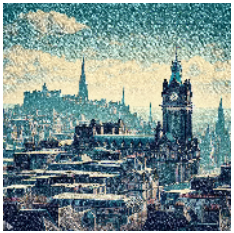
Advanced Topics in Machine Learning (deep generative modelling)

Lecture 8: Diffusion models I

Nikolay Malkin

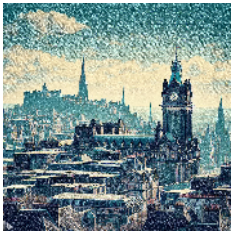
10 March 2026

Dynamics-based generative models in practice



'Edinburgh from Calton Hill, pointillist style'

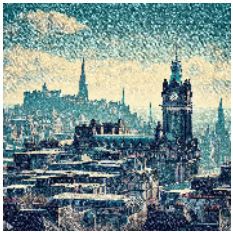
Dynamics-based generative models in practice



'Edinburgh from Calton Hill, pointillist style'

[Janner et al., ICML'22]

Dynamics-based generative models in practice



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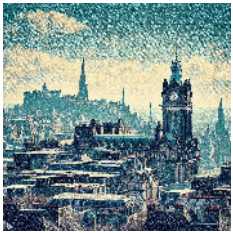

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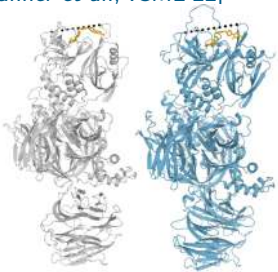

AlphaFold 3

Dynamics-based generative models in practice

[Zhang and Gienger, 2024]

Outline of weeks 8-10

What is a diffusion model, how to understand it from different perspectives, and where to use it in practice:

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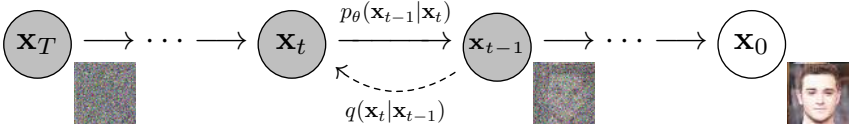
What is a diffusion model, how to understand it from different perspectives, and where to use it in practice:

- **Lecture 8:** Diffusion models are hierarchical latent variable models / deep VAEs



[Ho et al., 'Denoising diffusion probabilistic models']

Outline of weeks 8-10

What is a diffusion model, how to understand it from different perspectives, and where to use it in practice:

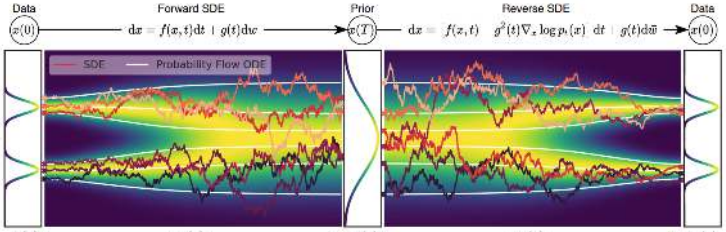
- **Lecture 8:** Diffusion models are hierarchical latent variable models / deep VAEs
- **Lecture 9:** Diffusion models are score-based models

[Song et al., 'Generative modeling by estimating...' blog post]

Outline of weeks 8-10

What is a diffusion model, how to understand it from different perspectives, and where to use it in practice:

- **Lecture 8:** Diffusion models are hierarchical latent variable models / deep VAEs
- **Lecture 9:** Diffusion models are score-based models
- **Lecture 10:** Diffusion models are continuous-time processes



[Song et al., 'Score-based generative modeling. . . ']

Outline of Lecture 8

- Historical overview
- Review of latent variable models
- Diffusion models as hierarchical generative models
  - Evaluation and likelihood estimation
  - Latent variable model perspective

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Historical overview

The principles have not changed much.

