5. Diffusion Models

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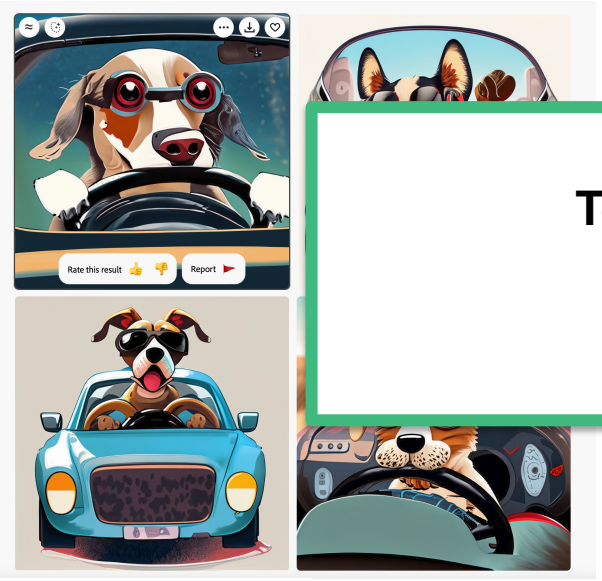
Diffusion models: what's the hype about?

Diffusion Models **Beat GANs** on Image Synthesis Dharwal & Nichol, OpenAI, 2021

Diffusion models: what's the hype about?

Adobe Firefly (Beta)

Diffusion models: what's the hype about?



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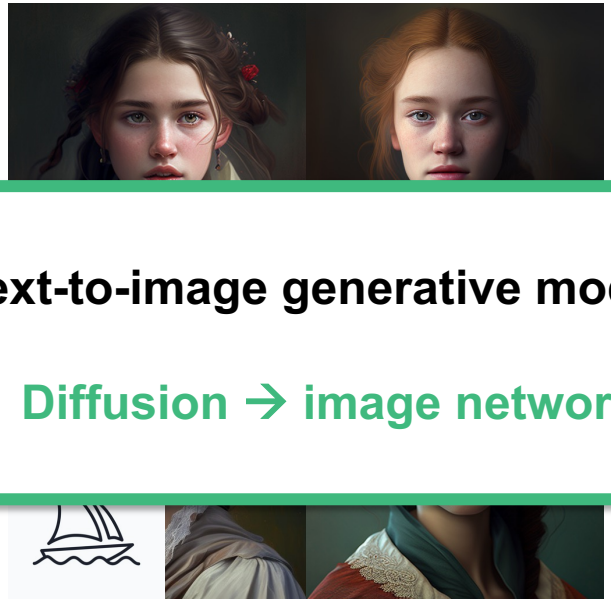


Text-to-image generative models

Diffusion → image network

Diffusion models: and the technology?

Developer: **OpenAI**

Release: Jan 2021 (v1), Jul 2022 (v2)

Tech: diffusion model conditioned on CLIP image embeddings

Developer: **StabilityAI**

Release: Aug 2022

Tech: latent diffusion model with CLIP ViT-L/14 text encoder

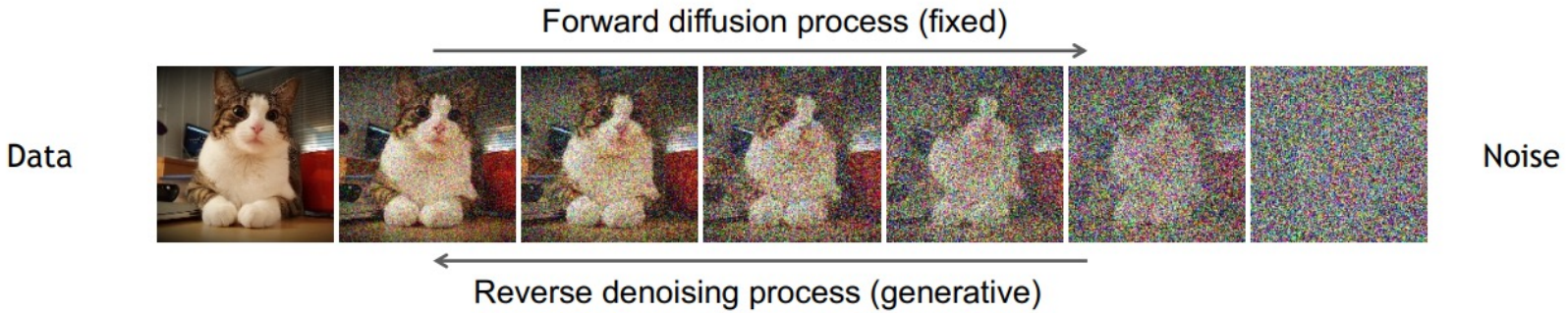
Developer: **Midjourney**

Release: Feb 2022 (v1), Mar 2023 (v5)

Tech: not disclosed fully

Diffusion models: intuition

*Family of neural networks that can learn to **generate images by gradually refining a Gaussian Noise realization** and making it more and more into a real image at each timestep*



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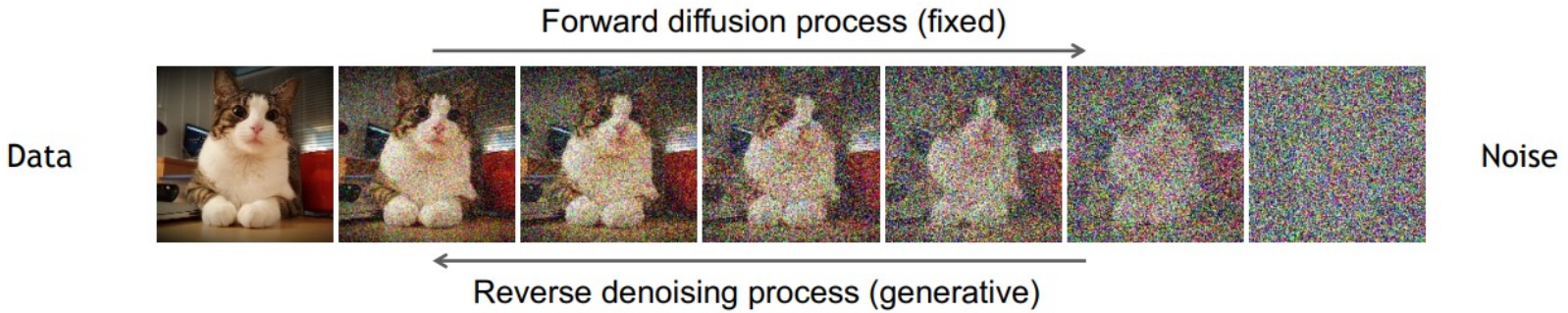


