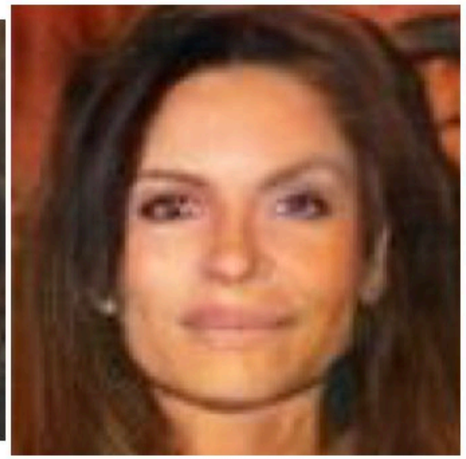
Machine Learning I
MATH60629A

Modern Generative Models
— Week #11

Rapid evolution of (image) generation capability

2014

2015



2016

2017

2018

P(image)

https://twitter.com/goodfellow_ian/status/1084973596236144640/photo/1

Conditional Generation

image

$P(\text{image} \mid \text{text})$

text

A photo of a raccoon
wearing an astronaut helmet,
looking out of the window at night.

https://imagen.research.google/

Why generate images?

- Scientific challenge (difficult question)
- To use wherever images are used (visualizations, video games, presentations, ads, etc.)
- Human-in-the-loop design

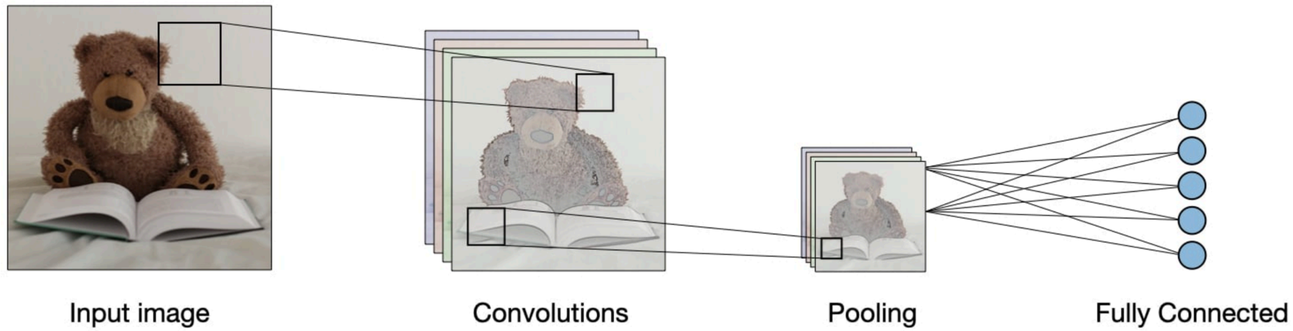
Today’s Plan*

- “Predict” an image
- Generative Models
  - Images (P(x)):
    - Frameworks: Variational auto-encoders (VAEs), Generative Adversarial Networks (GANs)
  - Images conditioned on text (P(x | y)) :
    - Dall-E 2, Imagen

* Slides are mostly from David Berger

Convolution Neural Network (CNN) — Recall

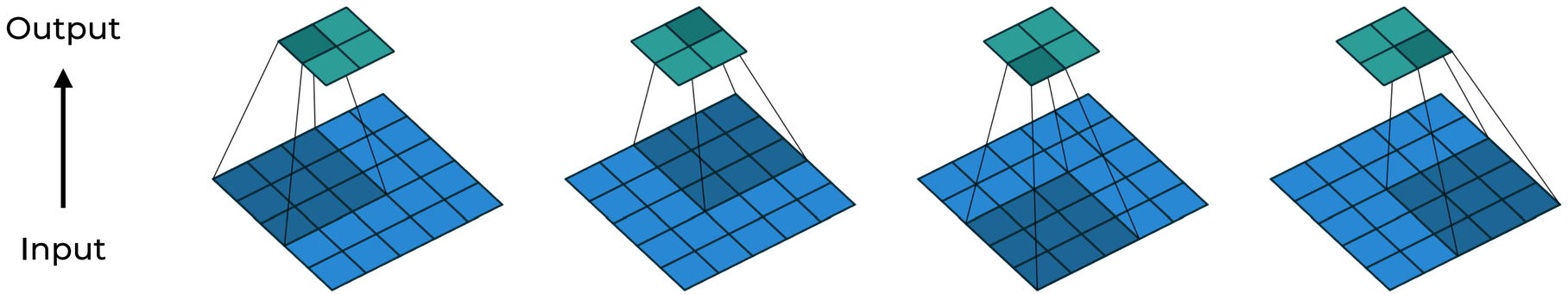
- Séries of layers (blocs): convolutions + pooling
  - Each layer reduces the dimensionality of the representation



 https://stanford.edu/~shervine/teaching/cs-230/cheatsheet-convolutional-neural-networks

Convolution

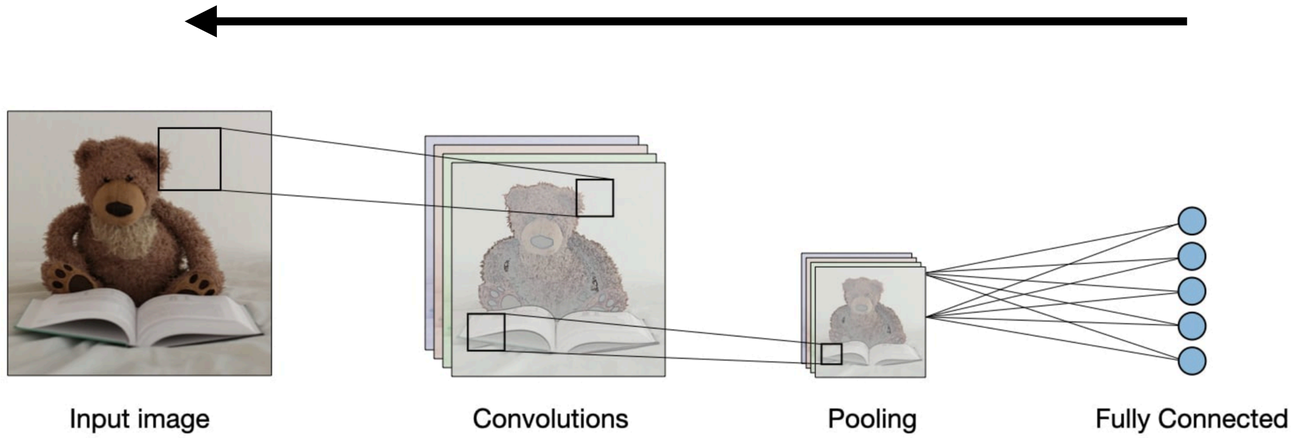
- **Input: 5 x 5**
- **Filter (kernel): 3 x 3. Stride 2.**
- **Output: 2 x 2**



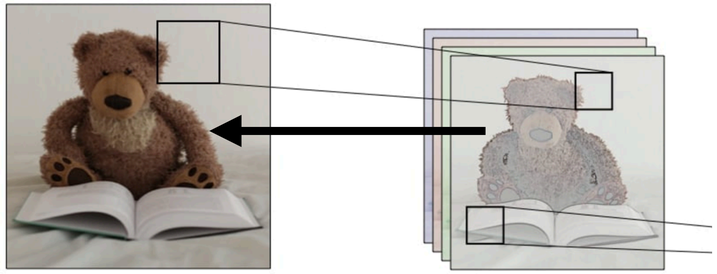
https://arxiv.org/pdf/1603.07285

“Reverse” a convolution network

- Each layers increases the dimensionality of the incoming representation



- (Note: this is in fact the same operation as done by backdrop in a CNN.)

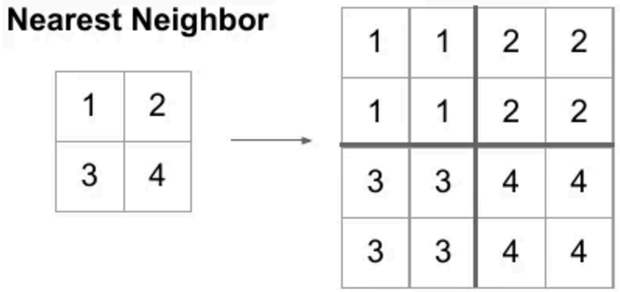


Input image

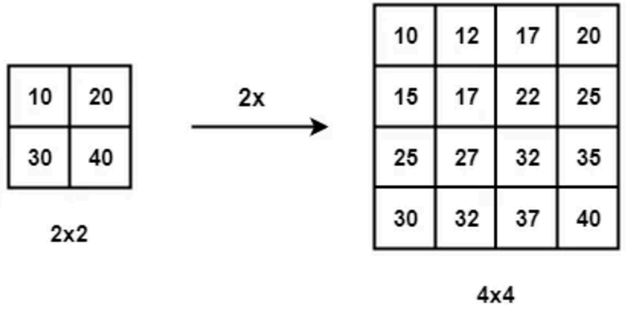
Convolutions

Interpolation

1. Repetition



2. (Bi-)linear interpolation

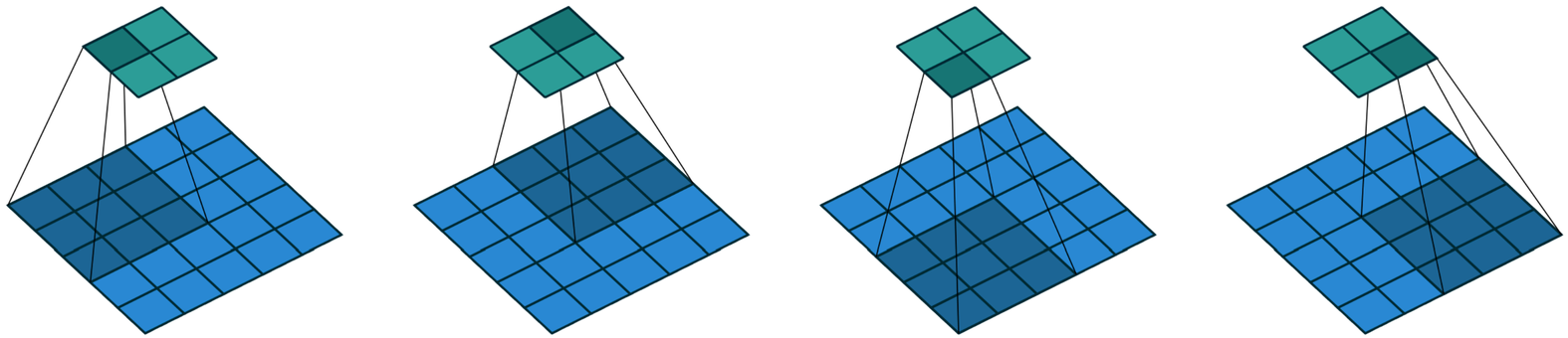


- No parameters to learn

Transposed Convolution

- Useful to generate images or increase the resolution of an image (like in movies)
- Input: 2 x 2
- Filter: 3 x 3. Stride 1.
- Output: 3 x 3