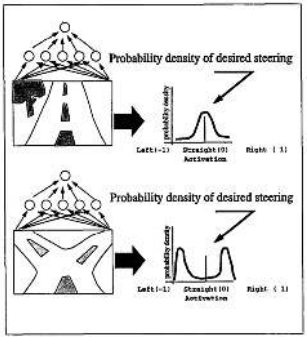
Historical overview

- Early ‘90s: proposals to model dynamics in neural activations
  - Combined two ideas from statistical physics: neural nets / connectionist models and diffusion processes / SDEs

COGNITIVE SCIENCE **17,** 463–496 (1993)

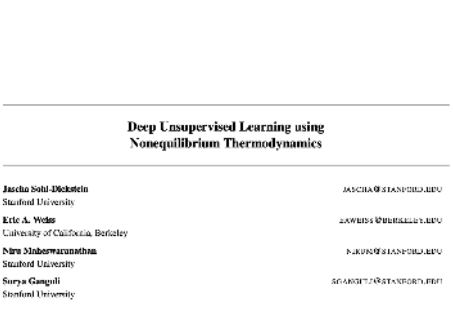
Learning Continuous Probability Distributions with Symmetric Diffusion Networks

JAVIER R. MOVELLAN
University of California, San Diego
JAMES L. MCCLELLAND
Carnegie Mellon University



Historical overview

- deep learning revolution (better hardware and algorithms) ...
- 2015: first deep generative model based on diffusion



Deep Unsupervised Learning using
Nonequilibrium Thermodynamics

Jascha Sohl-Dickstein
Stanford University
JASCHA@STANFORD.EDU

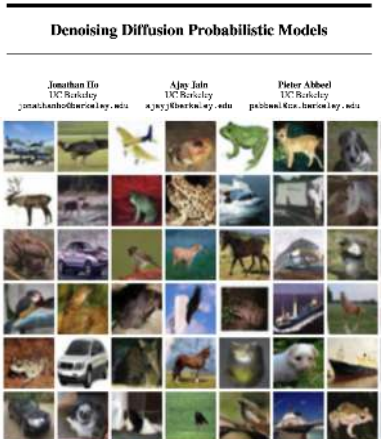
Eric A. Weiss
University of California, Berkeley
EAWEISS@BERKELEY.EDU

Niru Maheswaranathan
Stanford University
NIRUM@STANFORD.EDU

Surya Ganguli
Stanford University
SGANGULI@STANFORD.EDU

Historical overview

- 2020–2021: new training techniques and architectures make diffusion models competitive



Historical overview

- 2020–2021: new training techniques and architectures make diffusion models competitive

Diffusion Models Beat GANs on Image Synthesis

Prafulla Dhariwal*
OpenAI
prafulla@openai.com

Alex Nichol*
OpenAI
alex@openai.com

Historical overview

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- 2015: first deep generative model based on diffusion
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- deep learning revolution (better hardware and algorithms) . . .
- 2015: first deep generative model based on diffusion
- 2020–2021: new training techniques and architectures make diffusion models competitive
- 2022–: continued improvements in modeling, efficiency, and applications

Historical overview

Discrete, compositional, and symbolic representations through attractor dynamics

Andrew J. Nam[*]
Princeton University
Princeton, NJ
andrewnam@princeton.edu

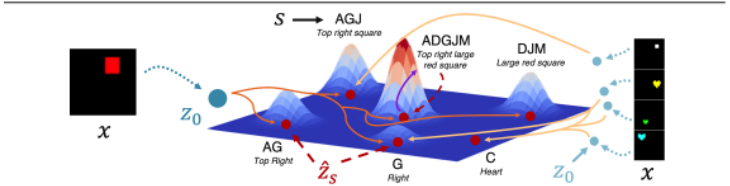
Eric Elmoznino
Mila, Université de Montréal
Montréal, QC, Canada
eric.elmoznino@mila.quebec

Nikolay Malkin[†]
University of Edinburgh
Edinburgh, Scotland, UK
nmalkin@inf.ed.ac.uk

James L. McClelland
Stanford University
Stanford, CA
jlmcc@stanford.edu

Yoshua Bengio[‡]
Mila, Université de Montréal
Montréal, QC, Canada
yoshua.bengio@mila.quebec

Guillaume Lajoie[†]
Mila, Université de Montréal
Montréal, QC, Canada
guillaume.lajoie@mila.quebec



- Historical overview
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- Diffusion models as hierarchical generative models
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  - Latent variable model perspective

Latent variable models

Generative models with **latent variables** z: To approximate π_{data} by a model p, model a joint distribution $p_\theta(x, z)$ over observed x and latent z to satisfy

$$p_\theta(x) = \int_z p_\theta(x, z)\, dz \approx \pi_{\text{data}}(x)$$

Latent variable models

Generative models with **latent variables** z: To approximate π_{data} by a model p, model a joint distribution $p_\theta(x, z)$ over observed x and latent z

$$z \xrightarrow{p_\theta(x|z)} x \qquad p_\theta(x) = \int_z p_\theta(z) p_\theta(x \mid z)\, dz$$

'Ancestral' sampling of x:

- Sample the latent z from a distribution $p_\theta(z)$.
- Sample x from $p_\theta(x \mid z)$.