Both training and generation

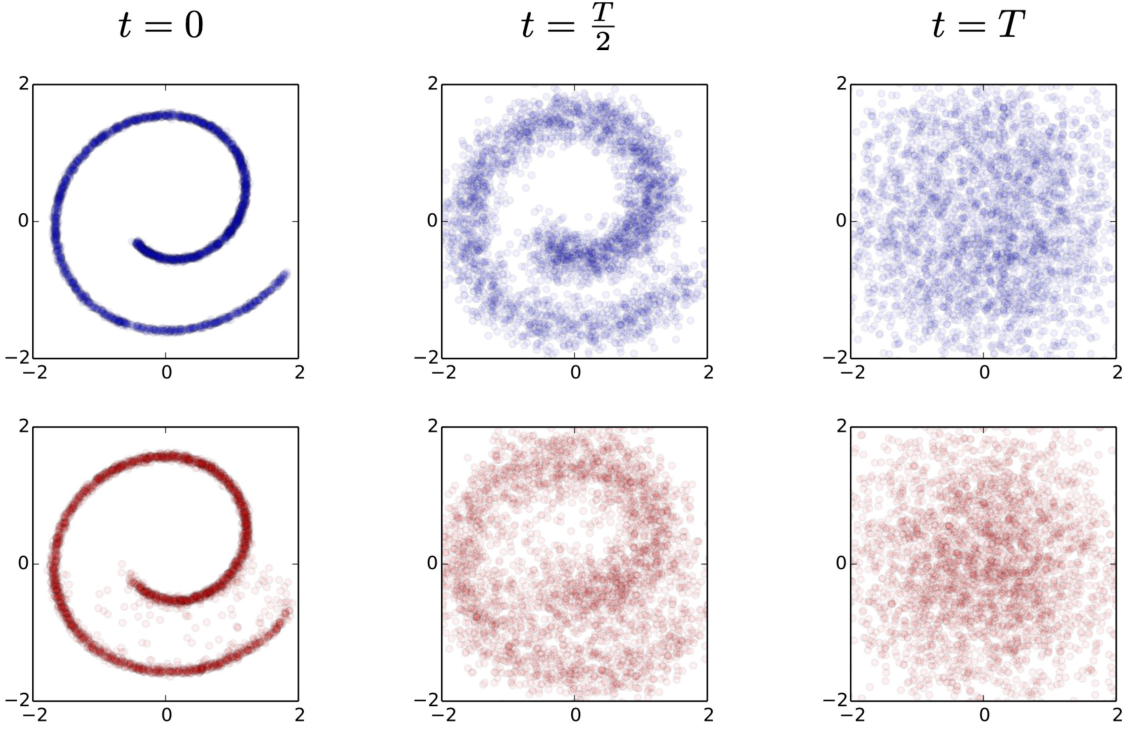
Normalizing Flows: intuition

The forward trajectory

$q(\mathbf{x}_{0:T})$

The reverse trajectory

$p_\theta(\mathbf{x}_{0:T})$

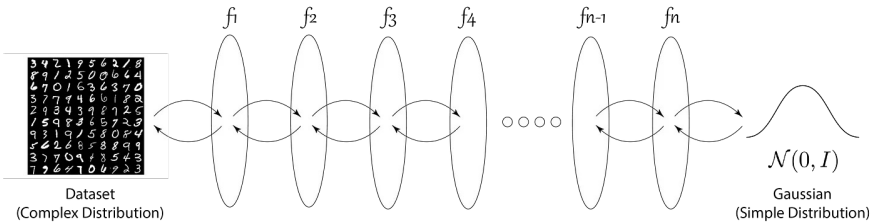


Sohl-Dickstein et al. (2015)

Diffusion models vs NFs

Diffusion models and NFs look similar at first.

Both operate in **2 directions**: one making something complex (image) into something simple (noise) and one doing the opposite.



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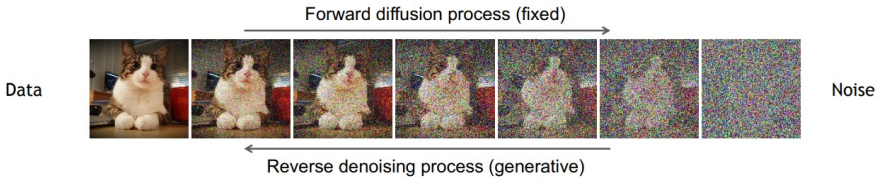

Diffusion model

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But there are some **fundamental differences:**

- No need for **invertible transformations** in DMs
- **Simpler training process** for DMs (no log-det of Jacobian)
- **Only sampling** for DMs

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Diffusion models: 3 in 1

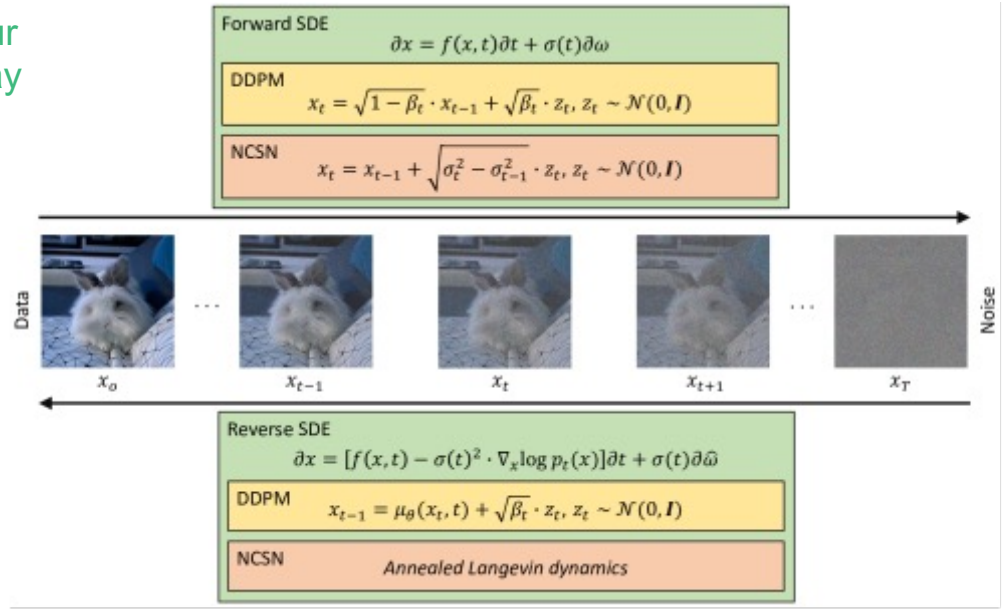
Different ways to achieve the same goal (unified lately into unique framework)

DDPMs
(Denoising Diffusion Probabilistic Models)

Most of our focus today

NCSNs
(Noise Conditioned Score Networks)

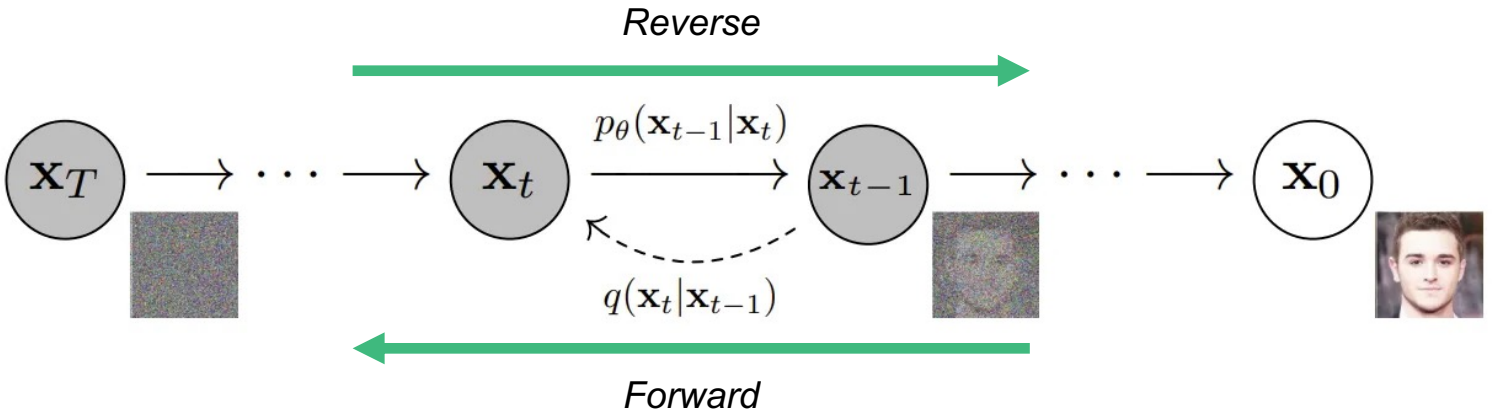
SDEs
(Stochastic differential equations)



Denoising Diffusion Probabilistic Models

Forward: inspired from non-equilibrium thermodynamics, Markov chain of diffusion steps to **slowly add random noise to data until output is pure noise – fixed**

Reverse: reversed Markov chain to **slowly remove noise** and generate outputs that belong to the distribution of training data - **learned**



