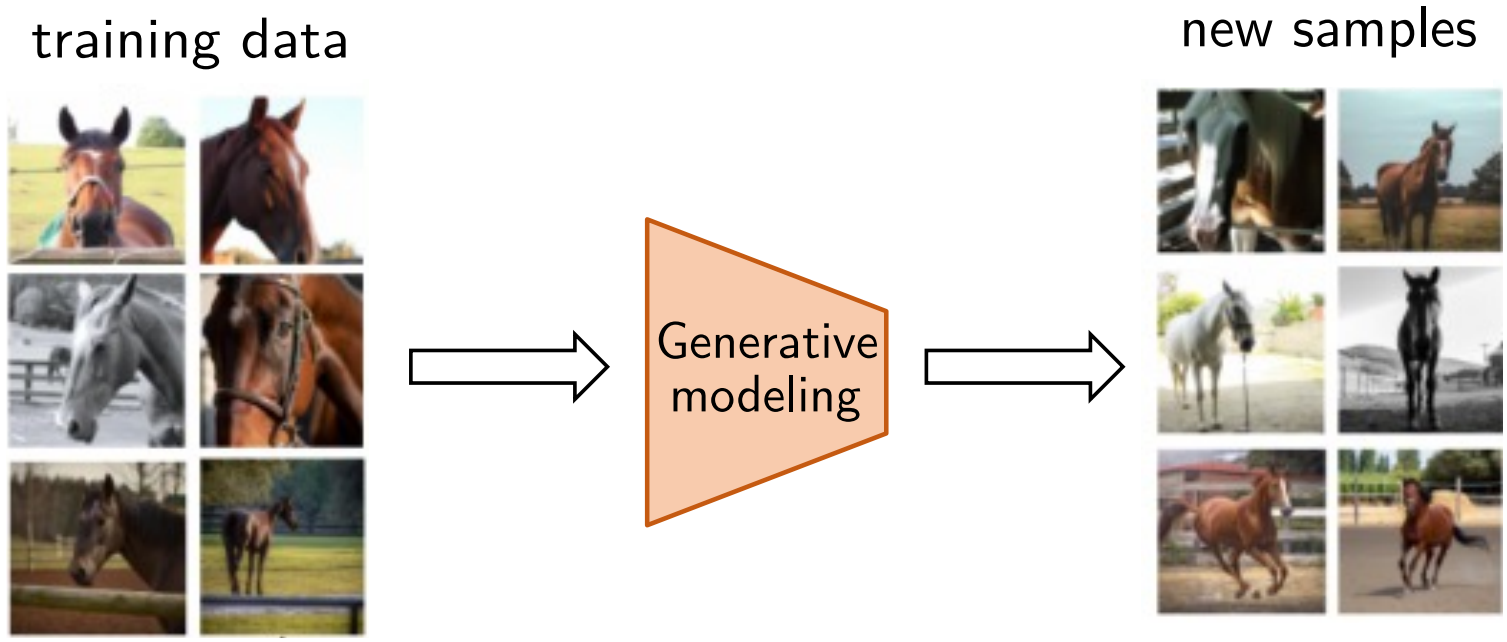
Yuxin Chen
UPenn

Generative modeling

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 modeling



- 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 $Y \sim p_{\text{data}}$

Inspired by nonequilibrium thermodynamics

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

Diffusion models

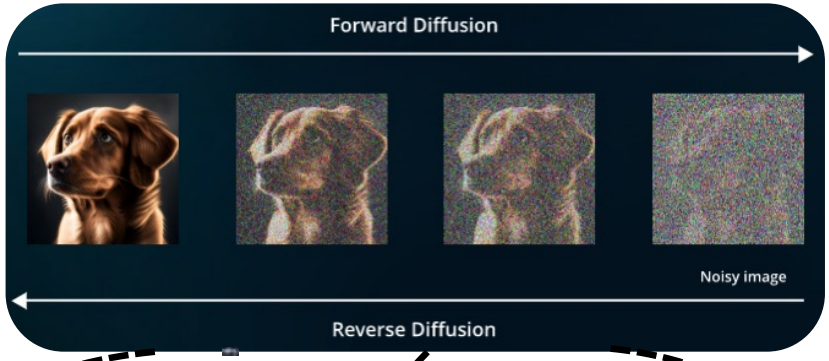
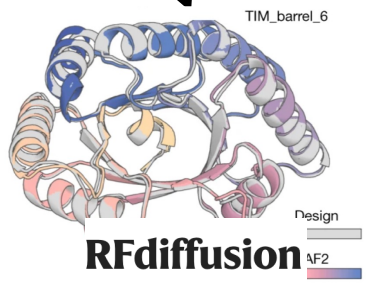
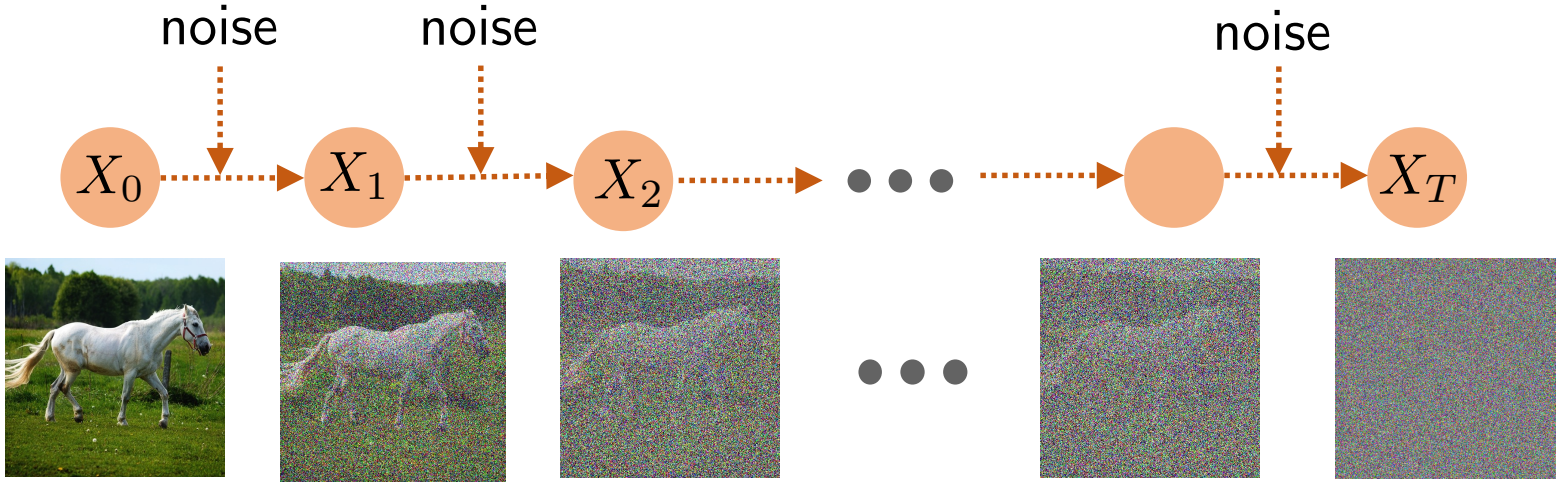


