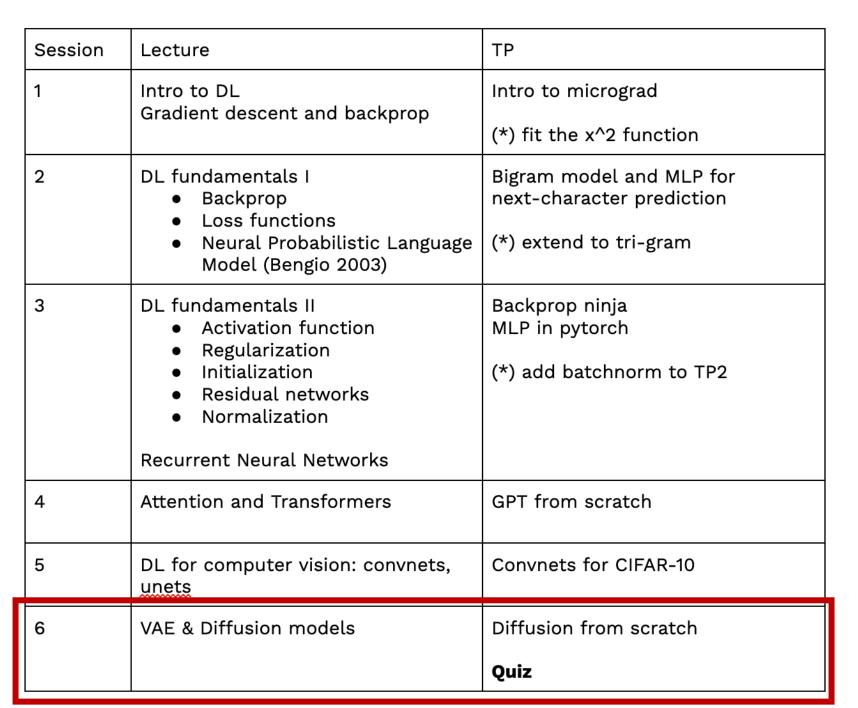
Deep learning

Unpacking Transformers, LLMs and image generation

Session 6



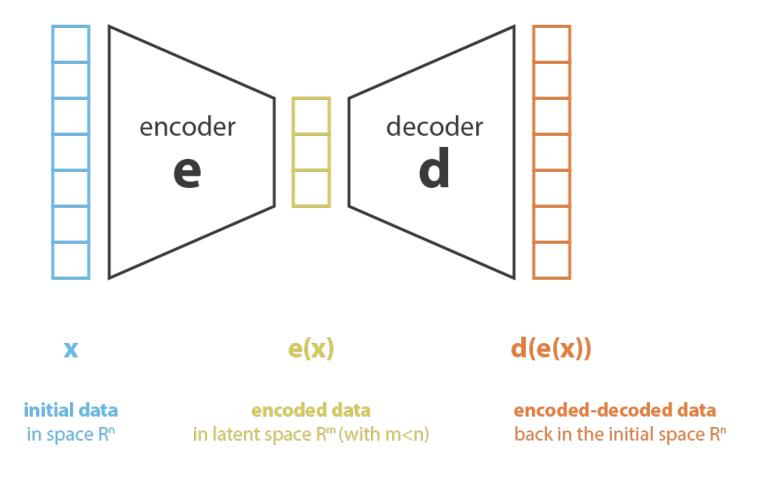




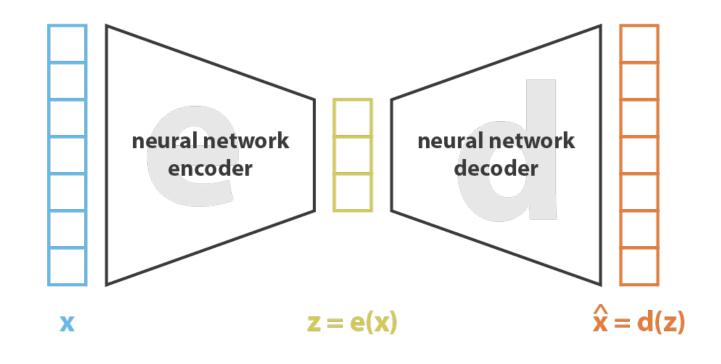
Agenda for today

- 1. VAEs
- 2. Diffusion

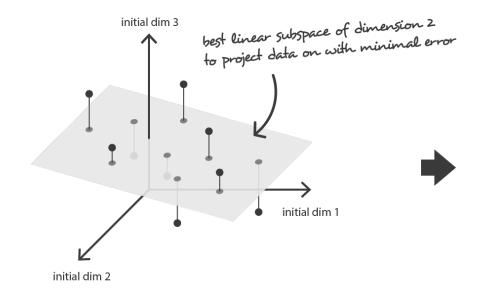
Auto-encoders



x = d(e(x)) | lossless encoding no information is lost when reducing the number of dimensions



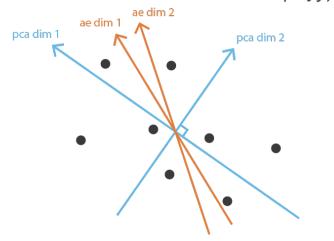