Markov chain refresher

A sequence of events in which the probability of each event depends only on the state attained in the **previous event**:

$$q(x_T|x_{T-1}, x_{T-2}, .., x_0) = q(x_T|x_{T-1})$$

x_T is independent from $x_{T-2}, .., x_0$

DDPMs: forward

Starting from a training sample $x_0 \sim q(x)$ (subscript: diffusion step), we define the diffusion process as follows (i.e., write x_t with $t = 1,2,..T$ as function of x_{t-1}):

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

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Normal distribution (since we keep adding Gaussian noise)

Mean and covariance of conditional distribution

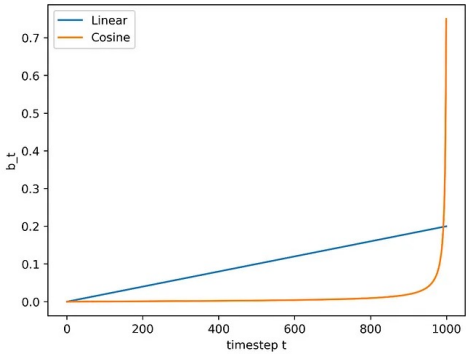
DDPMs: forward

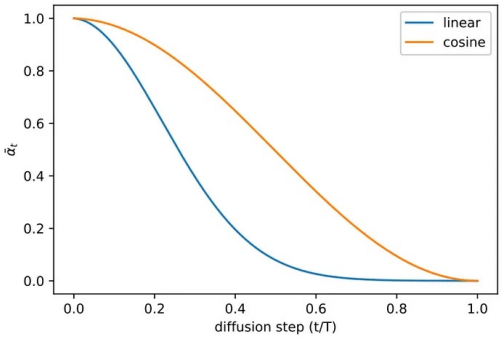
Noise variance changes over steps (**variance scheduler**):

$$0 < \beta_1 < \beta_2 < \ldots < \beta_T < 1$$

$$\alpha_t := 1 - \beta_t$$

$$\bar{\alpha}_t := \Pi_{s=1}^{t} \alpha_s$$





DDPM paper (Ho et al., 2020): linear scheduler with $\beta_1 = 1e^{-4}, \beta_{T=1000} = 0.02$ (always small compared to $\boldsymbol{x}_0 \in [-1,1]$)

Improved DDPM paper (Nichol and Dhariwal, 2021): cosine-based scheduler (near-linear drop in the middle of the training process and smaller changes at both ends)

DDPMs: forward

Using the **reparametrization trick** (remember VAEs!), we can write

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

More importantly, we can find a **closed-form solution for x_t directly from x_0** (much cheaper than generating all steps – T=1000 in DDPM paper!)

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + (1-\bar{\alpha}_t)\epsilon$$

DDPMs: forward

Derivation:

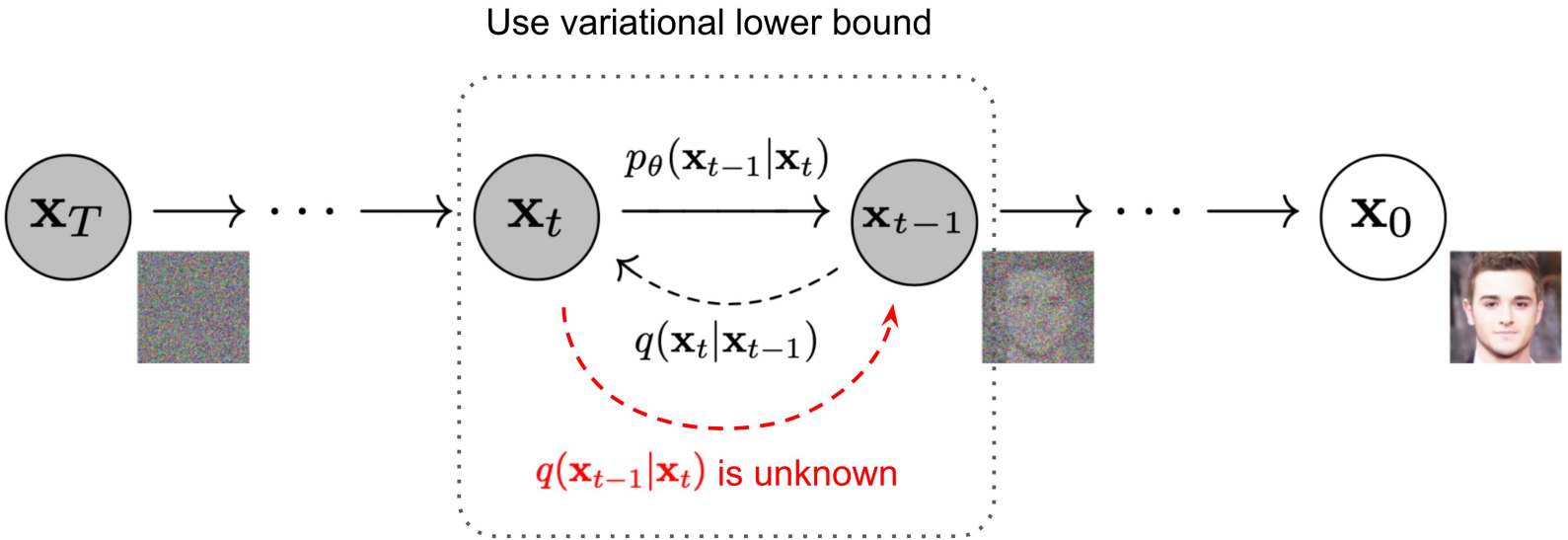
$$
\begin{aligned}
\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} && \text{;where } \boldsymbol{\epsilon}_{t-1}, \boldsymbol{\epsilon}_{t-2}, \cdots \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \\
&= \sqrt{\alpha_t\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\boldsymbol{\epsilon}}_{t-2} && \text{;where } \bar{\boldsymbol{\epsilon}}_{t-2} \text{ merges two Gaussians (*).} \\
&= \dots \\
&= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon} \\
q(\mathbf{x}_t|\mathbf{x}_0) &= \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})
\end{aligned}
$$

(*) Recall that when we merge two Gaussians with different variance, $\mathcal{N}(\mathbf{0}, \sigma_1^2\mathbf{I})$ and $\mathcal{N}(\mathbf{0}, \sigma_2^2\mathbf{I})$, the new distribution is $\mathcal{N}(\mathbf{0}, (\sigma_1^2 + \sigma_2^2)\mathbf{I})$. Here the merged standard deviation is $\sqrt{(1-\alpha_t) + \alpha_t(1-\alpha_{t-1})} = \sqrt{1-\alpha_t\alpha_{t-1}}$.

From https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

DDPMs: reverse

If we knew $q(\boldsymbol{x}_{t-1}|x_t)$, we could run the reverse process by sampling noise for $\boldsymbol{x}_T$ and slowly removing it… **but we do not know this probability!**