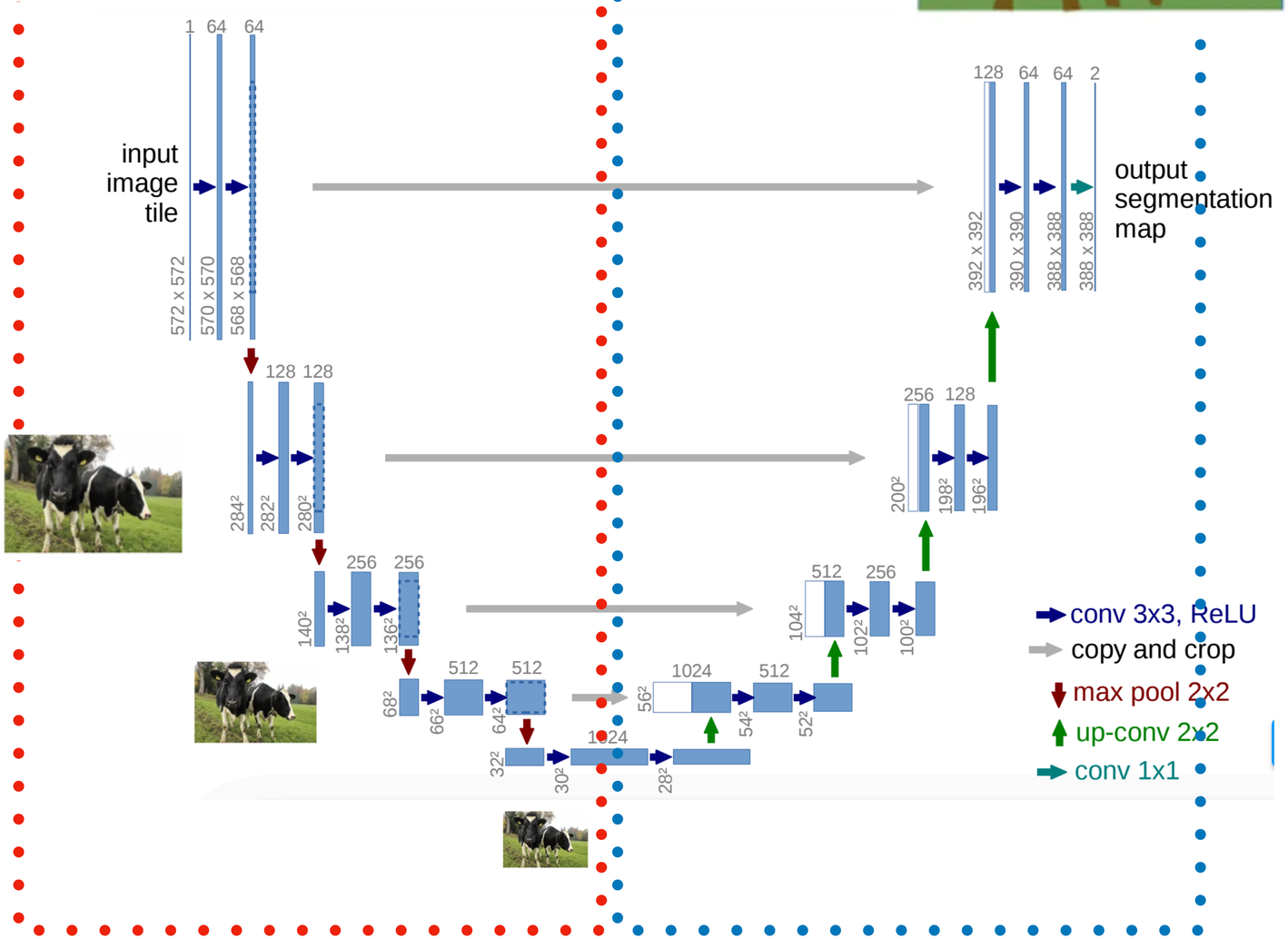
Input



Output

- If we write down a convolution as a matrix operation (by vectorizing the image), then the reverse operation is multiplying by the transpose (hence the name)

U-Nets



- Encoder-Decoder Architecture
  - Encoder: Obtain a representation of the image (classic CNN without the classification output)
  - Decoder: From the representation, obtain an image
  - Connections between the encoder and decoder allow for precise localization
- up-conv ->transposed convolution (for example)
- Proposed for segmentation
- Has become standard for image generation

U-Nets: https://arxiv.org/pdf/1505.04597

https://wiki.cloudfactory.com/docs/mp-wiki/key-principles-of-computer-vision/upsampling-and-downsampling-techniques-in-machine-learning

Generative models

- A U-Net can obtain a representation from an image, but it does not have a probabilistic interpretation
- A generative model is a method for parametrizing $P(x)$ — unsupervised

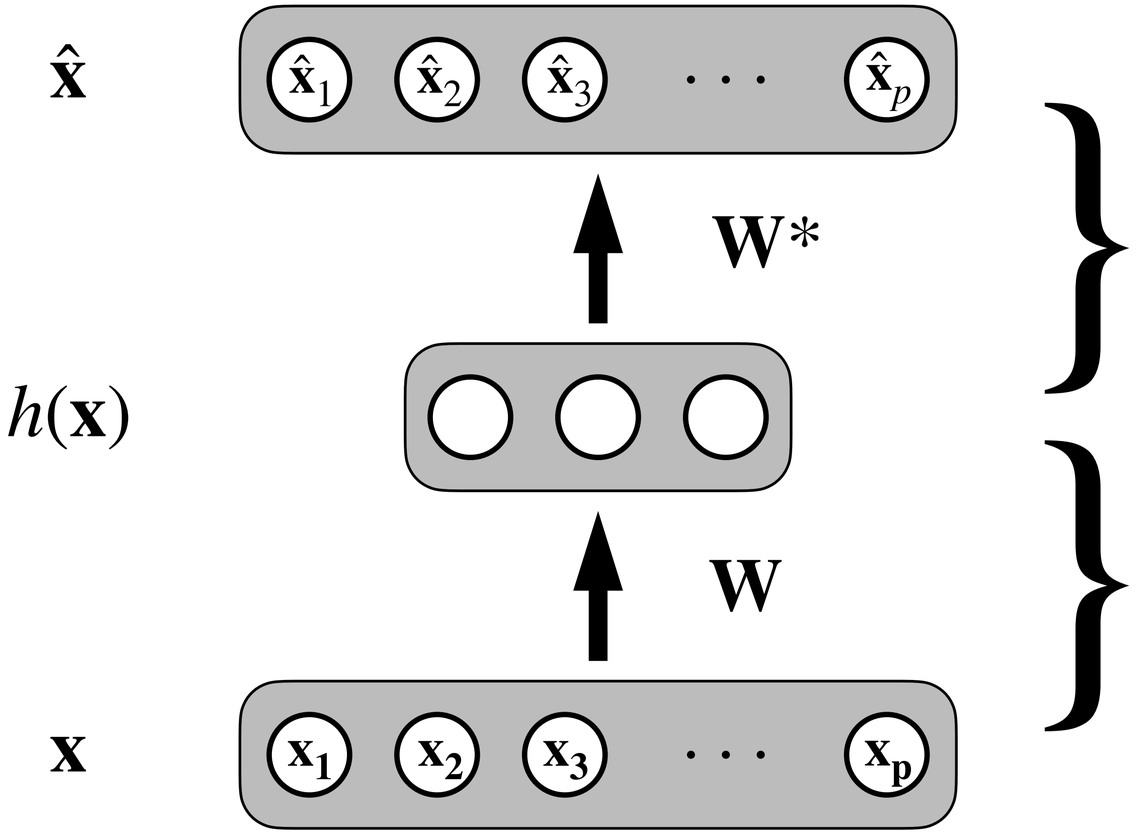
Why are generative models (often) probabilistic?

- Allows different types of evaluation
  - For example, the probability of an image according to the model: $P_\theta(x_{\text{new}})$
- Can obtain samples $x \sim P_\theta(x)$
- Quantifies uncertainty
- It has been popular recently to parametrize distributions with neural networks (think of a softmax layer) — these are not always proper generative models

Auto-Encoder (AE)

Auto-encoder - Recall

For an AE with a single hidden layer:



Decoder

$$\hat{\mathbf{x}} = o(\hat{\mathbf{a}}(\mathbf{x})) = o(\mathbf{W}^* h(\mathbf{x}) + \mathbf{b}^*)$$

Encoder

$$h(\mathbf{x}) = g(\mathbf{a}(\mathbf{x})) = g(\mathbf{W}\mathbf{x} + \mathbf{b})$$

Variational Auto-encoder (VAE)

* Understanding these models precisely requires concepts that are beyond our class. Here, we aim for familiarization with the terms and an intuitive understanding.

Variational Auto-Encoder - Motivation

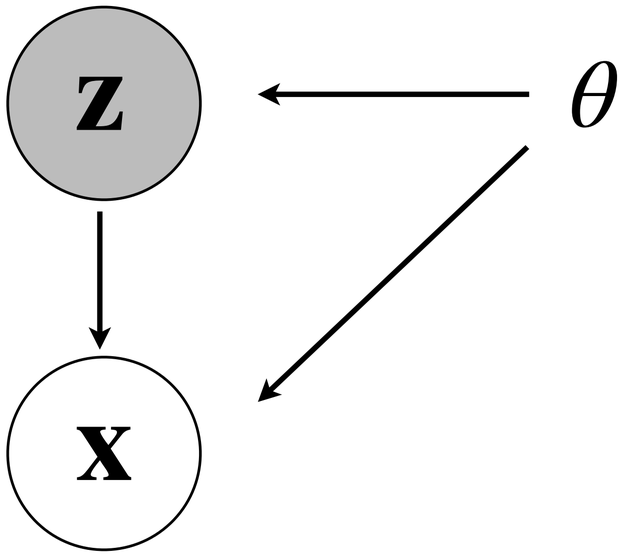
Idea:

- The data are generated conditioned on a random variable (Z):

$$\mathbb{P}_\theta\left(\mathbf{x} \mid \mathbf{z}\right)$$

You can think of Z has an embedding.
VAEs will learn a prior P(z) and
a posterior P(z|x) over it.

Graphical representation



Question:

- How do we learn such a distribution?

Variational Auto-Encoder - Motivation

Partial answer:

- A “good” model should maximize the likelihood of the data P(x)
- Bayes, provides us with two possibilities:

$$\mathbb{P}_\theta(\mathbf{x}) = \int_{\mathbf{z}} \mathbb{P}_\theta(\mathbf{z} \mid \mathbf{x}) \mathbb{P}_\theta(\mathbf{x}) d\mathbf{z}$$

$$\mathbb{P}_\theta(\mathbf{x}) = \int_{\mathbf{z}} \mathbb{P}_\theta(\mathbf{x} \mid \mathbf{z}) \mathbb{P}_\theta(\mathbf{z}) d\mathbf{z}$$

Problem:

- The posterior can be intractable.
- The integral is intractable.