image generation

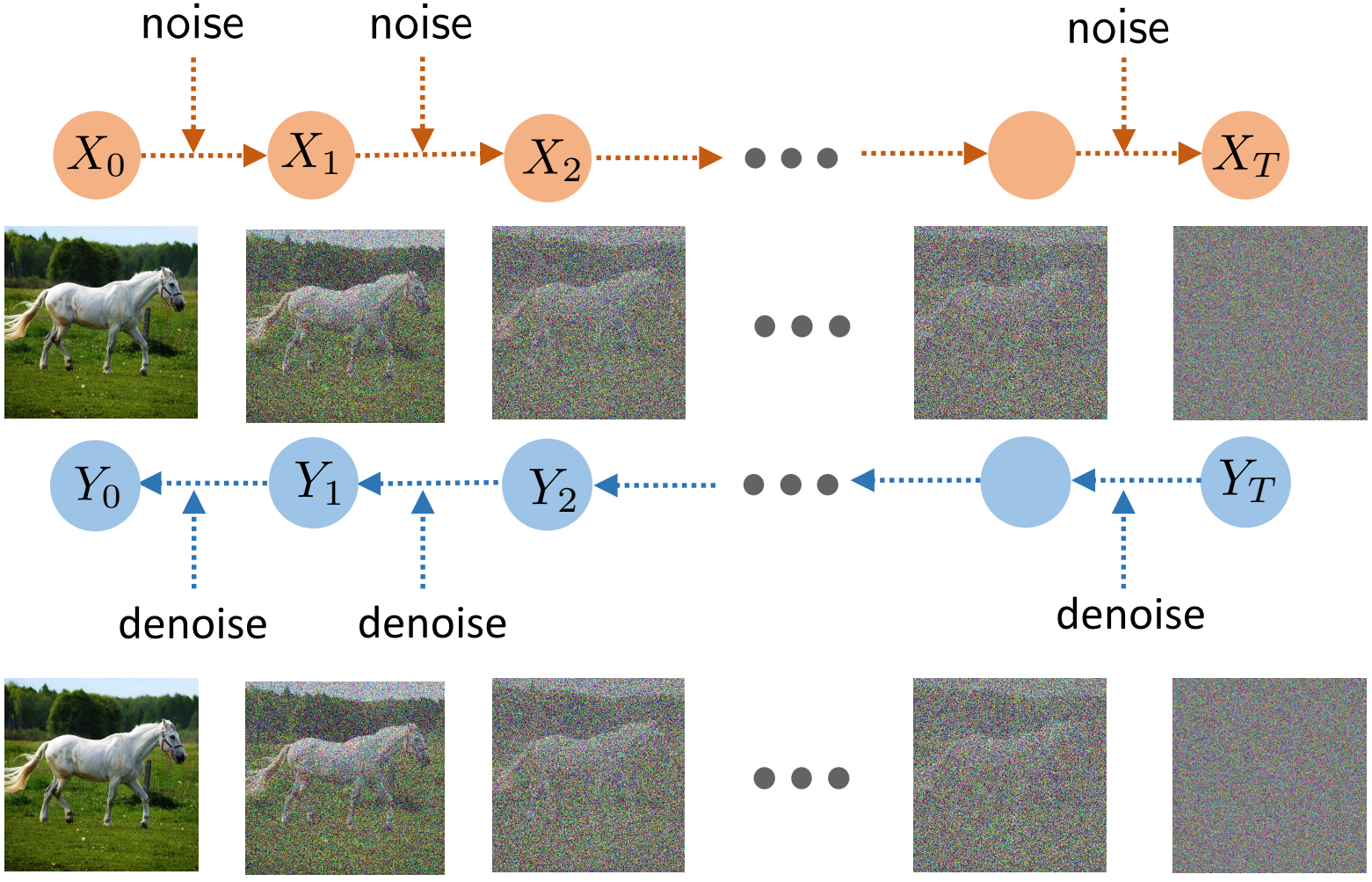
video generation



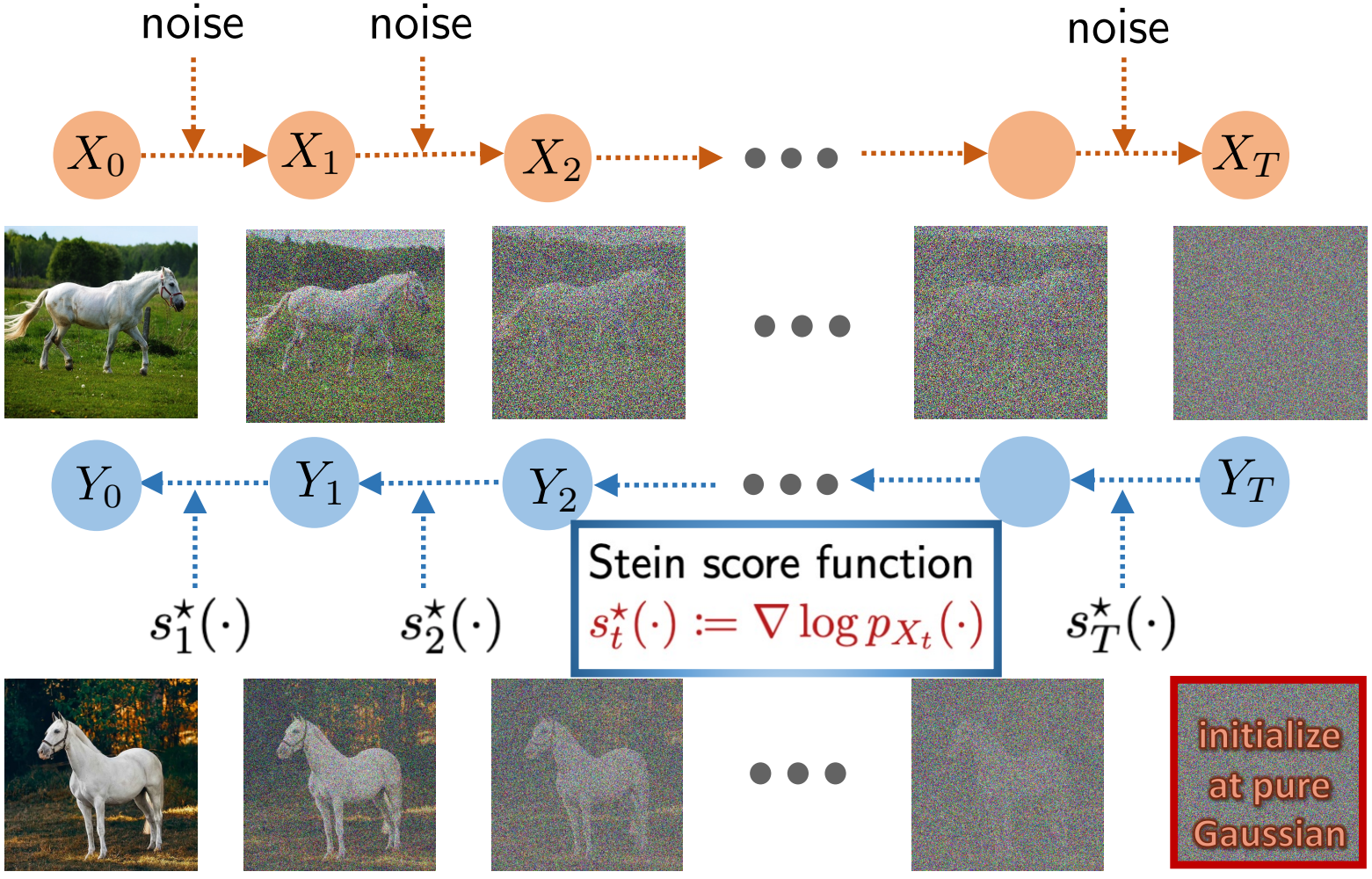
protein design



- **forward process:** diffuse data into noise



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



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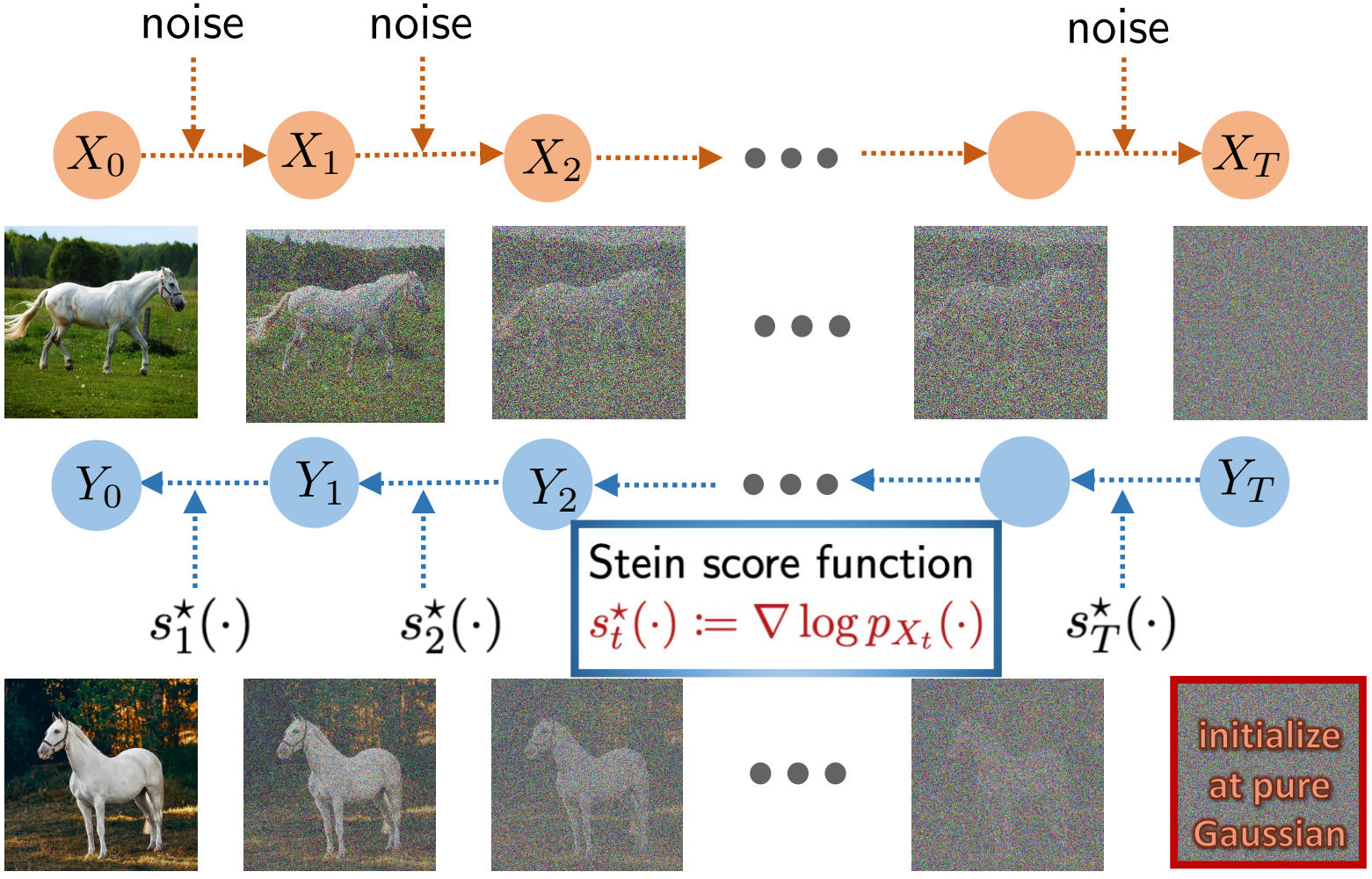