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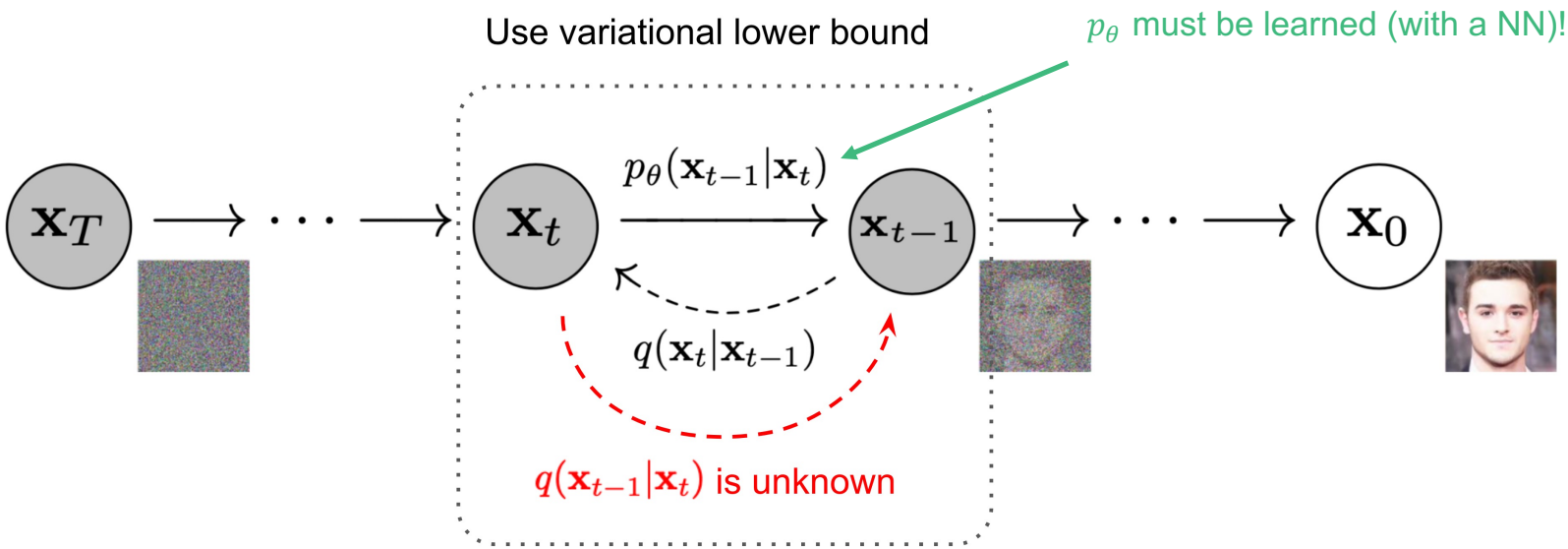

DDPMs: reverse

Assuming that $q(\boldsymbol{x}_{t-1}|x_t)$ is **Gaussian** (true for small β_t), we could just learn its mean and covariance

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \Sigma_\theta(\mathbf{x}_t, t))$$

Parametrized Mean and covariance of conditional distribution

t is additionally fed to the network so it can learn to behave differently during the reverse process

DDPMs: reverse

Assuming only that $q(\boldsymbol{x}_{t-1}|x_t)$, is **Gaussian** (true for small β_t) we could just learn its mean and covariance

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DDPM paper: fixed covariance $\Sigma_\theta(\mathbf{x}_t, t) = \sigma_t^2 \mathbf{I} \quad \sigma_t^2 = \beta_t \quad or \quad \sigma_t^2 = \bar{\alpha}_t$

Improved DDPM paper: learned covariance

DDPMs: reverse

The combination of $q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})$ and $\mathrm{p}_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ can be seen as **VAE**

→ use the **ELBO** to minimize negative log-likelihood

Overall training loss (since we can sample each step independently, **we can optimize random terms of the loss**):

$$L = L_0 + L_1 + ... + L_T$$

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Treated a bit specially…

KL divergence of 2 gaussians → L2 loss!

$$\|\epsilon - \epsilon_\theta(\mathbf{x}_t, t)\|^2 = \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\epsilon, t)\|^2$$

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DDPMs: reverse (simplified derivation)

1. Write expression for L_t $(t = 1, .., T-1)$ losses

$$L_t = D_{\mathrm{KL}}(q(\mathbf{x}_t|\mathbf{x}_{t+1}, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_t|\mathbf{x}_{t+1}))$$

Extra conditioning on x_0 to make it tractable

Given 2 gaussians, there is closed-form solution:

$$L_t = \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\|\boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)\|_2^2}\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_\theta(\mathbf{x}_t, t)\|^2\right]$$

DDPMs: reverse (simplified derivation)

2. Need to write an expression for the mean of $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ to know what $\mathrm{p}_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ has to learn:

Bayes Rule

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) = q(\mathbf{x}_t|\mathbf{x}_{t-1},\mathbf{x}_0)\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)}$$

$$\propto \exp\Big(-\frac{1}{2}\Big(\frac{(\mathbf{x}_t-\sqrt{\alpha_t}\mathbf{x}_{t-1})^2}{\beta_t}+\frac{(\mathbf{x}_{t-1}-\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0)^2}{1-\bar{\alpha}_{t-1}}-\frac{(\mathbf{x}_t-\sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\Big)\Big)$$

$$=\exp\Big(-\frac{1}{2}\Big(\frac{\mathbf{x}_t^2-2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1}+\alpha_t\mathbf{x}_{t-1}^2}{\beta_t}+\frac{\mathbf{x}_{t-1}^2-2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0\mathbf{x}_{t-1}+\bar{\alpha}_{t-1}\mathbf{x}_0^2}{1-\bar{\alpha}_{t-1}}-\frac{(\mathbf{x}_t-\sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\Big)\Big)$$

$$=\exp\Big(-\frac{1}{2}\Big(\Big(\frac{\alpha_t}{\beta_t}+\frac{1}{1-\bar{\alpha}_{t-1}}\Big)\mathbf{x}_{t-1}^2-\Big(\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t+\frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0\Big)\mathbf{x}_{t-1}+C(\mathbf{x}_t,\mathbf{x}_0)\Big)\Big)$$

Write mean out…

DDPMs: reverse (simplified derivation)

2. Need to write an expression for the mean of $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ to know what $\mathrm{p}_\theta(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ has to learn:

$$\tilde{\beta}_t = 1/(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}) = 1/(\frac{\alpha_t - \bar{\alpha}_t + \beta_t}{\beta_t(1-\bar{\alpha}_{t-1})}) = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t$$

$$\begin{aligned}
\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) &= (\frac{\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0)/(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}) \\
&= (\frac{\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0)\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 \quad \longleftarrow \text{Using } \mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + (1-\bar{\alpha}_t)\epsilon
\end{aligned}$$

$$= \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

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\end{aligned}$$

$$= \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right) \leftarrow$$

This is **why we cannot directly reverse the process directly** (outside of training we do not know $\boldsymbol{\epsilon}_t$)

DDPMs: reverse (simplified derivation)

3. Plug the derived mean of $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)$ into the loss

$$
\begin{aligned}
L_t &= \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{1}{2\|\boldsymbol{\Sigma}_\theta(\mathbf{x}_t,t)\|_2^2}\|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t,\mathbf{x}_0)-\boldsymbol{\mu}_\theta(\mathbf{x}_t,t)\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{1}{2\|\boldsymbol{\Sigma}_\theta\|_2^2}\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t-\frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)-\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t-\frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,t)\right)\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{(1-\alpha_t)^2}{2\alpha_t(1-\bar{\alpha}_t)\|\boldsymbol{\Sigma}_\theta\|_2^2}\|\boldsymbol{\epsilon}_t-\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,t)\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{(1-\alpha_t)^2}{2\alpha_t(1-\bar{\alpha}_t)\|\boldsymbol{\Sigma}_\theta\|_2^2}\|\boldsymbol{\epsilon}_t-\boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t,t)\|^2\right]
\end{aligned}
$$

Empirically found in DDPM paper

DDPMs: algorithm

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
6: **until** converged

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

In practice done in batches, each sample has different t (to learn different stages of denoising at same time)

DDPMs: algorithm

$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0)$: mean of $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0)$