Variational Auto-Encoder - Motivation

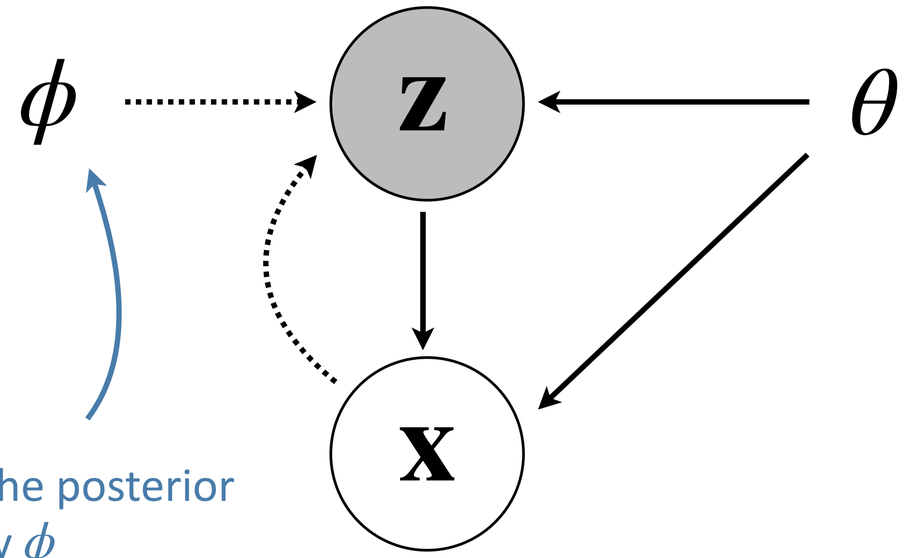
Let’s explore the first problem:

- The posterior can be intractable:

$$\mathbb{P}_\theta(\mathbf{x}) = \int_{\mathbf{z}} \mathbb{P}_\theta(\mathbf{z} \mid \mathbf{x}) \mathbb{P}_\theta(\mathbf{x}) d\mathbf{z}$$

Idea:

- We could approximate the real posterior to make it tractable



The approximation of the posterior would be parametric by ϕ

Variational Auto-Encoder - Formalism

We can obtain a bound on the log-likelihood of $\mathbf{x}$:

$$\log p_\theta(\mathbf{x}) \geq -\mathrm{KL}\{q_\phi(\mathbf{z} \mid \mathbf{x}) \mid\mid q_\phi(\mathbf{z})\} + \log p_\theta(\mathbf{x} \mid \mathbf{z}),$$

Where:

- We're trying to the distance between the posterior $q_\phi(\mathbf{z} \mid \mathbf{x})$ and the prior $q_\phi(\mathbf{z})$.
- While maximizing the conditional log-likelihood of $\mathbf{x}$.

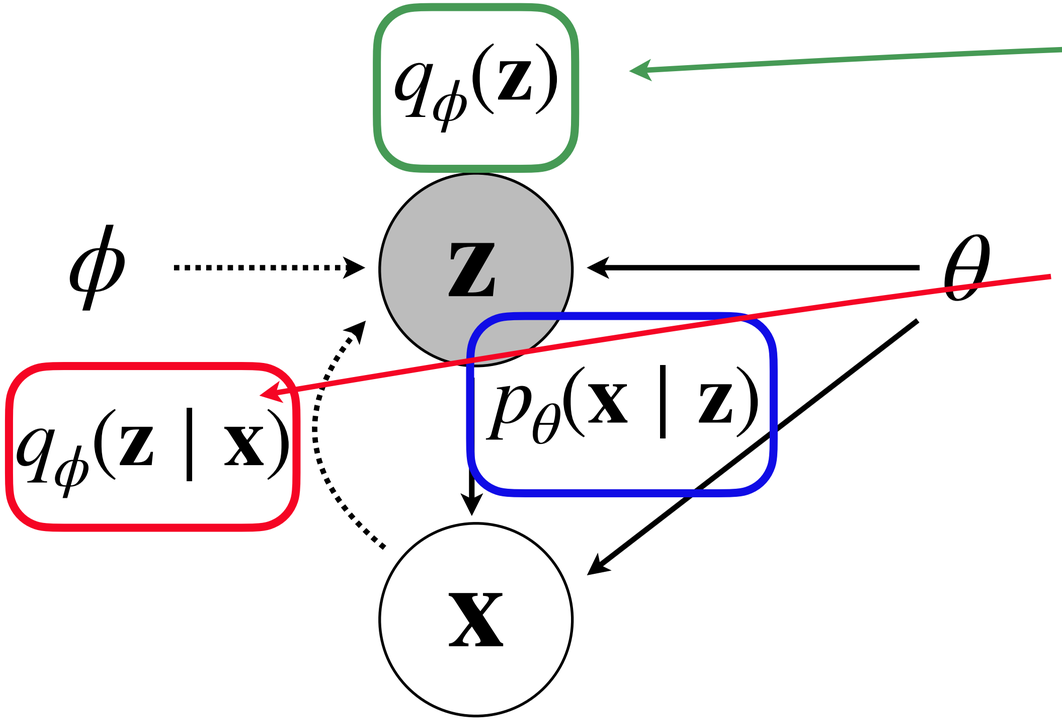
Question:

- How do we do this in practice?

Variational Auto-Encoder - Formalism

$$\log p_\theta(\mathbf{x}) \geq -\mathrm{KL}\{q_\phi(\mathbf{z} \mid \mathbf{x}) \,||\, q_\phi(\mathbf{z})\} + \log p_\theta(\mathbf{x} \mid \mathbf{z}),$$

Graphical view:



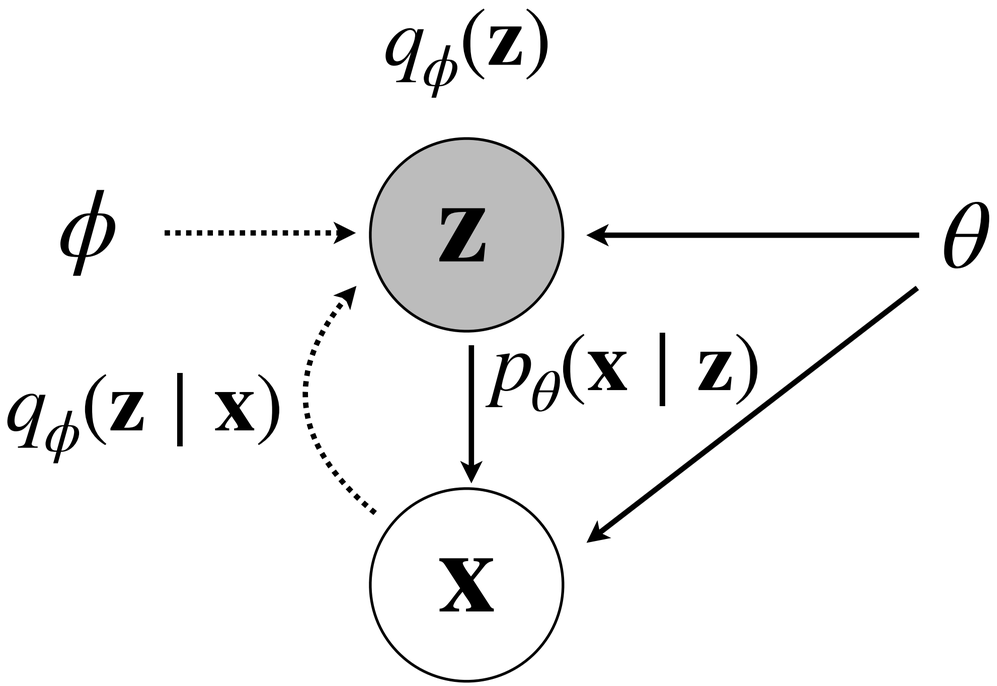
We suppose the prior follows a particular distribution

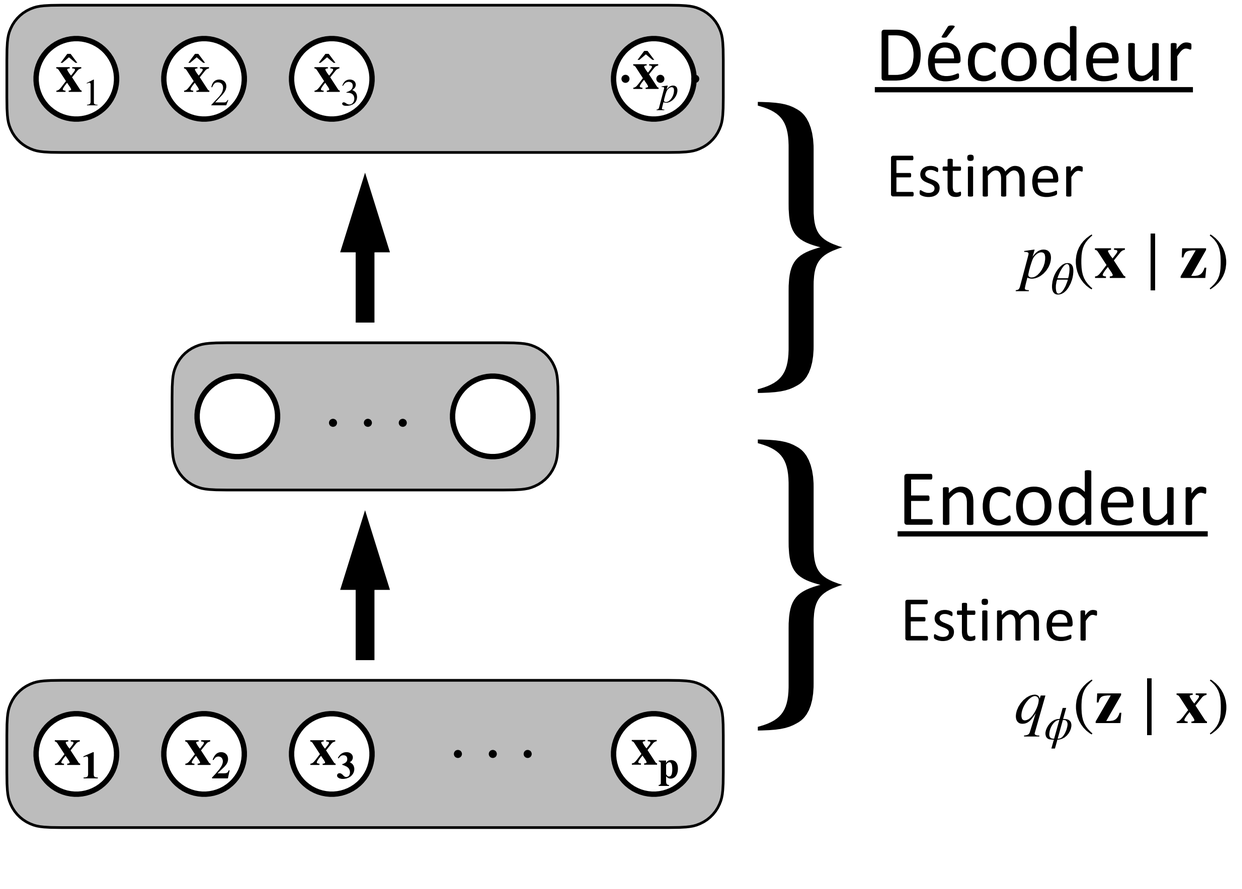
(e.g., a zero-mean Gaussian)

We suppose the posterior follows an unknown distribution parametrizes by a neural network

Variational Auto-encoders

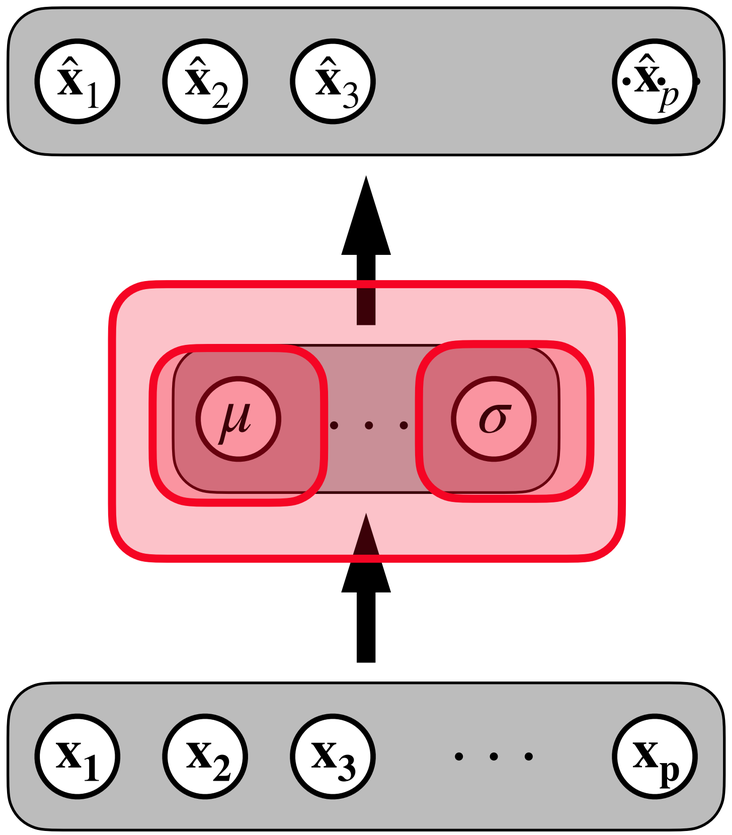
We can estimate these parameters using an auto encoder:





Variational Auto-encoders

Reparametrize the hidden layer:



Decode

Estimate $p_\theta(\mathbf{x} \mid \mathbf{z})$

Encoder

Estimate $q_\phi(\mathbf{z} \mid \mathbf{x})$

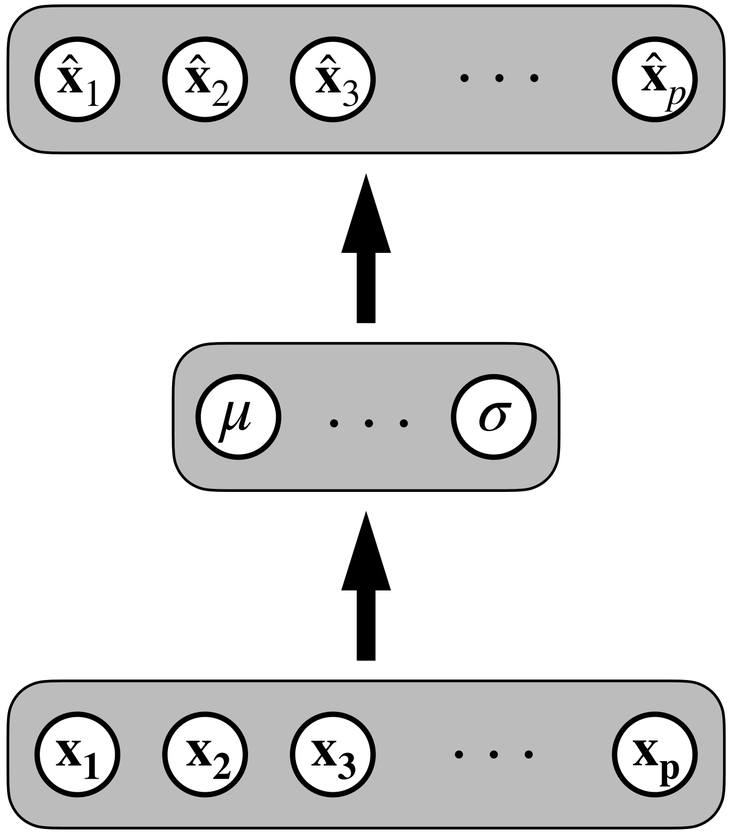
Suppose that $q_\phi(\mathbf{z} \mid \mathbf{x}) \sim \mathcal{N}(\mu, \sigma^2)$.

Then we can write $z = \mu + \sigma\epsilon$ où $\epsilon \sim \mathcal{N}(0,1)$.

Now, learning means estimating parameters μ et σ!

Variational Auto-encoders

VAEs are a way to train a generative model



Decoder

Estimate

$$p_\theta(\mathbf{x} \mid \mathbf{z})$$

Encoder

Estimate

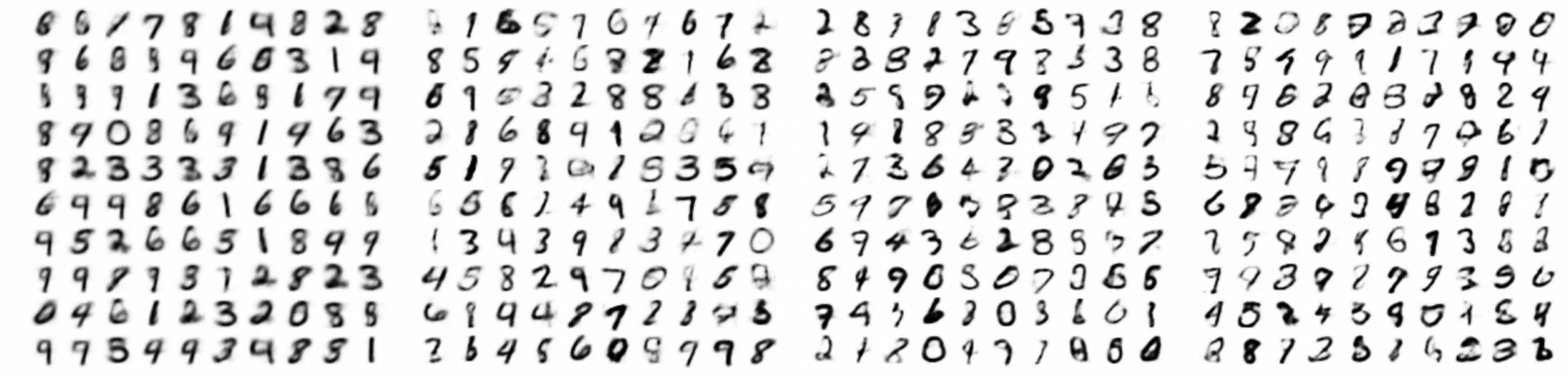
$$q_\phi(\mathbf{z} \mid \mathbf{x})$$

Steps:

1. Train the model to learn:
   - $p_\theta(\mathbf{x} \mid \mathbf{z})$
   - $q_\phi(\mathbf{z} \mid \mathbf{x}) \sim \mathcal{N}(\mu, \sigma^2)$
2. Generate ϵ et obtain $z \sim P(z)$.
3. Obtain $\mathbf{x}$ from $p_\theta(\mathbf{x} \mid \mathbf{z})$.

Variational Auto-encoders

Example: Generating numbers (range 0—9)



Multivariate Normal ($\mathbb{R}^2$)

Multivariate Normal ($\mathbb{R}^5$)

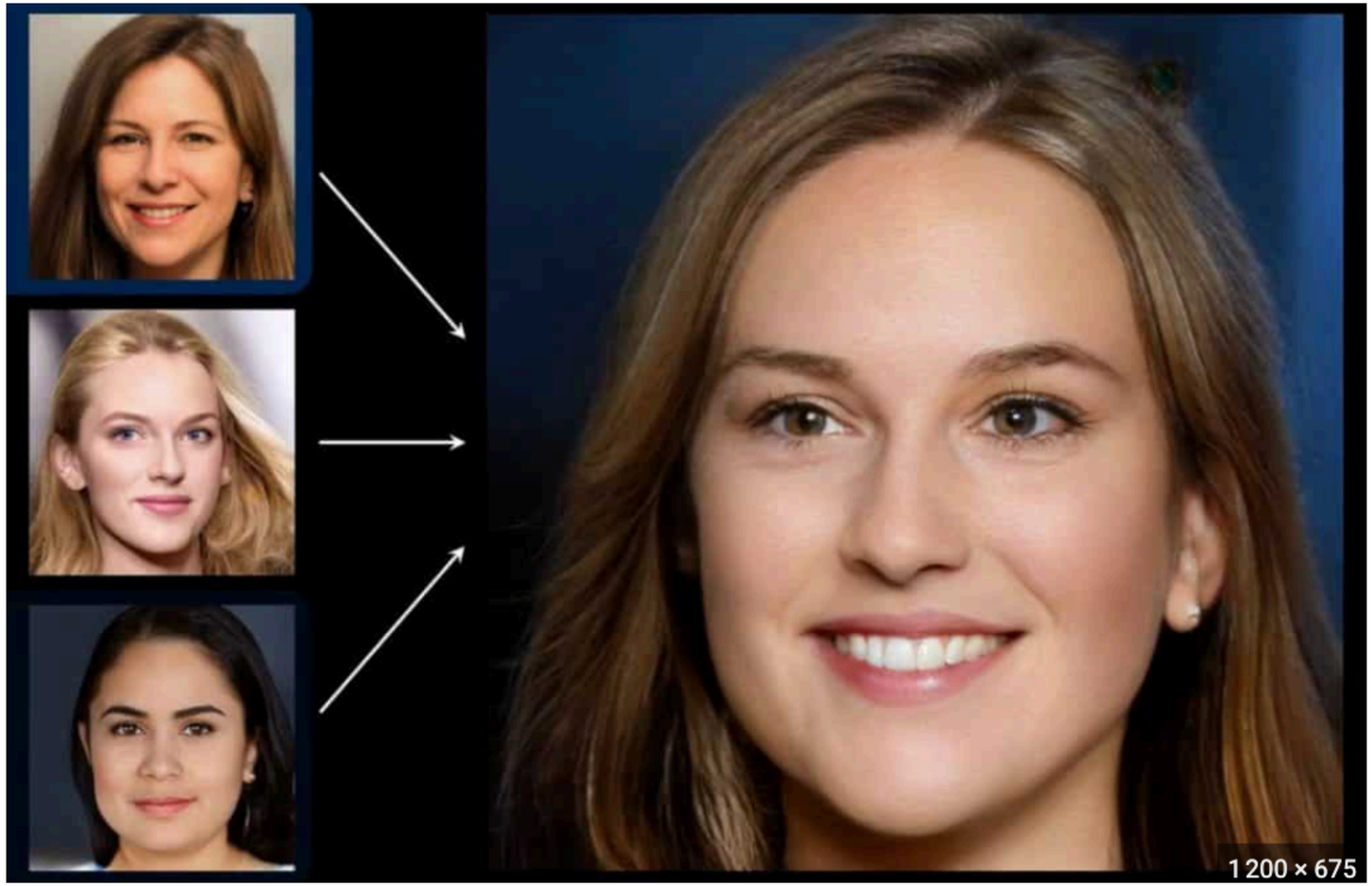
Multivariate Normal ($\mathbb{R}^{10}$)

Multivariate Normal ($\mathbb{R}^{20}$)

Generative Adversarial Networks (GANs)

