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BIOSINF

Generative Models

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Content

1. Intro

Let's have some fun with generative models!

Try these websites

- `https://thispersondoesnotexist.com`
- `https://ai-vs-real.com`
- `https://britannicaeducation.com/blog/quiz-real-or-ai/`

Discriminative vs Generative

Discriminative Models

- **Goal:** Learns a decision boundary.
- **Models:** The conditional probability $p(y|x)$.
- **Tasks:** Classification, Segmentation, Information Retrieval, *etc.*
- **Examples:** Logistic Regression, SVMs, FFC.

Discriminative vs Generative

Generative Models

- **Goal:** Learns the underlying data distribution.
- **Models:** The joint probability $p(x, y)$ or the marginal $p(x)$.
- **Tasks:** Generation, translation, editing, *etc.*
- **Examples:** VAEs, GANs, Diffusion Models.

Study Case: ChatGPT – where generative meets discriminative

What does GPT stand for?

- GPT stands for **G**enerative **P**re-trained **T**ransformer.
- **Generative:** Its primary purpose is to *generate* new text that is statistically similar to the data it was trained on. It creates content, rather than just classifying or analyzing it.
- **Pre-trained:** The model is first trained on a massive, unlabeled dataset. This *pre-training* phase teaches it grammar, facts, reasoning abilities, and stylistic patterns. It's later *fine-tuned* or *down-streamed* for specific tasks like instruction following.
- **Transformer:** This is the specific neural network architecture it uses. The Transformer is exceptionally good at handling long sequences of data.

Study Case: ChatGPT – where generative meets discriminative

How does ChatGPT work?

- At its heart, a GPT model is a sophisticated next-token predictor $\rightsquigarrow$ **discriminative**.
- Given a sequence of text (*prompt*), its fundamental job is to predict the most probable next word (or, more accurately, *token*).
- For example, given the input *The cat sat on the...*, the model's goal is to output a probability distribution over its entire vocabulary, with a high probability assigned to tokens like *mat*, *floor*, or *couch*.
- By repeatedly predicting the next token and appending it to the input it can generate long, coherent sequences of text one token at a time $\rightsquigarrow$ **generative**.

2. AutoEncoders

AutoEncoders (AEs)

What is an AE?

- An **autoencoder** is an **unsupervised** neural network trained to perform a simple task: **reconstruct its own input**.
- It consists of two (or three) main parts:
  - An **encoder**, $\mathcal{E}$, which maps the input x to a compressed latent representation $z = \mathcal{E}(x)$.
  - A **bottleneck**, which contains the compressed latent representation, sometimes further processing or guiding/conditioning it.
  - A **decoder**, $\mathcal{D}$, which reconstructs the input from the latent code, $\hat{x} = \mathcal{D}(z) = \mathcal{D}(\mathcal{E}(x))$.
- The network is trained to minimize a **reconstruction loss**, $\mathcal{L}(x, \hat{x})$.

The Importance of the Bottleneck

All-shaped bottleneck

- **Complete bottleneck:** the dimension of the latent is equal to that of the input: $\dim(x) = \dim(z)$
  Does this cause any problems?

- **Overcomplete bottleneck:** $\dim(z) \gg \dim(x)$
  Is this useful for anything?

- **Undercomplete bottleneck:** $\dim(z) \ll \dim(x)$
  Now we're talking!

Where AE shines...

What are AE used for?

- **Dimensionality Reduction:** The latent code z is a low-dimensional version of x, useful for compression or visualization.
- **Feature Extraction:** The encoder can be used as a pre-trained feature extractor for a down-stream supervised task.
- **Anomaly Detection:** A model trained on normal data will have a high reconstruction error for anomalous inputs.
- **Image Denoising:** The AE is a natural fit for denoising, and the encoder/decoder pair can be used for restoration.

...and its limitations.

Underlying problems

- **Irregular latent:** Some parts might be unused, other overly-used.
- **GIGO:** Sampling a random point in the latent might result in *garbage* results.
- **Not generational:** Can only encode/decode existing data $\rightsquigarrow$ unable to produce new samples!

The VAE: A Generative Approach

No more fixed points!

- A VAE is a **probabilistic generative model** built with an autoencoder-like architecture.
- Instead of mapping an input to a single point z, the encoder maps it to a **probability distribution** over the latent space.
- Specifically, the encoder outputs the parameters (mean μ and variance σ^2) of a Gaussian distribution.
- The latent code z is then *sampled* from this distribution, $z \sim \mathcal{N}(\mu, \sigma^2)$.

The Evidence Lower Bound (ELBO)

From data to probabilities

- The goal is to maximize the log-likelihood of the data, $\log p(x)$.
- Instead, we maximize a lower bound on it, known as the **Evidence Lower Bound (ELBO)**.

$$\log p_\theta(x) \geq \underbrace{\mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)]}_{\text{Reconstruction Term}} - \underbrace{D_{KL}(q_\phi(z|x)||p(z))}_{\text{Regularization Term}}$$

- **Reconstruction Term:** How well does the decoder reconstruct the input, given a sample from the latent distribution?
- **Regularization Term (KL Divergence):** How much does our learned latent distribution $q_\phi(z|x)$ diverge from a simple prior (usually $\mathcal{N}(0, I)$)? This forces the latent space to be well-structured.

Still not generative enough

Stochastic sampling step

- **Problem:** How to do backprop on stochastic sampling?
- **Answer:** We include it in the model input!

What we replace, exactly?

