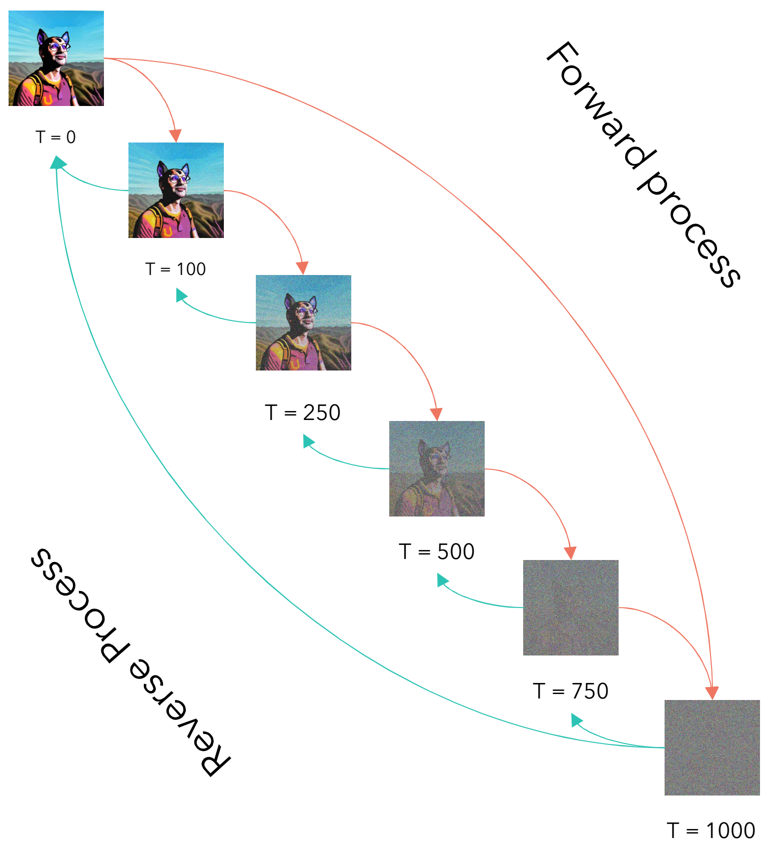


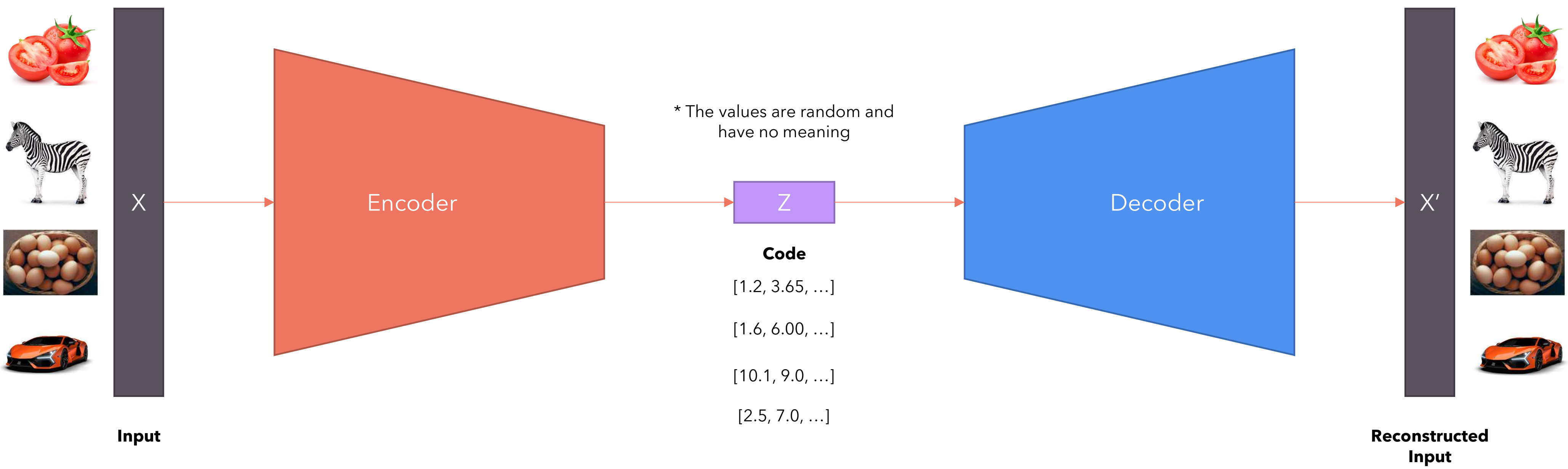

```python
def get_loss(self, batch, batch_idx):
    """
    Corresponds to Algorithm 1 from (Ho et al., 2020).
    """
    # Get a random time step for each image in the batch
    ts = torch.randint(0, self.t_range, [batch.shape[0]], device=self.device)
    noise_imgs = []
    # Generate noise, one for each image in the batch
    epsilons = torch.randn(batch.shape, device=self.device)
    for i in range(len(ts)):
        a_hat = self.alpha_bar(ts[i])
        noise_imgs.append(
            (math.sqrt(a_hat) * batch[i]) + (math.sqrt(1 - a_hat) * epsilons[i])
        )
    noise_imgs = torch.stack(noise_imgs, dim=0)
    # Run the noisy images through the U-Net, to get the predicted noise
    e_hat = self.forward(noise_imgs, ts)
    # Calculate the loss, that is, the MSE between the predicted noise and the actual noise
    loss = nn.functional.mse_loss(
        e_hat.reshape(-1, self.in_size), epsilons.reshape(-1, self.in_size)
    )
    return loss
```