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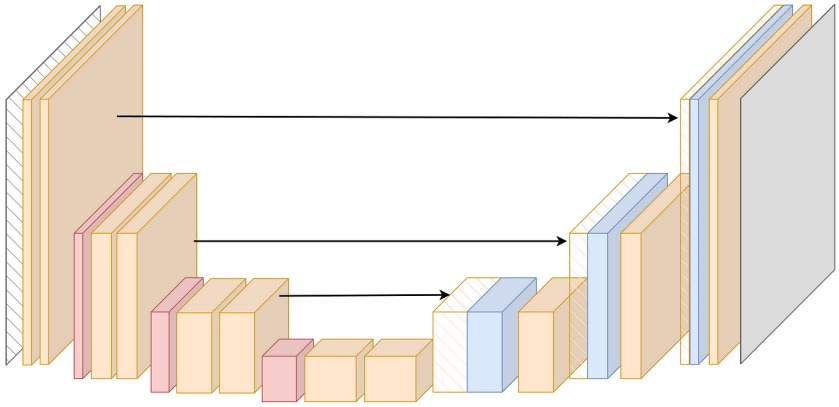
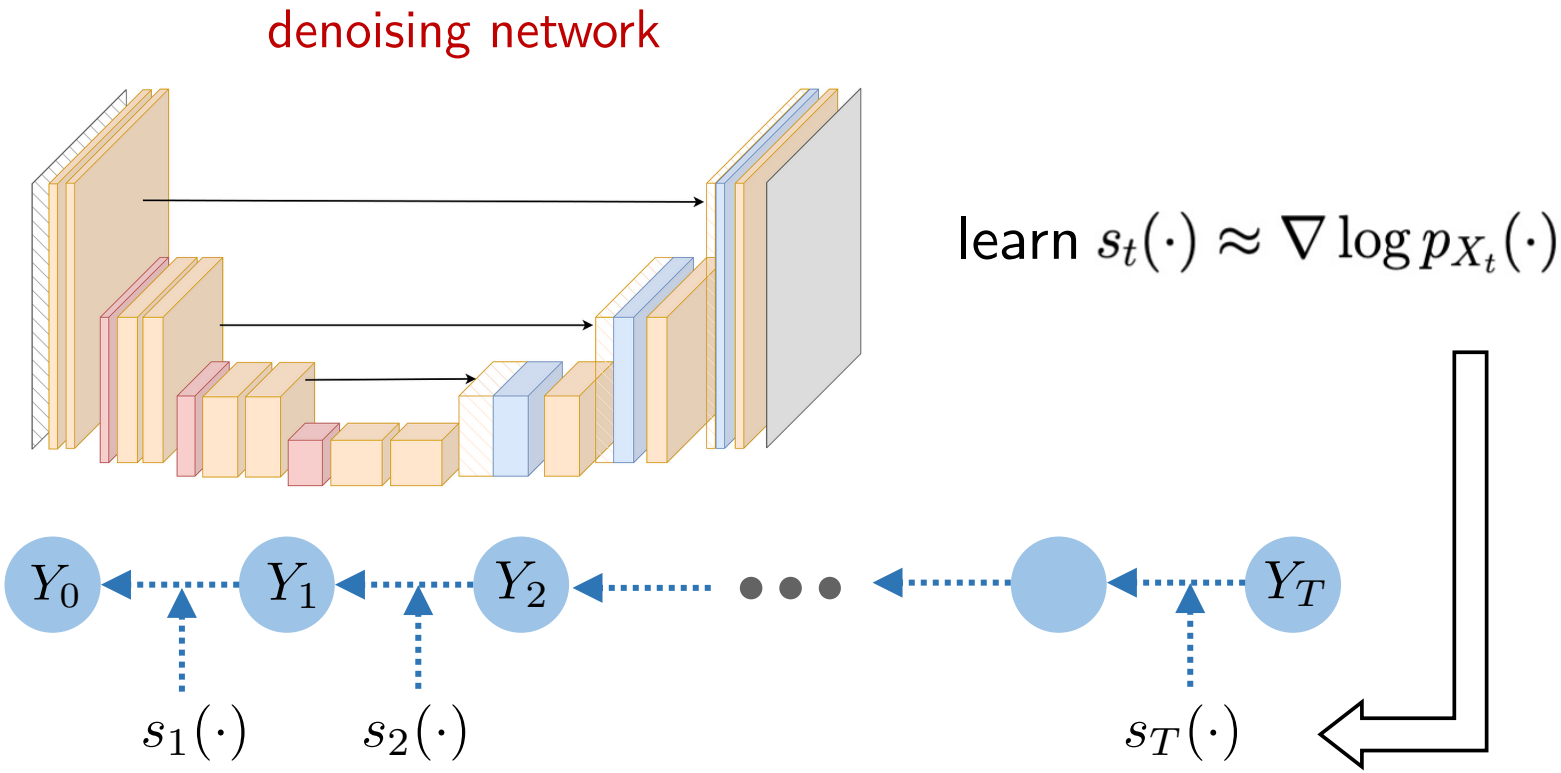
Goal: $Y_t \overset{\mathrm{d}}{\approx} X_t, \quad t = T, \cdots, 1$

denoising network



learn $s_t(\cdot) \approx \nabla \log p_{X_t}(\cdot)$

1. **score learning/matching:** learn estimates $s_t(\cdot)$ for $\nabla \log p_{X_t}(\cdot)$



1. **score learning/matching:** learn estimates $s_t(\cdot)$ for $\nabla \log p_{X_t}(\cdot)$
2. **data generation:** sampling w/ the aid of score estimates $\{s_t(\cdot)\}$

Towards mathematical theory for diffusion models

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

Towards mathematical theory for diffusion models

- hard to develop full-fledged **end-to-end** theory
- "divide-and-conquer": score learning $\overset{\text{✂ decouple}}{\leftarrow \not\rightarrow}$ sampling

Two mainstream approaches

Denoising Diffusion Probabilistic Models

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Pieter Abbeel
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DENOISING DIFFUSION IMPLICIT MODELS

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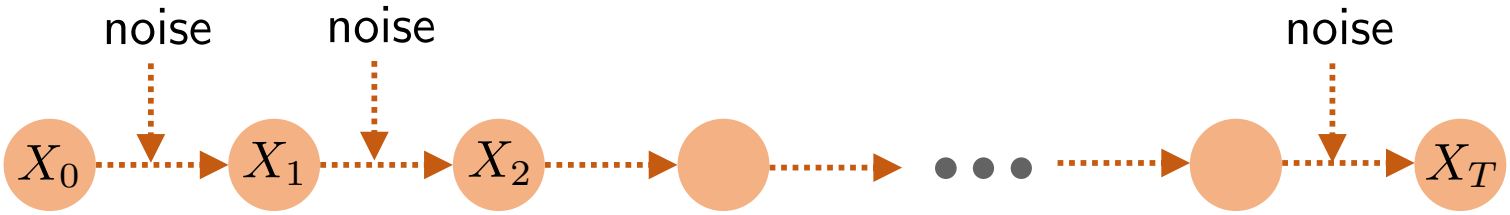
DDPM vs. DDIM