- Instead of directly sampling the latent

$$z \sim \mathcal{N}(\mu, \sigma^2)$$

- We sample some noise ϵ and add it to our z:

$$z = \mu_\phi(x) + \sigma_\phi(x) \odot \epsilon$$

VQ-VAE: Discrete Latent Spaces

The most modern approach

- The encoder outputs a vector, which is then replaced by the nearest vector from a learnable **codebook** (dictionary) of embeddings.
- This quantization step leads to higher-fidelity reconstructions.
- A more powerful model can then be trained over the discrete latent codes to create a strong conditional generative model.

Summary: AE vs. VAE

Autoencoder (AE)

- Deterministic
- Learns a point-estimate latent code
- Simple reconstruction loss
- Good for compression, anomaly detection
- Not generative

Variational Autoencoder (VAE)

- Probabilistic / Generative
- Learns a distribution over latent space
- Complex ELBO loss (Reconstruction + KL)
- Good for data generation, learning smooth representations
- More complex to train

3. Generative Adversarial Networks

What is a GAN?

Definition

A Generative Adversarial Network is an **implicit generative model**. It learns to generate data without defining a probability density function $p(x)$.

But... how?

It learns through a **two-player**, **zero-sum** game between:

- A **Generator (G)**: An *art forger* that takes random noise z (from a simple prior distribution like a Gaussian) and tries to create realistic data samples $G(z)$.
- A **Discriminator (D)**: An *art critic* or *detective* that is a binary classifier. It tries to distinguish between real data samples from the training set and fake samples from the generator.

The two networks are trained in opposition: G gets better by fooling D, and D gets better by seeing more convincing fakes from G.

Let's visualize them

The Minimax Objective Function

GAN loss function

The training process is a minimax game described by the following objective:

$$\min_G \max_D V(D,G) = \underbrace{\mathbb{E}_{x\sim p_{data}(x)}[\log D(x)]}_{\text{D wants to maximize this}} + \underbrace{\mathbb{E}_{z\sim p_z(z)}[\log(1-D(G(z)))]}_{\text{D wants to maximize this}}$$

Taking turns

- **The Discriminator's Turn ($\max_D$)**: This is equivalent to a standard binary cross-entropy loss where the label for real data is 1 and for fake data is 0.
- **The Generator's Turn ($\min_G$)**: G Minimization happens when $D(G(z))$ is high (i.e., when D is fooled into thinking fake samples are real).

Convergence and Divergence

Optimal Discriminator

For a fixed G, we want:

$$D^*(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)},$$

where:

- If the sample is real: $D^*(x) \approx 1$
- If the sample is fake: $D^*(x) \approx 0$

Optimal Generator

For a fixed D, we want:

$$p_{data}(x) = p_g(x) \rightsquigarrow D(x) = \frac{1}{2},$$

meaning that the discriminator is maximally confused.

The Unstable Equilibrium

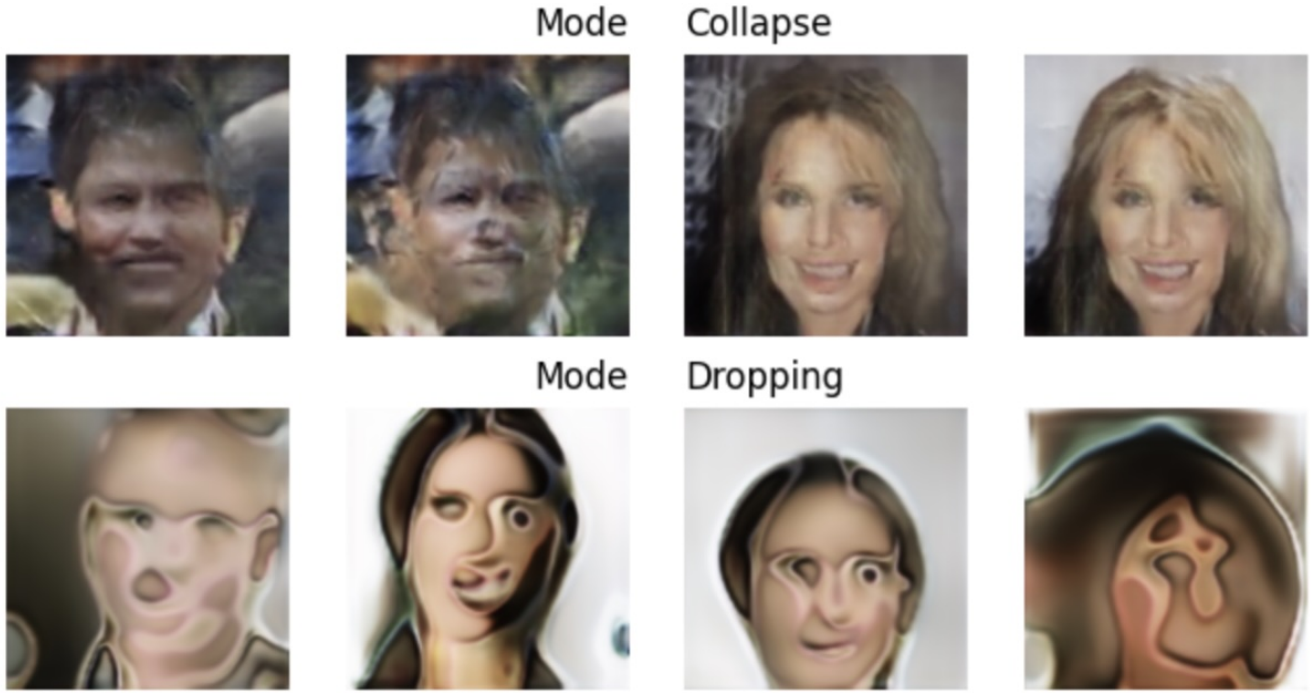
Why we cant achieve Nash equilibrium

- We do not have a straight-forward loss function, optimizing two networks at the same time $\rightsquigarrow$ unstable training
- One network (discriminator) learns much quicker than the other (generator)

What is stoping us?