Denoising Diffusion Probabilistic Models (DDPM)

Umar Jamil

Video: https://youtu.be/I1sPXkm2NH4

What is an Autoencoder?

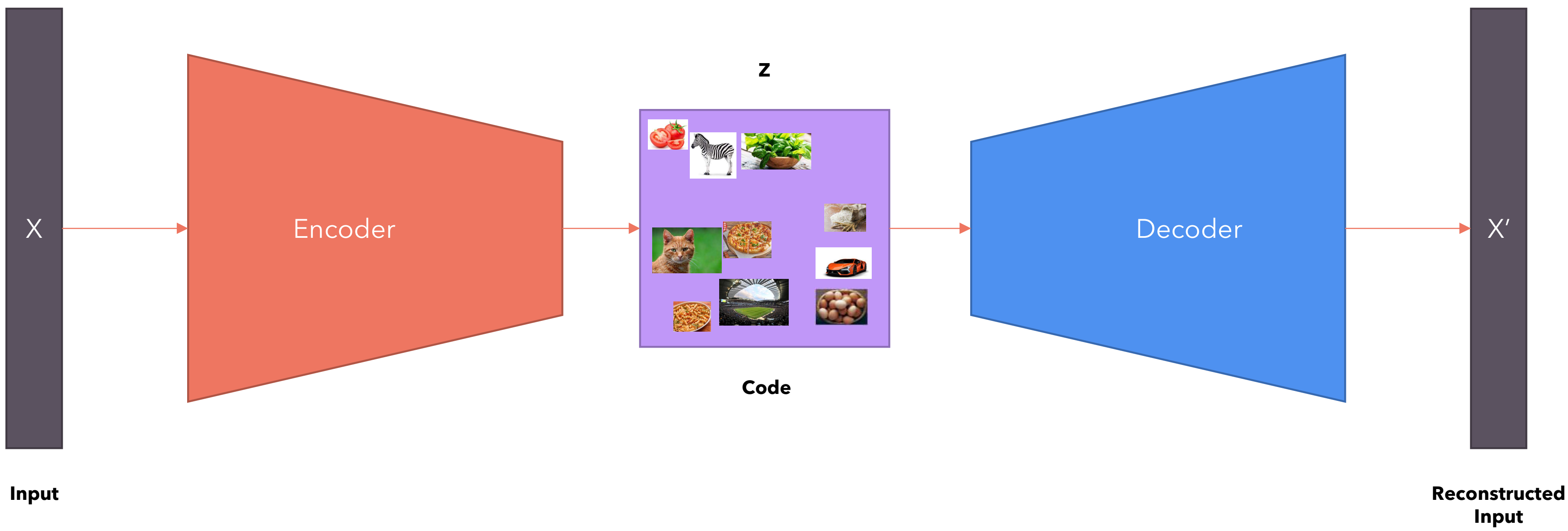


Main task: Compress data

Umar Jamil - https://github.com/hkproj/pytorch-ddpm

What's the problem with Autoencoders?