GANs - Introduction

Well-known for image generation



Historical note

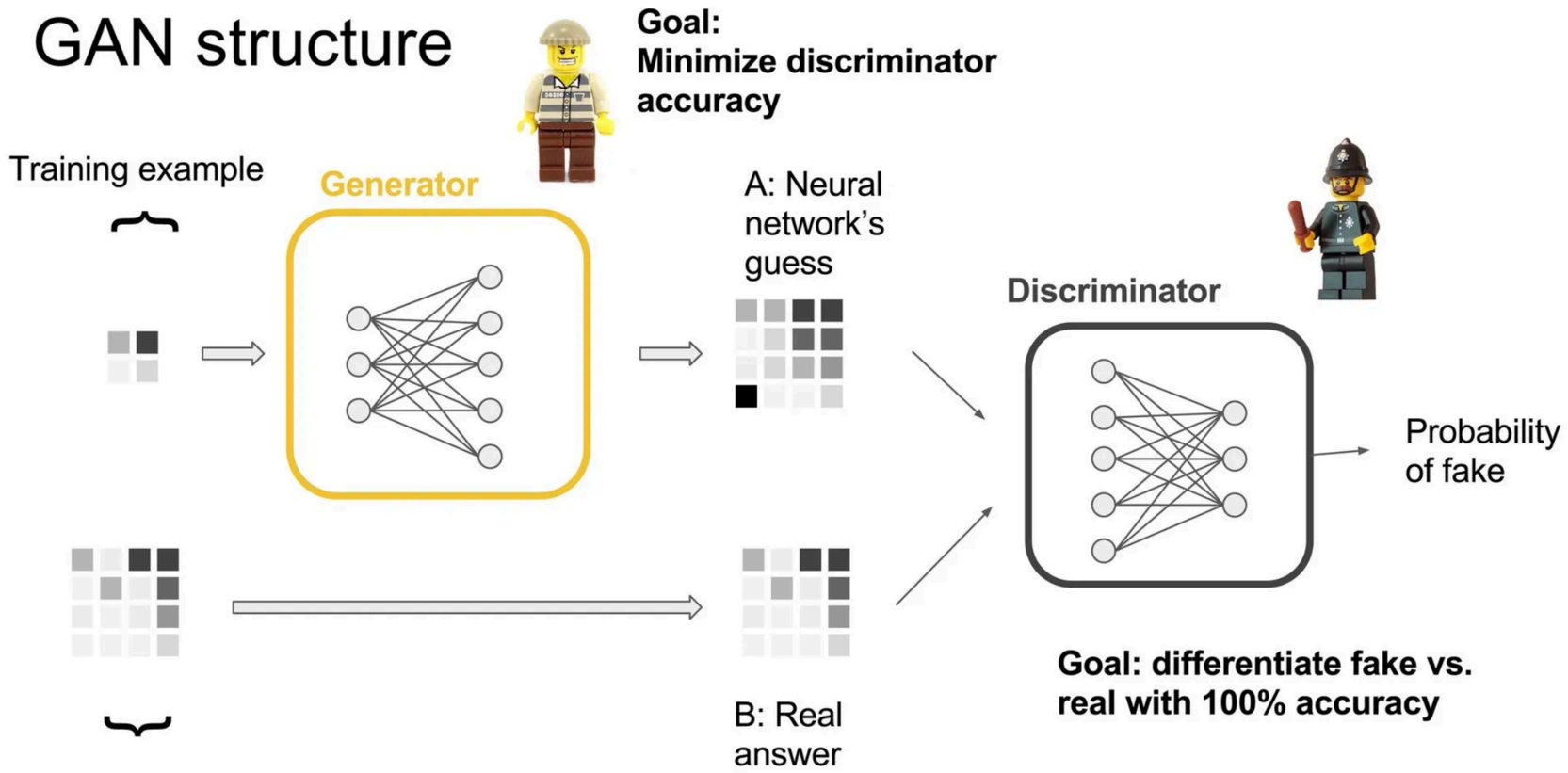
- Framework for learning a generative model (for example, an “inverted” CNN)
- Developed by researchers at Université de Montréal (2014)
- The first to generate high-quality complex images
- Have been (mostly?) replaced by diffusion models
  - The study of GANs has provided insights into 2-player (min-max) optimization

GANs — Intuition

- Two neural networks (players a game)
  - Generator: The first player. It learns to generate a (good) image
  - Discriminator: The second player, learns to recognize (discriminate) good images from bad images
- The game (at each round):
  - The second player receives an image. It must determine whether the image comes from the generator or from the training data
    - Depending on the response, the players update (their weights)

GANS — Introduction

Visually:



GANs - formalism

$$\boldsymbol{x} \sim \mathbb{P}_r$$

Data

GANs - objectives

GANs have two objectives (one for each player)

- The output of D is “1” for real and “0" for fake.

Objective of the discriminator

$$\max_D \mathop{\mathbb{E}}_{\boldsymbol{x}\sim\mathbb{P}_r}[\log(D(\boldsymbol{x}))] + \mathop{\mathbb{E}}_{\tilde{\boldsymbol{x}}\sim\mathbb{P}_g}[\log(1 - D(\tilde{\boldsymbol{x}}))].$$

Objective of the generator

$$\max_G \mathop{\mathbb{E}}_{\tilde{\boldsymbol{x}}\sim\mathbb{P}_g}[\log(D(\tilde{\boldsymbol{x}}))].$$

where:

$\mathbb{P}_r$ Is the distribution that “generates” the real data

$\mathbb{P}_g$ Is the distribution generating data

$\tilde{\boldsymbol{x}} = G(\boldsymbol{z}), \quad \boldsymbol{z} \sim p(\boldsymbol{z})$ Where z follows a normal (e.g.)

GANs - formalism

The game is framed as a two players game between the discriminator and the generator

$$\min_G \max_D \mathop{\mathbb{E}}_{\boldsymbol{x}\sim\mathbb{P}_r}[\log(D(\boldsymbol{x}))] + \mathop{\mathbb{E}}_{\tilde{\boldsymbol{x}}\sim\mathbb{P}_g}[\log(1 - D(\tilde{\boldsymbol{x}}))].$$

where:

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Training GANs in practice alternates between training D and G

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**

  for k steps **do**

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
  - Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right) \right].$$

  end for

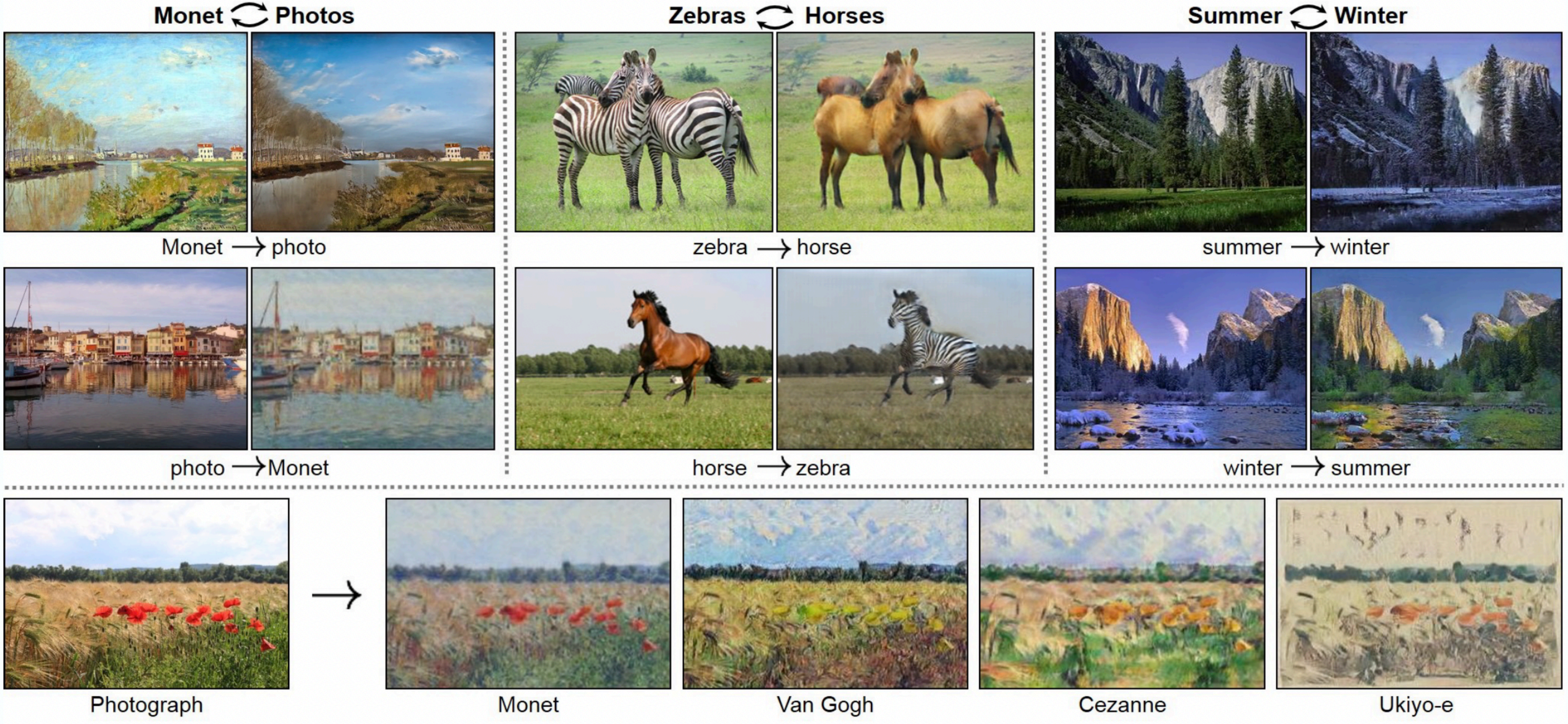
  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

end for

The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

GANs - Varia


Monet ⇄ Photos
Zebras ⇄ Horses
Summer ⇄ Winter
Monet → photo
zebra → horse
summer → winter
photo → Monet
horse → zebra
winter → summer
Photograph
Monet
Van Gogh
Cezanne
Ukiyo-e

DALL-E 2
(As an example of using a diffusion model)

https://arxiv.org/pdf/2204.06125v1

DALL-E

an espresso machine that makes coffee from human souls, artstation

panda mad scientist mixing sparkling chemicals, artstation

a corgi's head depicted as an explosion of a nebula

a dolphin in an astronaut suit on saturn, artstation

a propaganda poster depicting a cat dressed as french emperor napoleon holding a piece of cheese

a teddy bear on a skateboard in times square

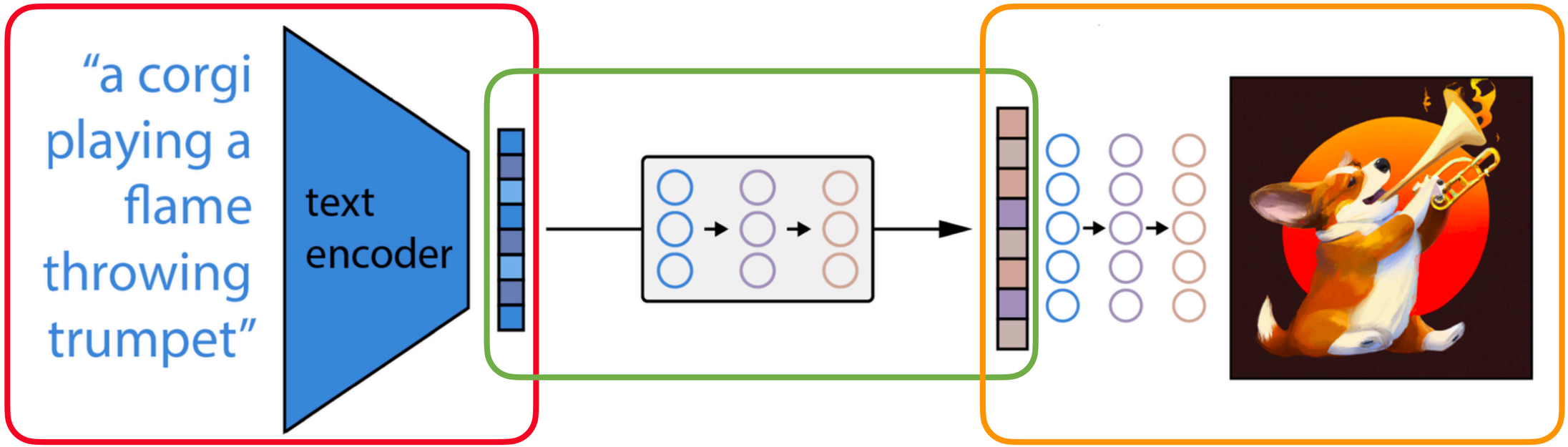
DALL-E - Overview

"a corgi playing a flame throwing trumpet"

1. Input, a sentence (*prompt*) of the image we want to create
2. This prompt is encoded in a (latent) representation
3. Transform this representation in an image representation (image space) — not shown
4. Decode the image representation into an actual image

