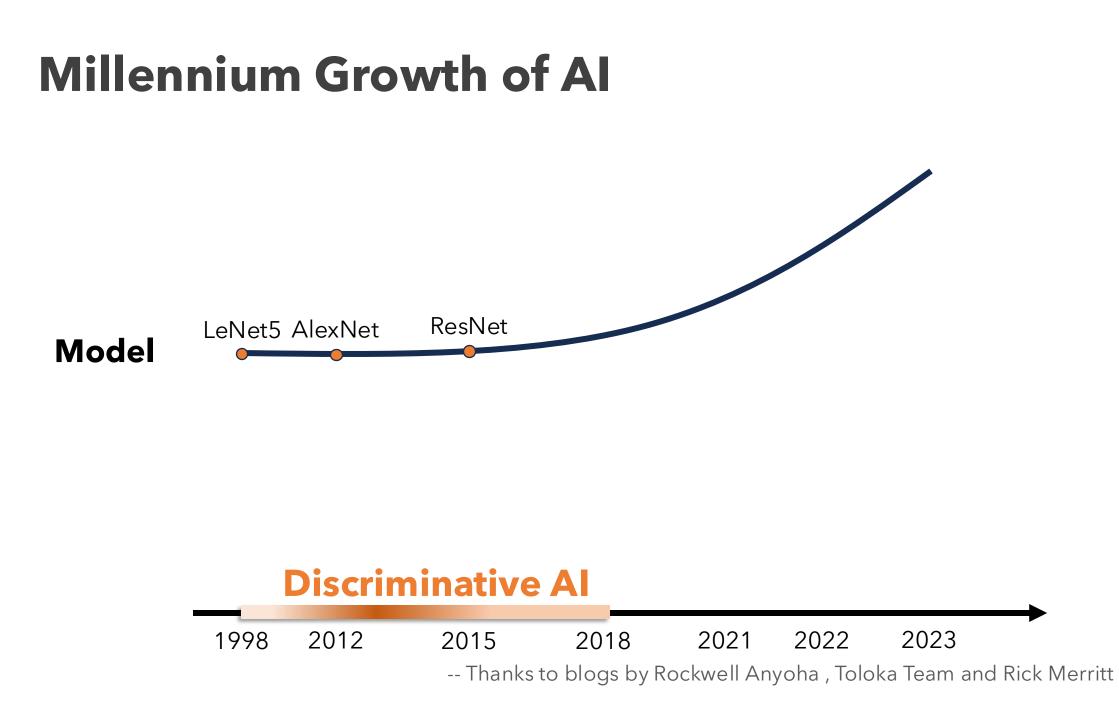
An Optimization Perspective on Guidance for Fine-Tuning Diffusion Models

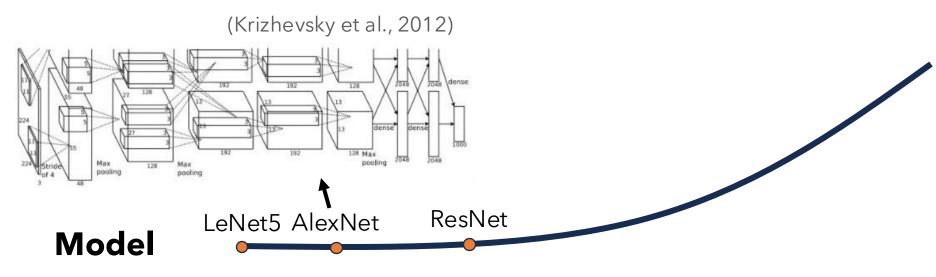
Minshuo Chen

Industrial Engineering & Management Sciences

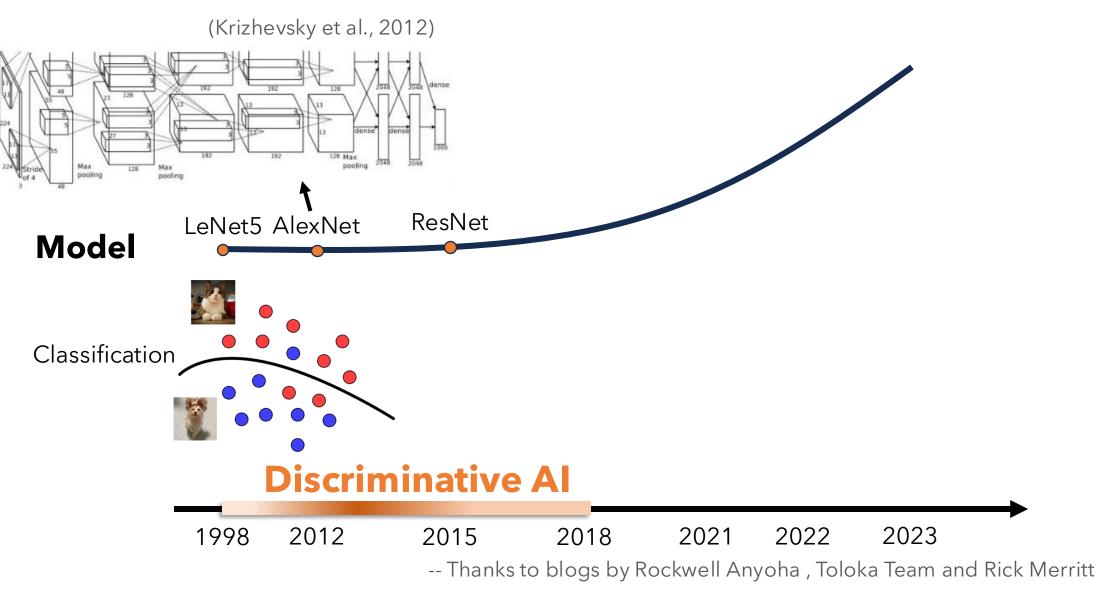


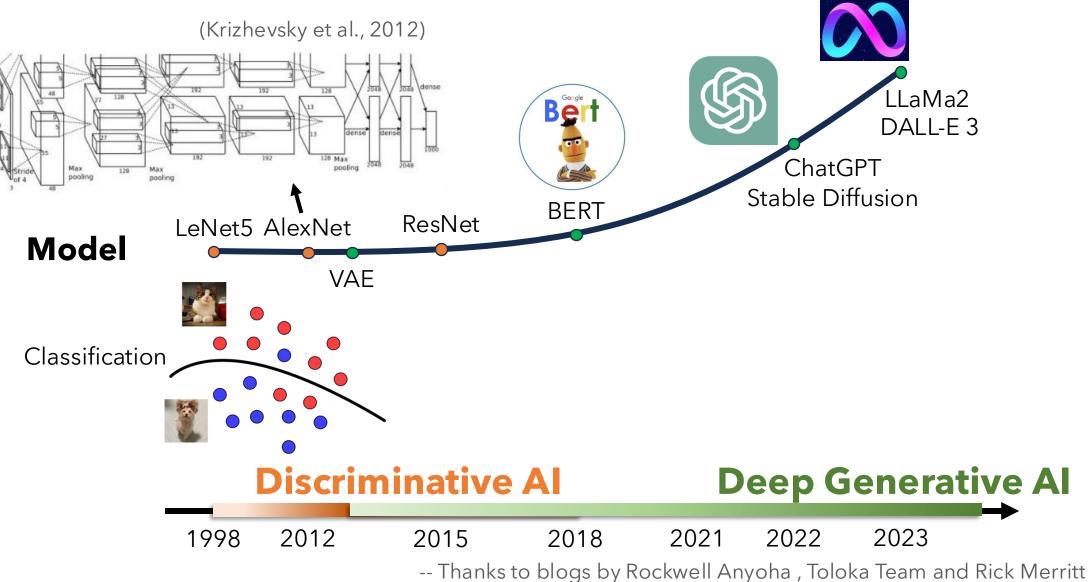
Joint work with Yingqing Guo, Zihao Li, Kaixuan Huang, Hui Yuan, Yukang Yang, Yinyu Ye, and Mengdi Wang