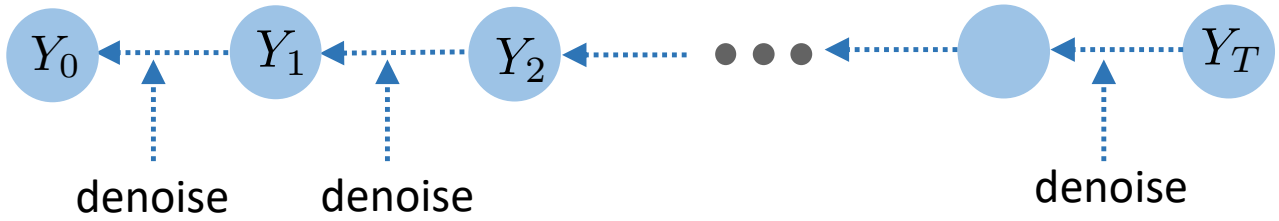


forward process: $X_0 \sim p_{\text{data}}$ (target distribution)

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

- $\beta_t := 1 - \alpha_t$ controls variance of injected noise

DDPM vs. DDIM



— *Ho, Jain, Abbeel '20*

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

DDPM

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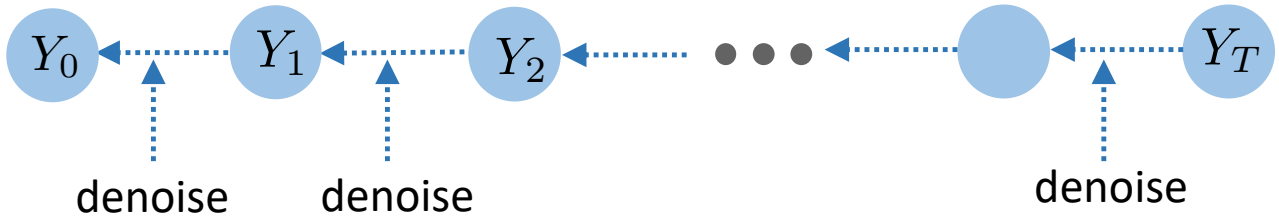

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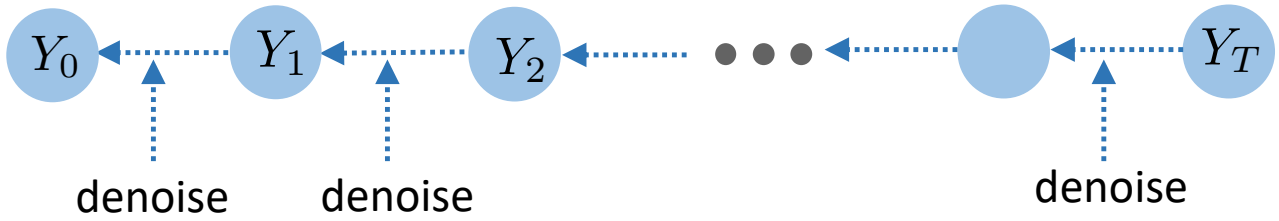
$$Y_T \sim \mathcal{N}(0, I_d)$$

$$Y_{t-1} = \frac{1}{\sqrt{\alpha_t}}\Big(\underbrace{Y_t + \eta_t^{\text{ddpm}} s_t(Y_t)}_{\text{deterministic}} + \underbrace{\sigma_t^{\text{ddpm}} \mathcal{N}(0, I_d)}_{\text{stochastic}}\Big), \quad t = T, \cdots, 1$$

DDPM vs. DDIM



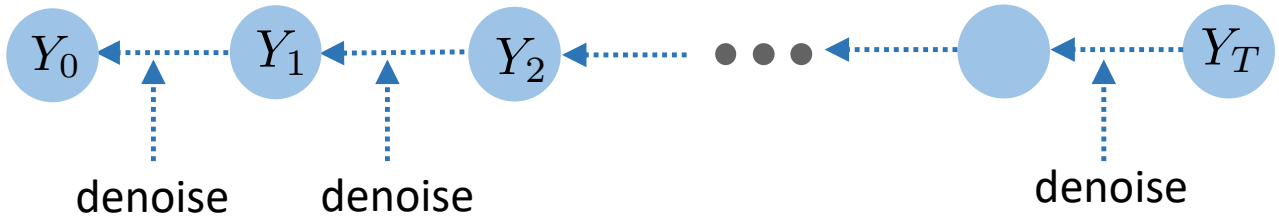
— *Song, Meng, Ermon '20*

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

2. A deterministic sampler: **denoising diffusion implicit models**

DDIM; or probability flow ODE

DDPM vs. DDIM



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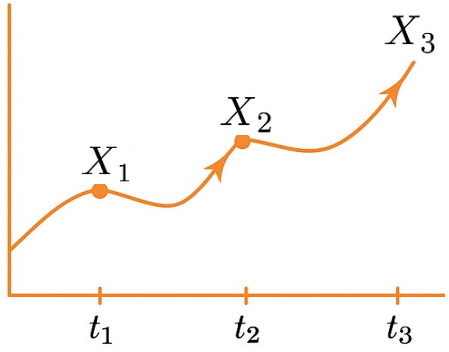
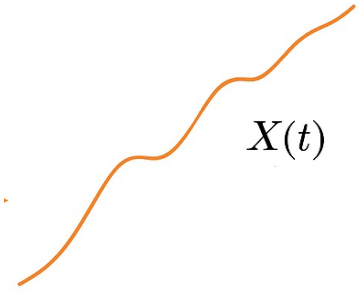
Interpretations from lens of SDE/ODE



discrete-time



continuous-time

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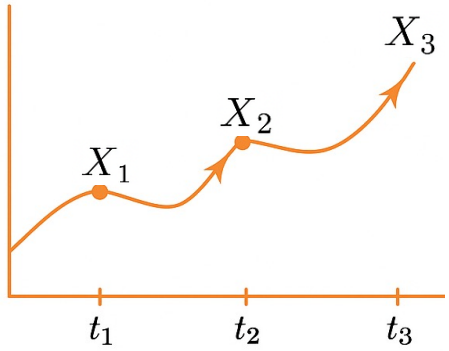

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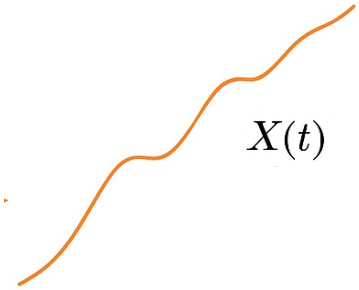

continuous-time

forward process

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

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

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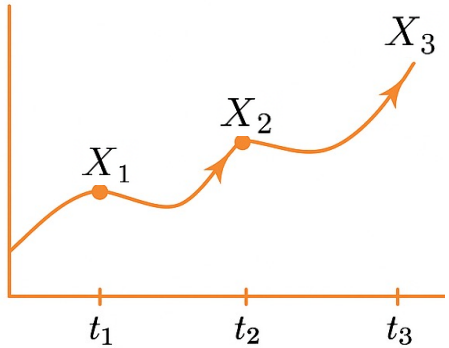

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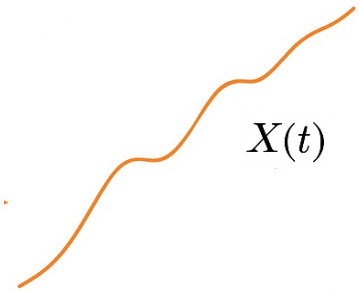

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- $\exists$ reverse-time SDE w/ same path distribution (Anderson '82)

$$\mathrm{d}Y_t = \left(Y_t + 2\boldsymbol{s}^\star_{T-t}(Y_t)\right)\beta(T-t)\mathrm{d}t + \sqrt{2\beta(T-t)}\,\mathrm{d}W_t$$

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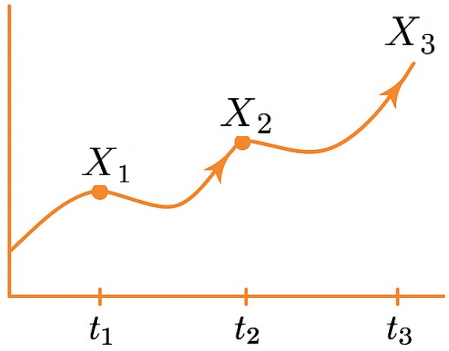

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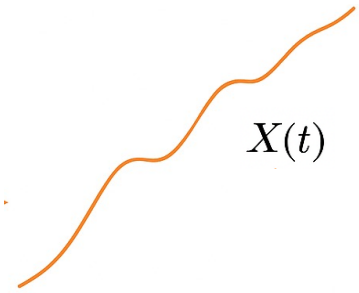

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$$\xrightarrow{\text{time discretization}} \text{DDPM}$$

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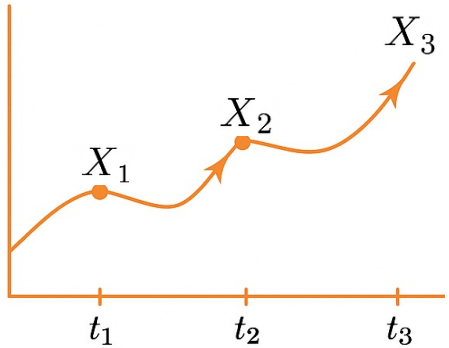