The code learned by the model **makes no sense**. ~~That is, the model can just assign any vector to the inputs without the numbers in the vector representing any~~ pattern. The model doesn't capture any **semantic relationship** between the data.



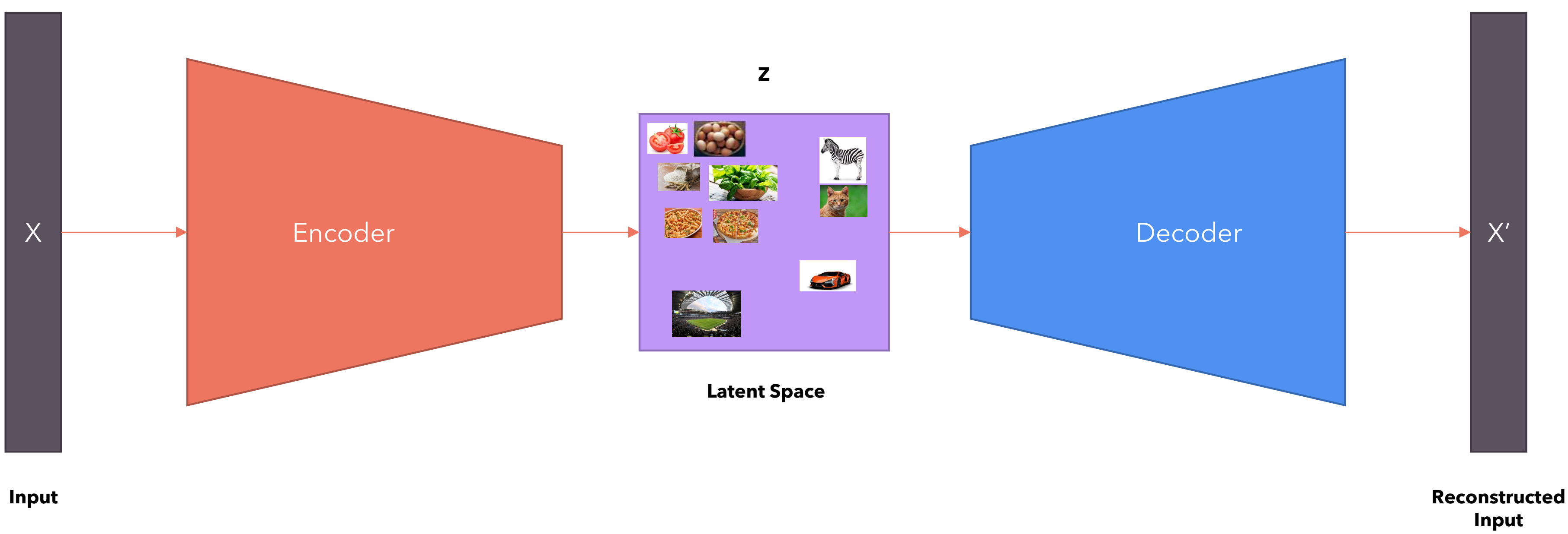
VAE learns a latent space
Params of multivariate dist
Aims to capture relationships in data.

Can sample from latent space to identify concepts.

Umar Jamil - https://github.com/hkproj/pytorch-ddpm

Introducing the Variational Autoencoder

The variational autoencoder, instead of learning a code, learns a "**latent space**". The latent space represents the parameters of a (multivariate) distribution.