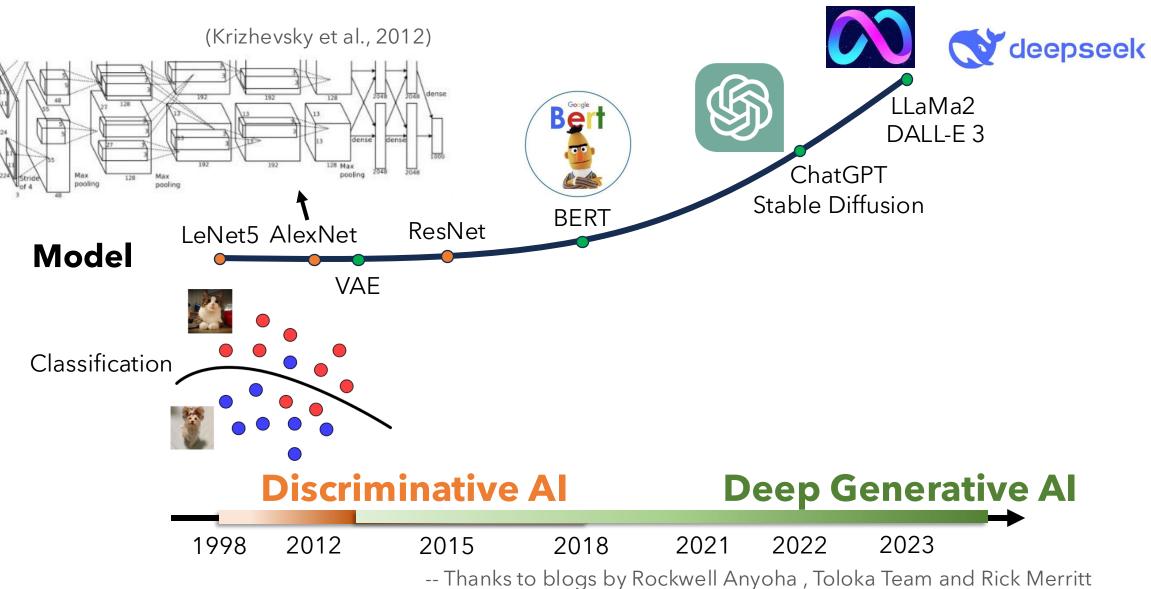


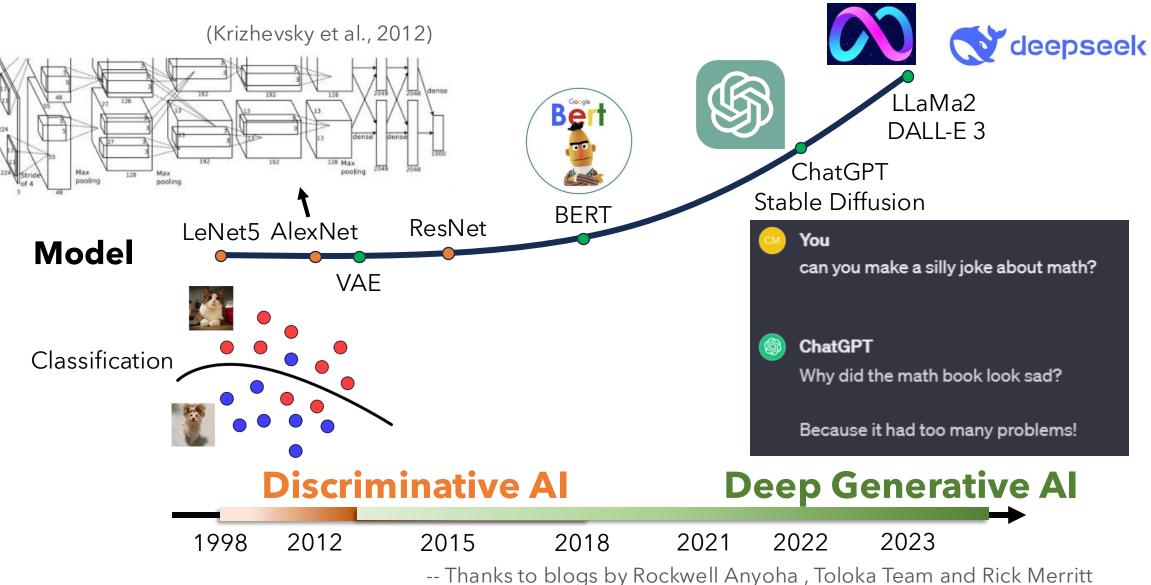




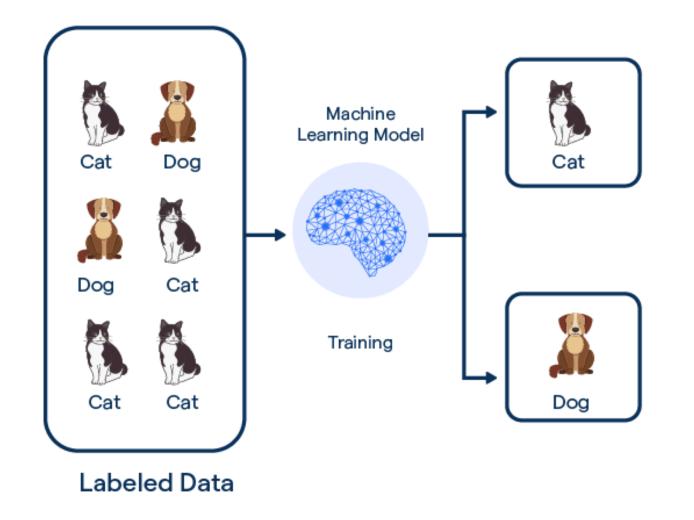






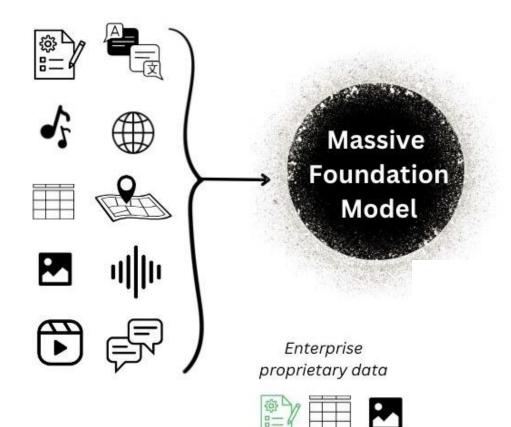


-- Thanks to blogs from BotPenguin and Humanloop

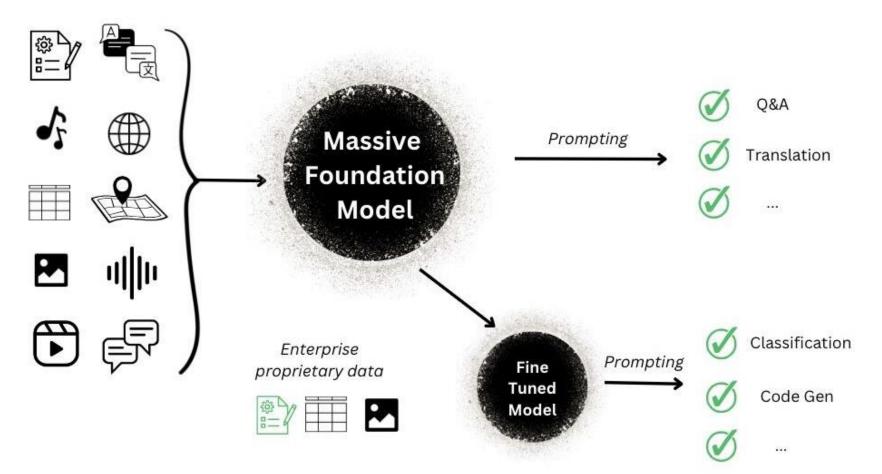


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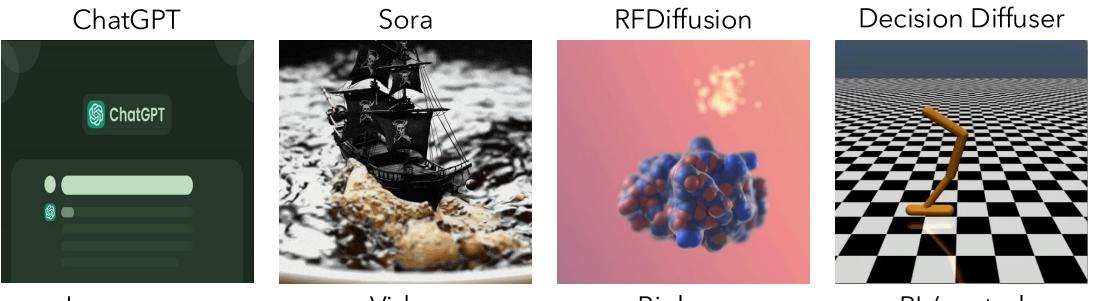
Massive external data



Massive external data



-- Thanks to blogs from BotPenguin and Humanloop

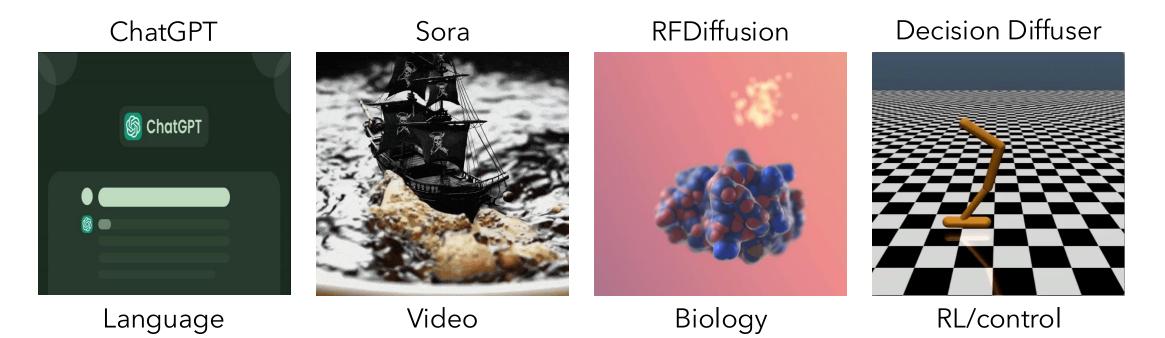


Language

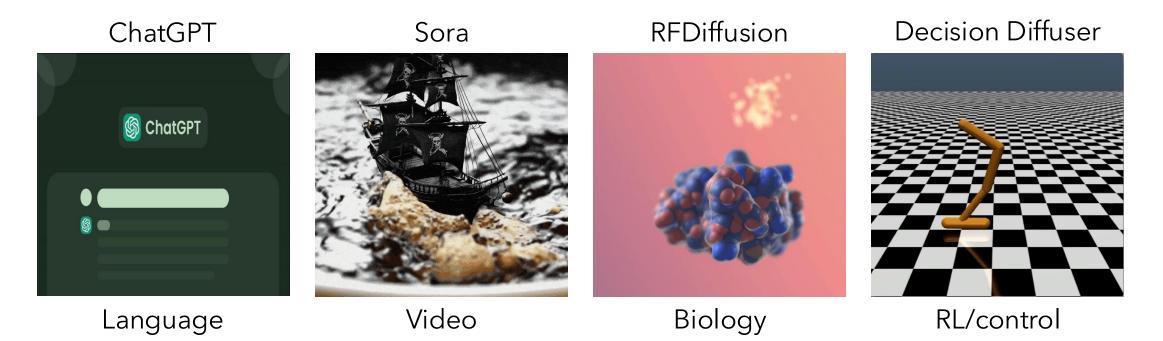
Video

Biology

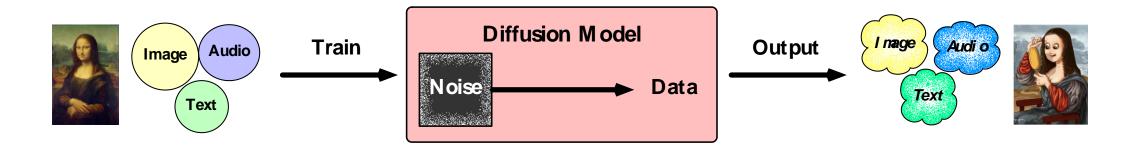
RL/control

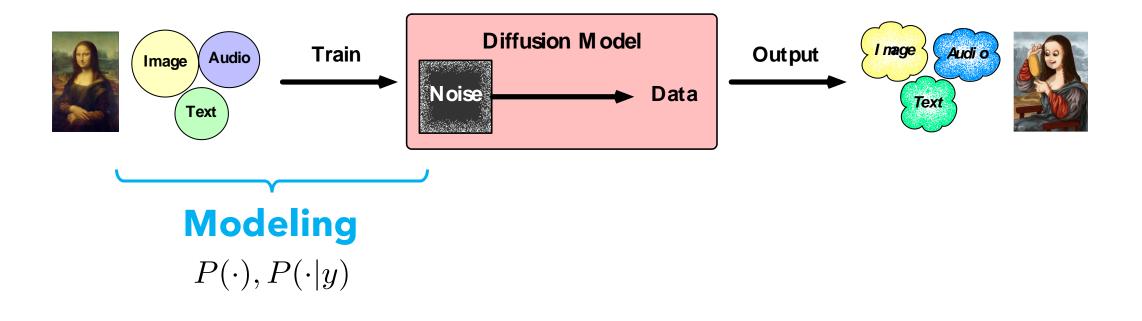


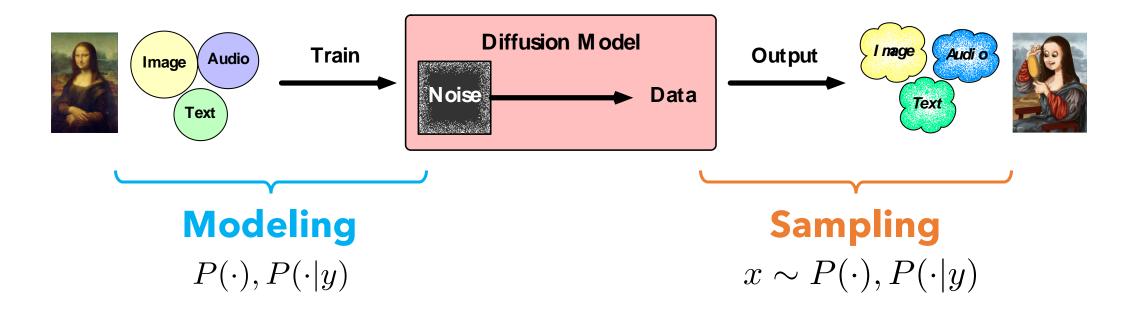
• Adapter (Houlsby et al., 2019), LoRA (Hu et al., 2022), Supervised fine-tuning (Ouyang et al., 2022), RLHF (Ouyang et al., 2022), Distillation (Poole et al., 2022), ...

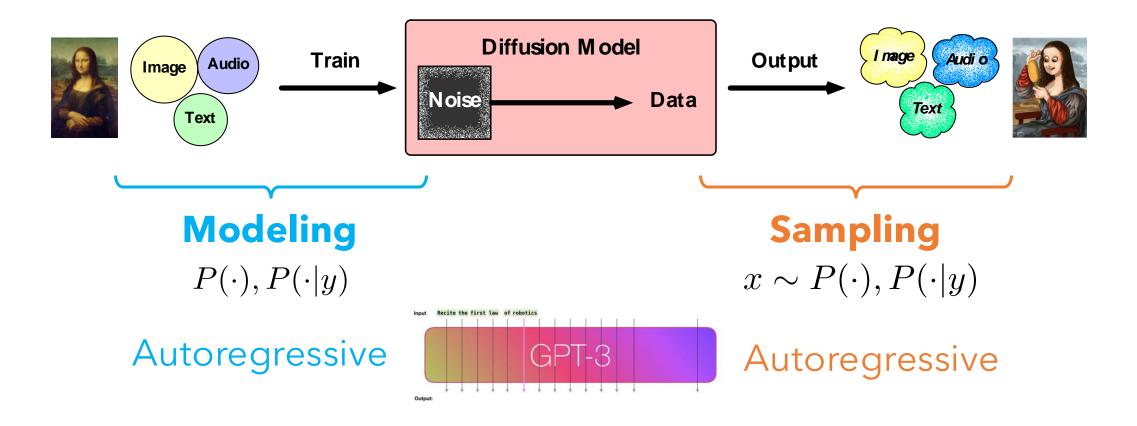


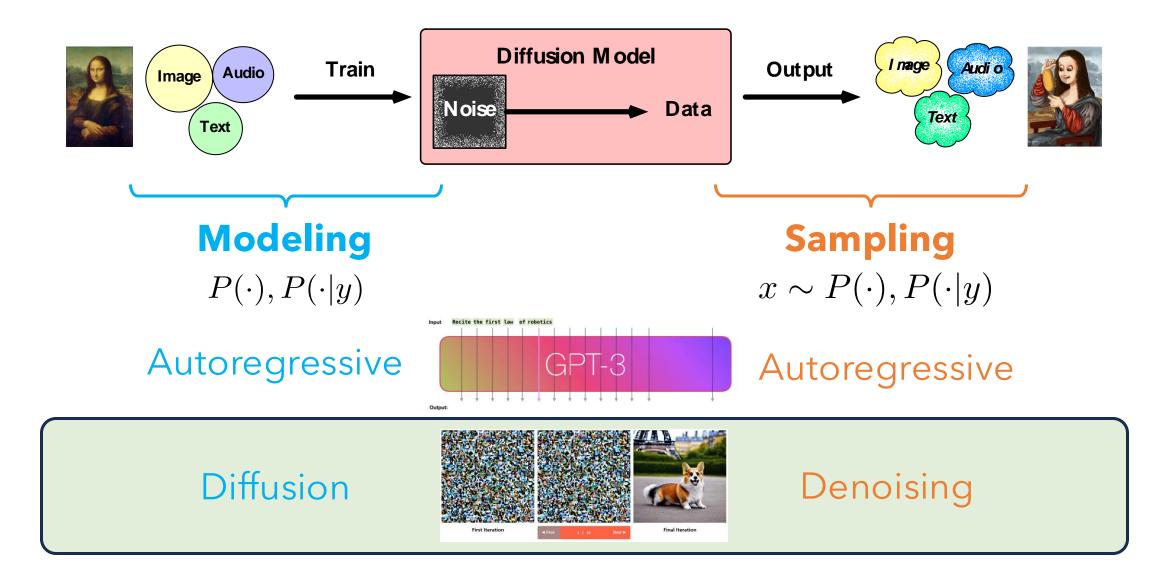
- Adapter (Houlsby et al., 2019), LoRA (Hu et al., 2022), Supervised fine-tuning (Ouyang et al., 2022), RLHF (Ouyang et al., 2022), Distillation (Poole et al., 2022), ...
- Gap: Methodology focused; limited theoretical guarantees