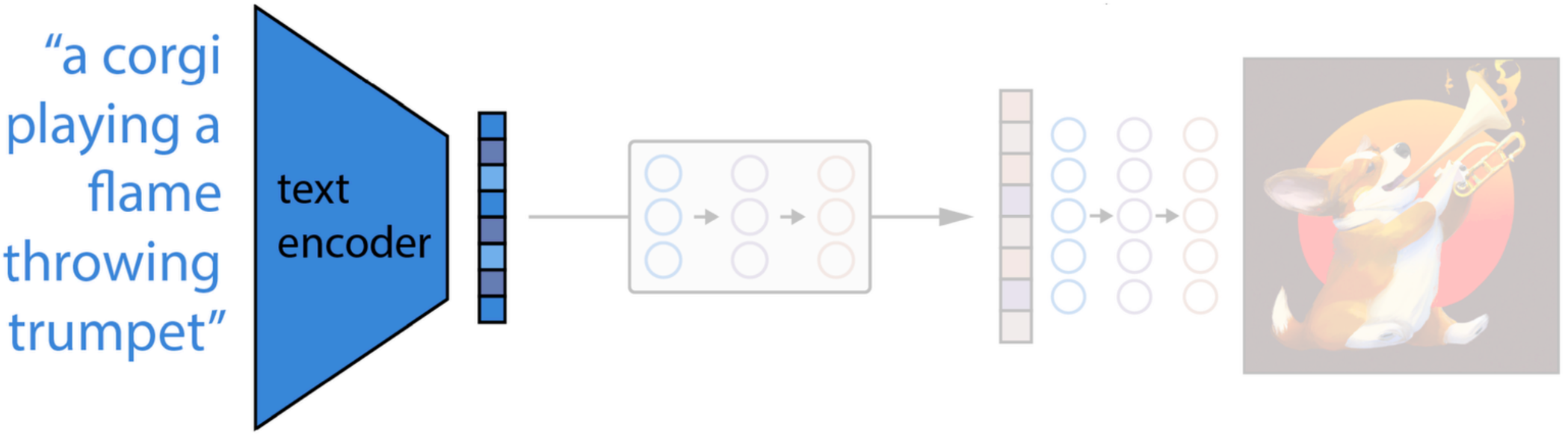
DALL-E - Overview

Each step uses specific techniques:

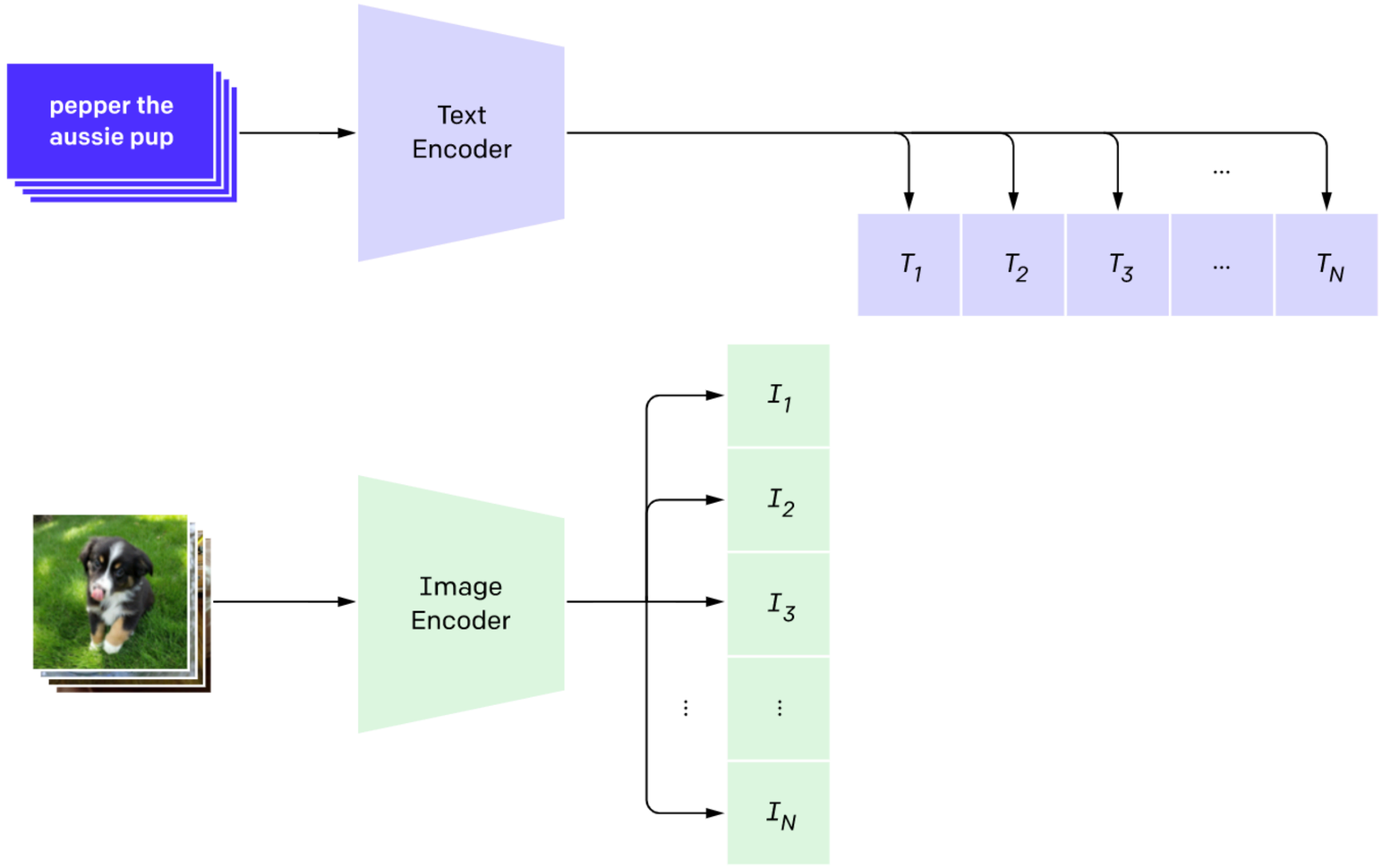


1. Contrastive Language-Image Pre-training (CLIP)
2. Generation of an image using a diffusion model
3. Learn the latent representations of text and images
4. Wrap-it up!

DALL-E - CLIP

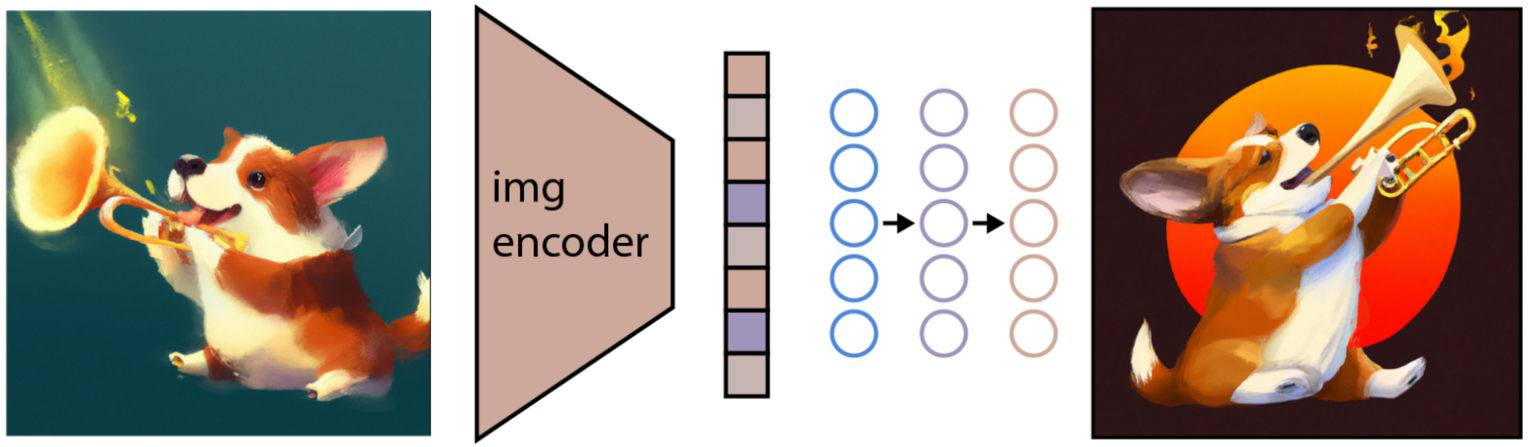


DALL-E - CLIP



1. Learn latent representations of text T_i and images I_i
   - From a batch of size N
2. Similarity measure
   - $\max T_i I_i$
3. Dissimilarity measure
   - $\min T_i I_j \quad \forall j \neq i$
4. Maximize the similarities and minimize the dissimilarities

DALL-E - Diffusion Models



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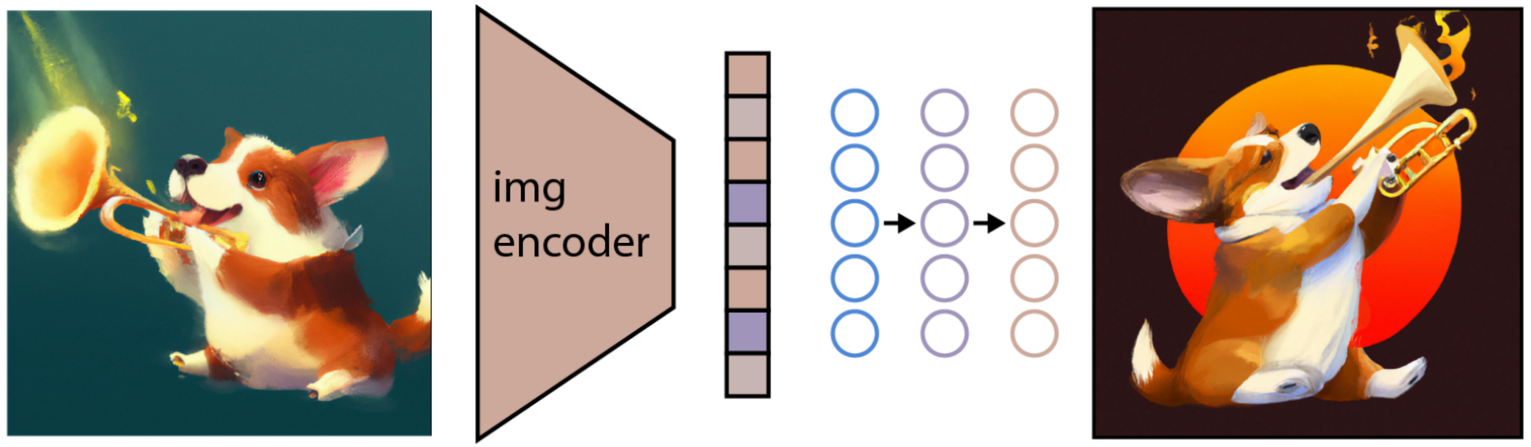
DALL-E - Diffusion Model

Idea:

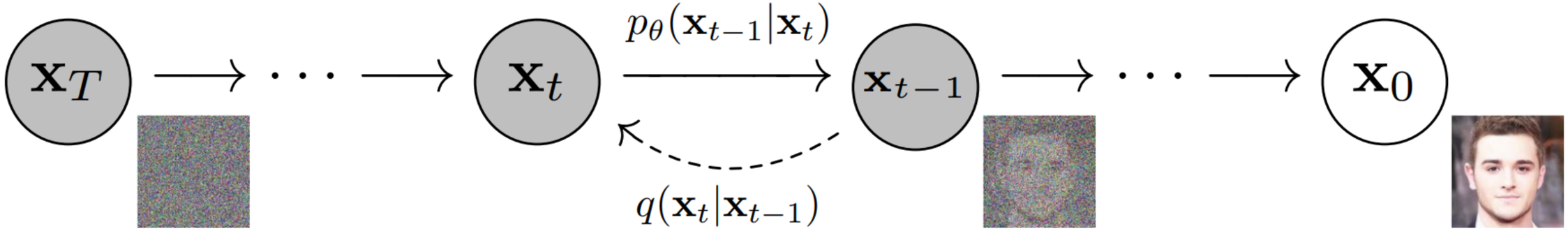
- From an image (left), generate other similar ones
- This is where diffusion models are used