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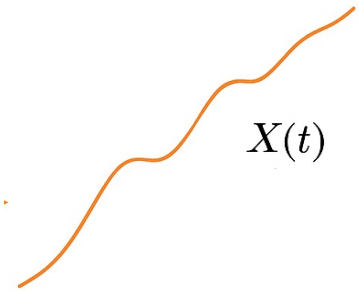

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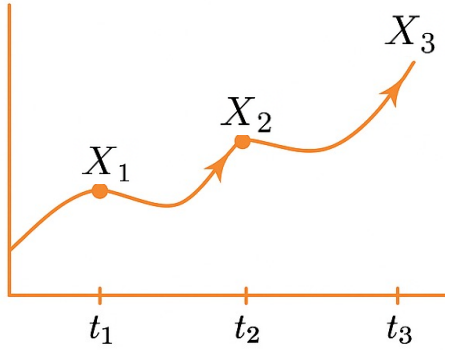

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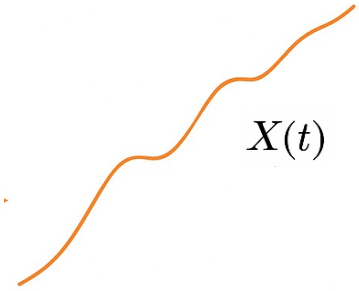

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time discretization $\longrightarrow$ DDIM

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

— *almost no restriction on target data distributions*

A small sample of convergence theory

- Lee, Lu, Tan '22
- Chen, Chewi, Li, Li, Salim, Zhang '22
- Chen, Lee, Lu '22
- Lee, Lu, Tan '23
- Chen, Daras, Dimakis '23
- Chen, Chewi, Lee, Li, Lu, Salim '23
- Benton, De Bortoli, Doucet, Deligiannidis '23
- Li, Wei, Chen, Chi '23
- Benton, Deligiannidis, Doucet '23
- Cheng, Lu, Tan, Xie '23
- Tang '23
- Li, Wei, Chi, Chen '24
- Li, Yan '24a, '24b
- Azangulov, Deligiannidis, Rousseau '24
- Potaptchik, Azangulov, Deligiannidis '24
- Huang, Wei, Chen '24
- Gao, Zhu '24
- Huang, Huang, Lin '24
- Li, Jiao '24
- Li, Di, Gu '24
- Liang, Ju, Liang, Shroff '24
- Tang, Zhao '24
- Liang, Huang, Chen '25
- Li, Cai, Wei '25
- Tang, Yan '25
- Yu, Yu '25
- Gentiloni-Silveri, Ocello '25
- ...

Assumptions: target data distribution p_{data}

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- can also be replaced by $\mathbb{E}[\|X_0\|_2] \leq T^{c_M}$ for large const c_M

A glimpse of existing convergence theory

DDPM:

$$\mathsf{KL}\big(p_{X_1} \,\|\, p_{Y_1}\big) \lesssim d/T + \varepsilon_{\mathsf{score}}^2 \quad \text{(Benton et al. '23)}$$

$$\mathsf{TV}\big(p_{X_1}, p_{Y_1}\big) \lesssim d/T + \varepsilon_{\mathsf{score}} \quad \text{(Li, Yan '24)}$$

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- **iteration complexity:** d/ε (assuming accurate scores)
  to yield $\mathsf{TV} \le \varepsilon$
  - Pinsker inequality ($\mathsf{TV} \le \sqrt{\frac{1}{2}\mathsf{KL}}$) is loose when bounding TV

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$\mathsf{TV}(p_{X_1}, p_{Y_1}) \lesssim d/T + \varepsilon_{\mathsf{score}}$ (Li, Yan '24)

DDIM: $\mathsf{TV}(p_{X_1}, p_{Y_1}) \lesssim d/T + \sqrt{d}\,\varepsilon_{\mathsf{score}} + d\varepsilon_{\mathsf{Jacobi}}$ (Li et al. '24)

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DDPM and DDIM are still slow . . .

— *Song, Meng, Ermon '20*

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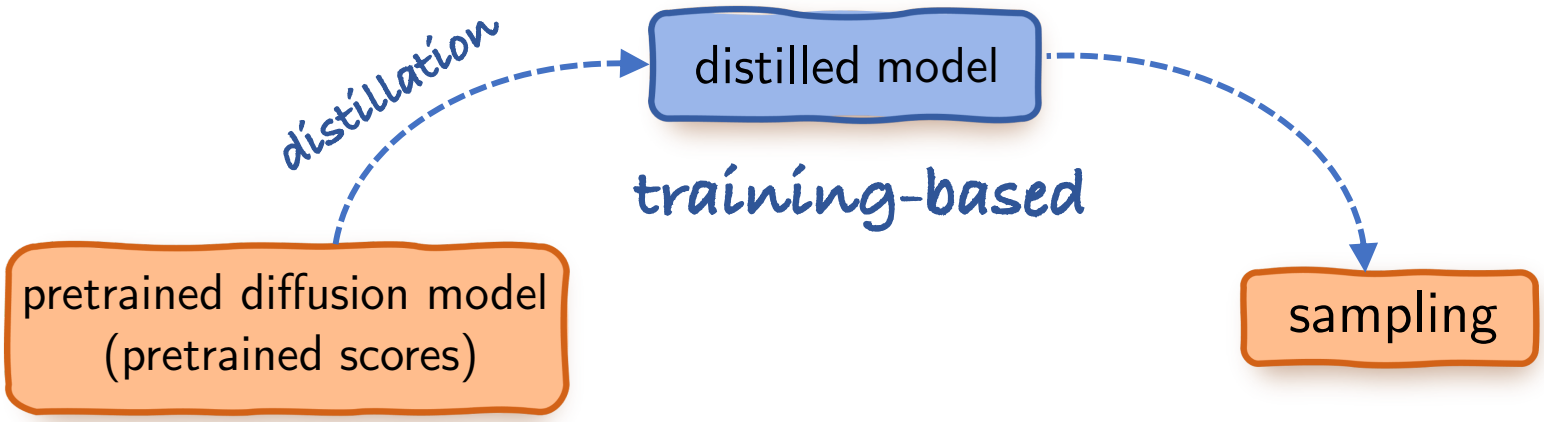
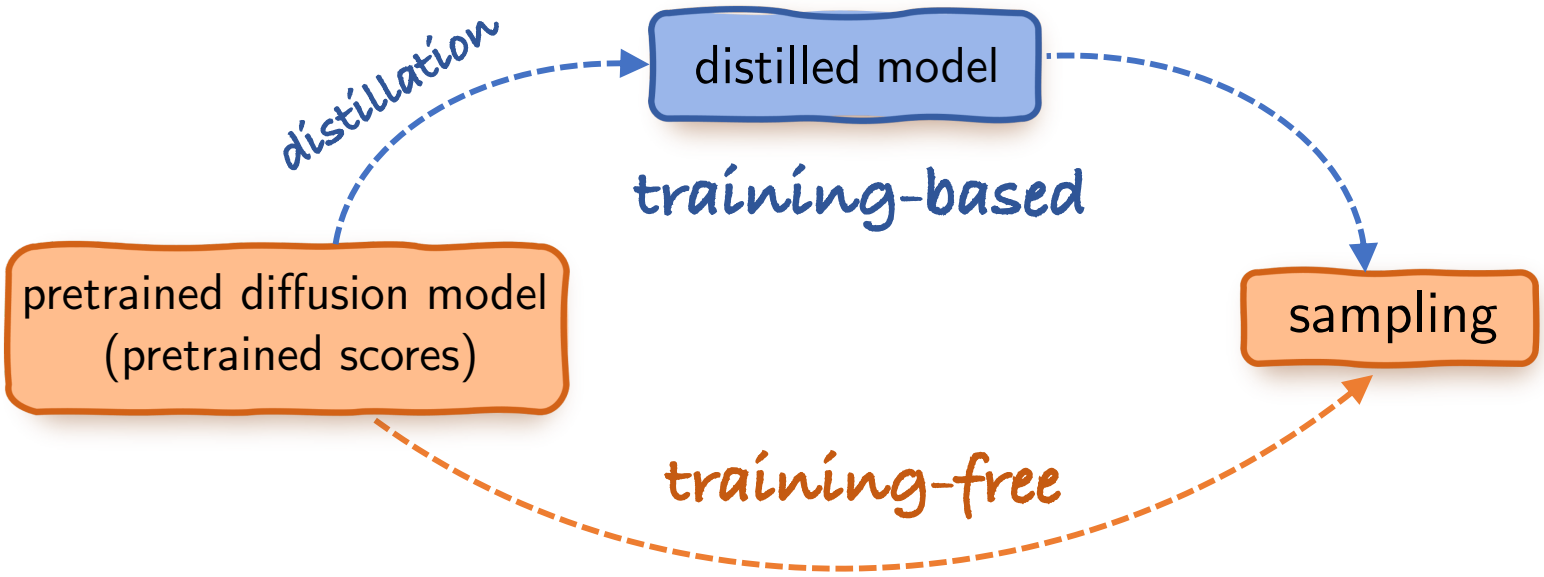
50K 32×32 images: DDPM (20h) *vs.* single-step GANs ($<$ 1min)

— *Song, Meng, Ermon '20*



- **training-based:** distill pre-trained diffusion model into another model that can be executed rapidly
  - e.g., progressive distillation, consistency model

requires additional training



- **training-free:** directly invoke pre-trained 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 sampler that is provably faster than DDIM/DDPM?