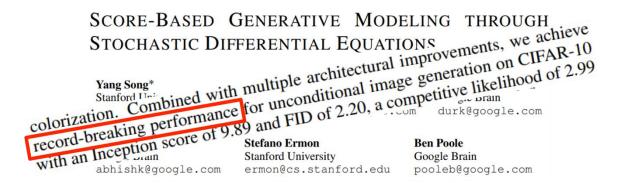


Diffusion Models Beat GANs on Image Synthesis

Prafulla Dhariwal* OpenAI prafulla@openai.com Alex Nichol* OpenAI alex@openai.com

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ImageNet Benchmark (Image Generation)

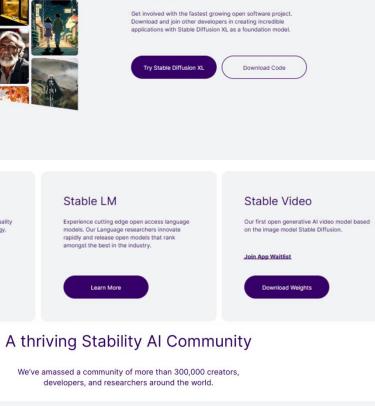
I	Rank	Model	FID ↓ Paper		Code	Result	Year	Tags 🖻
	1	DIT-XL/2 with CADS	1.70	CADS: Unleashing the Diversity of Diffusion Models through Condition-Annealed Sampling		Ð	2023	Diffusion
CIF	2	MAGVIT-v2	1.78	Language Model Beats Diffusion Tokenizer is Key to Visual Generation		Ð	2023	VAE/VQ-VAE Mask Prediction
	3	MDT-XL2	1.79	Masked Diffusion Transformer is a Strong Image Synthesizer	0	Ð	2023	VAE/VQ-VAE Diffusion
	4	Discriminator Guidance	1.83	Refining Generative Process with Discriminator Guidance in Score-based Diffusion Models	0	Ð	2022	Diffusion
	5	RDM	1.87	Relay Diffusion: Unifying diffusion process across resolutions for image synthesis	0	Ð	2023	Diffusion
	6	ViT-XL	2.06	Efficient Diffusion Training via Min-SNR Weighting Strategy	0	Ð	2023	Diffusion
	7	VDM++	2.12					Diffusion
	8	StyleSAN-XL	2.14	SAN: Inducing Metrizability of GAN with Discriminative Normalized Linear Layer	0	Ð	2023	GAN

ImageNet Benchmark (Image Generation)

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Rank	Model	FID 4	Paper	Cod	
1	DiT-XL/2 with CADS	1.70	CADS: Unleashing the Diversity of Diffusion Models through Condition-Annealed Sampling		
2	MAGVIT-v2	1.78	Language Model Beats Diffusion Tokenizer is Key to Visual Generation		
3	MDT-XL2	1.79	Masked Diffusion Transformer is a Strong Image Synthesizer	C	Stable Audio
4	Discriminator Guidance	1.83	Refining Generative Process with Discriminator Guidance in Score-based Diffusion Models	C	Generate music and sound effects in high quality using cutting-edge audio diffusion technology.
5	RDM	1.87	Relay Diffusion: Unifying diffusion process across resolutions for image synthesis	C	Try Stable Audio
6	VIT-XL	2.06	Efficient Diffusion Training via Min-SNR Weighting Strategy	C	A
7	VDM++	2.12			10M
8	StyleSAN-XL	2.14	SAN: Inducing Metrizability of GAN with Discriminative Normalized Linear Layer	Ç	Global users just two months after its release

stability.ai



270,000

Stable Diffusion's Discord

channel Members

+170M

Clipdrop SDXL

Images generated with

Stable Diffusion XL

400M

Images generated using Stability Al's API

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Generative AI imagines new protein structures

"FrameDiff" is a computational tool that uses generative AI to craft new protein structures, with the aim of accelerating drug development and improving gene therapy.

Rachel Gordon | MIT CSAIL July 12, 2023





Biology is a wondrous yet delicate tapestry. At the heart is DNA, the master weaver that encodes proteins, responsible for orchestrating the many biological functions that sustain life within the human body. However, our body is akin to a finely tuned instrument, susceptible to losing its harmony. After all, we're faced with an ever-changing and relentless natural world: pathogens, viruses, diseases, and cancer.

stability ai n) Cod Stable Diffusion XL Get involved with the fastest growing open software project. Models Download and join other developers in creating incredible applications with Stable Diffusion XL as a foundation model Try Stable Diffusion XI Download Code r is Kev to Stable Audio Stable LM Stable Video Generate music and sound effects in high quality Experience cutting edge open access language Our first open generative AI video model based using cutting-edge audio diffusion technology. models. Our Language researchers innovate on the image model Stable Diffusion. rapidly and release open models that rank amongst the best in the industry. Join App Waitlist Learn more cross Try Stable Audi Learn More Download Weigh A thriving Stability AI Community ahtina We've amassed a community of more than 300,000 creators, developers, and researchers around the world.

Global users just two months after its release

10M

Stable Diffusion's Discord channel Members

270,000

Images generated with Clipdrop SDXL

+170M

Images generated using Stability Al's API

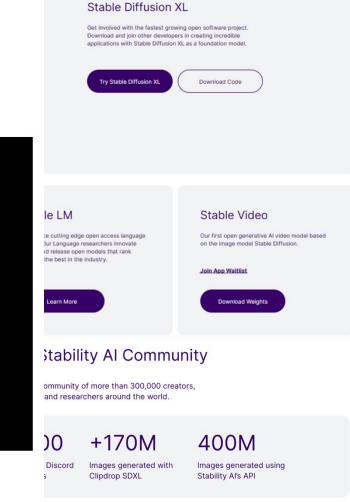
400M

Generative AI imagines new prDiffusion models are now "FrameDiff" is a computational tool that uses generating turbocharging reinforcement improving gene therapy. learning systems Stable Diffusion XL Rachel Gordon | MIT CSAIL July 12, 2023 Download and join other developers in creating incredible By Ben Dickson - March 4, 2024 Like 75 Try Stable Diffusion X Download Code Facebook V Linkedin Reddlt in le LM e cutting edge open access language our Language researchers innovate d release open models that rank the best in the industry.

Biology is a wondrous yet delicate tapestry. At the heart is encodes proteins, responsible for orchestrating the many within the human body. However, our body is akin to a fine

losing its harmony. After all, we're faced with an ever-chan *This article is part of our coverage of the latest in AI research*. pathogens, viruses, diseases, and cancer.

Image generated with Bing Image Creator



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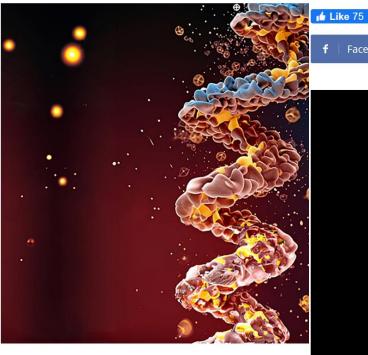
Generative AI imagines new prDiffusion models are ARTIFICIAL INTELLIGENCE

"FrameDiff" is a computational tool that uses go protein structures, with the aim of accelerating turbocharging reinfo AniPortrait: Audio-Driven Synthesis of improving gene therapy. **Photorealistic Portrait Animation** learning systems

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By Ben Dickson - March 4, 2024

Facebook



Published 3 days ago on May 3, 2024



Over the years, the creation of realistic and expressive portraits animations from static images and audio has found a range of applications including gaming, digital media, virtual reality, and a lot more. Despite its potential application, it is still difficult for developers to create frameworks capable of generating highquality animations that maintain temporal consistency and are visually captivating. A major cause for the complexity is the need for intricate coordination of lip movements, head positions, and facial expressions

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Dani Valevski^{*} Yaniv Leviathan^{*} Moab Arar^{*†} Shlomi Fruchter^{*} July 12, 1 Google Research Google Research Tel Aviv University Google DeepMind Over the years, the creation of realistic and expressive portraits animations from static images and audio

Diffusion Models Are Real-Time Game Engines s of

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Gen Diffusion Models Are Real-Time Game Engines s of "Fram protei improv

Large Language Diffusion Models

Shen Nie^{1*†} Fengqi Zhu^{1*†} Zebin You^{1†} Xiaolu Zhang^{2‡} Jingyang Ou¹ Jun Hu^{2‡} Jun Zhou² Yankai Lin^{1‡} Ji-Rong Wen¹ Chongxuan Li^{1‡¶}

Abstract

Rachel (July 12, 1

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Biology is

encodes

Autoregressive models (ARMs) are widely regarded as the cornerstone of large language models (LLMs). We challenge this notion by introducing LLaDA, a diffusion model trained from scratch under the pre-training and supervised finetuning (SFT) paradigm. LLaDA models distriwithin the human body. However, our body is akin to a fine

Mattematics ARC-C GSM8K TruthfulQA Math and audio Despite ing high-MMLU se for the

complexity is the need for intricate coordination of lip movements, head positions, and facial expressions

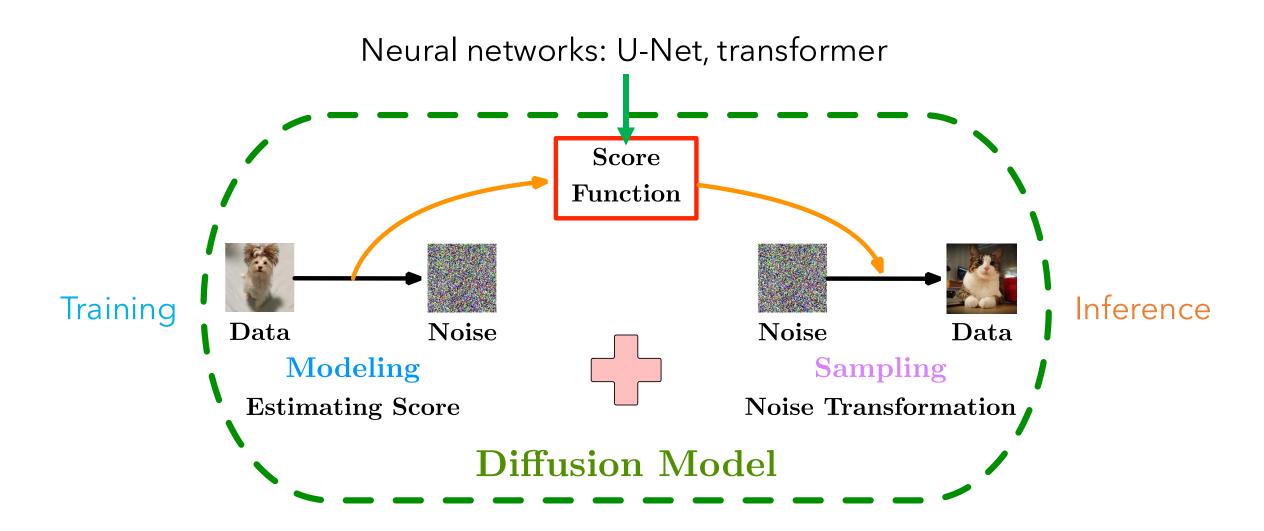
losing its harmony. After all, we're faced with an ever-chan This article is part of our coverage of the late to craft a visually compelling effect. pathogens, viruses, diseases, and cancer.