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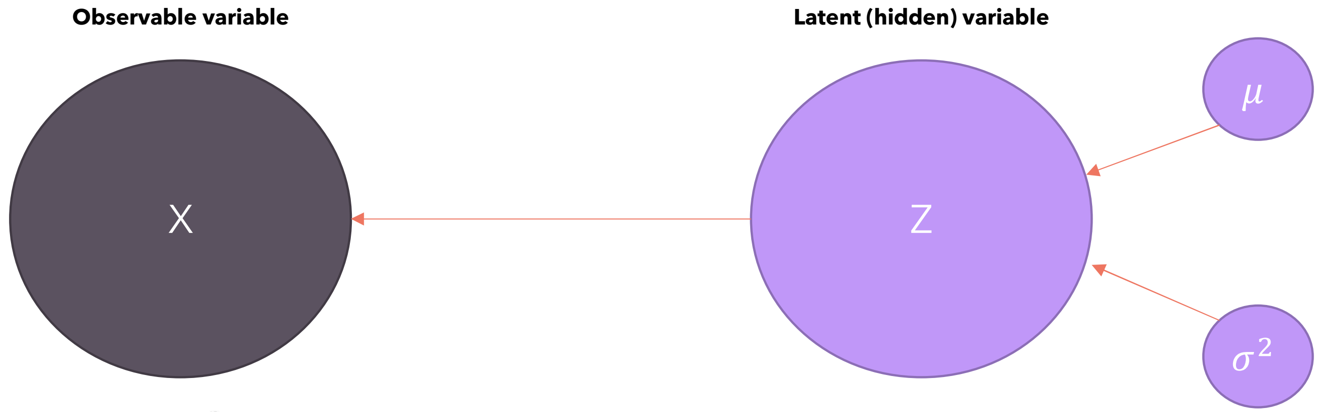
Why is it called latent space?



[8.67, 12.8564, 0.44875, 874.22, …]

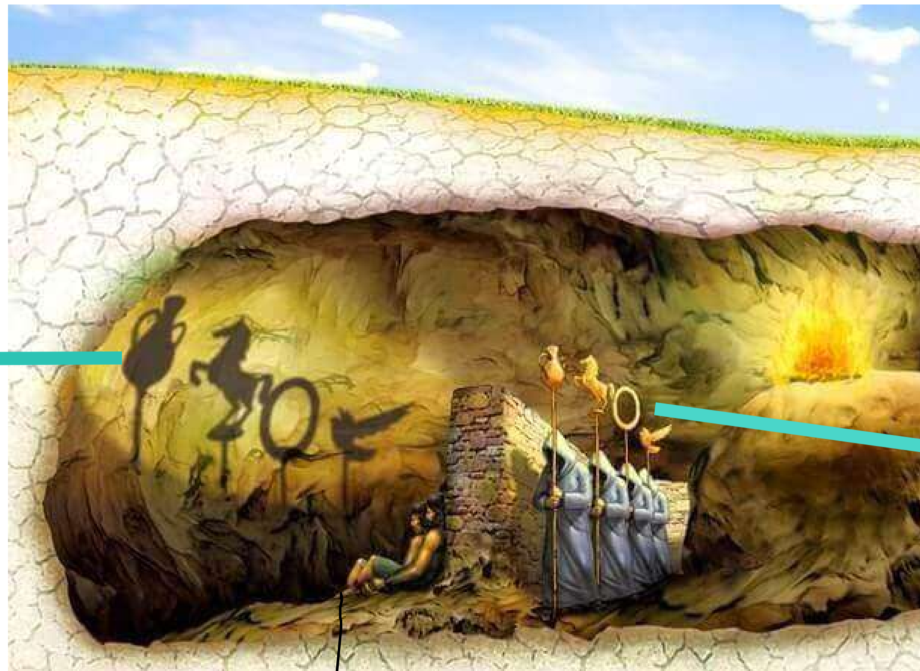
[4.59, 13.2548, 1.14569, 148.25, …]

[1.74, 32.3476, 5.18469, 358.14, …]

z cannot be observed, but we want to infer some properties of it.

Plato's allegory of the cave

Observable variable



Latent (hidden) variable

[8.67, 12.8564, 0.44875, 874.22, …]

[4.59, 13.2548, 1.14569, 148.25, …]

[1.74, 32.3476, 5.18469, 358.14, …]

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People born & lived all life in cave
Cannot leave cave. Chained inside.

They observe shadows on the wall, & believe it is real.
Eg:- Observe horse, bird, etc.

We know these are actually projections of objects.
Outside people can actually see the objects.
Data → Observed variable. It is conditioned on latent variable

For diffusion model

We assume that the outside people themselves didn't have access to the real object, but observed some projection of the object. They were also always in the cave.

Cave-ception!

Can't see anything

Each step can only see data from the previous step.