- **Vanishing gradients:** The generator gradients are too low when the discriminator becomes too powerful.
- **Oscillation:** The loss function fluctuates without finding a local minima $\rightsquigarrow$ generator and discriminator do not improve
- **Generator starts cheating:**
  - Reproduces only a small set of examples $\rightsquigarrow$ **mode collapse**
  - Reproduces similar features in all its data $\rightsquigarrow$ **mode dropping**

Visualizing Failure



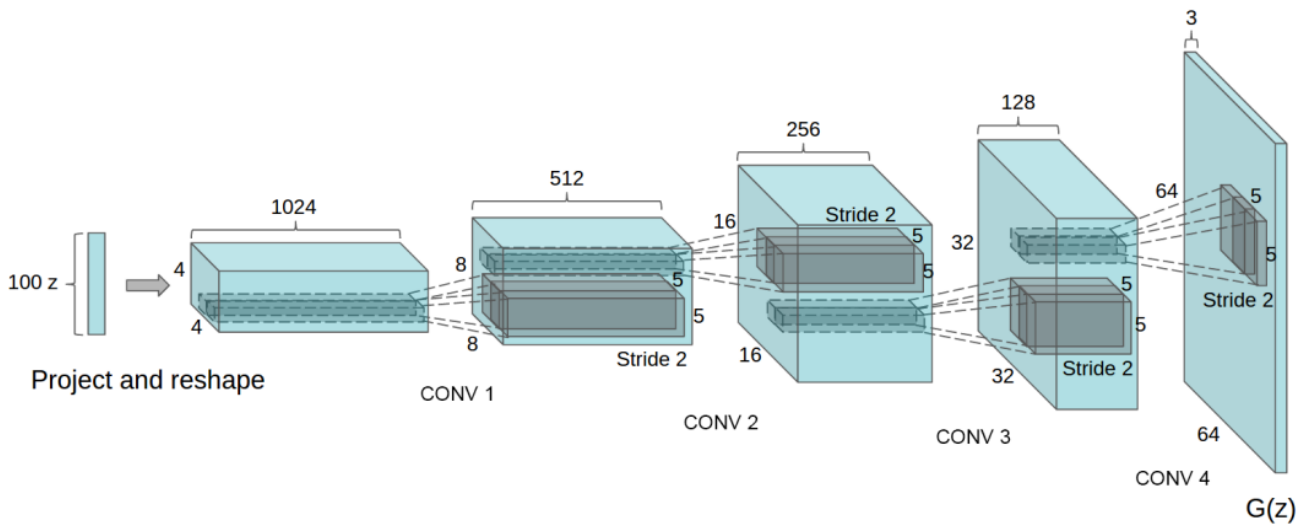
First implementation: DCGAN

Key Innovations

- **All convolutional Net:** Both the generator and discriminator are fully-convolutional, learning specific down samplings/up samplings.
- **Batch Normalization:** Stabilizes training by normalizing distributions after each layer, allowing proper gradient flow.

Impact

- First high quality image generation model
- Latent spaces has a structure, allowing for latent interpolation.



Making Training Stable: WGAN

Key Innovations

- **Critic, not Discriminator:** Replace the final prediction with a *realness* score, not a real/fake prediction. This new score is used to tell the Generator *how far* it is from the actual sample.
- **Better loss:** Replaced the standard GAN loss with Wasserstein distance (*i.e. minimum energy to "move" from a distribution to another)*. This new loss is used jointly with the *realness* score to optimize the networks.
- **Weights clipping:** Proposes a method for stabilizing the training, especially in the Discriminator, slowing it down and making it more robust to mode collapse.

Impact

- Showcases that GANs can be trained in a more stable manner.

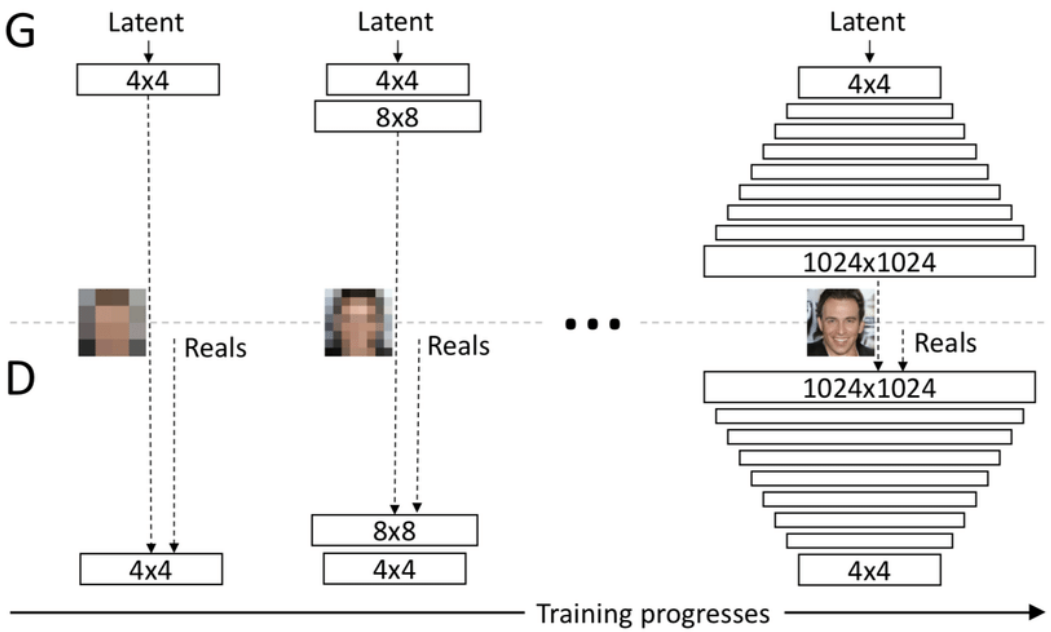
Iterations Makes Perfections: PGAN

Key Innovations

- **Start small:** Generate HQ samples iteratively, by first producing low-res ones, refine and then upscale!
- **Adding layers:** During training, once a plateau is reached, more layers are added to increase the resolution.