- Introduction to diffusion models
- Conditional models and guidance
- Guiding diffusion models in offline and online settings
- Future directions

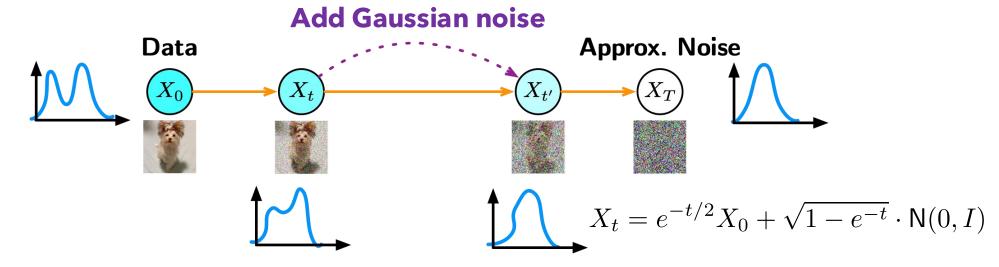
Diffusion Model and Guidance

Overview of Diffusion Models

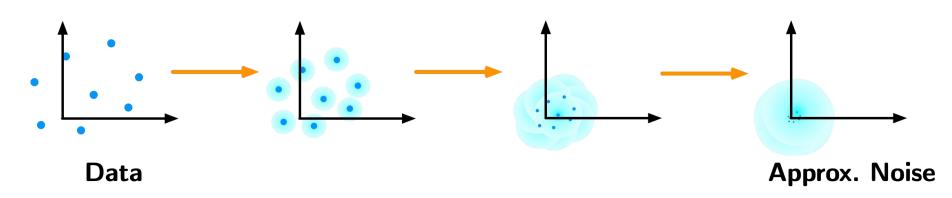


Forward Process - Noise Corruption

• Noise corruption process $dX_t = -\frac{1}{2}X_t dt + dW_t$

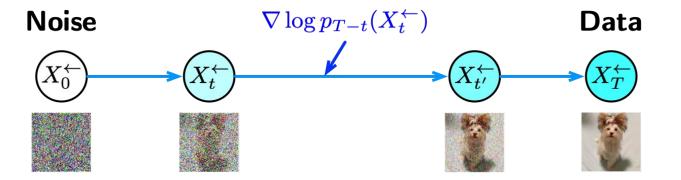


• The noise corruption



Backward Process - Sample Generation

• Time reversal in distribution



• The math (Anderson, 1982; Haussmann and Pardoux, 1986)

Forward $dX_t = -\frac{1}{2}X_t dt + dW_t$ Theorem Later such as the as a smooth further that as a smooth further tha

Theorem. Let x_t be the process described by (3.3), and suppose $f(\cdot, \cdot)$ and $g(\cdot, \cdot)$ are such as to guarantee the existence of the probability density $p(x_n, t)$ for $t_0 \le t \le T$ as a smooth and unique solution of its associated Kolmogorov equation. Suppose further that an t-vector process \tilde{w}_i is defined by $\tilde{w}_n = 0$ and

$$\mathbf{d}\bar{w}_{t}^{k} = \mathbf{d}w_{t}^{k} + \frac{1}{p(x_{h},t)}\sum_{i}\frac{\partial}{\partial x_{t}^{i}}\left[p(x_{h},t)g^{ik}(x_{h},t)\right]\mathbf{d}t,$$
(3.10)

and that the forward Kolmogorov equation associated with the joint process (x_b, \bar{w}_t) yields a smooth and unique solution in $t > t_0$ for $p(x_b, \bar{w}_b, t)$ and in $t > s \ge t_0$ for $p(x_b, \bar{w}_b, t, \bar{w}_b, s)$. Then

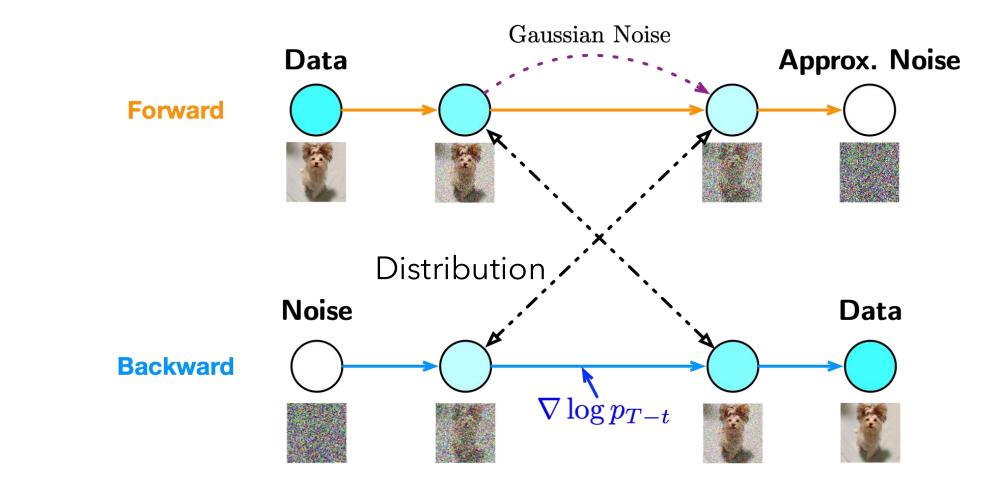
(i) x_t and $\bar{w}_t - \bar{w}_s$ are independent for all $t \ge s \ge t_0$.

(ii) With \vec{x}_t the minimal σ -algebra with respect to which x_s for $s \ge t$ and \vec{w}_s for $s \ge t$ are measurable, conditions (3.4) and (3.5) hold. (iii) A reverse time model for x_s is defined by

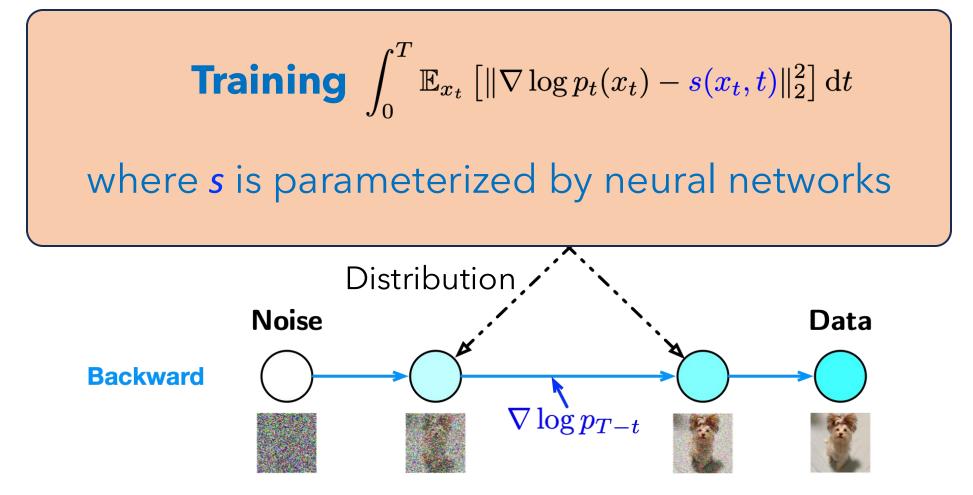
$$\mathbf{d}\mathbf{x}_t = \bar{f}(\mathbf{x}_t, t) \, \mathbf{d}t + g(\mathbf{x}_t, t) \, \mathbf{d}\bar{w}_t \tag{3.11}$$

 $\bar{f}^{i}(x_{b},t) = f^{i}(x_{b},t) - \frac{1}{p(x_{b},t)} \sum_{l \in \mathcal{A}} \frac{\partial}{\partial x_{l}^{i}} [p(x_{b},t)g^{ik}(x_{b},t)g^{lk}(x_{b},t)].$ (2.12)

Forward and Backward Coupling



Forward and Backward Coupling



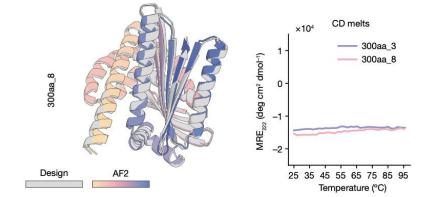
From P(x) to P(x|y)

• Text-to-image generation (Black et al., 2023)

— Prompt Alignment: a raccoon washing dishes —

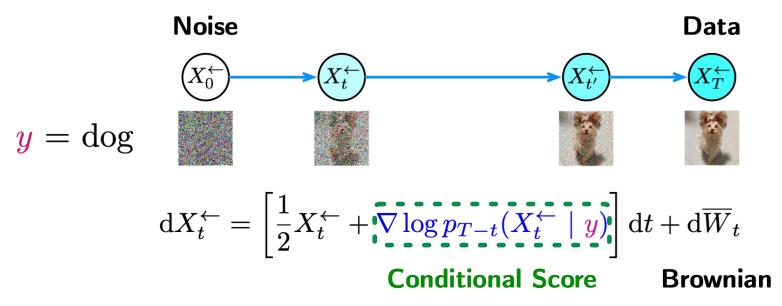


• Protein generation with biochemical properties (Watson et al., 2023; Gruver et al., 2023)



Conditional Diffusion Models

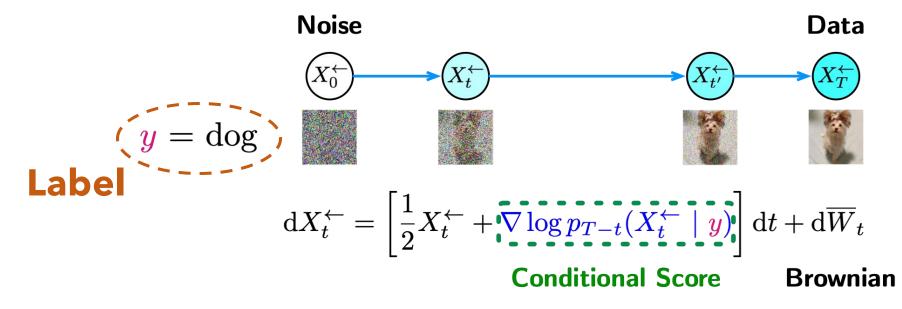
• Conditioned sample generation for a given label



-- More in the survey: M. Chen, S. Mei, J. Fan, and M. Wang. "Challenges and Opportunities of Diffusion Models for Generative AI". National Science Review 2024

Conditional Diffusion Models

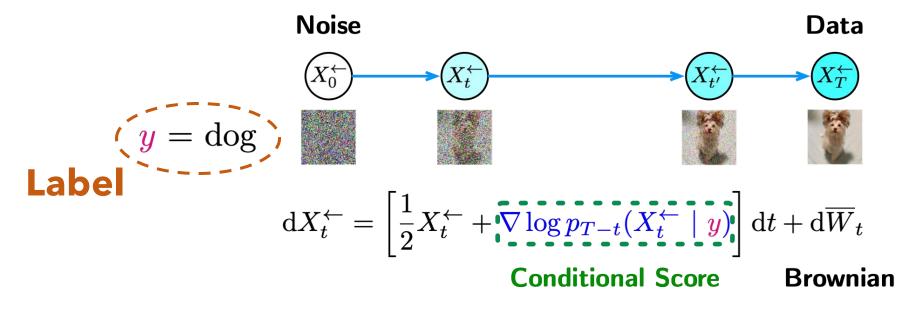
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Conditional Diffusion Models

• Conditioned sample generation for a given label



- Diffusion models can handle diverse conditional information, e.g., text prompts, partial images, etc.
- The key is to scalably estimate the conditional score

-- More in the survey: M. Chen, S. Mei, J. Fan, and M. Wang. "Challenges and Opportunities of Diffusion Models for Generative AI". National Science Review 2024

Conditional Score and Guidance

$$\nabla_x \log p_t(x_t|y) = \nabla_x \log \frac{p_t(x_t, y)}{p_t(y)}$$
$$= \nabla_x \log p_t(x_t) p_t(y|x_t) - \underbrace{\nabla_x \log p_t(y)}_{= \nabla_x \log p_t(x_t) + \nabla_x \log p_t(y|x_t)}$$

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• Bayes' rule defines **guidance**

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• When y is a label, guidance is gradient of classification logit; known as the *classifier guidance* (Dhariwal & Nichol, 2021)

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- Beyond labels? (Ho & Salimans, 2022; Bansal et al., 2023)

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- Beyond labels?



(Ho & Salimans, 2022; Bansal et al., 2023)

Role of Guidance I ---- To Optimize

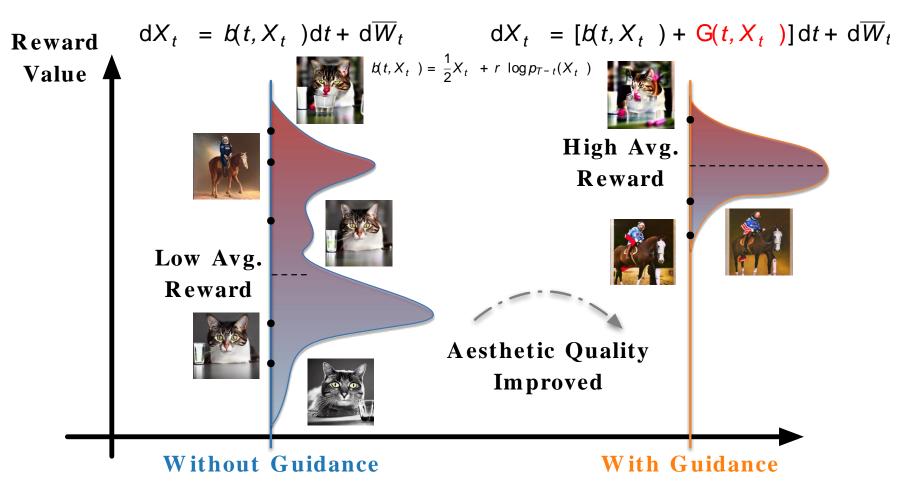
• Abstract the task-specific objective as a reward function *f*

Role of Guidance I ---- To Optimize

- Abstract the task-specific objective as a reward function f
- Guidance is to optimize reward by generating solutions