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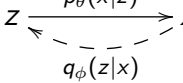

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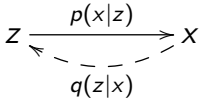
'Ancestral' sampling of x:

- Sample the latent z from a distribution $p_\theta(z)$.
- Sample x from $p_\theta(x \mid z)$.

The posterior over z, by Bayes' rule (we often approximate it by a $q_\phi(z \mid x)$):

$$p_\theta(z \mid x) = \frac{p_\theta(z) p_\theta(x \mid z)}{p_\theta(x)} \propto p_\theta(z) p_\theta(x \mid z)$$

Latent variables ‘encode’ the data



The approximate posterior $q(z \mid x)$ (often a Gaussian in VAEs) stochastically ‘encodes’ the data x into a latent z

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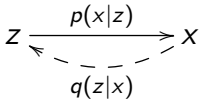

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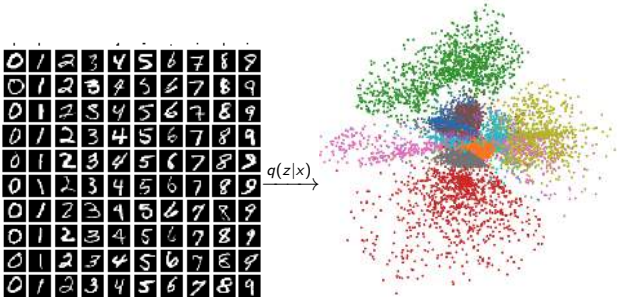
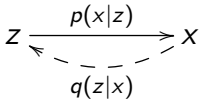


VAE latent space explorer

Latent variables ‘encode’ the data



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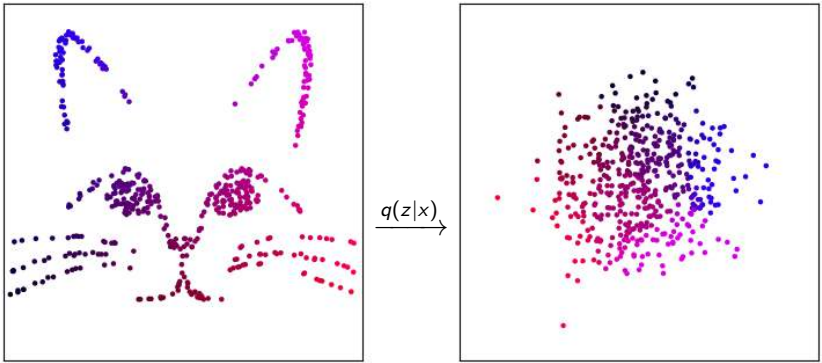

MLE training of latent variable models

Given a dataset $\{x_i\}_{i=1}^N$, we want to maximise

$$\sum_i \log p_\theta(x_i)$$

w.r.t. parameters of $p_\theta(z)$ and $p_\theta(x \mid z)$.

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- **Gibbs' inequality:** for any distribution $q_i(z)$,

$$\log p_\theta(x_i) = \log \int_z p_\theta(z) p_\theta(x_i \mid z)\, dz \geq \underbrace{\int_z q_i(z) \log \frac{p_\theta(z) p_\theta(x_i \mid z)}{q_i(z)}\, dz}_{\text{evidence lower bound (ELBO)}}$$

with equality when $q_i(z) = p_\theta(z \mid x_i) \propto p_\theta(z) p_\theta(x_i \mid z)$ (true posterior)

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$$= \log p_\theta(x) - \mathrm{KL}(q_i \,\|\, p_\theta(z|x_i)))$$