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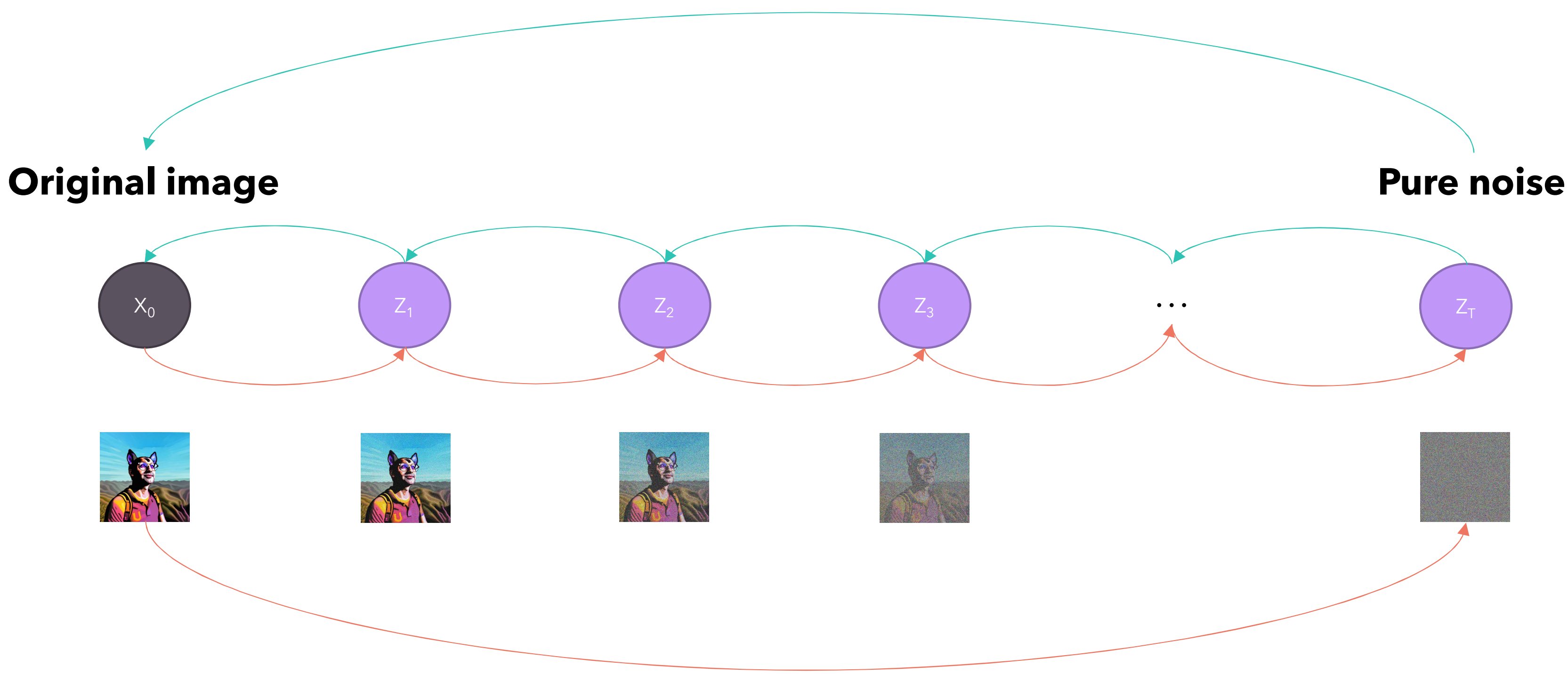
Reverse process: **Neural network**



Forward process: **Fixed**

Process of adding noise is forward process

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Since we don't know how to go from more noise to less noise, we train a neural network to do it.

Let's have fun with… math!

Just like with a VAE, we want to learn the parameters of the latent space

Reverse process **p**

2 Background

Diffusion models [53] are latent variable models of the form $p_\theta(\mathbf{x}_0) := \int p_\theta(\mathbf{x}_{0:T})\, d\mathbf{x}_{1:T}$, where $\mathbf{x}_1, \ldots, \mathbf{x}_T$ are latents of the same dimensionality as the data $\mathbf{x}_0 \sim q(\mathbf{x}_0)$. The joint distribution $p_\theta(\mathbf{x}_{0:T})$ is called the *reverse process*, and it is defined as a Markov chain with learned Gaussian transitions starting at $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$:

$$p_\theta(\mathbf{x}_{0:T}) := p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t), \qquad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \quad (1)$$