Diffusion Models

Idea:

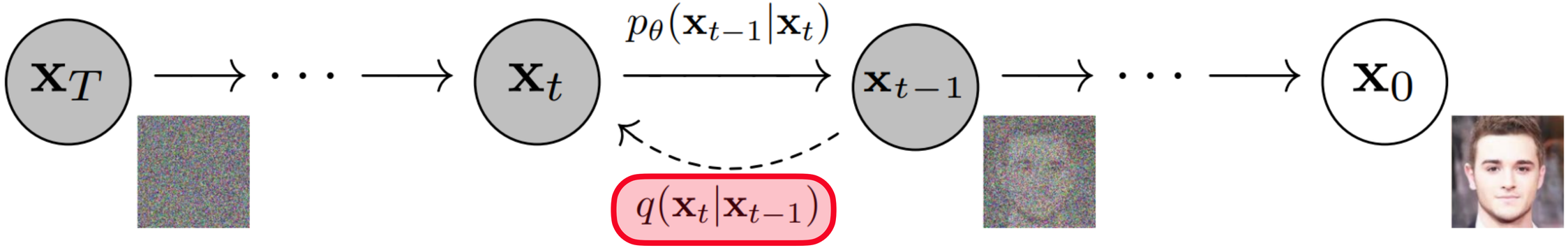
- Add noise incrementally to an image until it is pure white noise
- Denoise the image to obtain the original image
- If we know the noise mechanism, starting from white noise, we can then generate an image

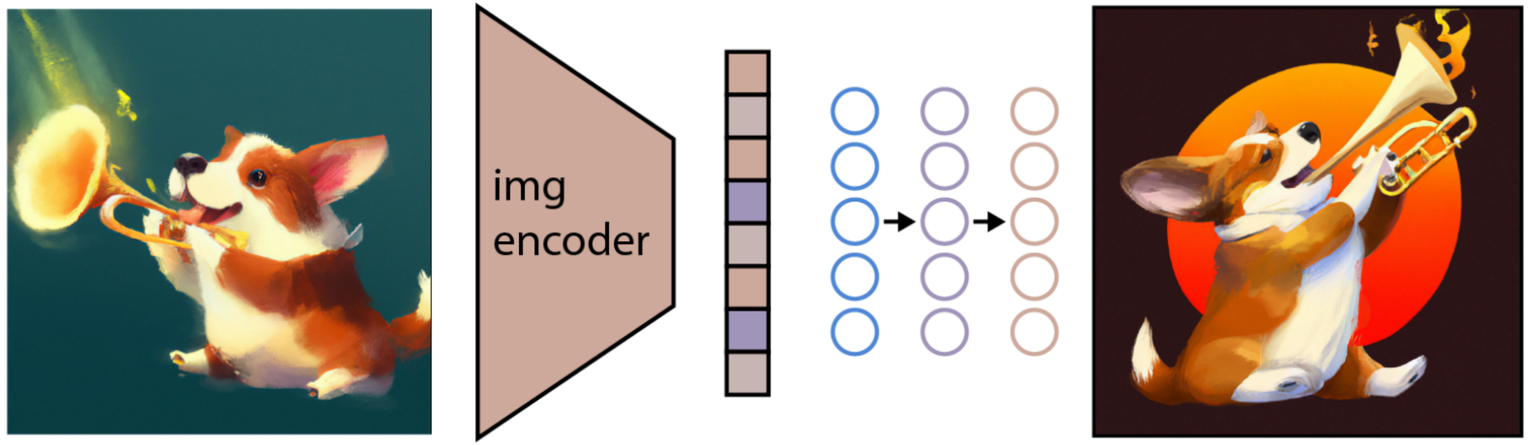


DALL-E - Diffusion Model

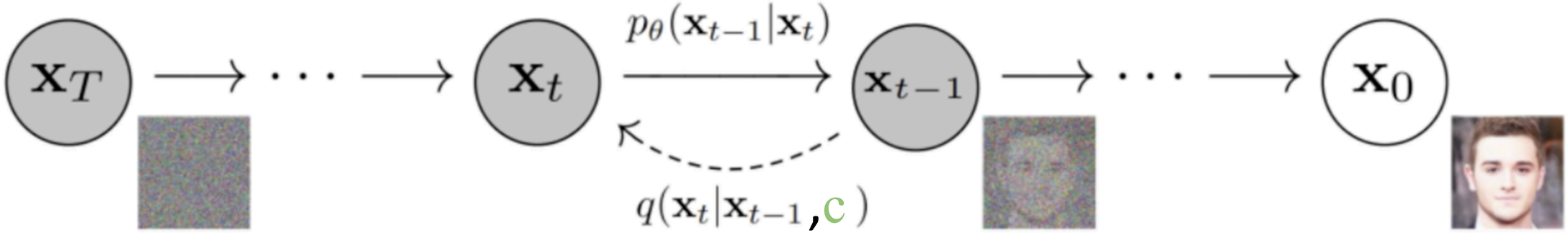
For text-to-image generation, we add information from the text

During the diffusion process





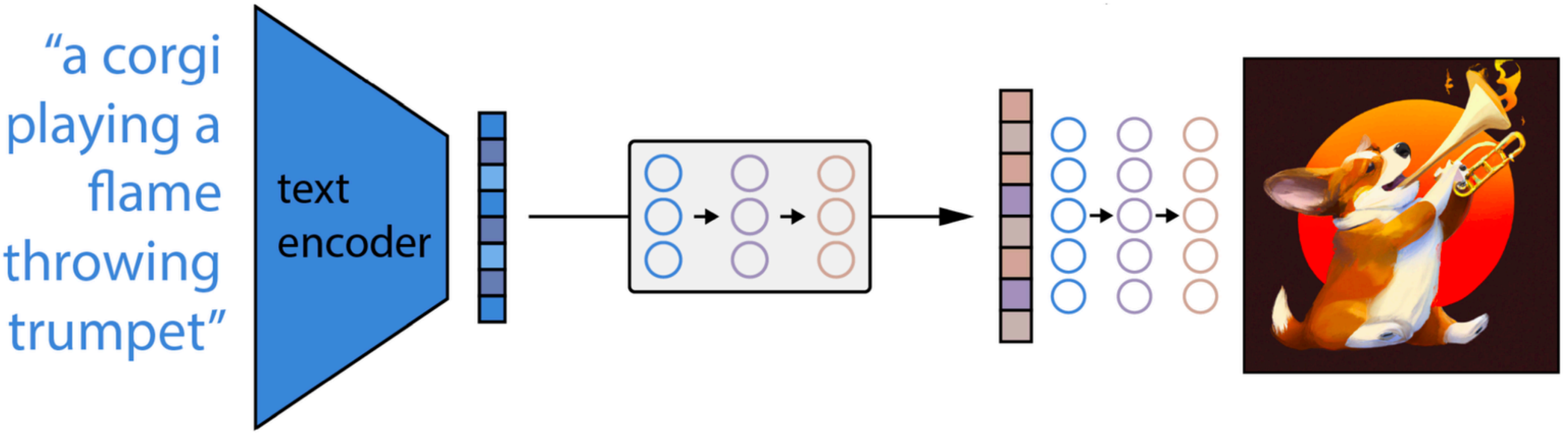
DALL-E



We use the text representation to condition the model

“Face face of a man with red hair”

DALL-E - Wrap-it up!



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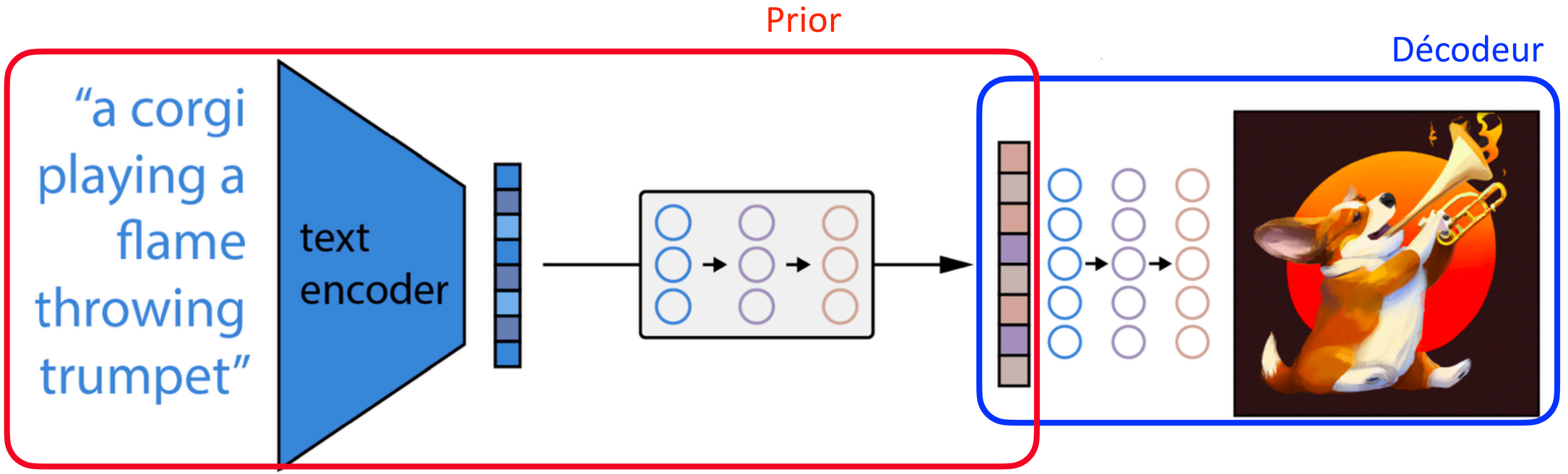
4. Wrap-it up!

DALL-E - Wrap-it up!