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  with equality when $q_i(z) = p_\theta(z \mid x_i) \propto p_\theta(z) p_\theta(x_i \mid z)$ (true posterior)
- Idea: to maximise $\log p(x^t)$, maximise the ELBO
  - $\rightsquigarrow$ **EM alg.** ("Maximum likelihood from incomplete data" [Dempster et al., 1977])

Gradient-based EM

Idea: to maximise $\log p_\theta(x_i)$, maximise the ELBO

$$\int_z q_i(z) \log \frac{p_\theta(z) p_\theta(x_i \mid z)}{q_i(z)} = \mathbb{E}_{z \sim q_i} \left[\log \frac{p_\theta(z) p_\theta(x_i \mid z)}{q_i(z)} \right]$$

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- **(Amortised) variational EM:** approximate q_i with a model $q_\phi(z \mid x_i)$ and train it to approximate the true posterior $p_\theta(z \mid x_i)$ (**E-step**)

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- Intuitively:
  - E-step: learn to encode x into z that explains it well
  - M-step: for data x, sample explanation z and learn to recover x from z

Hierarchical latent variable models

$$z_N \xrightarrow{p(z_{N-1}|z_N)} z_{N-1} \xrightarrow{p(z_{N-2}|z_{N-1})} \cdots \longrightarrow z_1 \xrightarrow{p(x|z_1)} x$$

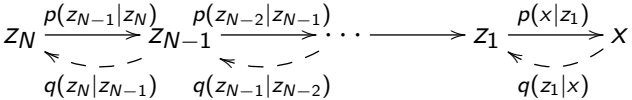
Hierarchical latent variable models

$$z_N \xrightarrow{p(z_{N-1}|z_N)} z_{N-1} \xrightarrow{p(z_{N-2}|z_{N-1})} \cdots \longrightarrow z_1 \xrightarrow{p(x|z_1)} x$$

We want to maximise

$$\log p(x) = \log \int p(z_N) p(z_{N-1} \mid z_N) \cdots p(z_1 \mid z_2)\, p(x \mid z_1)\, dz_1 \cdots dz_N$$

Hierarchical latent variable models



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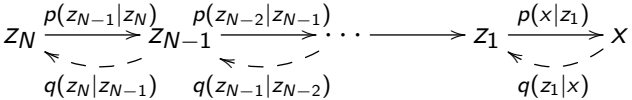
Introduce approximate posteriors $q(z_n \mid z_{n-1})$;

Hierarchical latent variable models



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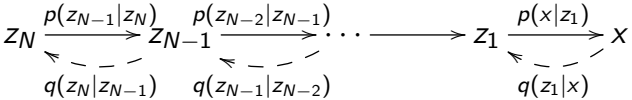
Introduce approximate posteriors $q(z_n \mid z_{n-1})$; hierarchical ELBO:

$$\log p(x) \geq \mathbb{E}_{z_1,\ldots,z_N \sim q(\cdots|x)} \left[\log \frac{p(z_N)p(z_{N-1} \mid z_N) \cdots p(x \mid z_1)}{q(z_1 \mid x) \ldots q(z_N \mid z_{N-1})} \right]$$

Hierarchical latent variable models



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To train the model given fixed q:

- Sample the latents from q in reverse order: $x \to z_1 \to \cdots \to z_N$
- Maximise $\log p$ in ancestral order w.r.t. parameters of p