loss =
$$||\mathbf{x} - \hat{\mathbf{x}}||^2 = ||\mathbf{x} - \mathbf{d}(\mathbf{z})||^2 = ||\mathbf{x} - \mathbf{d}(\mathbf{e}(\mathbf{x}))||^2$$



Data in the full initial space

In order to reduce dimensionality, PCA and linear autoencoder target, in theory, the same optimal subspace to project data on...

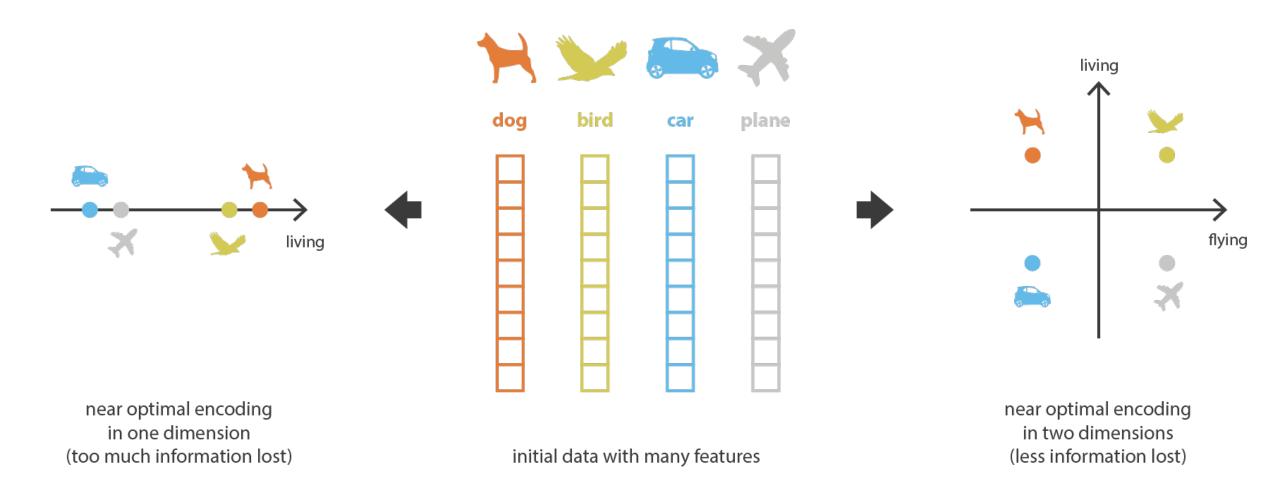
(contrarily to PCA, linear autoencoder can end up with any basis)