What distinguishes diffusion models from other types of latent variable models is that the approximate posterior $q(\mathbf{x}_{1:T}|\mathbf{x}_0)$, called the *forward process* or *diffusion process*, is fixed to a Markov chain that gradually adds Gaussian noise to the data according to a variance schedule $\beta_1, \ldots, \beta_T$:

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) := \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}), \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \quad (2)$$

Evidence Lower Bound **(ELBO)**

Training is performed by optimizing the usual variational bound on negative log likelihood:

$$\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] \le \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] = \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\ge1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L \quad (3)$$

Forward process **q**

The forward process variances β_t can be learned by reparameterization [33] or held constant as hyperparameters, and expressiveness of the reverse process is ensured in part by the choice of Gaussian conditionals in $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$, because both processes have the same functional form when β_t are small [53]. A notable property of the forward process is that it admits sampling $\mathbf{x}_t$ at an arbitrary timestep t in closed form: using the notation $\alpha_t := 1 - \beta_t$ and $\bar{\alpha}_t := \prod_{s=1}^{t} \alpha_s$, we have

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}) \quad (4)$$

Ho, J., Jain, A. and Abbeel, P., 2020. Denoising diffusion probabilistic models. Advances in Neural Information Processing Systems, 33, pp.6840-6851.

Markov chain of gaussian variables

$\beta \rightarrow$ seq of β is called schedule

p has param θ since we want to learn it.

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In forward process, we can directly go from original image to full noisy final image, without going through all intermediate steps.

$\alpha_t = 1 - \beta_t$ $\qquad \hat{\alpha}_t \rightarrow$ Product of all α from 1 to t

How to derive the loss function?

1. We start by writing our objective: we want to maximize the log likelihood of our data, $\log(p_\theta(x_0))$, marginalizing over all other latent variables.
2. We find a lower bound for the log likelihood, that is, $\log\big(p_\theta(x_0)\big) \geq ELBO$
3. We maximize the $ELBO$ (or minimize the negated term).

$$ELBO = E_q\left[-\log p(x_T) - \sum_{t\geq 1} \log \frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})}\right]$$

Maximize ELBO $\Rightarrow$ Maximize log likelihood.

Algorithm 1 Training

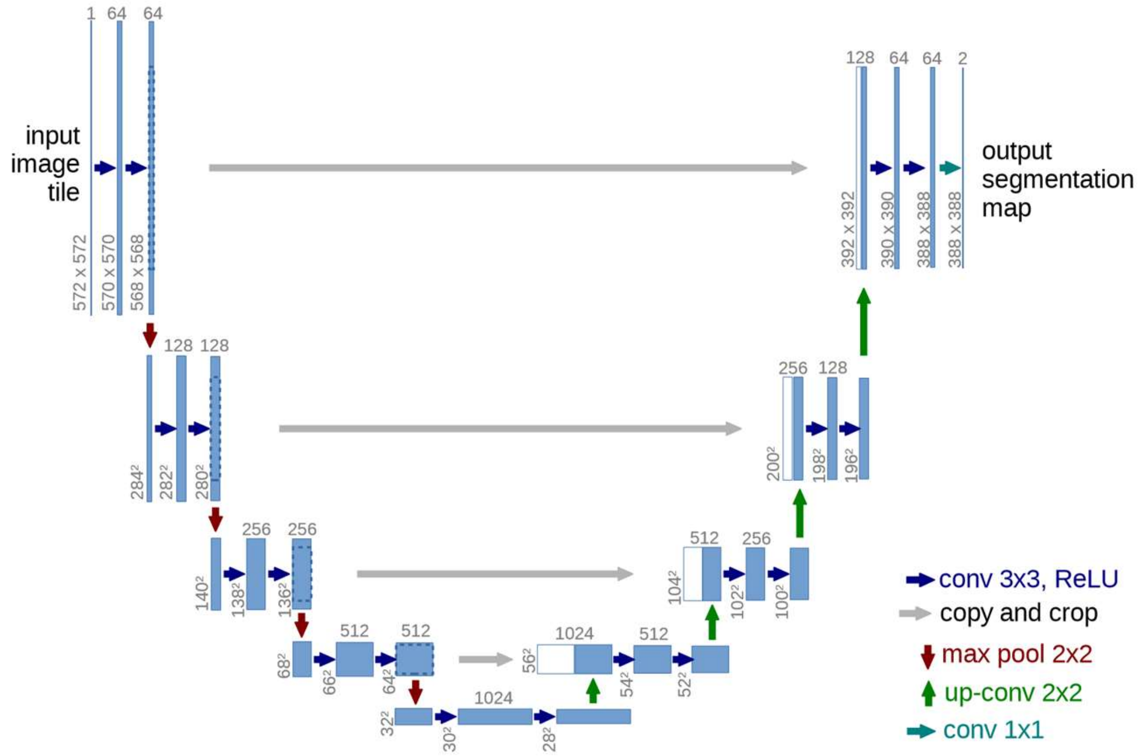
1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ We take a sample from our dataset
3: $t \sim \mathrm{Uniform}(\{1, \dots, T\})$ We generate a random number t, between 1 and T
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ We sample some noise
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
We add noise to our image, and we train the model to learn to predict the amount of noise present in it.
6: **until** converged