Discretization $\longleftrightarrow$ approximation

A starting point: equiv solution to probability flow ODE

$$\underbrace{Y^{\mathsf{ode}}_{\overline{\alpha}_{t-1}}}_{\text{represent } Y_{t-1}} = \frac{1}{\sqrt{\alpha_t}} \underbrace{Y^{\mathsf{ode}}_{\overline{\alpha}_t}}_{\text{represent } Y_t} + \underbrace{\int_{\overline{\alpha}_t}^{\overline{\alpha}_{t-1}} \frac{1}{\sqrt{\gamma^3}} s^\star_\gamma(Y^{\mathsf{ode}}_\gamma) \mathrm{d}\gamma}$$

where $s^\star_\gamma(x) := \nabla \log p_{\sqrt{\gamma} X_0 + \sqrt{1-\gamma}\mathcal{N}(0, I_d)}(x)$

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- can we approximate the integral by a few score evals?

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1st order approx: $s^\star_\gamma\left(Y^{\mathsf{ode}}_\gamma\right) \approx s^\star_{\overline{\alpha}_t}\left(Y^{\mathsf{ode}}_{\overline{\alpha}_t}\right) \approx s_t(Y_t)$

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$$\Longrightarrow \quad Y_{t-1} \approx \frac{1}{\sqrt{\alpha_t}}\left(Y_t + \frac{1-\alpha_t}{2} s_t(Y_t)\right) \qquad \text{original DDIM}$$

$$Y^{\mathsf{ode}}_{\overline{\alpha}_{t-1}} = \frac{1}{\sqrt{\alpha_t}} Y^{\mathsf{ode}}_{\overline{\alpha}_t} + \int_{\overline{\alpha}_t}^{\overline{\alpha}_{t-1}} \frac{1}{\sqrt{\gamma^3}} \underbrace{s^\star_\gamma\big(Y^{\mathsf{ode}}_\gamma\big)}_{\text{approximate by?}} \, \mathrm{d}\gamma$$

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$\frac{d}{\varepsilon}$ iterations; $\quad 1$ score eval per iteration $\qquad$ (DDIM)

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2nd order approx: (Li, Huang, Efimov, Wei, Chi, Chen '24)

$$\sqrt{\alpha_t} Y_{t-1} \approx Y_t + \frac{1-\alpha_t}{2} s_t(Y_t) + \frac{(1-\alpha_t)^2}{4(1-\alpha_{t+1})}\Big(s_t(Y_t) - \sqrt{\alpha_{t+1}} s_{t+1}(Y_{t+1})\Big)$$

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

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even higher-order approximation? for order K:

$$\frac{1}{\gamma^{3/2}} s^\star_\gamma(Y^{\mathsf{ode}}_\gamma) \approx \sum\nolimits_{0 \le i < K} \psi_i(\gamma) \frac{s_{\gamma_{t,i}}(Y^{\mathsf{ode}}_{\gamma_{t,i}})}{(\gamma_{t,i})^{3/2}}$$

- K anchor points: $\gamma_{t,0}, \ldots, \gamma_{t,K-1}$

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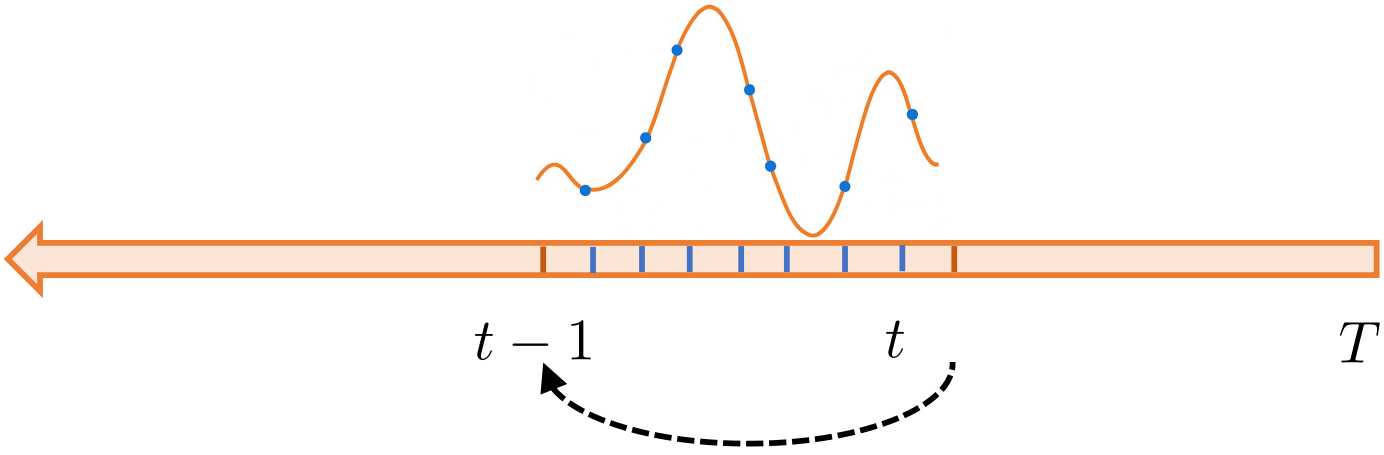
- Lagrange basis polynomial: $\psi_i(\gamma) := \frac{\prod_{i':i' \neq i} (\gamma - \gamma_{t,i'})}{\prod_{i':i' \neq i} (\gamma_{t,i} - \gamma_{t,i'})}$

Proposed K-th order sampler (Li et al. '25)



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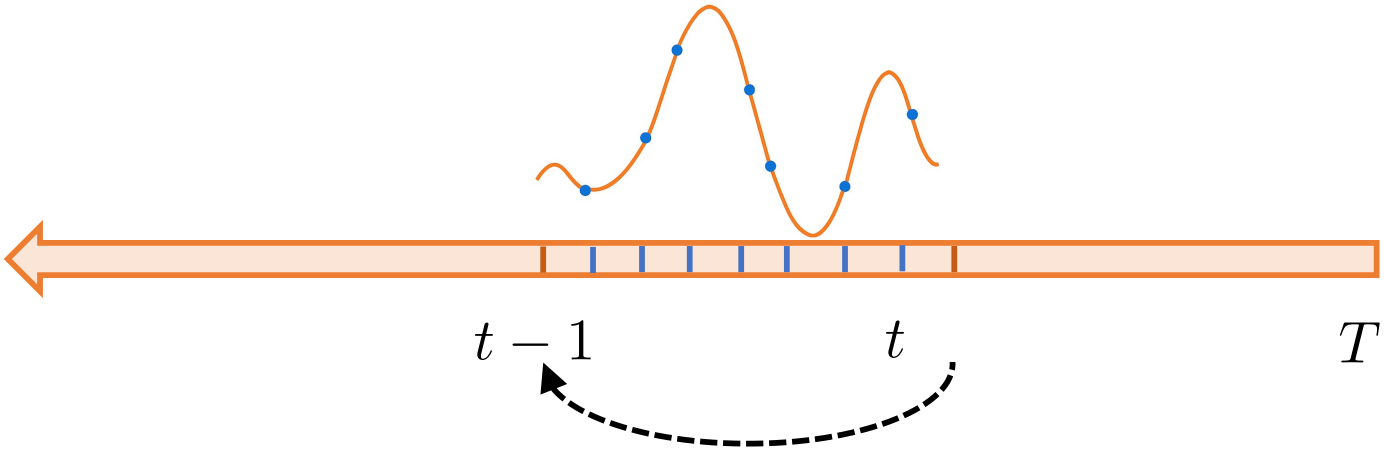