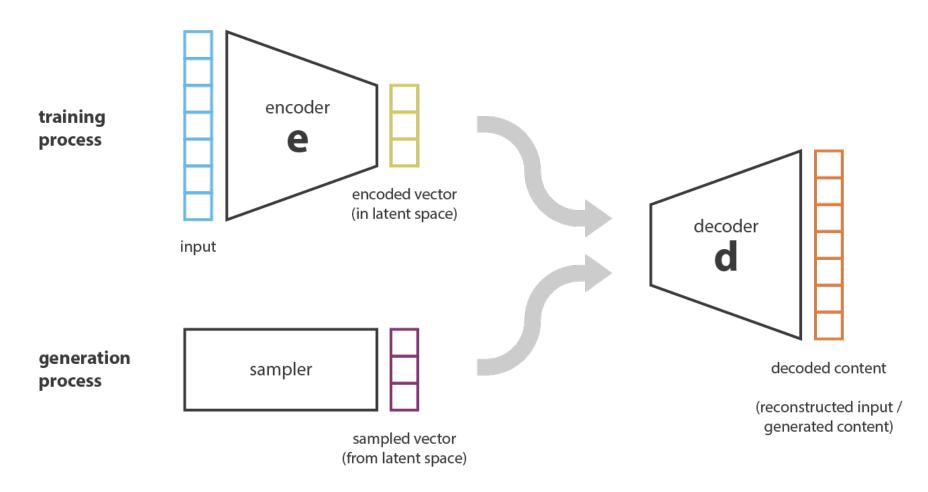
Data projected on the best linear subspace

... but not necessarily with the same basis due to different constraints (in PCA the first component is the one that explains the maximum of variance and components are orthogonal)

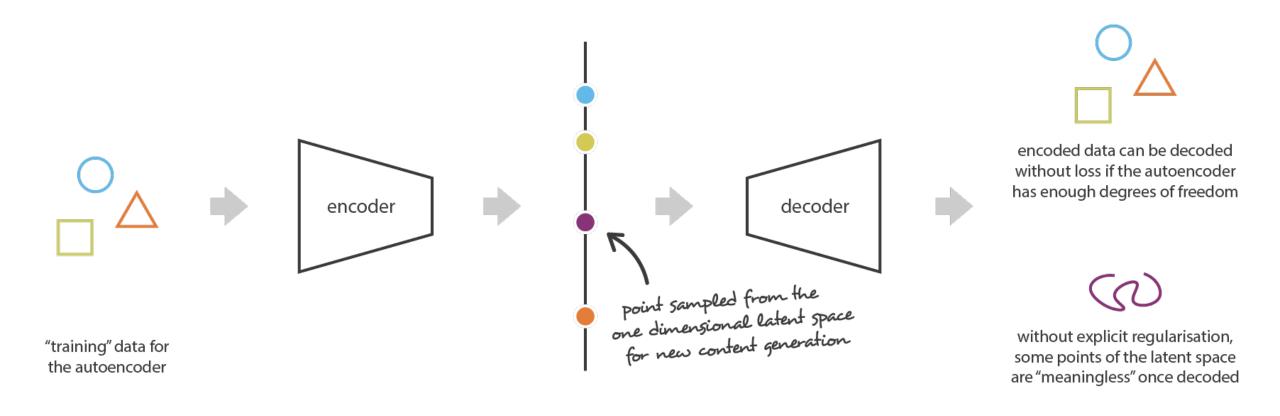
Auto-encoders



When reducing dimensionality, we want to keep the main structure there exists among the data.



In theory, auto-encoders can be used for data generation.

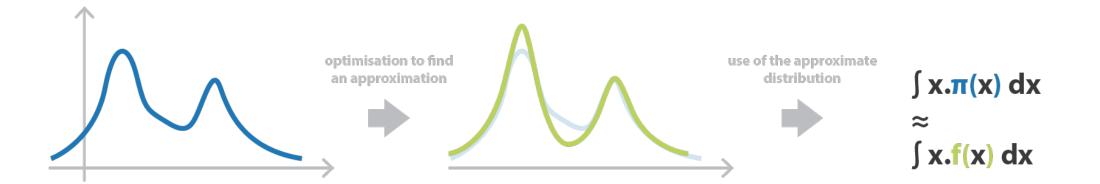


Irregular latent space prevent us from using autoencoder for new content generation.

Variational auto-encoders

A variational autoencoder can be defined as being an autoencoder whose training is regularised to avoid overfitting and ensure that the latent space has good properties that enable generative process.