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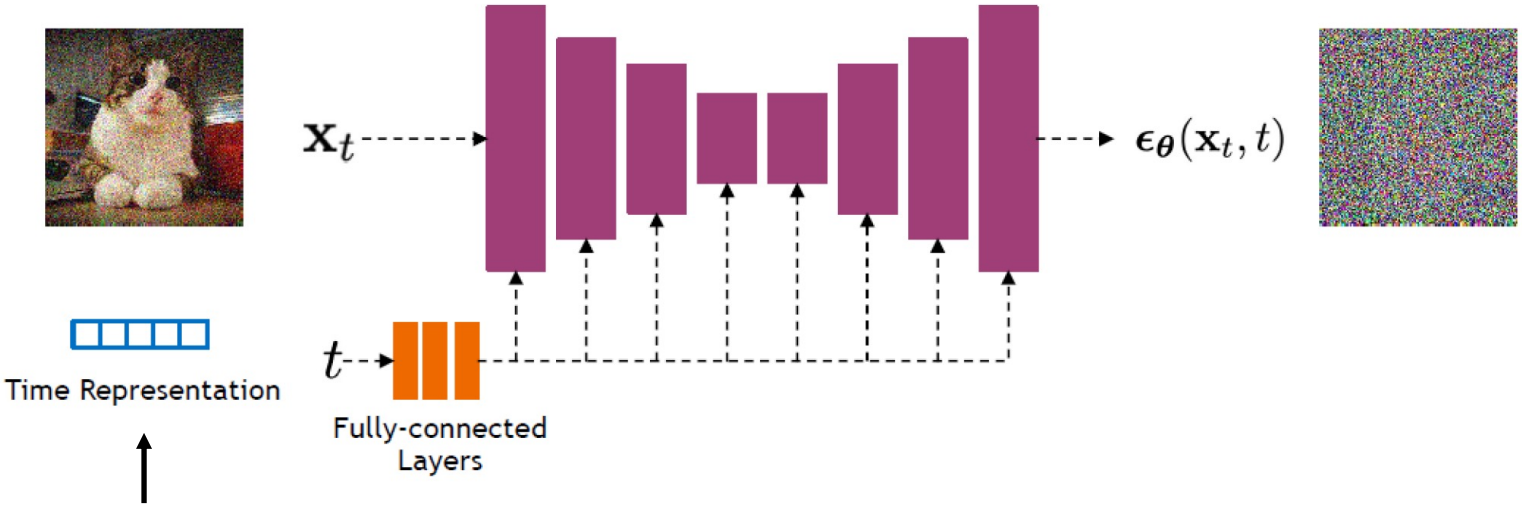
In practice done in batches, each sample has different t (to learn different stages of denoising at same time)

DDPMs: network architecture

Whilst this can be anything, a **UNet-like CNN architecture** is usually employed

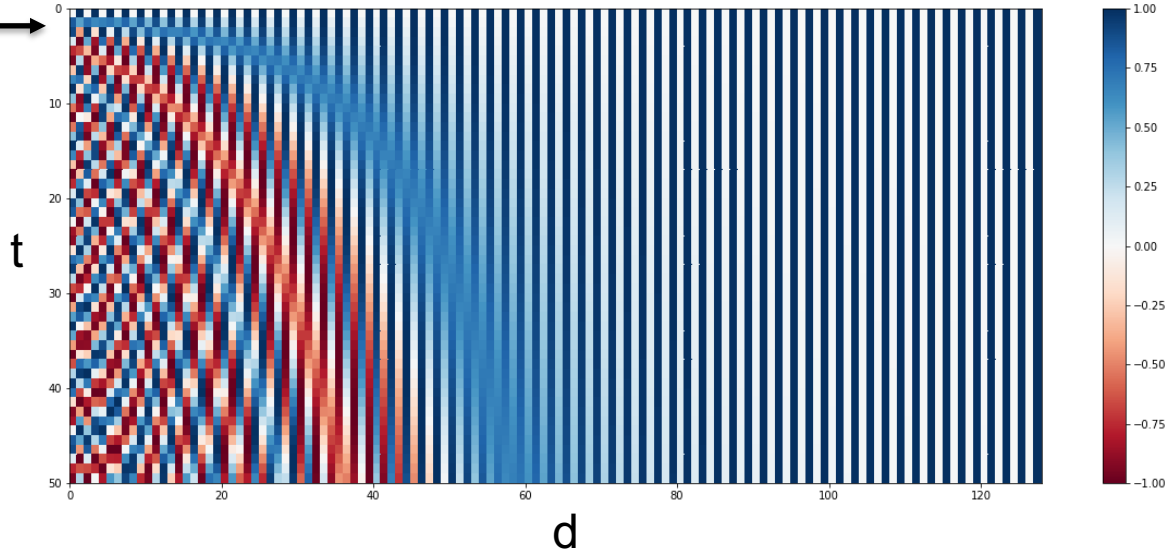


Sinusoidal positional embeddings or random Fourier features (added to channels)

Sinusoidal positional encoding

$$\overrightarrow{p_t} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_{d \times 1}$$

t=0



DDPMs: more details

- Covariance learning: instead of being fixed, it can be learned to improve the quality of the model (actually a vector $\mathbf{v}$ mixing β_t and $\tilde{\beta}_t$ is learned in Nichol & Dhariwal, 2021)

DDPMs: more details

- Covariance learning: instead of being fixed, it can be learned to improve the quality of the model (actually a vector $\mathbf{v}$ mixing β_t and $\tilde{\beta}_t$ is learned in Nichol & Dhariwal, 2021))

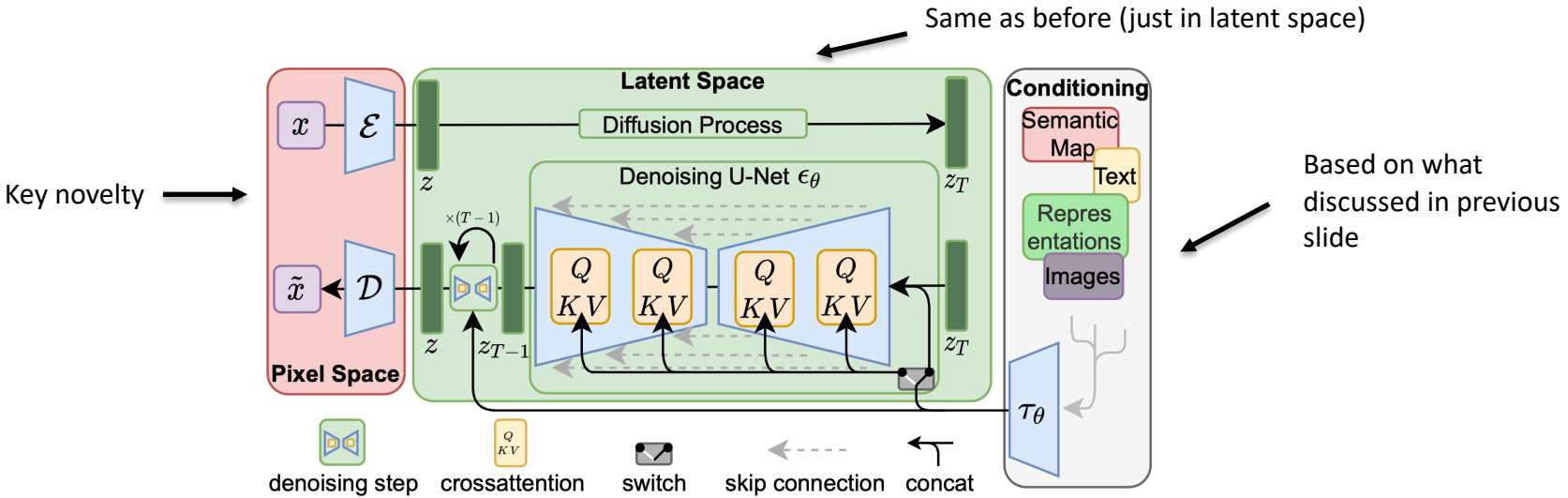
- Conditioning: can add class (if training with data with labels – e.g., ImageNet) or text prompt (or any descriptive representation, e.g., another image)

- **Classifier guided diffusion:** train classifier on noisy images and use its gradient to guide diffusion reverse process towards class of interest.
- **Classifier-free guidance:** learn both an unconditional and conditional diffusion process with one network and choose which one to use at generation time

DDPMs: more details

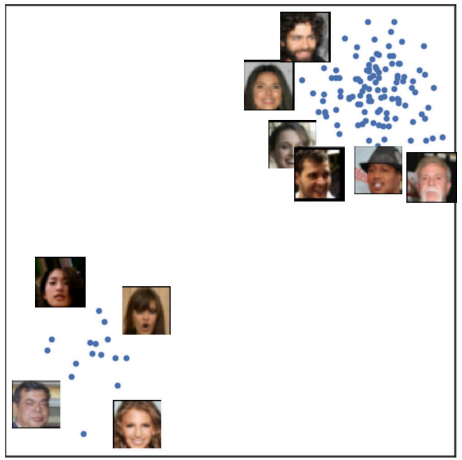
- Speed-up:

- to sample a subset of steps from T to 0 in generation, one can learn a direct noise map from any t to 0 - DDIMs (Denoising Diffusion Implicit Models)
- can learn the diffusion process in a latent space – LDM (Latent Diffusion Models)



NCSNs: an alternative approach

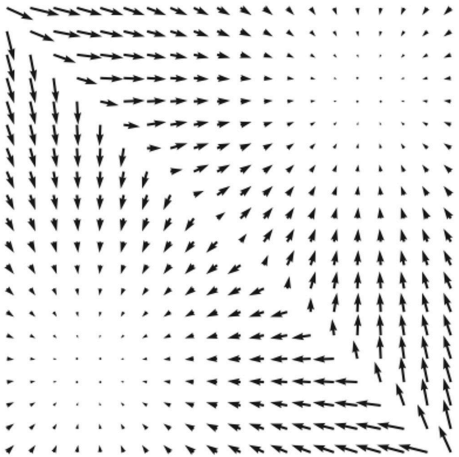
An alternative approach which relies on the **score function** and **Langevin dynamics.**



Data samples

$$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p(\mathbf{x})$$

score matching



Scores

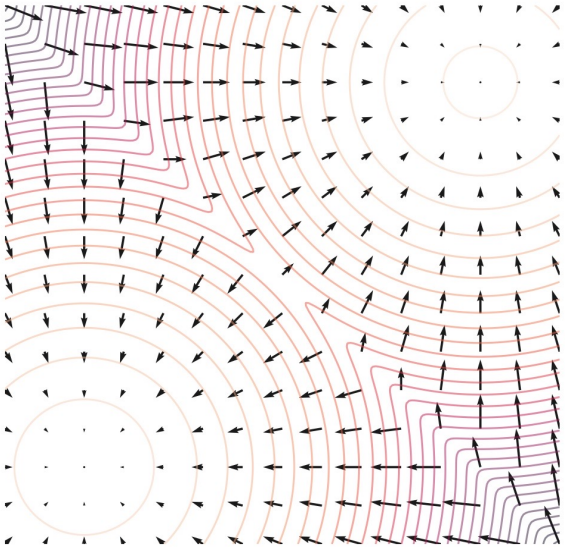
$$\mathbf{s}_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p(\mathbf{x})$$

Langevin dynamics

New samples

NCSNs: an alternative approach

Score function corresponds to the gradient of log-likelihood



$$\nabla_{\mathbf{x}} log p(\mathbf{x})$$

NCSNs: an alternative approach

Ideally we would like to model $p(\boldsymbol{x})$ directly (by maximizing its log-likelihood):

$$\underset{\theta}{\operatorname{argmax}}\ logp(\mathbf{x})$$

We can write it in an exponential form and learn the parameters:

$$p_\theta(\mathbf{x}) = \frac{e^{-f_\theta(\mathbf{x})}}{Z_\theta}$$

Normalization factor such as

$$\int p_\theta(\mathbf{x})d\mathbf{x} = 1$$

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Intractable (must be evaluated in learning process)

NCSNs: an alternative approach

By learning a score based model, the normalizing factor is side-stepped

$$s_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} log p_\theta(\mathbf{x}) = -\nabla_{\mathbf{x}} log f_\theta(\mathbf{x}) - \cancel{\nabla_{\mathbf{x}} log Z_\theta} = -\nabla_{\mathbf{x}} log f_\theta(\mathbf{x})$$

The learning process minimizes the **Fisher divergence** between the model and the data distributions:

$$E_p[\|s_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} log p(\mathbf{x})\|_2^2] \longleftarrow$$ **Score matching methods!**

NCSNs: an alternative approach

The generation process becomes simple – i.e., gradient ascent on $p(\boldsymbol{x})$:

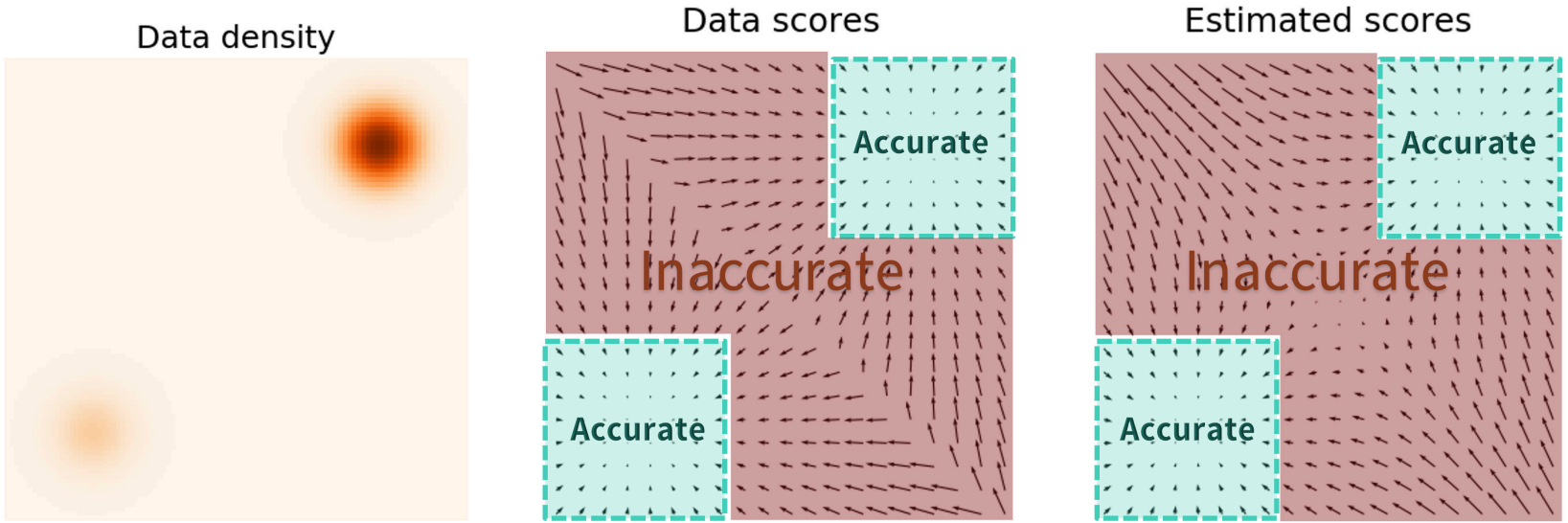
$$\mathbf{x}_{i+1} = \mathbf{x}_i + \epsilon \underbrace{\nabla_{\mathbf{x}} log p(\mathbf{x})}_{\approx\ s_\theta(\mathbf{x}_{i+1})} + \sqrt{2\epsilon}\mathbf{z}_i$$

Indirect/learned access to the score function

Note: this is not pure gradient ascent (would not sample the distribution as it is deterministic) → Langevin dynamics = stochastic version of gradient ascent

NCSNs: where is the connection with DDPMs?