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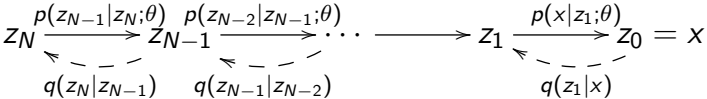
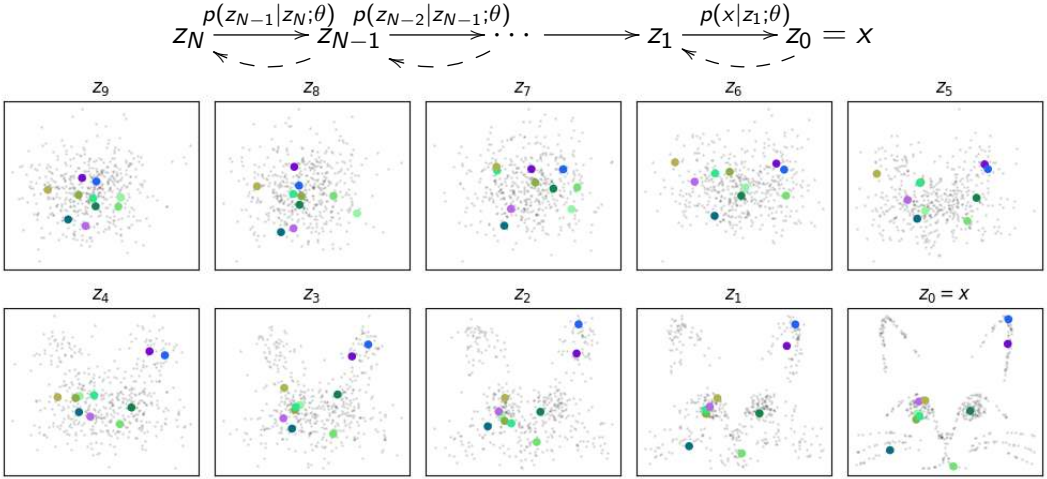
Diffusion models are deep VAEs with fixed encoder

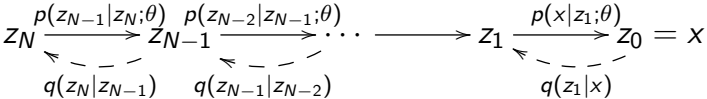


- Diffusion models (typically) fix the distributions $q(z_n \mid z_{n-1})$
  - Typically to adding isotropic Gaussian noise: $q(z_n \mid z_{n-1}) = \mathcal{N}(z_n; z_{n-1}, \sigma_n^2 I_d)$. . . or variants (next time)

Diffusion models are deep VAEs with fixed encoder



Diffusion models are deep VAEs with fixed encoder



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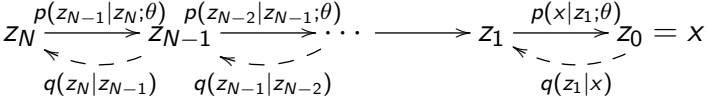

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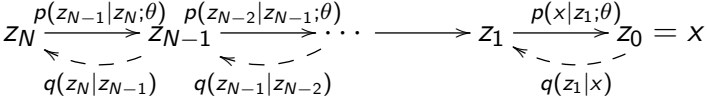

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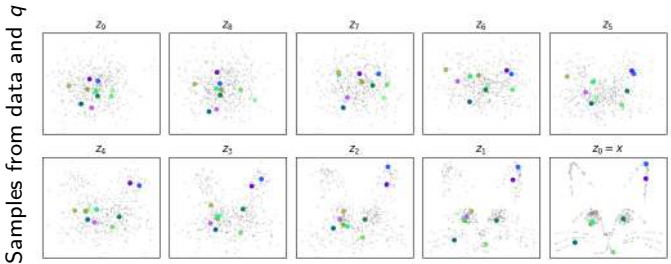
Training a diffusion model on 2D data

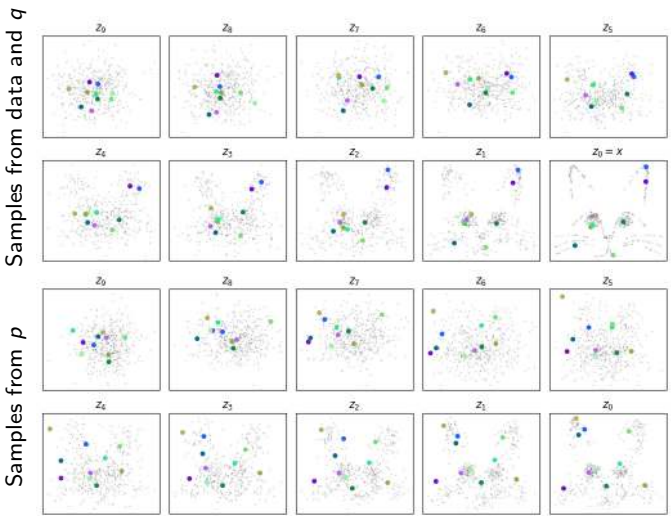
Posterior model
(noising)