Role of Guidance I ---- To Optimize

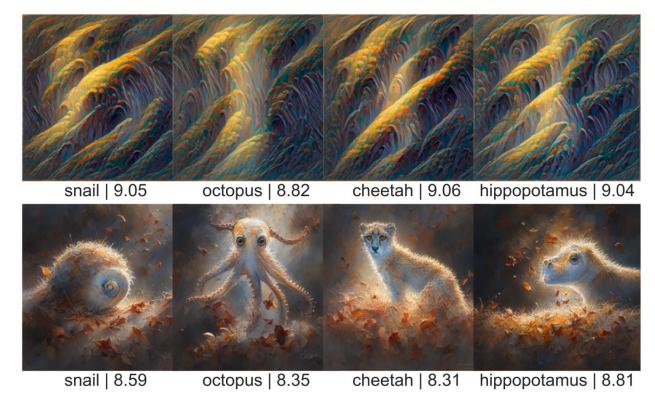
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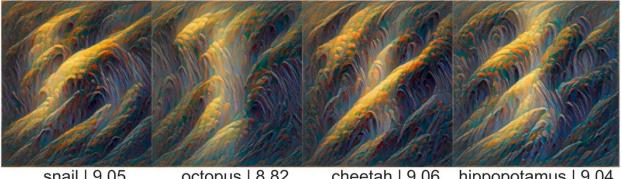
• Reward collapse is a common challenge (Ouyang et al., 2022; Song et al., 2023)

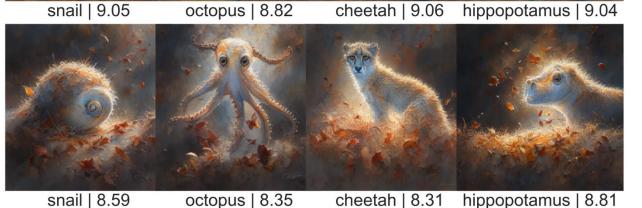
- Reward collapse is a common challenge (Ouyang et al., 2022; Song et al., 2023)
- Guidance also needs to preserve data fidelity

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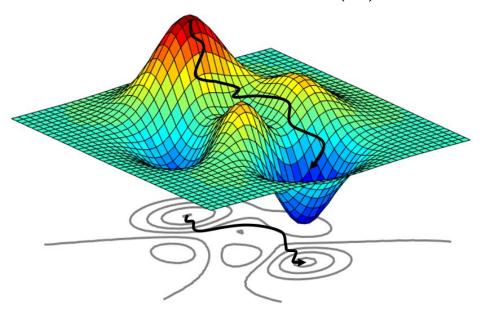
- Reward collapse is a common challenge (Ouyang et al., 2022; Song et al., 2023)
- Guidance also needs to preserve data fidelity





-- Figure from Uehara et al., (2024)

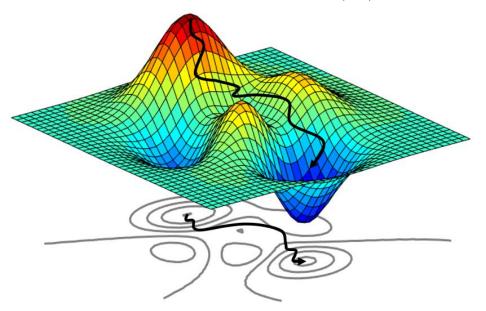
 $x^* \in \arg\max f(x)$



Generate solution $x \sim \mathbb{P}(\cdot \mid f(\cdot) = a)$

Complex landscape Data fidelity

 $x^* \in \arg\max f(x)$

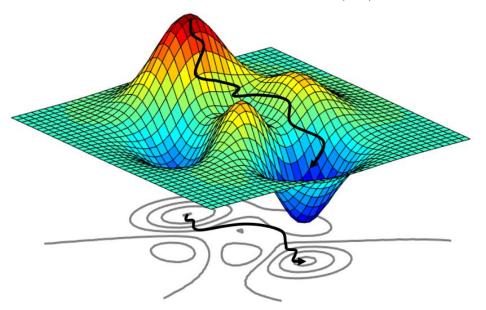


Generative Optimization

Generate solution $x \sim \mathbb{P}(\cdot \mid f(\cdot) = a)$

Complex landscape Data fidelity

 $x^* \in \arg\max f(x)$



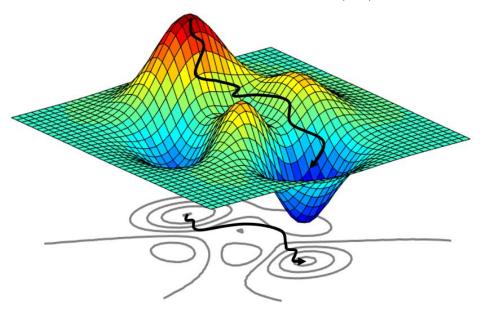
Generative Optimization

Generate solution $x \sim \mathbb{P}(\cdot \mid f(\cdot) = a)$

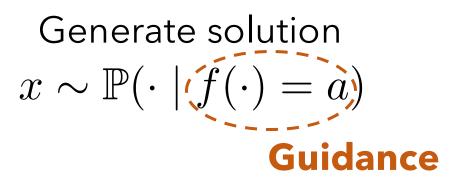
Complex landscape Data fidelity

Conditional distribution Guidance design

 $x^* \in \arg\max f(x)$



Generative Optimization



Complex landscape Data fidelity

Conditional distribution Guidance design

Offline with Logged Data:

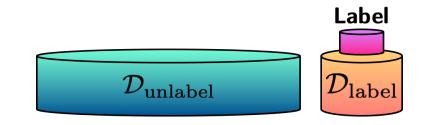
Can we learn a **conditional** diffusion model to generate **high-reward** high-fidelity data?

Problem Setup: Offline Reward Maximization

- ${\ensuremath{\cdot}}$ Given a training data set, generate new x
- Training data set

 $\mathcal{D}_{\text{unlabel}} = \{x_j\}_{j=1}^{n_{\text{unlabel}}}$ $\mathcal{D}_{\text{label}} = \{x_i, y_i = f^*(x_i) + \epsilon_i\}_{i=1}^{n_{\text{label}}}$ $\triangleright \ \epsilon_i \text{ is observation noise}$ $\triangleright f^* \text{ is reward function}$ $\triangleright x \text{ is in a linear subspace}$

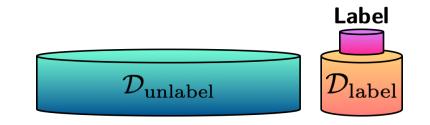
$$x = Az$$
 with $A \in \mathbb{R}^{D \times d}$ $z \in \mathbb{R}^d$



Problem Setup: Offline Reward Maximization

- ${\ensuremath{\cdot}}$ Given a training data set, generate new x
- Training data set

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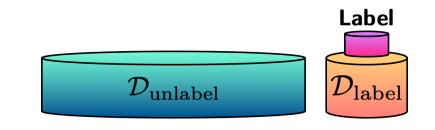
ϵ_i is observation noise
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 Example: a large collection of unlabeled protein structures;

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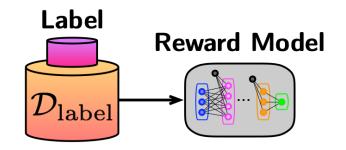
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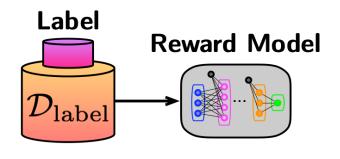


Off-policy bandit problem (Jin et al., 2021; Nguyen-Tang et al., 2021)

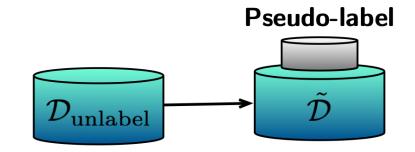
Example: a large collection of unlabeled protein structures; only a few has measured properties.



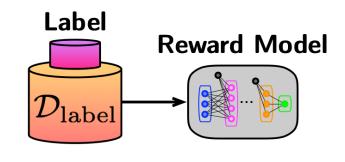
Step 1: Reward Learning



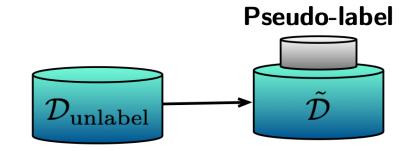
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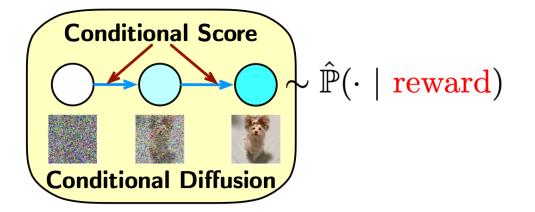
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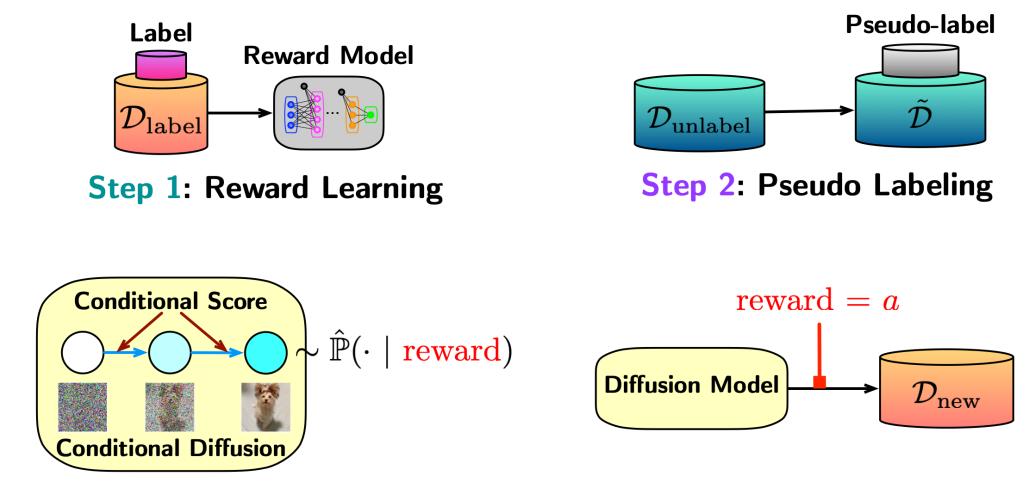
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Step 3: Conditional Diffusion Training

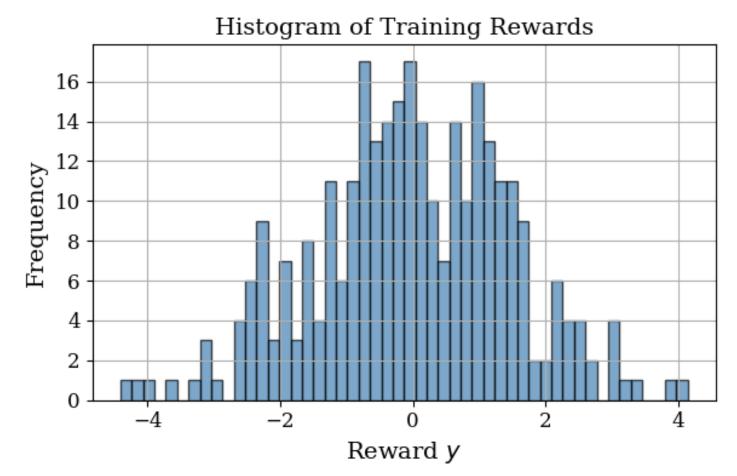


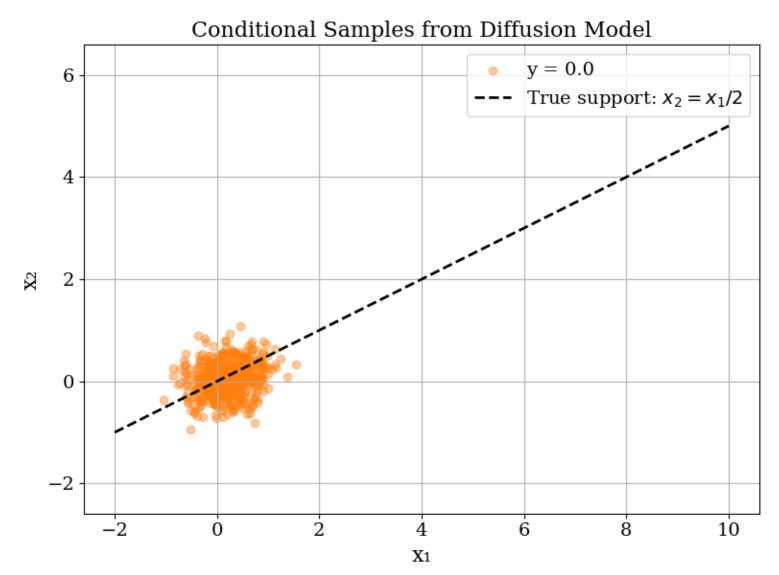
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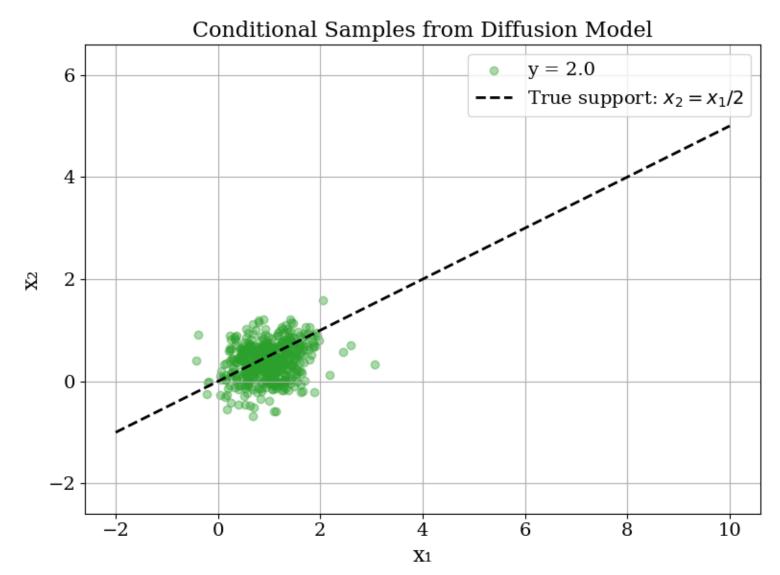
Step 4: Guided Generation