Impact

- First method to achieve 1024×1024 photorealistic images.



Adding disentanglement: StyleGAN

Key Innovations

- **Mapping Network:** Add a new module to process the z latents, creating a more meaningful (and disentangled) W space.
- **AdaIN:** Adaptive Instance Normalization uses the style codes from W to control the μ and σ of the features at each layer, resulting in different layers controlling features at different scales: first layers create general appearance while higher ones focus on finer details.

Impact

- Allowed image editing by combining different styles in the W space, with explicit control over coarse-to-fine details
- Achieves better quality and a more disentangled latent space, being a de-facto model in image generation.

Combining styles

Make them conditional: cGAN

Key Innovations

- **Conditional:** Adds information in the form of one-hot vectors to both the Generator and Discriminator.
- **Affects both models;** The Generator learns features specific to a class in the provided condition. The Discriminator is forced to predict the sample class (including a *fake* one).

Impact

- Was a foundation for conditioning generative models.
- Allowed finer control over the generation, not just a generic image.
- Almost free-cost, which is why later added to other GANs (such as StyleGAN-2)

Image-to-Image Translation: CycleGAN

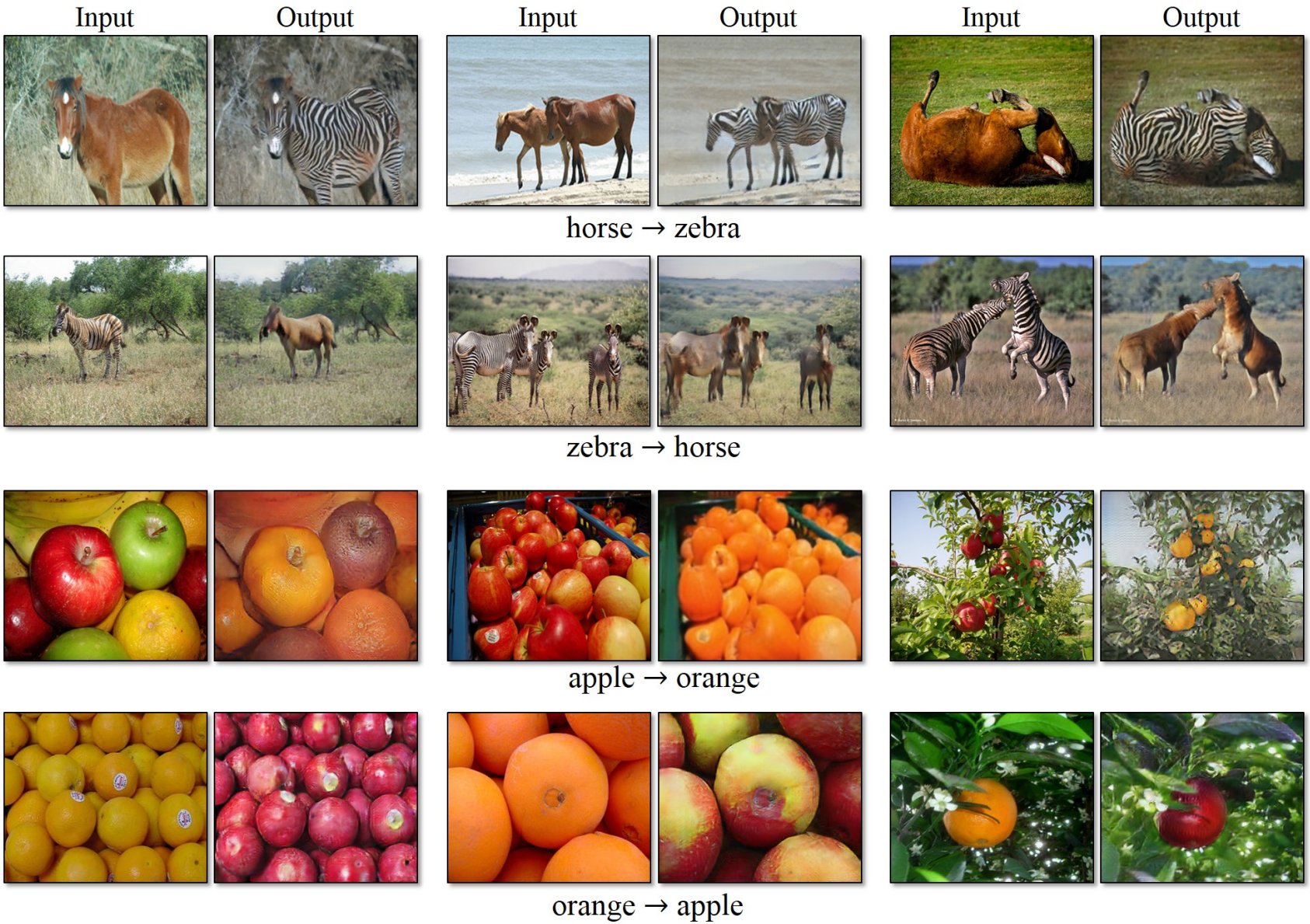
Key Innovations

- **Cycles:** Learns to translate between two sets of images: A and B, to morph images from one set to the other.
- **No paired data:** Does not require exact pairs of images, only two distinct but similar sets (*e.g.* zebra and horse, summer and winter, photos and paintings).
- **We have 2 GANS:** G_{AB} and G_{BA}, which are trained on *cyclic generation:* $\hat{x}_A = G_{BA}(G_{AB}(x_A))$

Impact

- Extens GANs to image-translation tasks.
- Allows for explicit changes without latent manipulation tricks or conditioning.