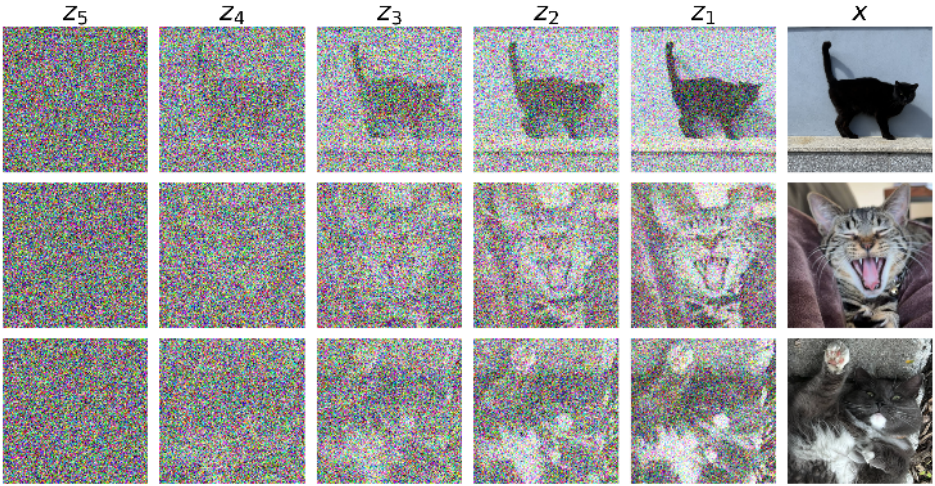
Training a diffusion model on 2D data

Posterior model (noising)

Generative model (denoising / reconstruction)



Scaling to images



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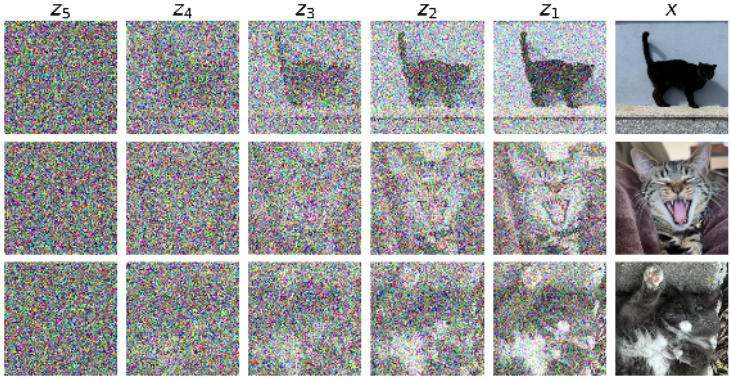

Generating cats with Gaussian $p(z_{n-1} \mid z_n)$ requires **hundreds** of steps

- But much fewer if the p distributions are more expressive
  e.g., [Xiao et al., 'Tackling the generative learning trilemma...']: train the p distributions as GANs!

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- Noise distribution $p(z_N)$ not usually trained (approximately Gaussian)
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  - Generalisations may lose one or both magic properties

Evaluation and tradeoffs

- Evaluation: log-likelihood using ELBO, or sample-based metrics

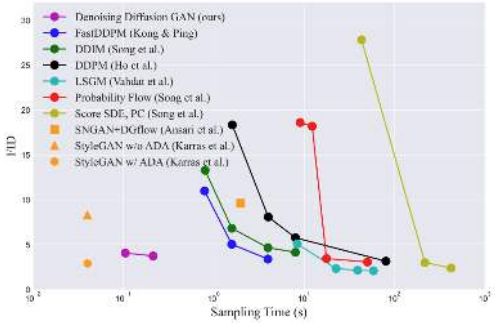

Figure 4: Sample quality vs sampling time trade-off.

[Xiao et al., 'Tackling the generative learning trilemma. . . ']

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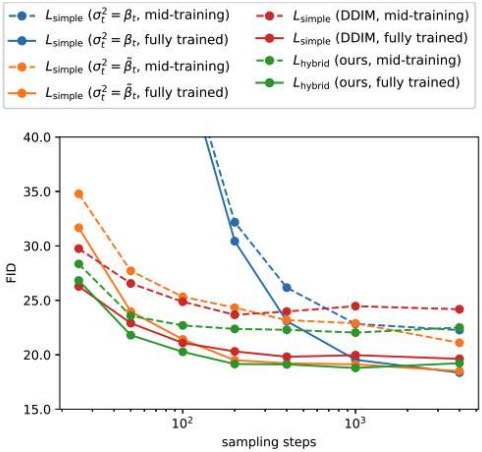

[Nichol&Dhariwal, 'Improved denoising...']