Idea:

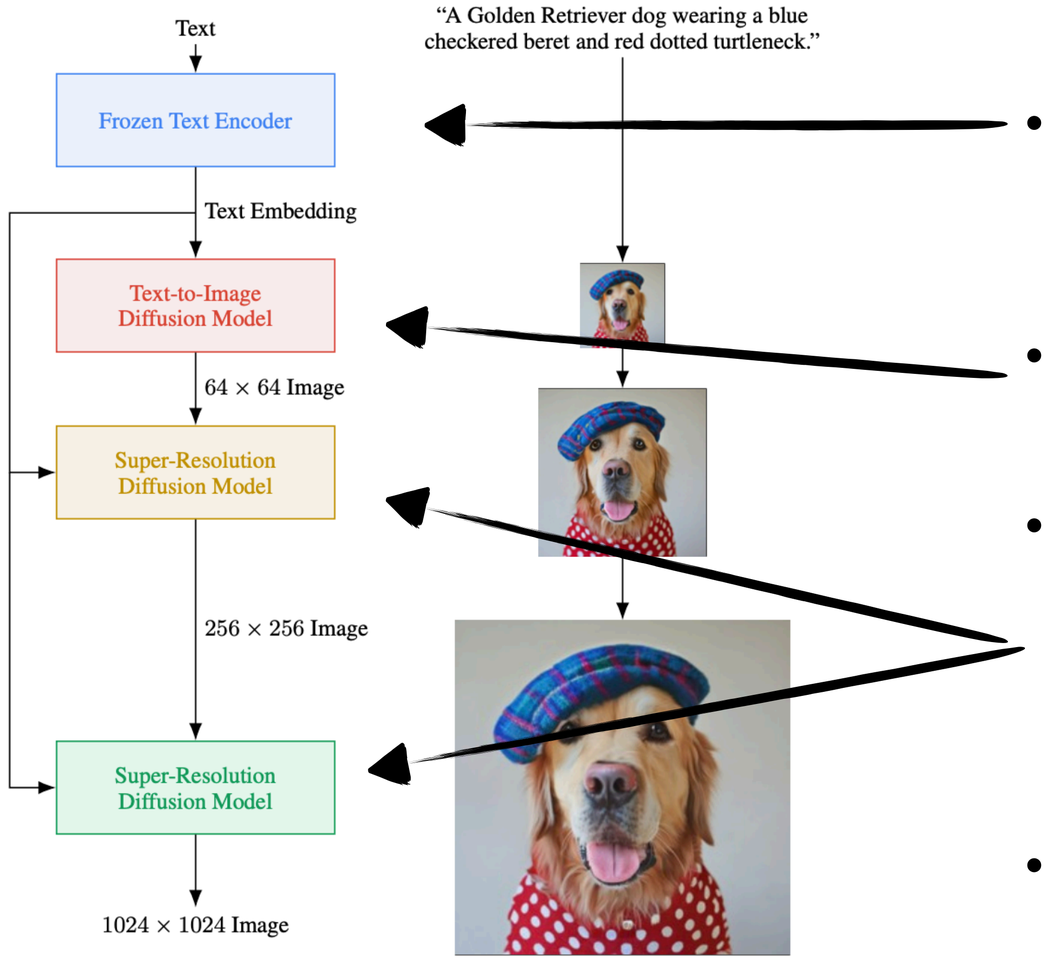
- Given (*x, y*) a tuple of an image *x* and text *y*.
- Given the representation of an image z.
- The distribution of the image given the text is:

$$P(x|y) = P(x, z_i|y) = P(x|z_i, y)P(z_i|y)$$

Imagen

https://imagen.research.google/

Architecture



- Uses a fixed and pertained encoder

  For example a transformer learned from a large-scale text dataset to predict the next word. **No image!**

- *Followed by a diffusion model to obtain a first image*
- Followed by a few other diffusion models to obtain images of higher and higher resolution
  - The diffusion models use an attention mechanism on the text representation
- The diffusion moles are parametrized using a U-Net

https://arxiv.org/pdf/2205.11487

« Classifier-free » guidance

- The diffusion model is trained using two objectives

  1. Generate images from the text

  2. (Also) Generate images

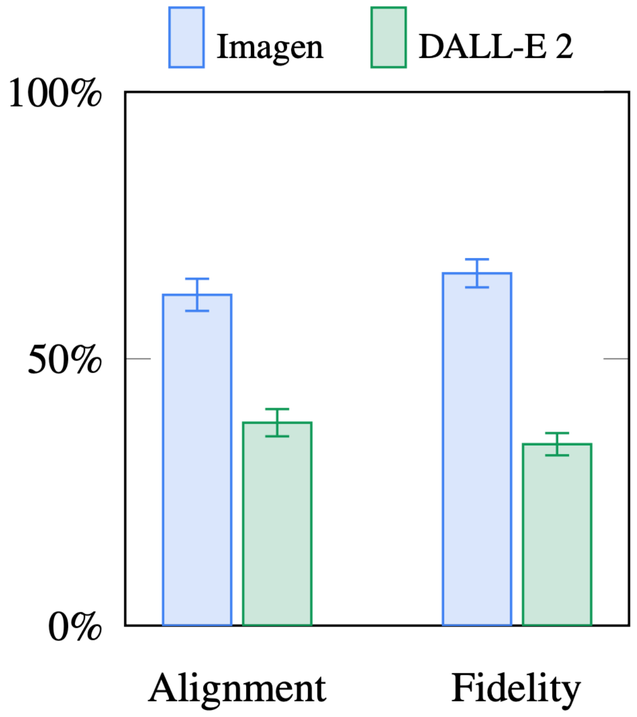
     - This allows to obtain high-quality images (1) that are diversified (2)

- Imagen proposes a method to ensure pixels don’t saturate during diffusion (somewhat similar problem to clipping in RNNs)

Before Imagen

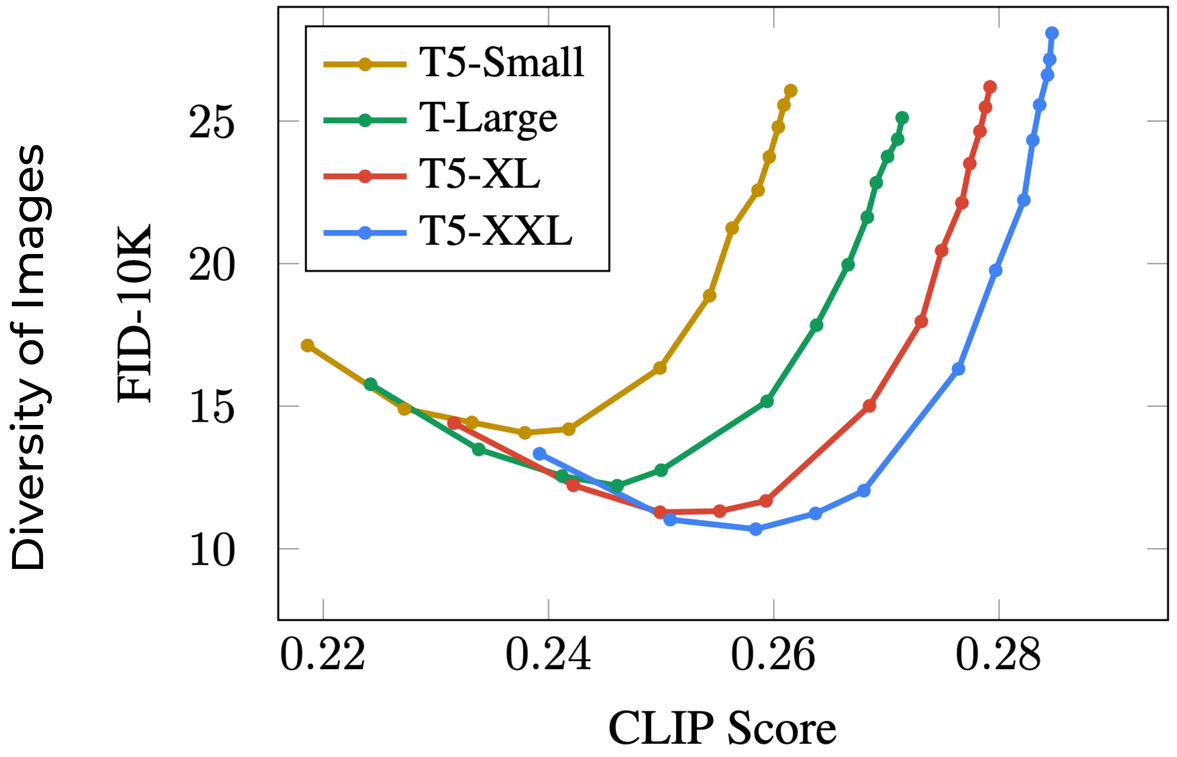
Imagen

Compared to Dall-E 2



- Better empirical performance (according to a human study)
  - “Alignment” -> “Does the caption accurately describe the above image”
  - “Fidelity” -> “Which image is more photorealistic”
- Users a simpler architecture (no CLIP)

The size of the text encoder is an important hyper-ammeter

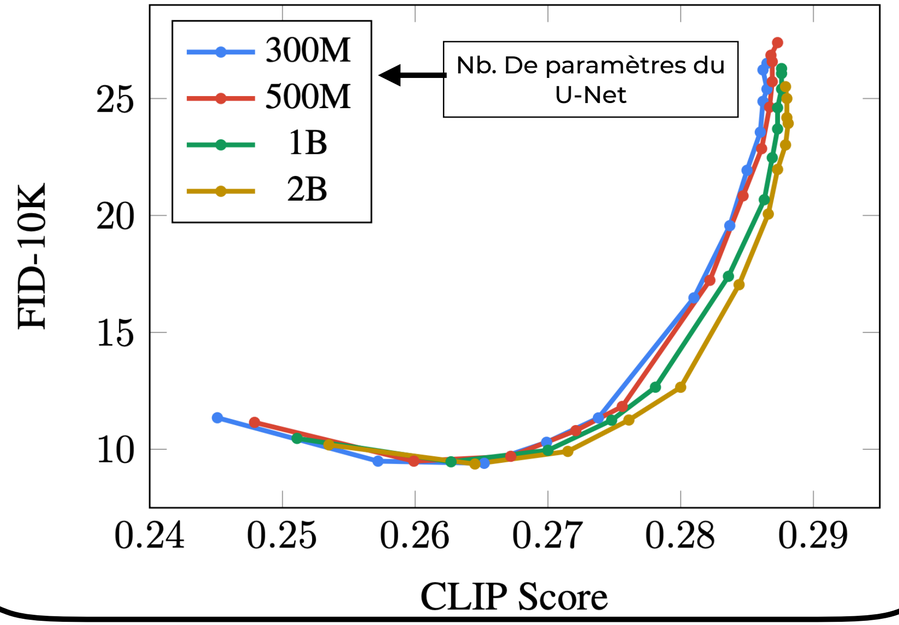


Alignment between images and the text

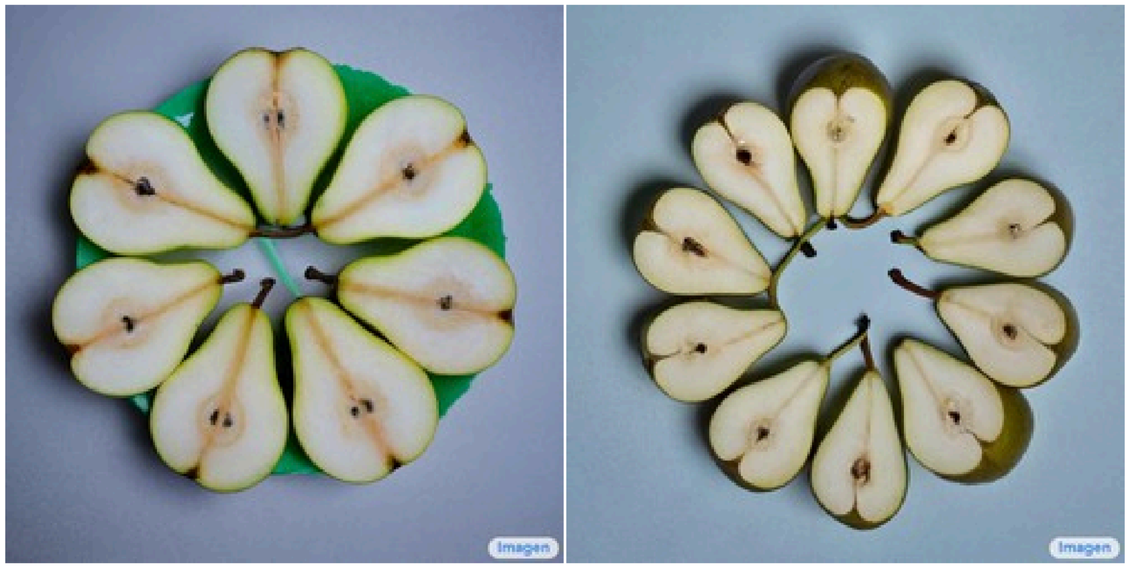
T5 XXL (2.6B)

- Trans. Encodeur-Decodeur
  - Uses only the encoder

Comparatively, the size of the image generation model is less important



Still far from perfect…



A pear cut into seven pieces arranged in a ring.

One cat and two dogs sitting on the grass.

- **E.g., operations that require counting and logic remain difficult**