CycleGAN in action



Applications: Where are GANs Used?

Usage in multiple domains:

- **Creative Arts & Design:** Generating novel artistic images, textures, and designs.
- **Data Augmentation & Simulation:** Creating synthetic data to train other machine learning models, especially in low-data domains like medical imaging. Generating realistic scenarios for training autonomous systems (e.g., self-driving cars).
- **Image Editing & Super-Resolution:** "Inpainting" missing parts of images, increasing image resolution.
- **Fashion & E-commerce:** Creating virtual try-ons and wrapping product images.

How about misuses?

- We better do not talk about this...

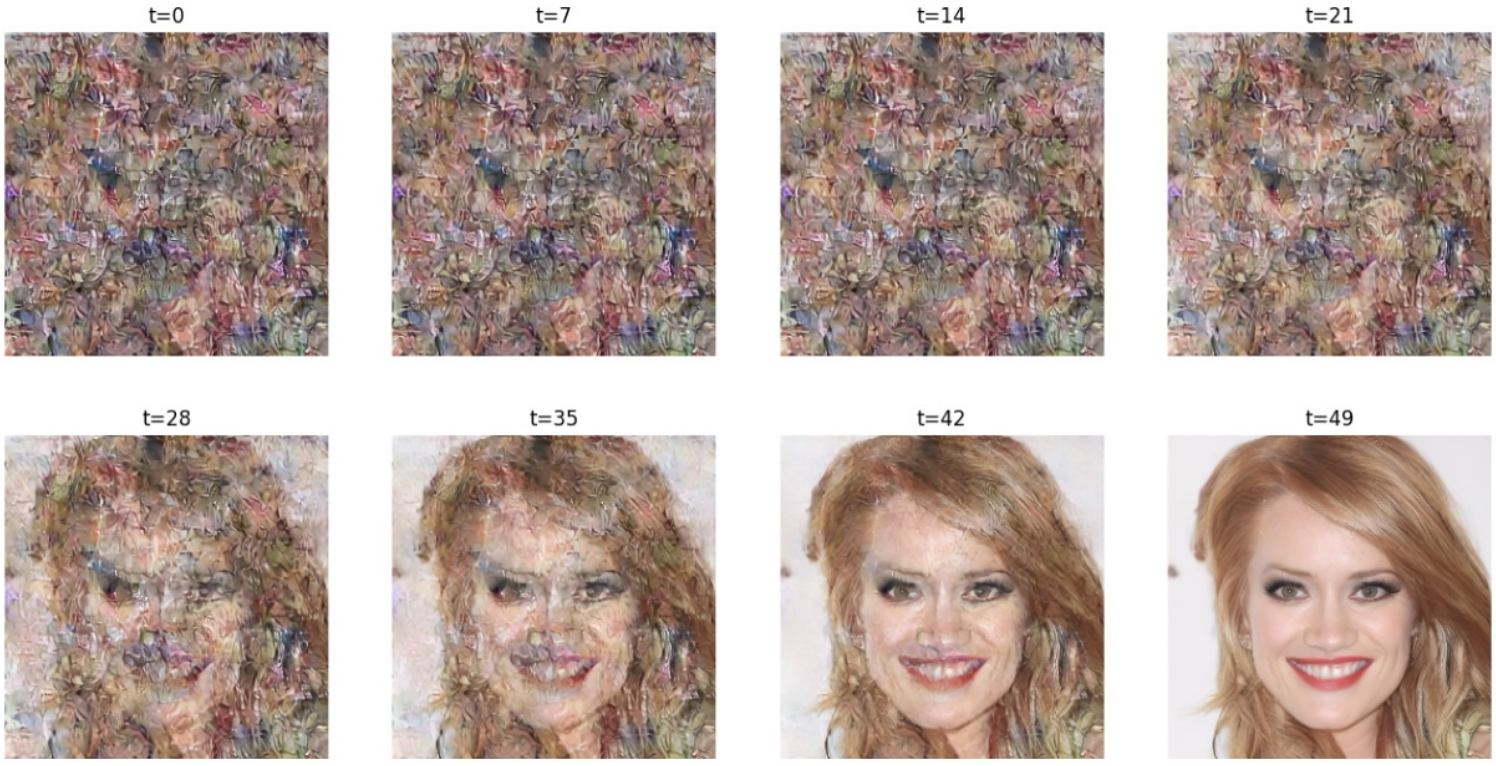
4. Diffusion Models

Diffusion Models

Intuition and Formulation

- Diffusion models are a class of generative models inspired by thermodynamics.
- They learn to generate data by reversing a gradual **noising process**.
- **The Two-Step Process:**
  1. **Forward Process (Fixed):** Systematically destroy structure in the data by gradually adding Gaussian noise over a series of steps. This is a fixed, non-learned process.
  2. **Reverse Process (Learned):** Train a neural network to reverse this process. The network learns to gradually denoise an image, starting from pure noise, to generate a clean sample.