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ We sample some noise
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** $\mathbf{x}_0$

We keep denoising the image progressively for T steps.

U-Net



Ronneberger, O., Fischer, P. and Brox, T., 2015. U-net: Convolutional networks for biomedical image segmentation. In *Medical Image Computing and Computer-Assisted Intervention–MICCAI 2015: 18th International Conference, Munich, Germany, October 5-9, 2015, Proceedings, Part III 18* (pp. 234-241). Springer International Publishing.

This is the model used to predict the reverse process

Some modifications:

⇒ Need to tell model what is at timestep t. How?

· → At each downsampling & upsampling operation, we concat the input vector with the position embedding (from transformers)

Training code

Algorithm 1 Training

1: **repeat**
2: $\quad \mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $\quad t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: $\quad$ Take gradient descent step on

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0}_{\text{Initial image}} + \underbrace{\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}_{\text{Noise}}, t) \right\|^2$$

6: **until** converged

```python
def get_loss(self, batch, batch_idx):
    """
    Corresponds to Algorithm 1 from (Ho et al., 2020).
    """
    # Get a random time step for each image in the batch
    ts = torch.randint(0, self.t_range, [batch.shape[0]], device=self.device)
    noise_imgs = []
    # Generate noise, one for each image in the batch
    epsilons = torch.randn(batch.shape, device=self.device)
    for i in range(len(ts)):
        a_hat = self.alpha_bar(ts[i])
        noise_imgs.append(
            (math.sqrt(a_hat) * batch[i]) + (math.sqrt(1 - a_hat) * epsilons[i])
        )
    noise_imgs = torch.stack(noise_imgs, dim=0)
    # Run the noisy images through the U-Net, to get the predicted noise
    e_hat = self.forward(noise_imgs, ts)
    # Calculate the loss, that is, the MSE between the predicted noise and the actual noise
    loss = nn.functional.mse_loss(
        e_hat.reshape(-1, self.in_size), epsilons.reshape(-1, self.in_size)
    )
    return loss
```

Umar Jamil - https://github.com/hkproj/pytorch-ddpm

Add noise to each input image at timestep t. Noise increases with t.

Rate of noise addition controlled by α.

Sampling code

Only inner loop code

Algorithm 2 Sampling

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

```python
def denoise_sample(self, x, t):
    """
    Corresponds to the inner loop of Algorithm 2 from (Ho et al., 2020).
    """
    with torch.no_grad():
        if t > 1:
            z = torch.randn(x.shape)
        else:
            z = 0
        # Get the predicted noise from the U-Net
        e_hat = self.forward(x, t.view(1).repeat(x.shape[0]))
        # Perform the denoising step to take the image from t to t-1
        pre_scale = 1 / math.sqrt(self.alpha(t))
        e_scale = (1 - self.alpha(t)) / math.sqrt(1 - self.alpha_bar(t))
        post_sigma = math.sqrt(self.beta(t)) * z
        x = pre_scale * (x - e_scale * e_hat) + post_sigma
        return x
```

The full code is available on GitHub!

Full code: https://github.com/hkproj/pytorch-ddpm

Special thanks to:
https://github.com/lucidrains/denoising-diffusion-pytorch for the U-Net Model
https://github.com/awjuliani/pytorch-diffusion/ for the Diffusion Model

Thanks for watching!
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