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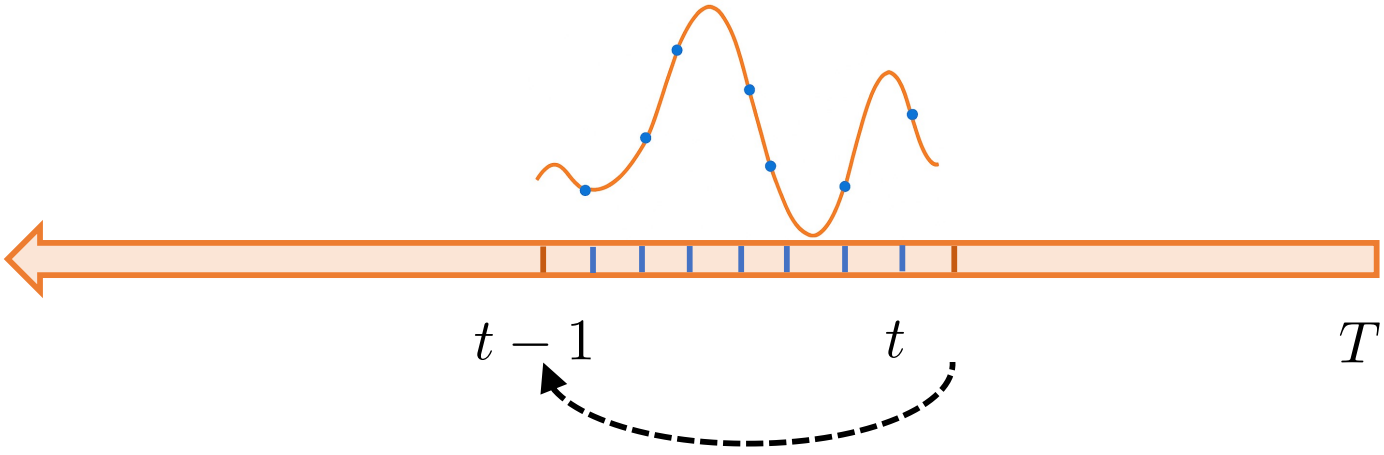

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K score evals per iteration; $\widetilde{O}(1)$ rounds of refinements

Convergence theory for our accelerated sampler

Theorem 1 (Li, Zhou, Wei, Chen '25)

Consider any $K = O(1)$. With perfect scores, our accelerated deterministic sampler yields $\mathsf{TV}(p_{X_1}, p_{Y_1}) \le \varepsilon$ *in*

$$\widetilde{O}\big(d^{1+2/K}/\varepsilon^{1/K}\big) \text{ iterations}$$

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- **# score function evaluations**: $\frac{d^{1+o(1)}}{\varepsilon^{1/K}}$
- outperforms vanilla DDIM (d/ε)
  - substantially improved ε-dependency
  - almost no loss in d-dependency;
- **minimal assumptions** on data distributions
  - see also Huang et al. '24, '25 (Runge-Kutta; stronger assumptions)

Summary

- nonasymptotic convergence theory for diffusion models
- provable training-free acceleration

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- nonasymptotic convergence theory for diffusion models
- provable training-free acceleration

Future directions:

- adaptive improvement under stylized statistical models
- design of high-order stochastic samplers
- parallelization

Papers

"Faster diffusion models via higher-order approximation," G. Li*, Y. Zhou*, Y. Wei, Y. Chen, `arXiv:2506.24042`, 2025

(*=equal contributions)

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 (for DDIM only):*

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

Assumptions: learning rates

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

- **learning rates:** for some consts $c_0, c_1 > 0$,

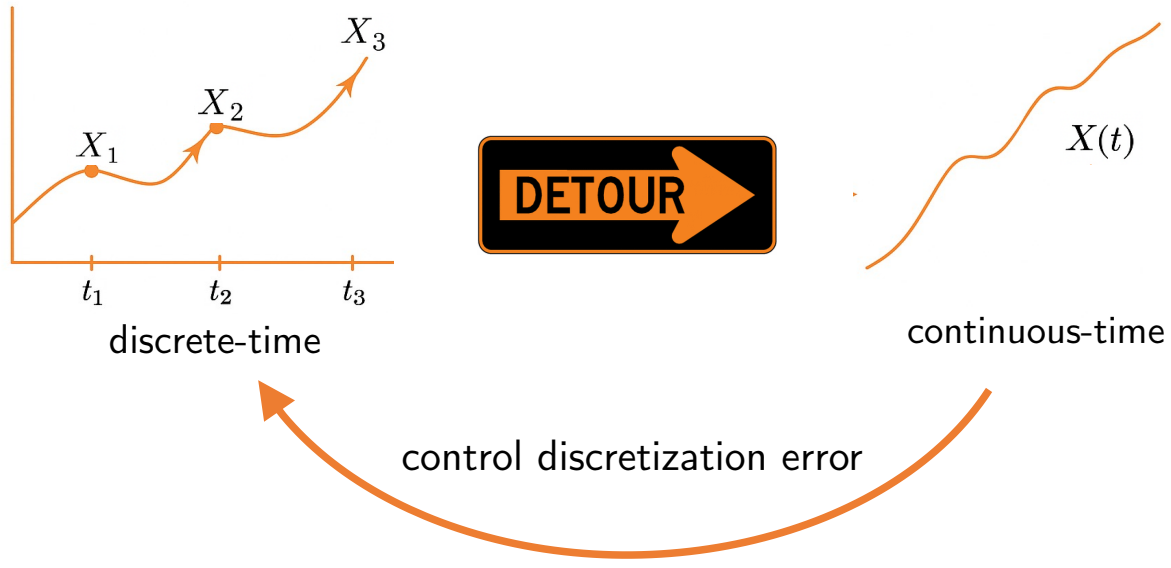
$$1 - \alpha_1 = \frac{1}{T^{c_0}}$$

$$1 - \alpha_t = \underbrace{\frac{c_1 \log T}{T} \min\left\{(1-\alpha_1)\left(1 + \frac{c_1 \log T}{T}\right)^t, 1\right\}}_{\text{2 phases: exp growth} \to \text{flat}}$$

Analysis strategy # 1 (for DDPM)

— *Chen, Chewi, Li, Li, Salim, Zhang '22, Chen, Lee, Lu '22, Tang, Zhao '24*

— *Benton, De Bortoli, Doucet, Deligiannidis '23, Huang, Wei, Chen '24*



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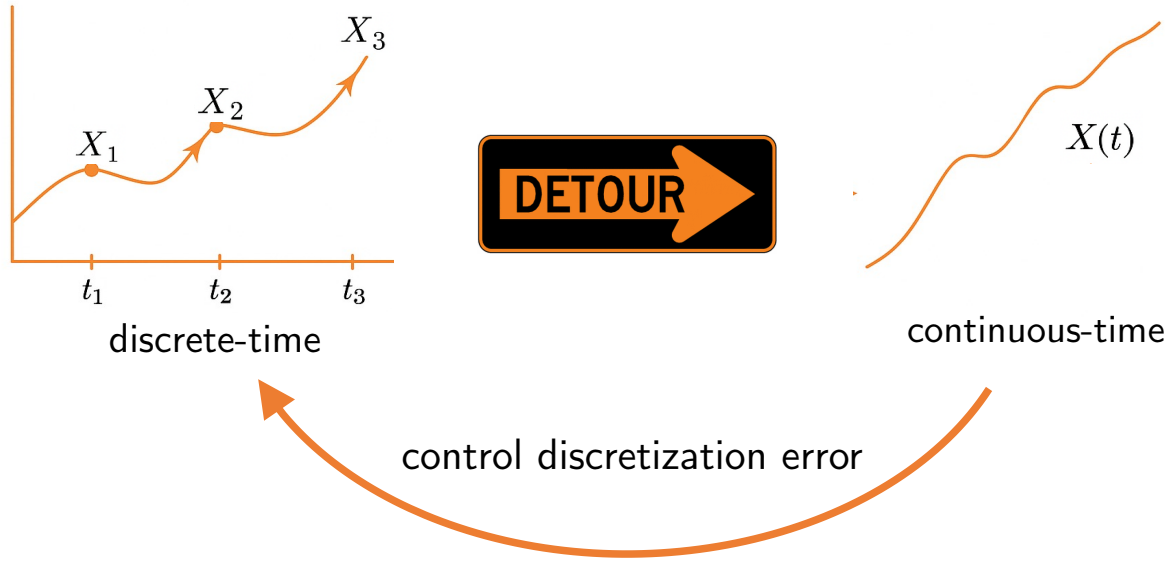

Analogy: (stochastic) gradient descent vs. gradient flow, TD learning via ODE

yields state-of-the-art KL-based theory for DDPM!