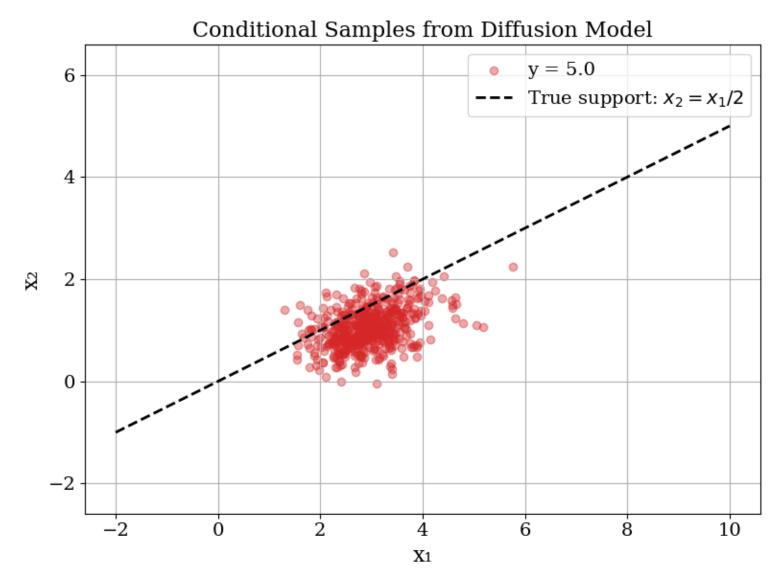
A Toy Example

- 2D data X with $X = [1, 0.5]^{\top} z$ for $z \sim N(0, 1)$
- Linear reward $Y = [1, 1]^{\top} x + \epsilon$

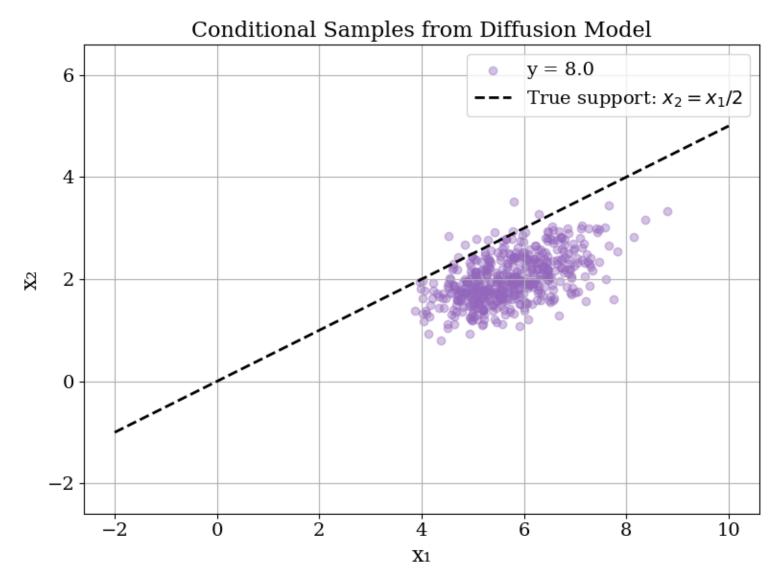




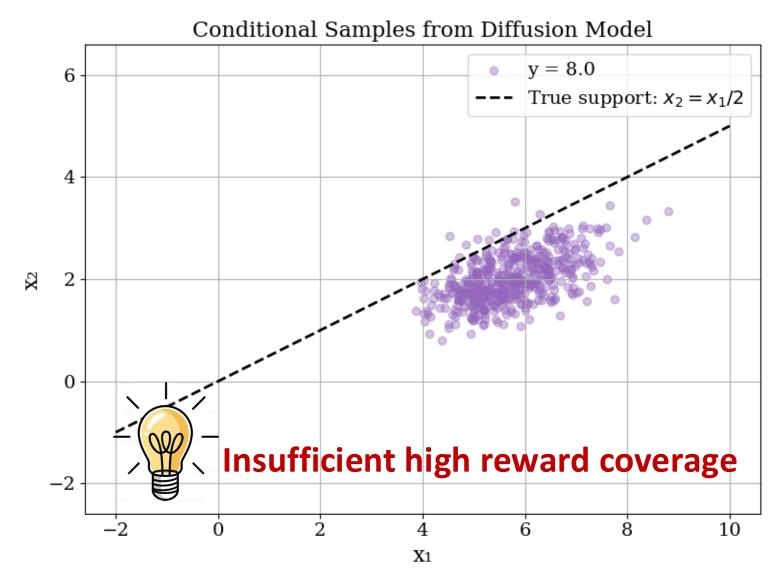




A Toy Example Cont'd: Good and Bad



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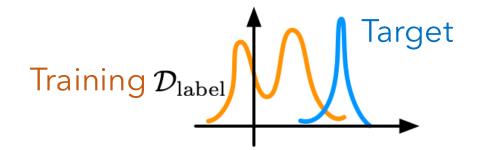
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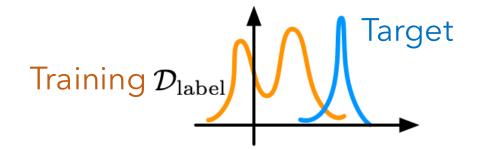


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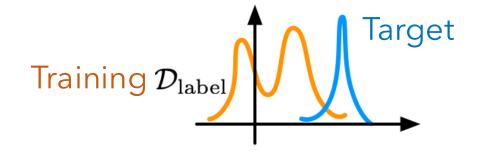
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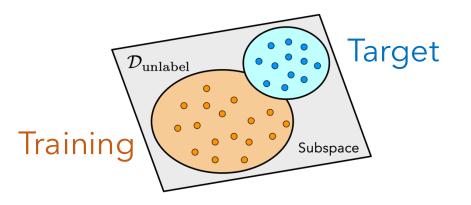


• Let a be the target reward of generation SubOpt(a) = a - Generated Average Reward

(Reward estimation error) • (Reward distribution shift)

(Conditional diffusion error) • (Diffusion distribution shift)





Theorem

✓ The sub-optimality satisfies

$$\texttt{SubOpt}(a) = \tilde{\mathcal{O}}\left(\sqrt{\text{Trace}\left(\hat{\Sigma}_{\lambda}^{-1}\Sigma_{a}\right)} \cdot \sqrt{\frac{d\log(n_{\text{label}})}{n_{\text{label}}}} + \min\{a, d\} \cdot \frac{a \cdot \text{poly}(D, d)}{n_{\text{unlabel}}}\right)$$

where $\hat{\Sigma}_{\lambda} = (X^{\top}X + \lambda I)/n_{\text{label}}$ for X the data matrix, $\lambda > 0$, and Σ_a is the covariance matrix of $P_a(\cdot | \text{ reward} = a)$.

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Match optimal off-policy bandit learning with representation learning (Jin et al., 2021; Nguyen-Tang et al., 2021)

Advantages of Offline Generative Opt.

✓ Meta algorithm provably generates samples of high reward and fidelity, in nonparametric settings.

$$\texttt{SubOpt}(a) = \tilde{O}\left(\kappa_1(a) \cdot n_{\text{label}}^{-\frac{\alpha}{d+2\alpha}} + \kappa_2(a) \cdot n_{\text{unlabel}}^{-\frac{2}{3(d+6)}}\right)$$

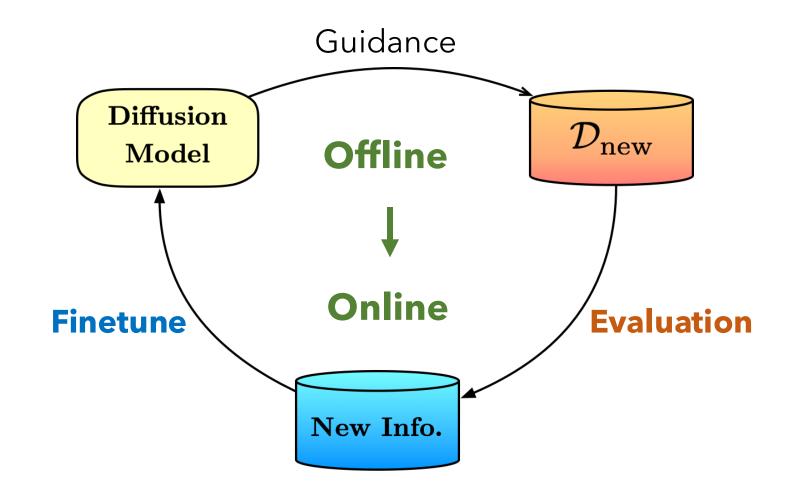
Generative optimization in offline:

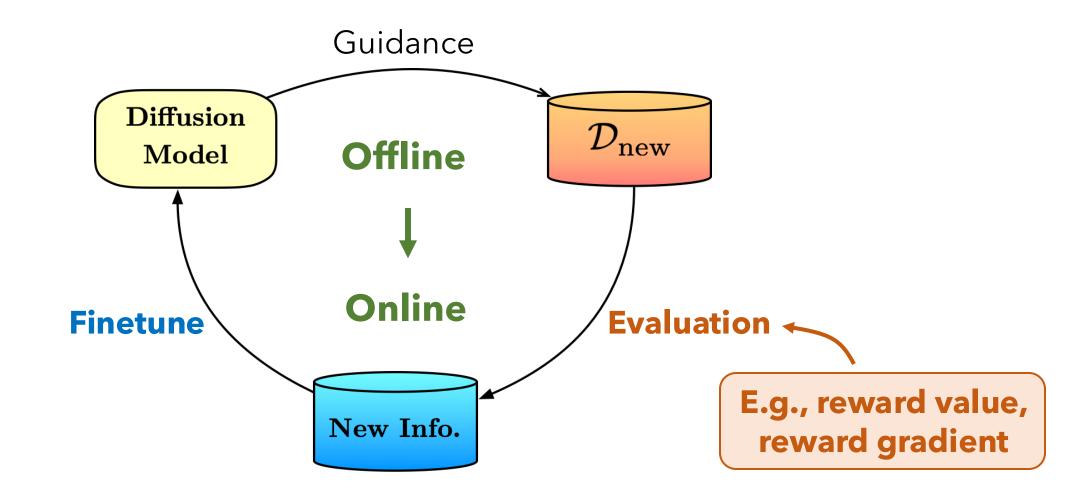
- ✓ Off-policy bandit optimality
- ✓ High-fidelity to subspace structures
- ✓ Efficiency: no curse of dimensionality

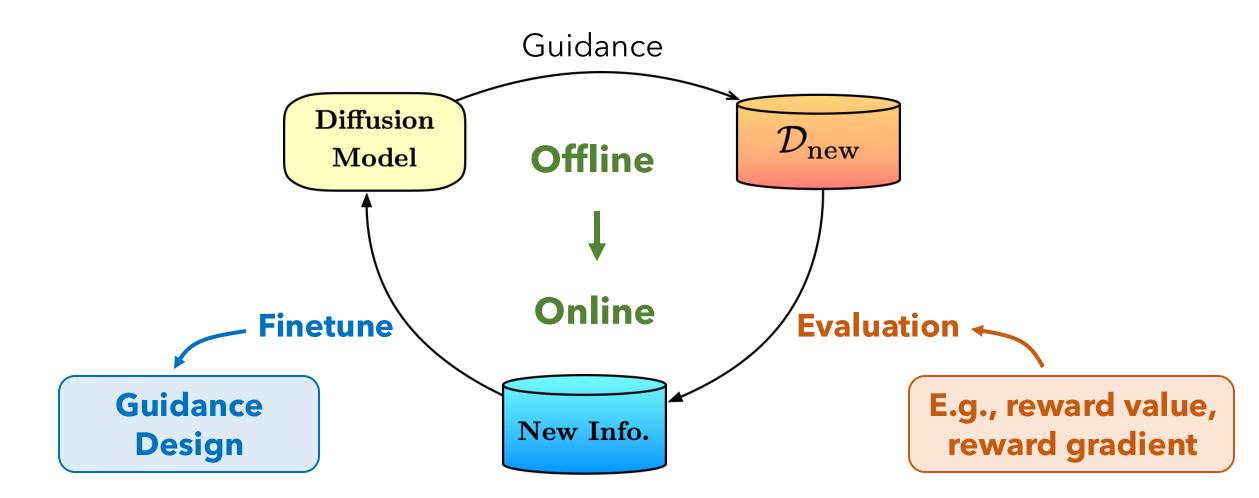
Online with Real-Time Feedback:

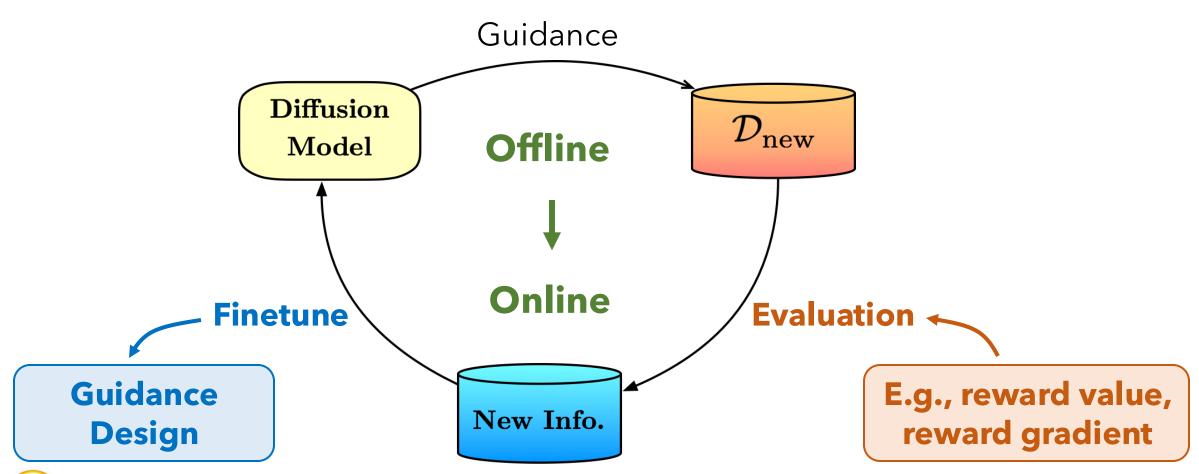
How can we **progressively** fine-tune a diffusion model to generate **max-reward high-fidelity** data?









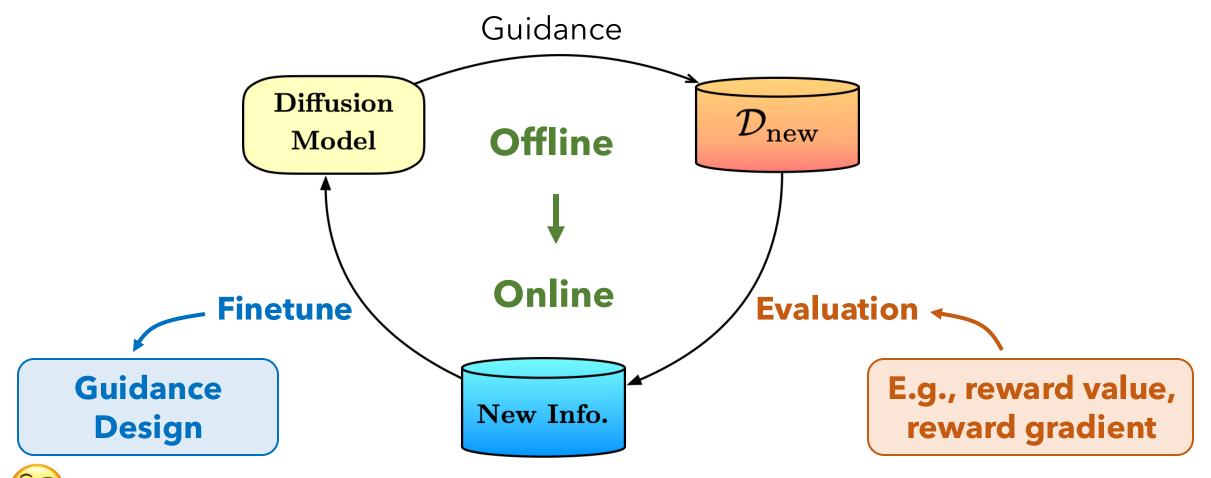




Form of guidance, computation, theoretical guarantees, ...

Stochastic control method

(Uehara et al., 2024; Han et al., 2024; Tang, 2024)



Form of guidance, computation, theoretical guarantees, ...

Definition In *general* settings, given a gradient vector g, define **gradient guidance** as

$$\mathsf{G}(x_t, t) = -\beta(t) \cdot \nabla_{x_t} \left(y - g^\top \mathbb{E}[X_0 | x_t] \right)^2$$

where $\beta(t)$ is some coefficient.

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$$Y = f(x) + \epsilon \qquad \text{with} \qquad \epsilon \sim \mathsf{N}(0, \sigma^2)$$

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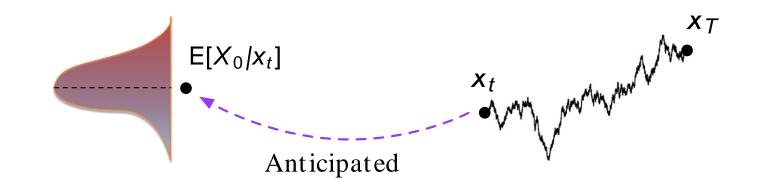
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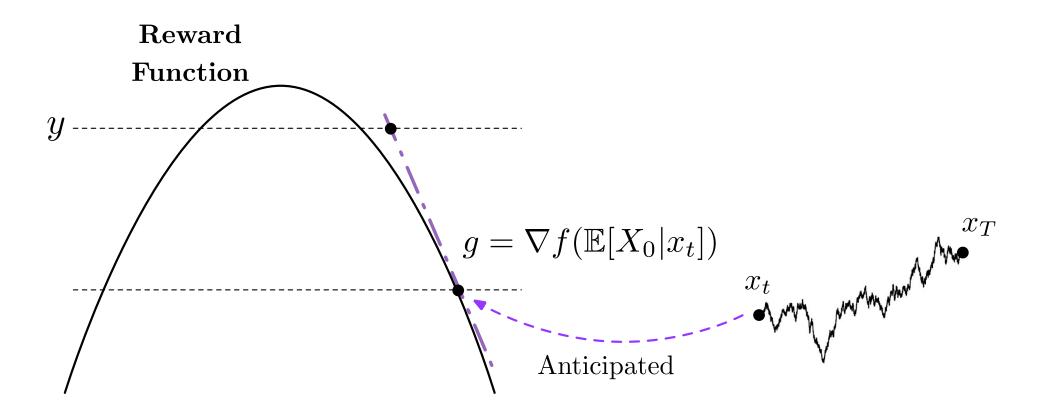
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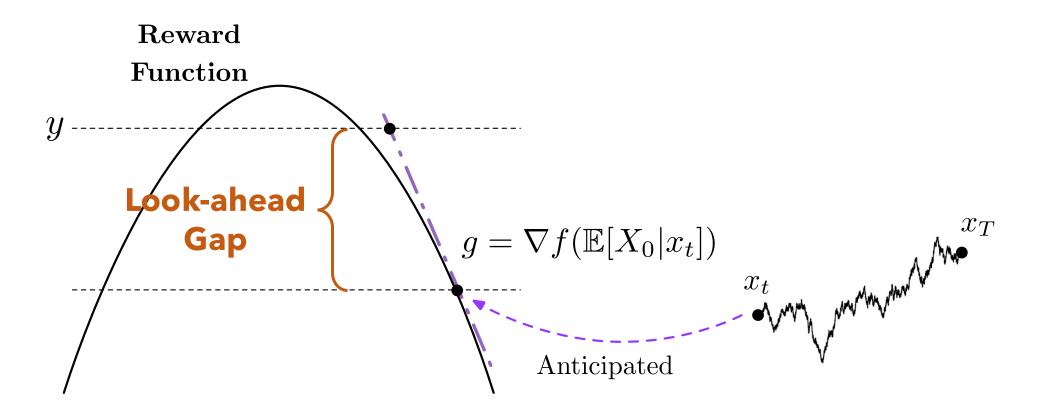
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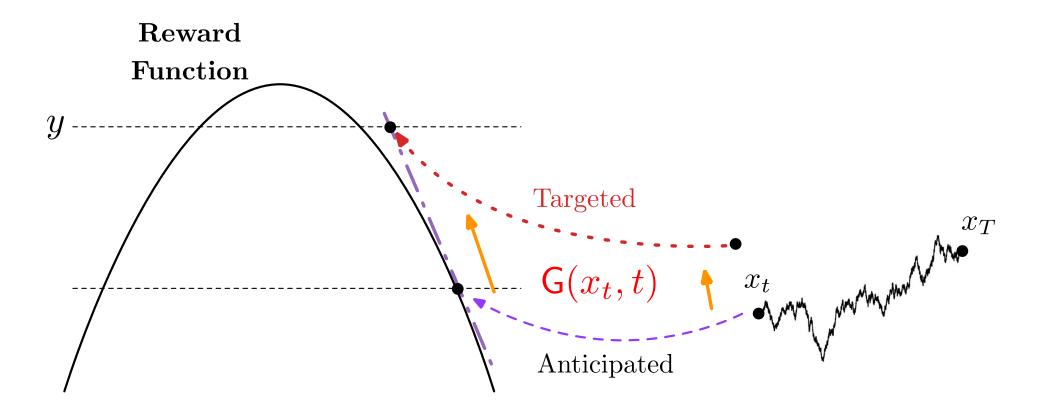
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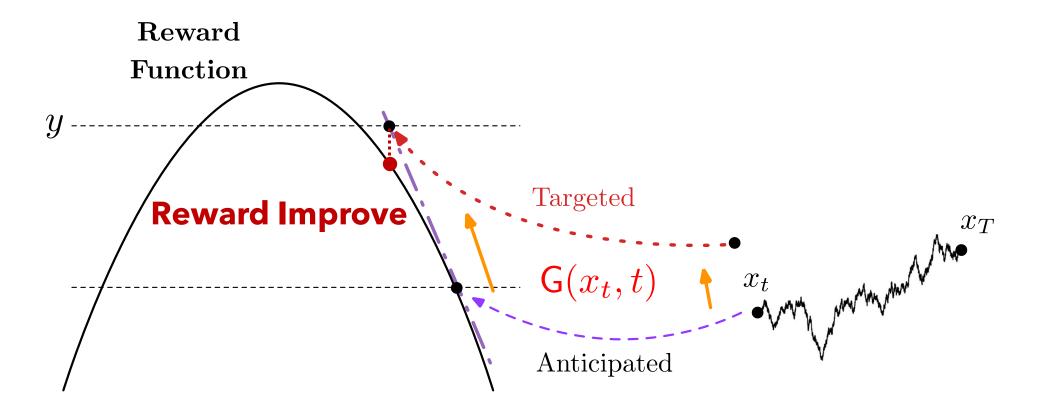
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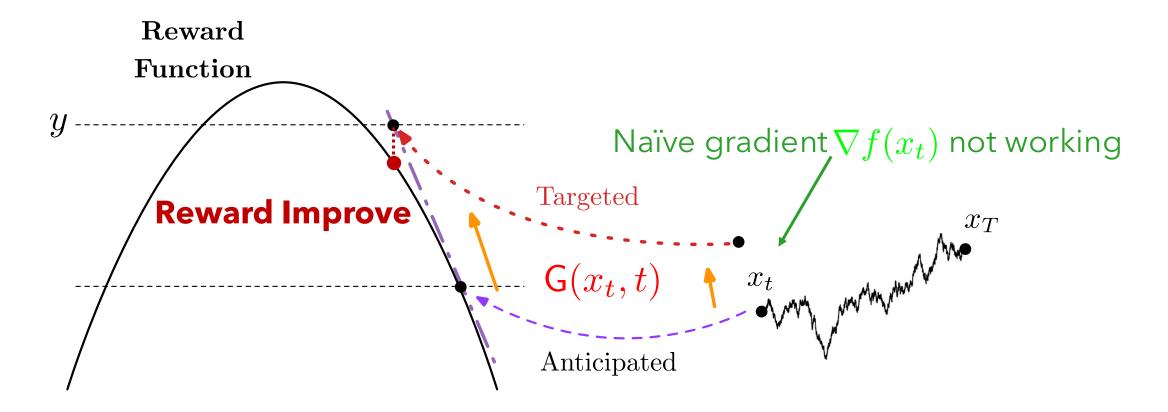












Gradient Guidance Preserves Structure

 Gradient guidance preserves subspace structures, but naïve gradient deviates from the subspace

 $\mathsf{G}(x_t, t) = -2\beta(t)(y - g^{\top} \mathbb{E}[X_0 | x_t]) \cdot (\nabla_{x_t} \mathbb{E}[X_0 | x_t]) \cdot g$