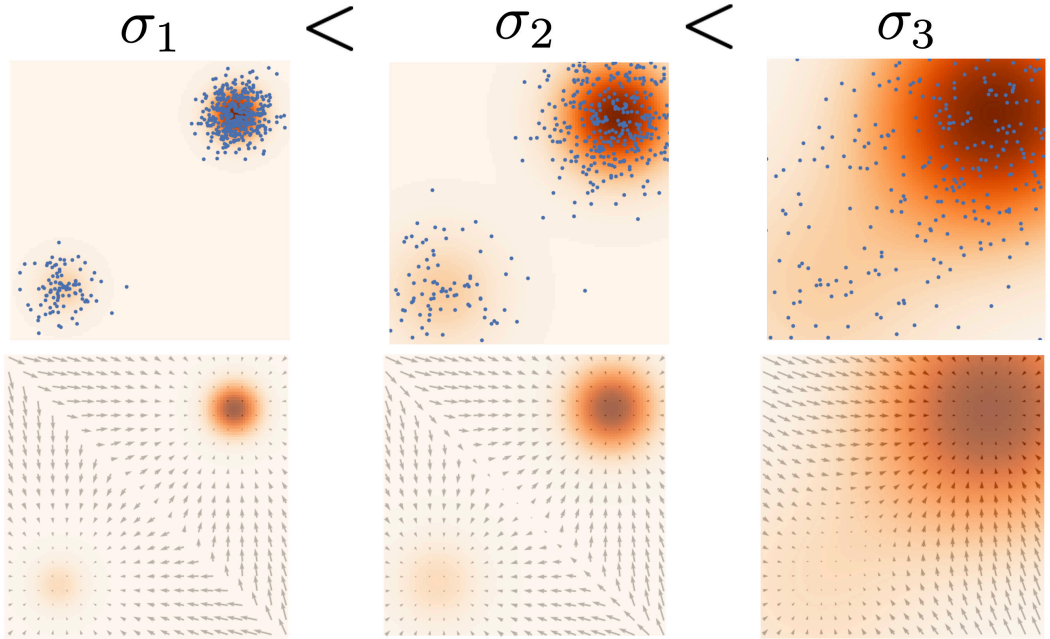
Turns out score functions cannot be stably learned in areas of low probs.



Source: https://yang-song.net/blog/2021/score/

NCSNs: where is the connection with DDPMs?

Solution: **perturb training data with different levels of noise** (=convolve/smooth underlying pdf)

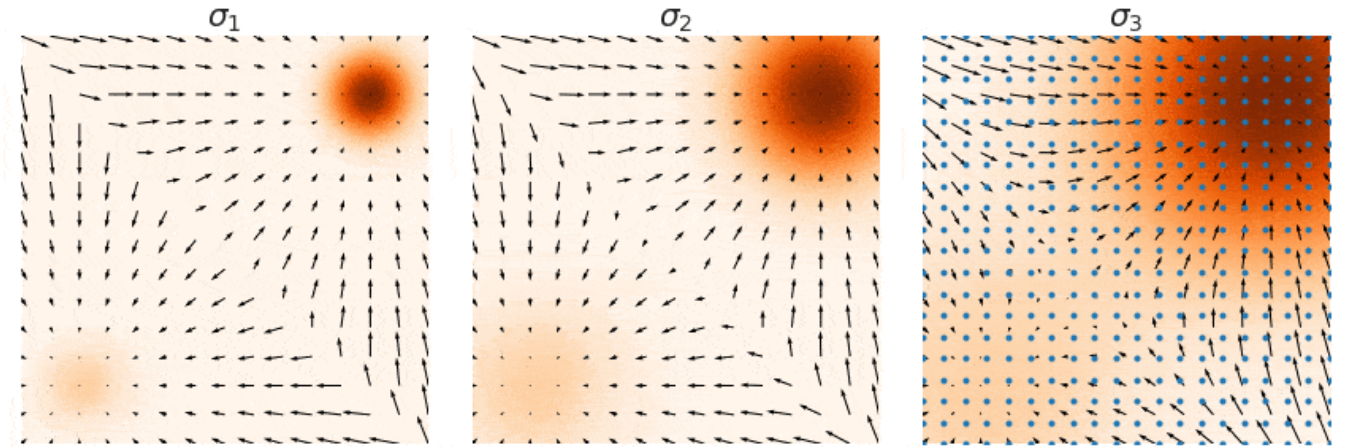


Source: https://yang-song.net/blog/2021/score/

Accurate reconstruction at all scales

NCSNs: where is the connection with DDPMs?

Solution: combine a **sequence of Langevin chains** with gradually decreasing noise scales.



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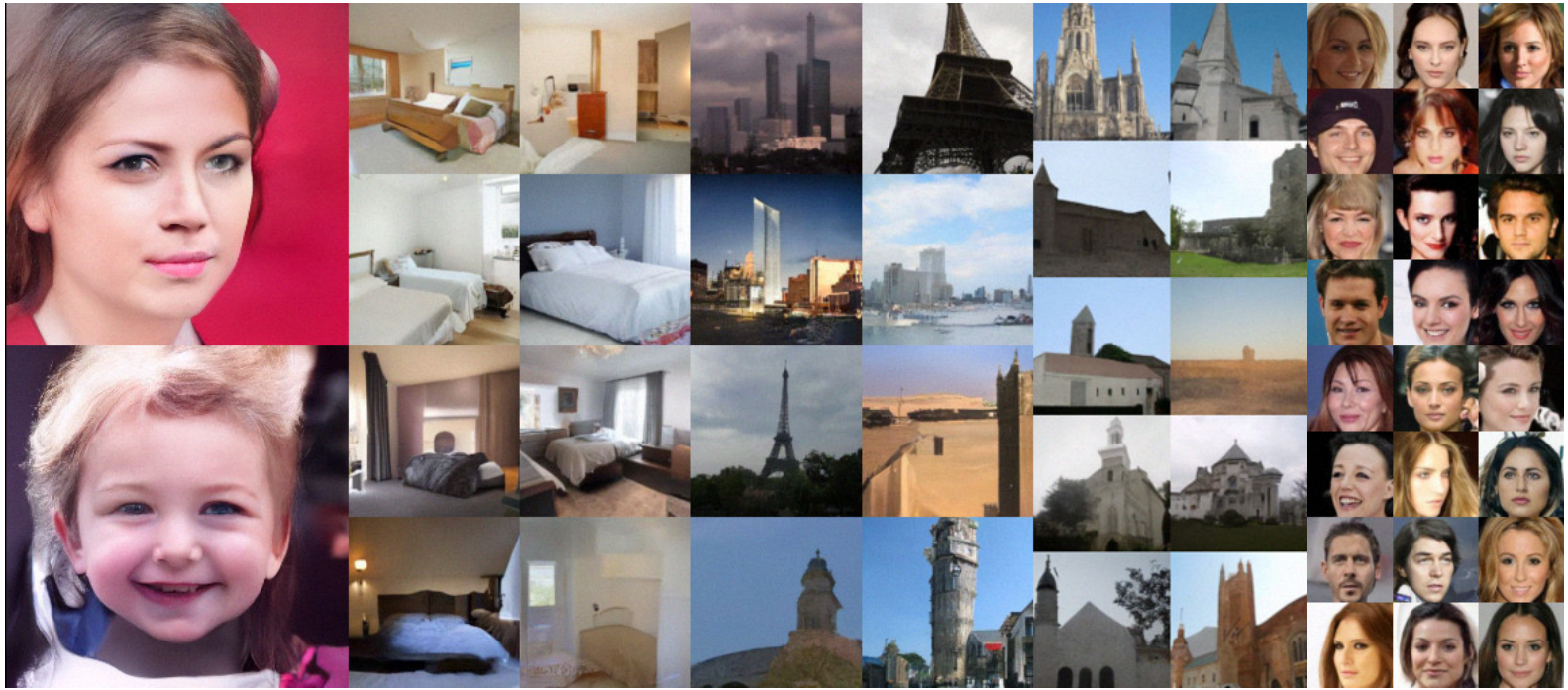
NCSNs: an alternative approach