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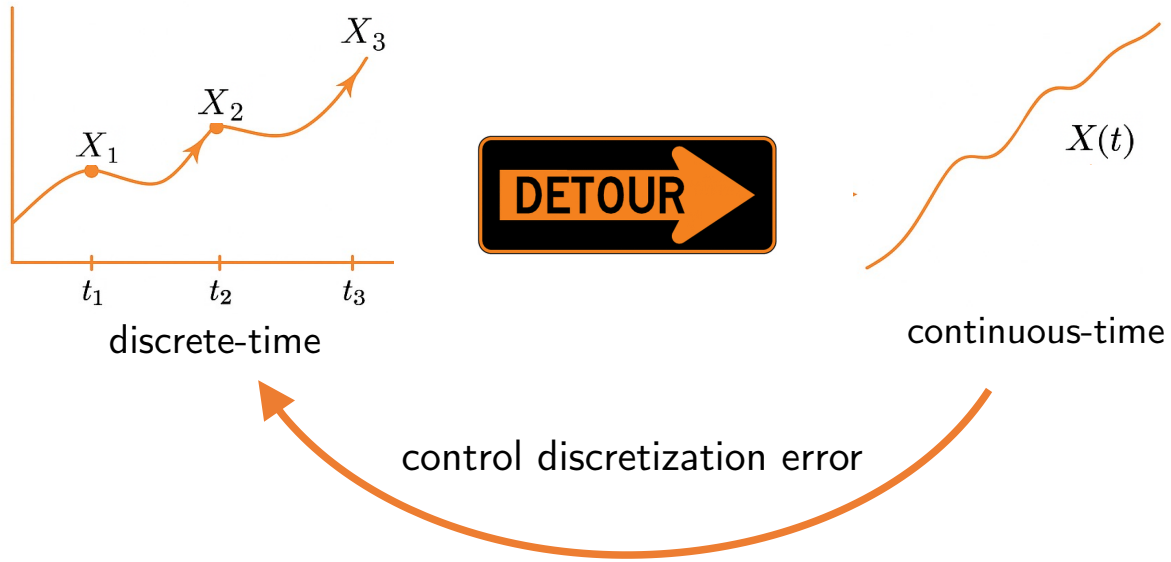

2 key steps:

- apply change of measure (e.g. Girsanov thm) to show

$$\mathsf{KL}\big(P^{\mathsf{true}} \,\|\, P^{\mathsf{ddpm}}\big) \le \int w(t) \underbrace{\mathbb{E}\Big[\big\|\mathsf{drift}^{\mathsf{true}}(t) - \mathsf{drift}^{\mathsf{ddpm}}(t)\big\|\Big]^2}_{\text{score error + discretization error}} \mathrm{d}t + \mathsf{small\text{-}term}$$

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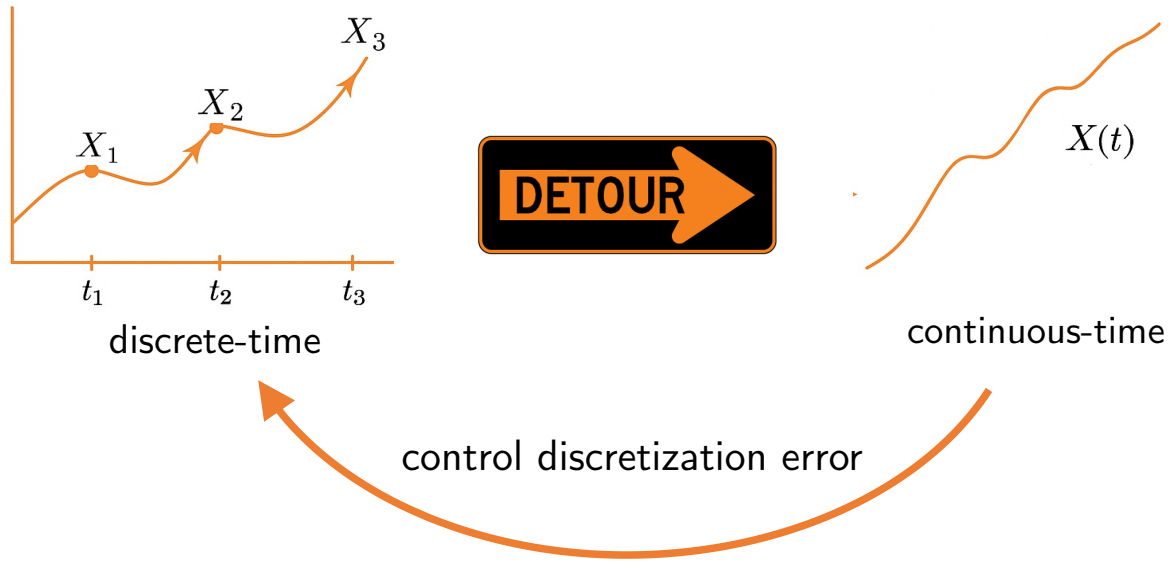

2 key steps:

- leverage stochastic localization to chacracterize

$$\text{discretization error} \overset{\text{link}}{\longleftrightarrow} \mathbb{E}\big[\mathrm{Cov}\big(X_0 \,|\, X_t\big)\big]$$

Analysis strategy # 2 (for DDIM & DDPM)

— *Li, Wei, Chen, Chi '24*, *Li, Wei, Chi, Chen '24*

— *Li, Yan '24*, *Liang, Huang, Chen '25*

Tackle discrete-time process directly & track changes of TV distance

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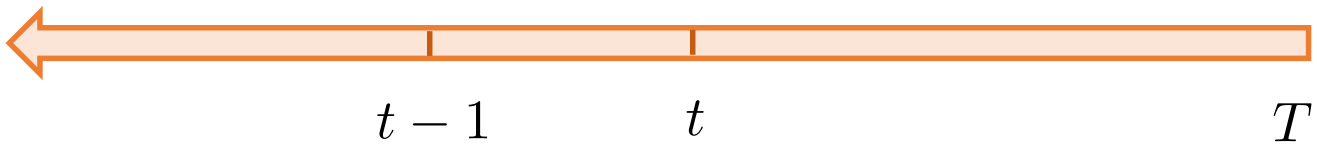

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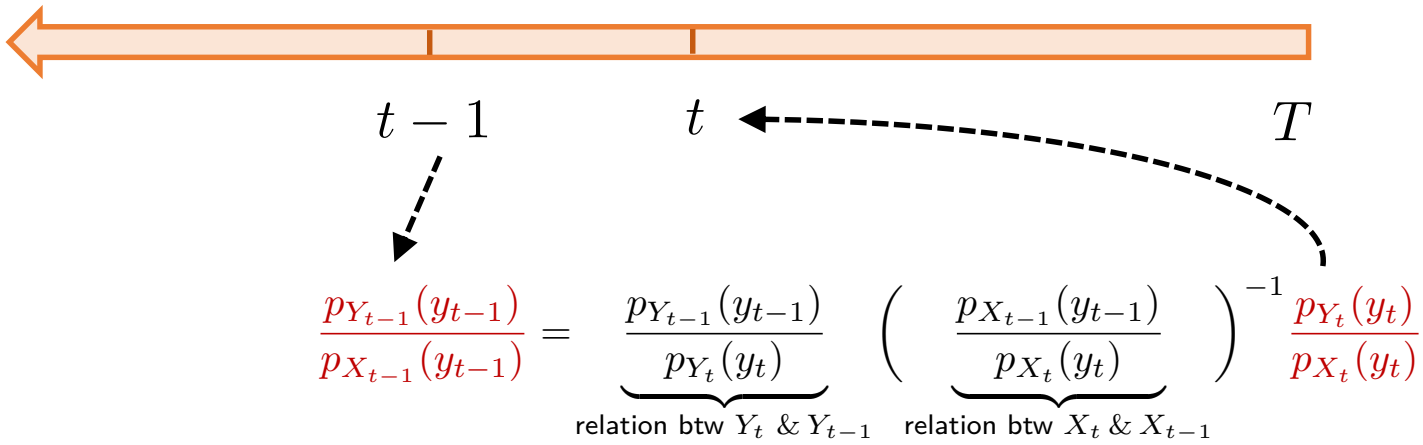
— Li, Wei, Chen, Chi '24, Li, Wei, Chi, Chen '24

— Li, Yan '24, Liang, Huang, Chen '25

Tackle discrete-time process directly & track changes of TV distance

$$\mathrm{TV}\big(p_{X_t}, p_{Y_t}\big) \approx 0 \quad \Longleftarrow \quad \frac{p_{Y_t}(y_t)}{p_{X_t}(y_t)} \approx 1 \quad \forall y_t \in \mathcal{E}_t \text{ (some "typical" set)}$$



Analysis strategy # 2 (for DDIM & DDPM)

— Li, Wei, Chen, Chi '24, Li, Wei, Chi, Chen '24

— Li, Yan '24, Liang, Huang, Chen '25

Tackle discrete-time process directly & track changes of TV distance

$$\mathrm{TV}\big(p_{X_t}, p_{Y_t}\big) \approx 0 \quad \Longleftarrow \quad \frac{p_{Y_t}(y_t)}{p_{X_t}(y_t)} \approx 1 \quad \forall y_t \in \mathcal{E}_t \text{ (some "typical" set)}$$