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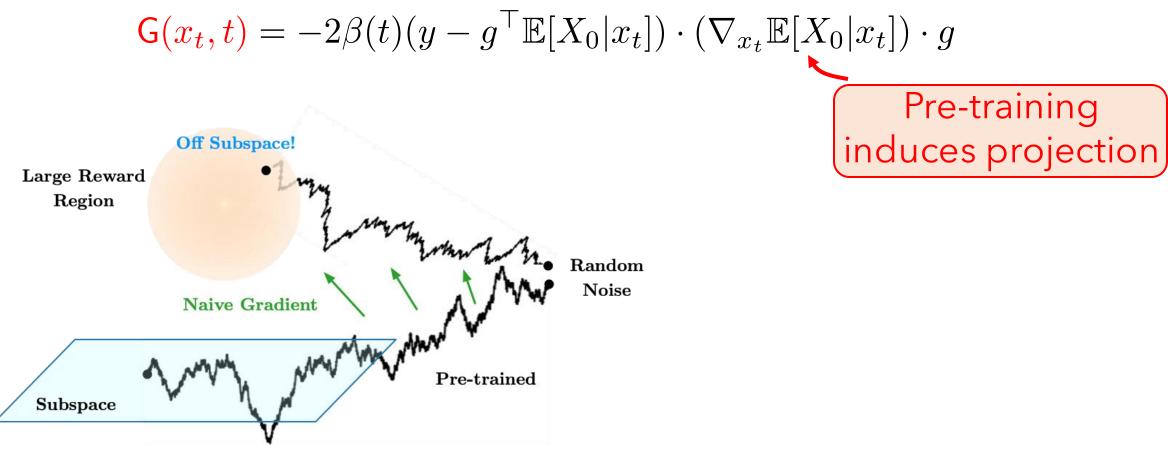
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Pre-training induces projection

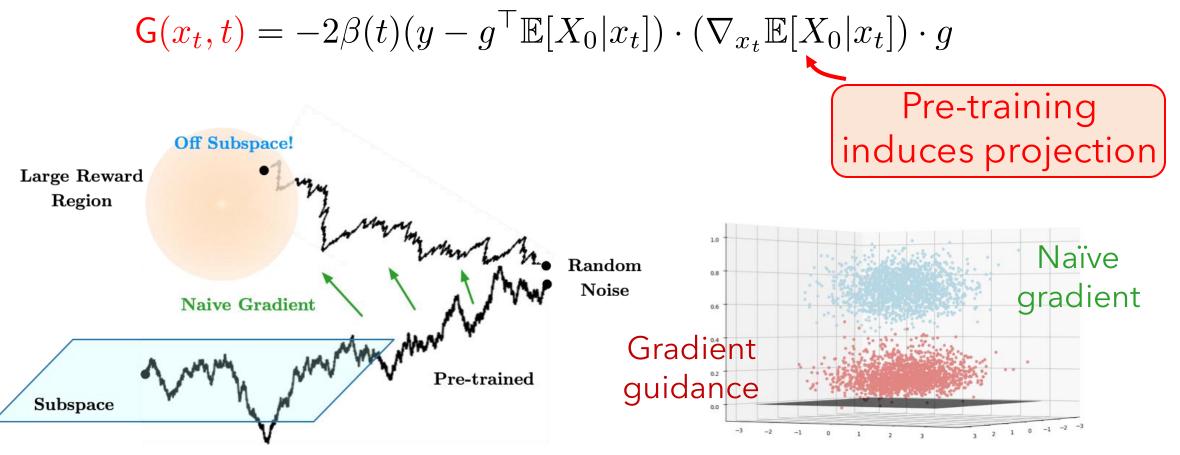
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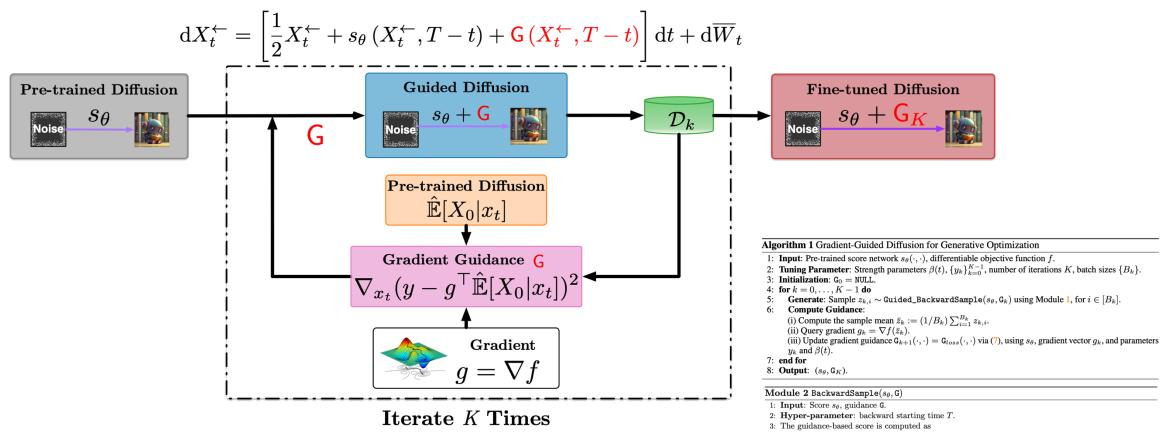
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- The gradient can be found by auto-differentiation
- Coefficient $\beta(t)$ is a tuning parameter, akin to a step size

Gradient Guidance Algorithm



 $s(x_t,t) = s_{\theta}(x_t,t) + \mathsf{G}(x_t,t),$

Sample from backward process:

$$\mathrm{d} X_t^{\leftarrow} = \left[\frac{1}{2}X_t^{\leftarrow} + s_\theta\left(X_t^{\leftarrow}, T-t\right) + \mathsf{G}\left(X_t^{\leftarrow}, T-t\right)\right]\mathrm{d} t + \mathrm{d} \overline{W}_t.$$

4: Output: $z = X_T^{\leftarrow}$.

Convergence to Regularized Optima

Theorem

Suppose the reward function is concave and *L*-smooth. Consider linear pre-trained score. With high probability, it holds $f(x_{A,\lambda}^*) - f(\mu_K) = \lambda (L/\lambda)^K \cdot \tilde{\mathcal{O}}(d)$

where $\lambda = O(L)$, μ_K is the mean of generated samples, and $x^*_{A,\lambda}$ is the maximizer of

$$x_{A,\lambda}^* = \arg\max_{x \in \text{subspace}} f(x) - \frac{\lambda}{2} \|x - \bar{\mu}_0\|_{\bar{\Sigma}_0^{-1}}^2$$

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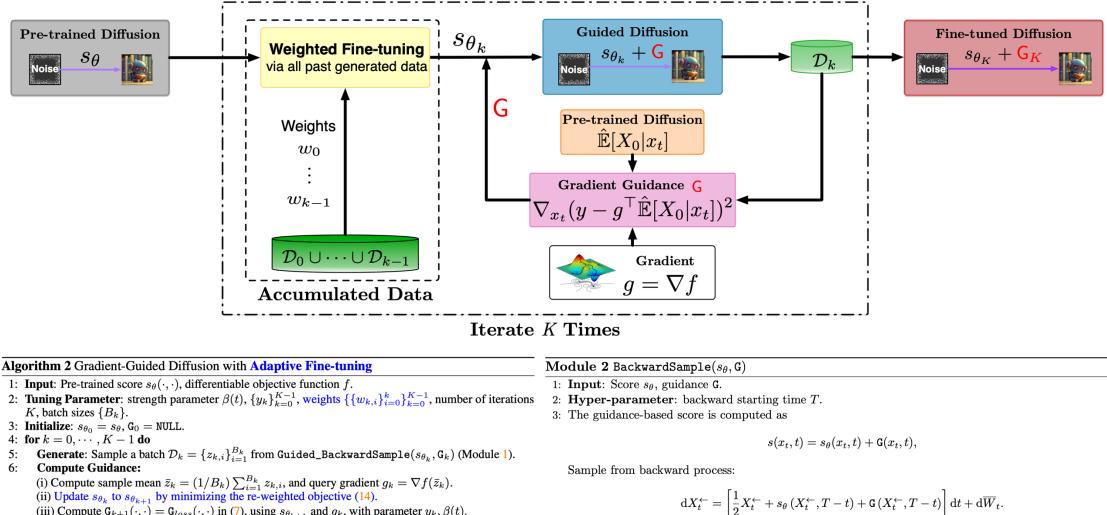
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Effective gradient-guided diffusion for optimization:

✓ Linear convergence and intrinsic dimension dependence
 ✓ Pre-training induces regularization

Algorithm with Adaptive Pre-trained Score



(ii) Update
$$s_{\theta_k}$$
 to $s_{\theta_{k+1}}$ by minimizing the re-weighted objective (14).

(iii) Compute
$$G_{k+1}(\cdot, \cdot) = G_{loss}(\cdot, \cdot)$$
 in (7), using $s_{\theta_{k+1}}$ and g_k , with parameter $y_k, \beta(t)$.

8: **Output:** $(s_{\theta_K}, \mathsf{G}_K)$.

4: Output: $z = X_T^{\leftarrow}$.

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Global Convergence with Adapted Score

Theorem

Suppose the reward function is concave and *L*-smooth. Consider adapting a linear pre-trained score. It holds that $f_A^* - f(\mu_K) = \tilde{\mathcal{O}} \left(dL^2 / K \right)$ where $f_A^* = \max_{x \in \text{subspace}} f(x)$ is the global maximum.

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Effective gradient-guided diffusion for optimization:

- ✓ 1/K **global** convergence
- ✓ **intrinsic** dimension dependence
- ✓ Preservation of subspace structure

-- Q. Ying, H. Yuan, Y. Yang, M. Chen, M. Wang. "Gradient Guidance for Diffusion Models", NeurIPS 2024

Numerical Results

- Reward function $f(x) = 10 (\theta^{\top}x 3)^2$
- Ambient dimension D = 64; subspace dimension d = 16

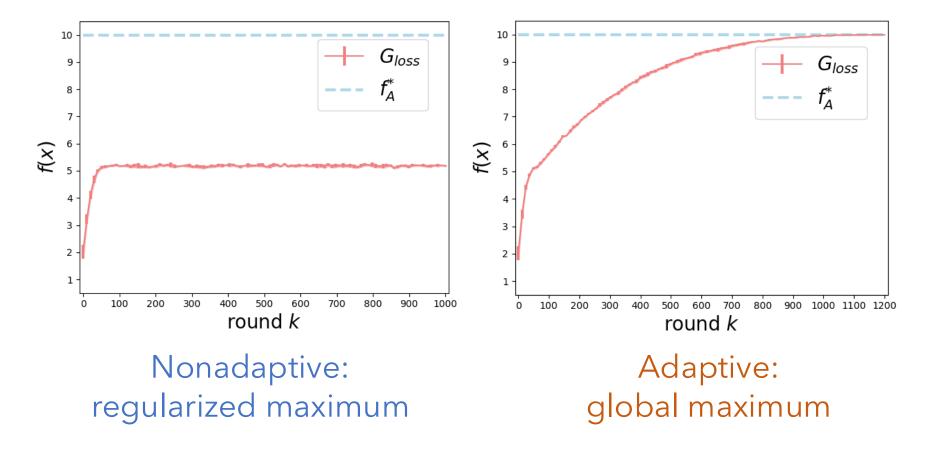
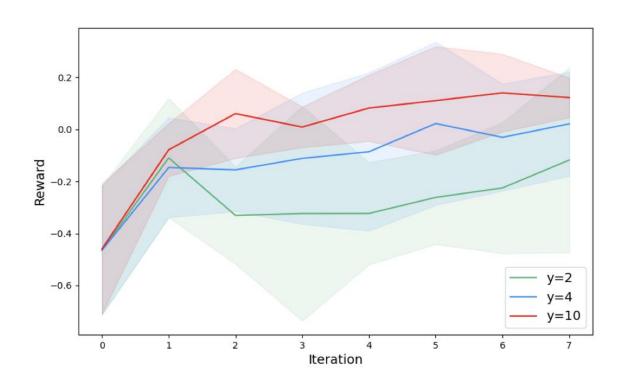
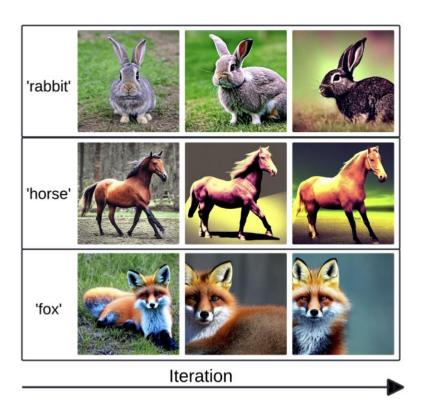


Image Generation

 Finetuing StableDiffusion v1.5 model (Rombach et al., 2022) on ImageNet





Take-Home Message and Future Directions

- We present methods for **adapting** diffusion models to an abstract reward function in both offline and online settings
- In the offline setting, diffusion models enjoy the **optimality** of off-policy bandits
- In the online setting, gradient guidance incorporates real-time feedback and enjoys **convergence** akin to first-order methods

 Beyond real-valued rewards, such as human preferences
 Noisy feedback, such as noisy reward gradients or contaminated gradients

 $\circ Nonconvex \ nonsmooth \ rewards$