Visualizing this process



Mathematical approach

Forward

- We start with a clean data sample $x_0 \sim p_{data}(x)$.
- We define a sequence of T noising steps (e.g., $T = 1000$). At each step t, we add a small amount of Gaussian noise according to a variance schedule β_t.
- We can sample x_t at any arbitrary timestep t directly from x_0, without iterating:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon, \quad \text{where } \epsilon \sim \mathcal{N}(0, I) \text{ and } \bar{\alpha}_t = \prod_{i=1}^{t}(1 - \beta_i)$$

Note: *The β_t values are not random! We chose them such that if we apply this process T times, x_T is approximately pure Gaussian noise ($x_T \approx \mathcal{N}(0, I)$).*

Mathematical approach II

Reverse

- The goal is to learn the reverse transition $p_\theta(x_{t-1}|x_t)$ which will undo the noising process at timestep t.
- This reverse transition is also a Gaussian, but with learned mean and fixed variance:

$$p_\theta(x_{t-1}|x_t) = x_t - \mathcal{N}(\mu_\theta(x_t, t), \beta_t I)$$

- The network's job is to predict the mean $\mu_\theta(x_t, t)$ of the slightly less noisy image x_{t-1}.

Note: *Since the reverse is also a Gaussian, the forward process is "locked". Choosing other distribution as a starting point (x_T) will not yield satisfactory results!*

DDPM: Let us simplify training

Objective function

- In theory, we can use the ELBO, similar to VAEs. However, it will be slower and inaccurate because of the high number of steps.
- Since the σ is fixed, predicting the μ_θ is similar to predicting the noise ϵ.
- This leads to an even simpler loss: $\mathcal{L}_2$:

$$\mathcal{L}_2 = \mathbb{E}_{t,x_0,\epsilon}\|\epsilon - \epsilon_{\text{pred}}\|^2 = \mathbb{E}_{t,x_0,\epsilon}\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)\|^2$$

Quite easy, actually!

1. Pick a random training image x_0, a timestep t and generate some noise ϵ
2. **Forward:** Create the noisy image x_t using the forward formula.
3. **Reverse:** Ask the neural network to predict ϵ from x_t and t.
4. The loss is the difference between the network's prediction and the actual noise.

The Denoising Network Architecture

UNet

- An encoder-decoder architecture with **skip connections** between corresponding layers in the encoder and decoder.
- Preserving low-level details (from skip connections) while capturing high-level semantics (from the bottleneck).
- **Timestep Information (t)** is typically encoded into a vector using sinusoidal positional embeddings.

Further Reading

It all depends what you want!

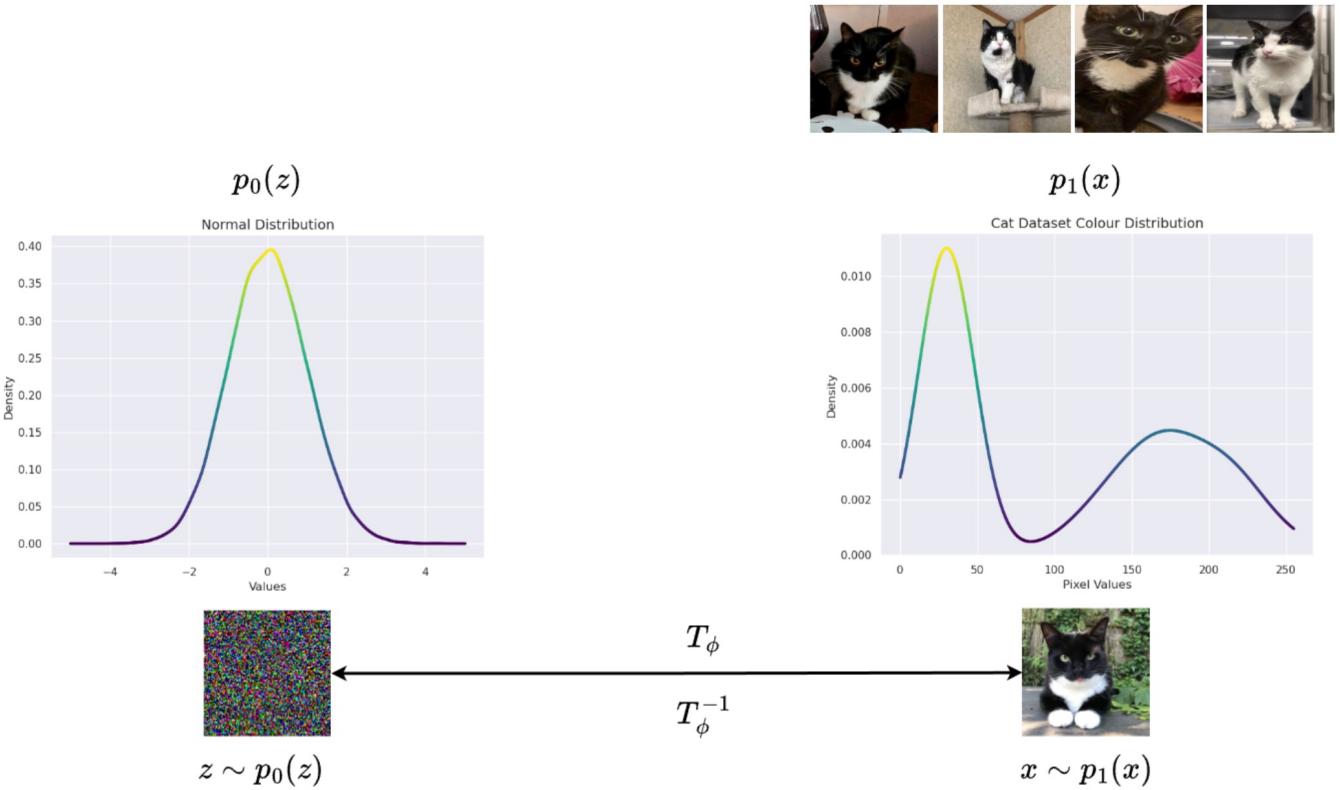
- Conditional Generation:
  - Contrastive Learning (CLIP, CLAP)
  - Latent Diffusion Models (LDMs)
  - Classifier-free guidance (CFG)
- Speeding up the process:
  - Denoising Diffusion Implicit Models (DDIM)
  - Latent Diffusion Models (LDMs)
  - Normalizing Flows (NF), Continuos NF, Flow Matching
- Applications:
  - Text-to-Image Generation: DALL-E, Stable Diffusion, Midjourney
  - Text/Image-to-Video: Sora, Lumiere
  - Text-to-Audio: AudioLDM, a-WaSP, Tango