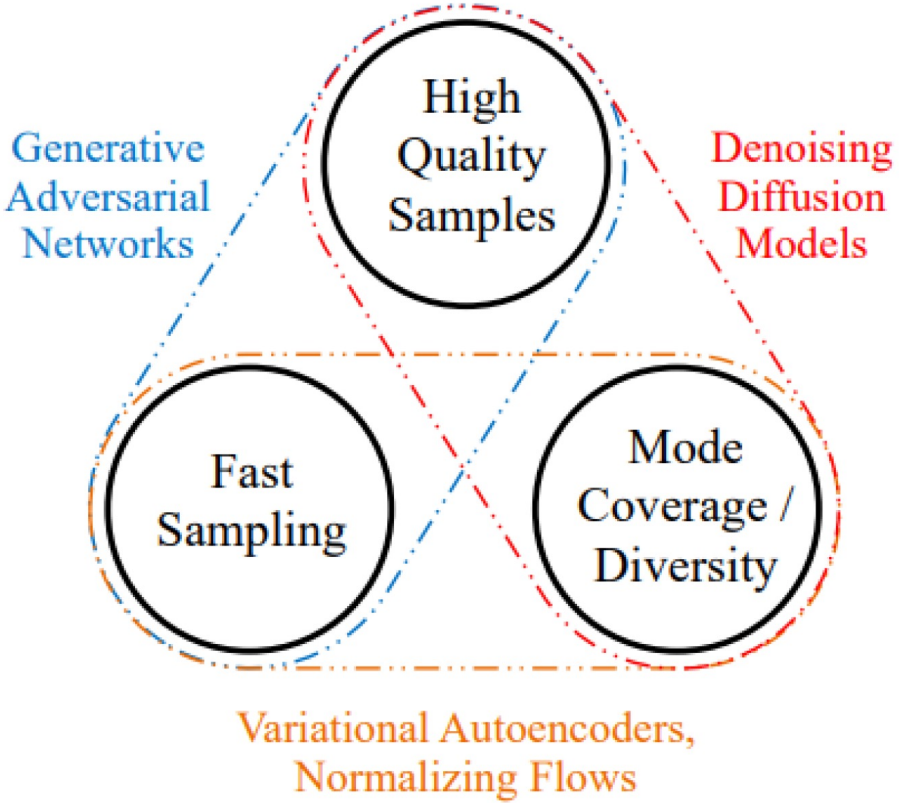
From NCSNv2 model

Trying out Diffusion models for free

A nice demo of stable diffusion (without code / fee):

https://huggingface.co/spaces/stabilityai/stable-diffusion

Wrapping up the week

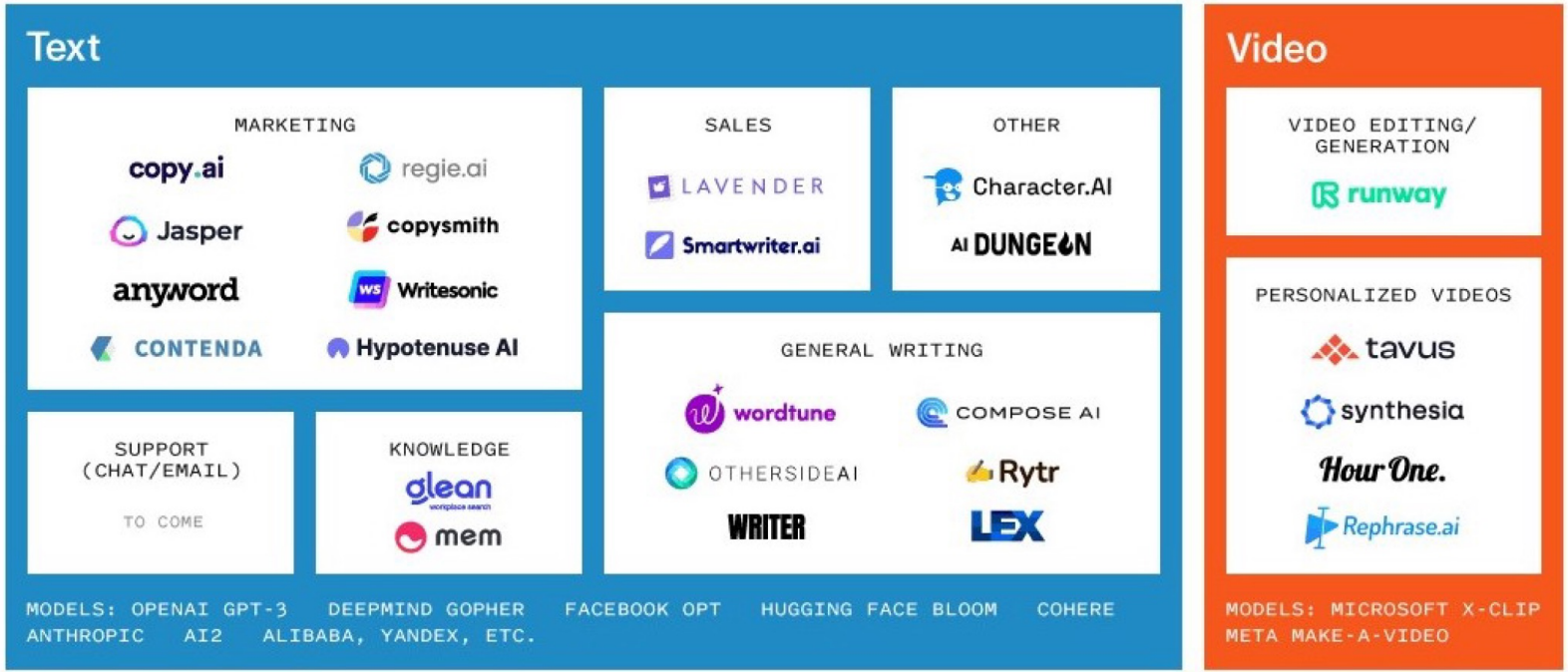


Generative learning trilemma

From: Tackling the Generative Learning Trilemma with Denoising Diffusion GANs

Wrapping up the week

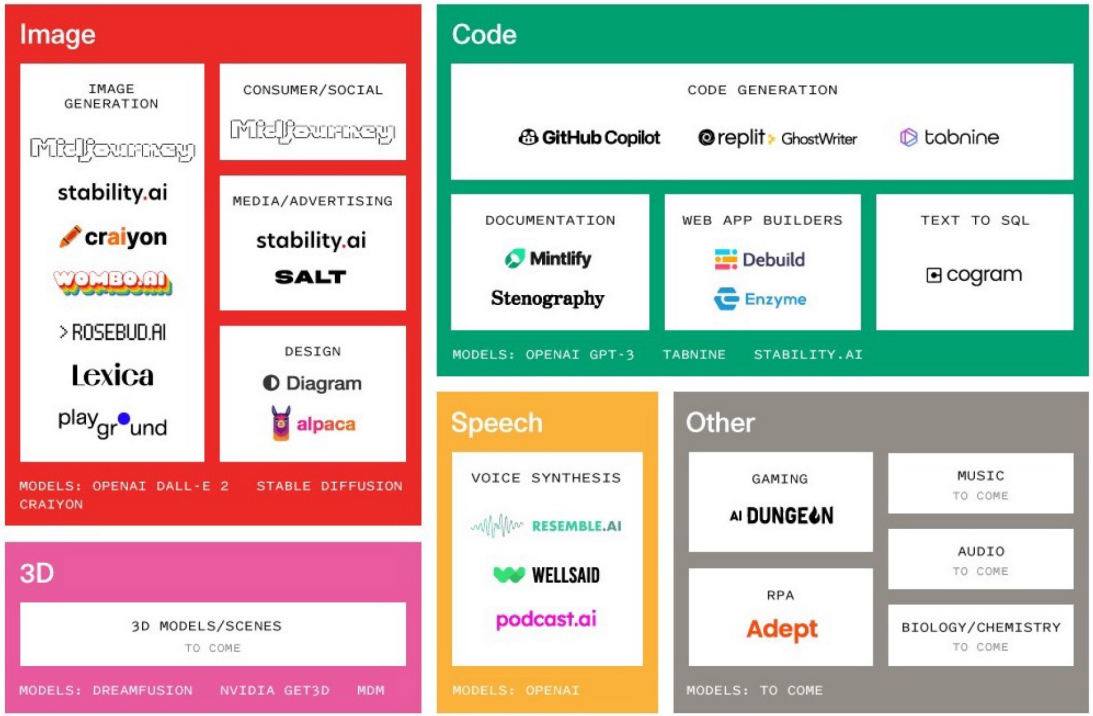
The Generative AI landscape



From Sonya Huang (@sonyatweetybird)

Wrapping up the week

The Generative AI landscape



From Sonya Huang (@sonyatweetybird)