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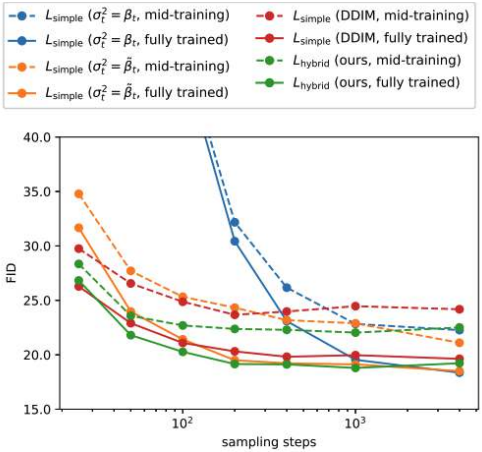

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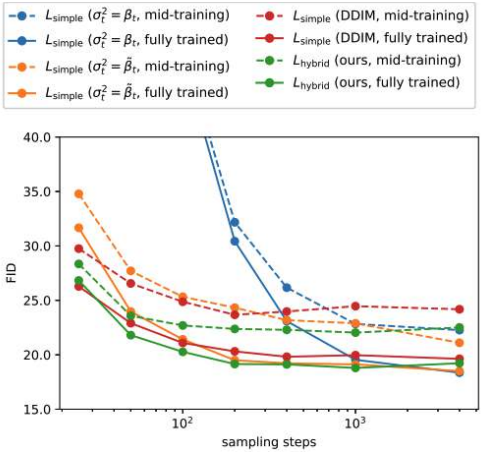

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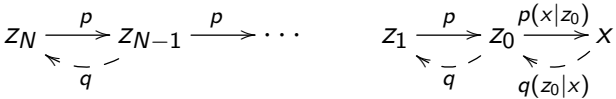
- **Latent diffusion:** separate learnt encoder and decoder for $z_0 \leftrightarrow x$ (most large-scale image models work this way)



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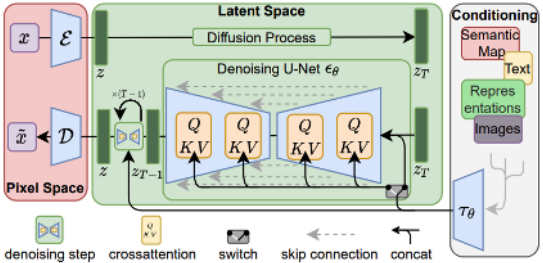
$$z_N \underset{q}{\overset{p}{\rightleftarrows}} z_{N-1} \underset{q}{\overset{p}{\rightleftarrows}} \cdots \qquad z_1 \underset{q}{\overset{p}{\rightleftarrows}} z_0 \underset{q(z_0|x)}{\overset{p(x|z_0)}{\rightleftarrows}} x$$



[Rombach et al., 'High-resolution image synthesis with latent diffusion models']

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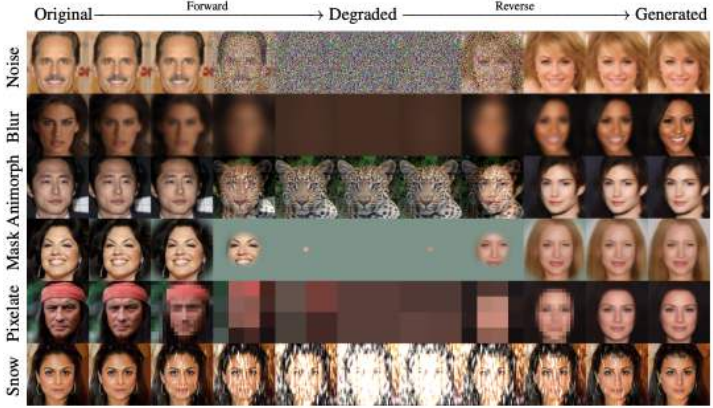

[Bansal et al., 'Cold diffusion. . . ']

Conclusion and looking forward

Next time:

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  - The magic properties + the right noising process are enough to train a diffusion model on moderately-sized image data

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- Conditioning and guidance

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