5. Flow-based Models

Intuition

What we are interested in

- Apply a random transformation to an image until it no longer makes sense.
- Apply the inverse transformation to noise until it starts making sense!



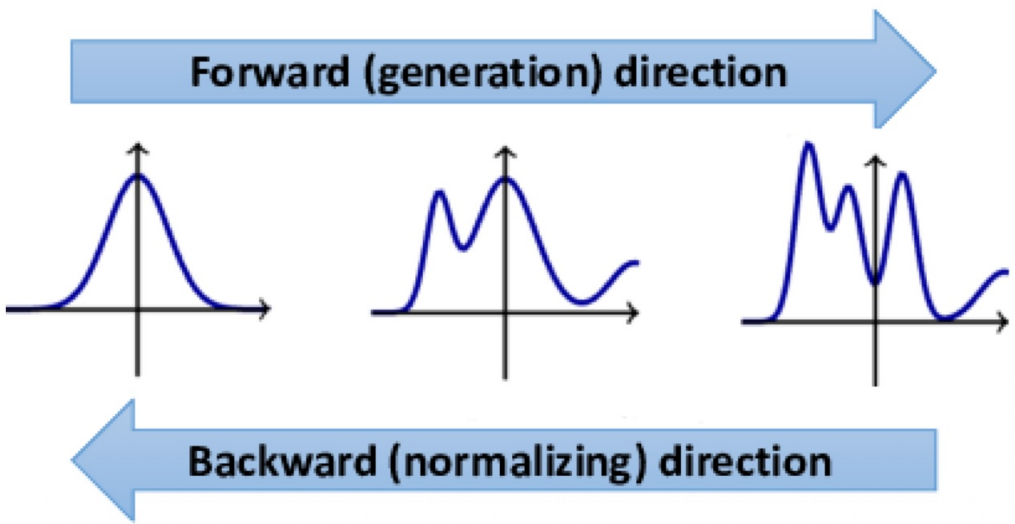
Is a single transformation enough?

Normalizing Flows

- Would you train a Neural Networks with a single layer?
- We can write T_ϕ as a composition of functions:

$$z_0 \xrightarrow{T_{\phi,1}} z_1 \xrightarrow{T_{\phi,2}} \cdots \xrightarrow{T_{\phi,i}} z_i \xrightarrow{T_{\phi,i+1}} \cdots \xrightarrow{T_{\phi,k}} z_k = x$$

with each $T_{\phi,i}$, $i \in [1, k]$ representing a different transformation.



Flow Matching

Linked with Continuous Normalizing Flows

- We can treat each transformation as a *change of state* of the previous one:

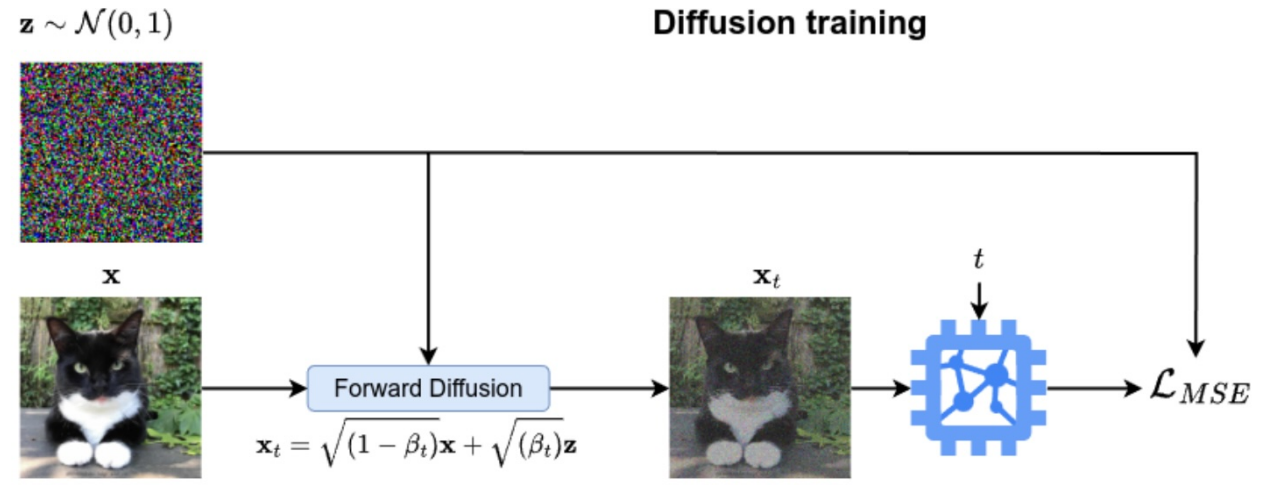
$$z_{k+1} = z_k + r_k(z_k)$$

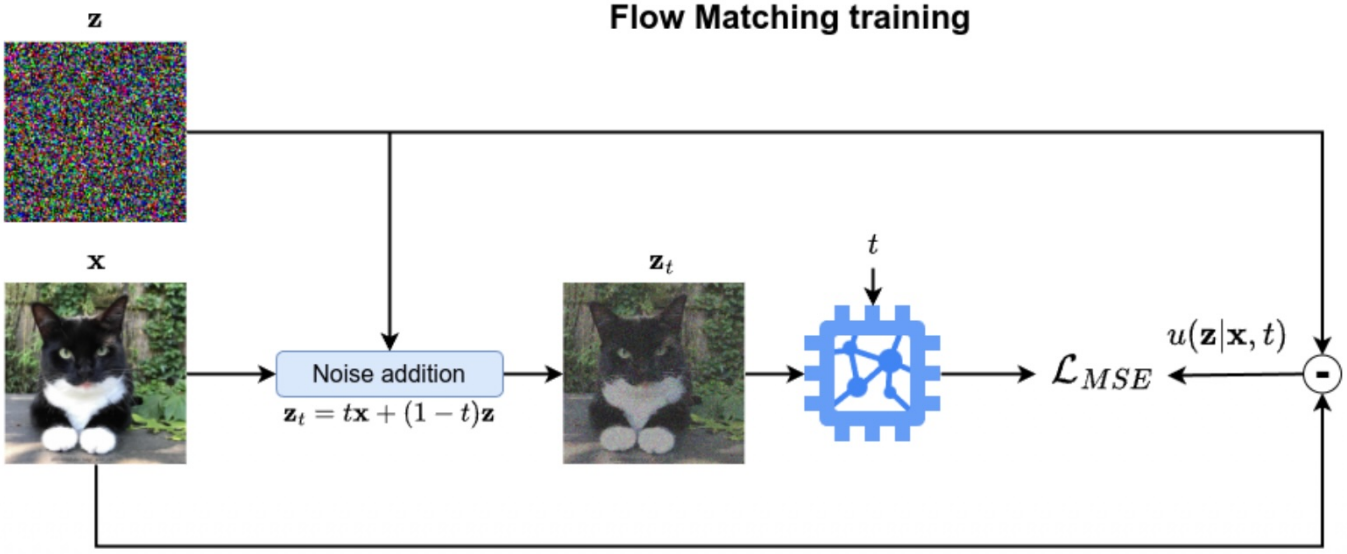
- If we consider $k \to \infty$:

$$\frac{\delta z_t}{\delta t} = r_t(z_t) = u(z_t, \phi, t)$$

- This is very similar to diffusion models...

Let's compare Diffusion and Flow Matching



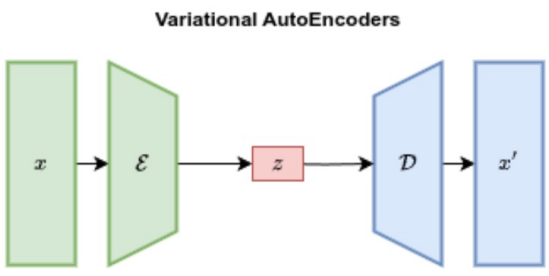


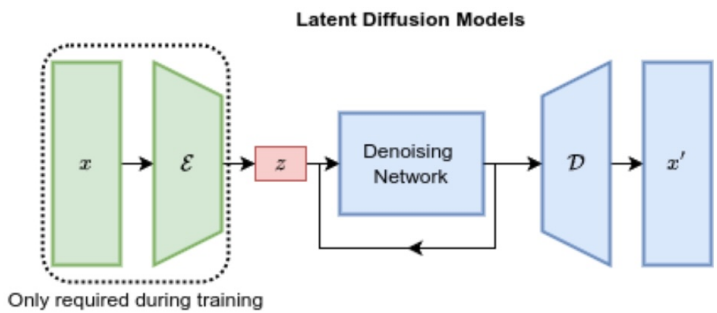
6. Conclusions

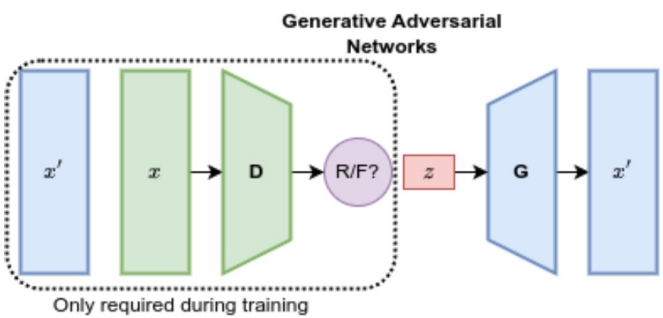
Summary

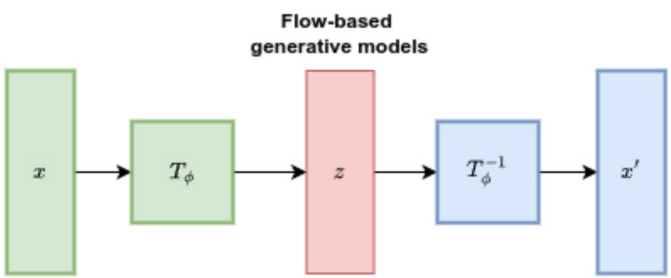
What we did today?

- We explored the theory behind **VAEs**, the adversarial dynamics of **GANs**, and the iterative refinement of **Diffusion Models**.
- We explored the **Generative Trilemma**.









Q&A

End of Course III.