Variational inference



Unnormalised distribution (π)

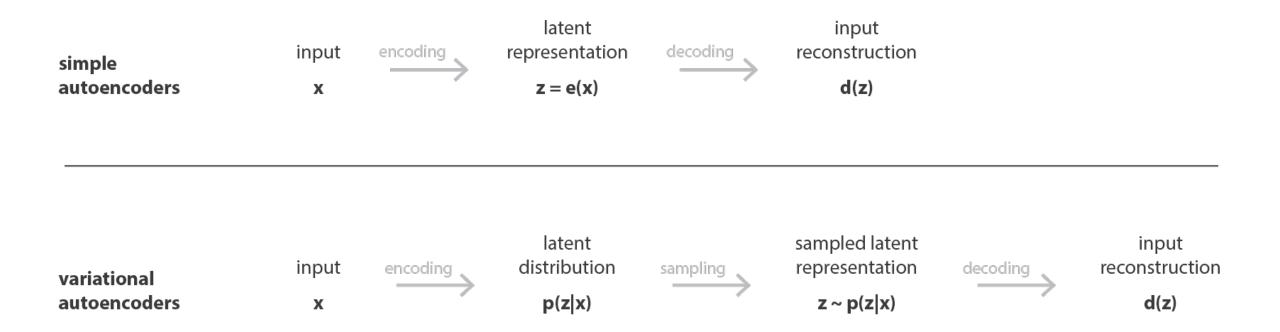
whose normalisation factor computation is intractable

Best approximation (f)

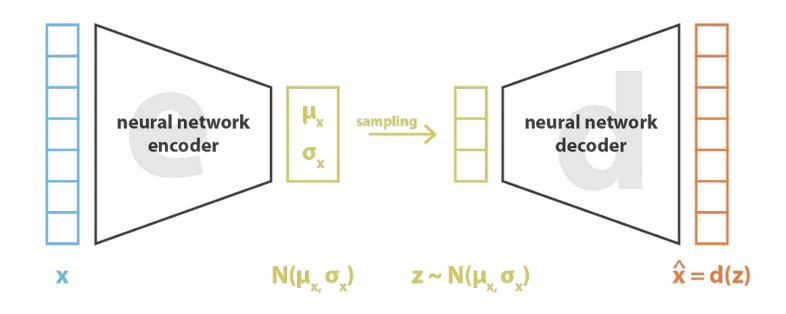
among a parametrised family, obtained by optimising over the family parameters and without proceeding to the normalisation **Approximate computations**

obtained by replacing the exact distribution by the approximate one

Variational Inference methods that consist in finding the best approximation of a distribution among a parametrised family.

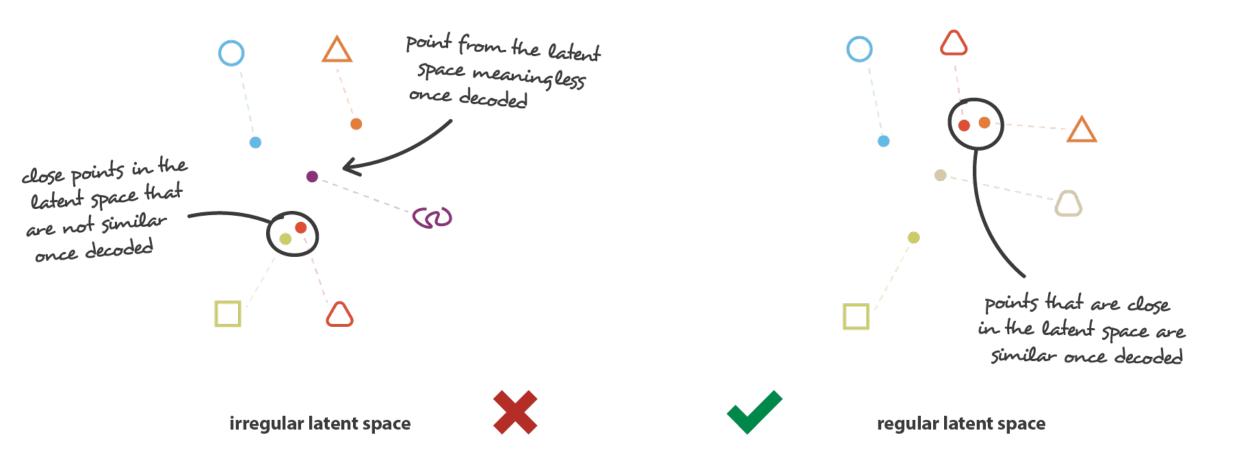


Difference between autoencoder (deterministic) and variational autoencoder (probabilistic).

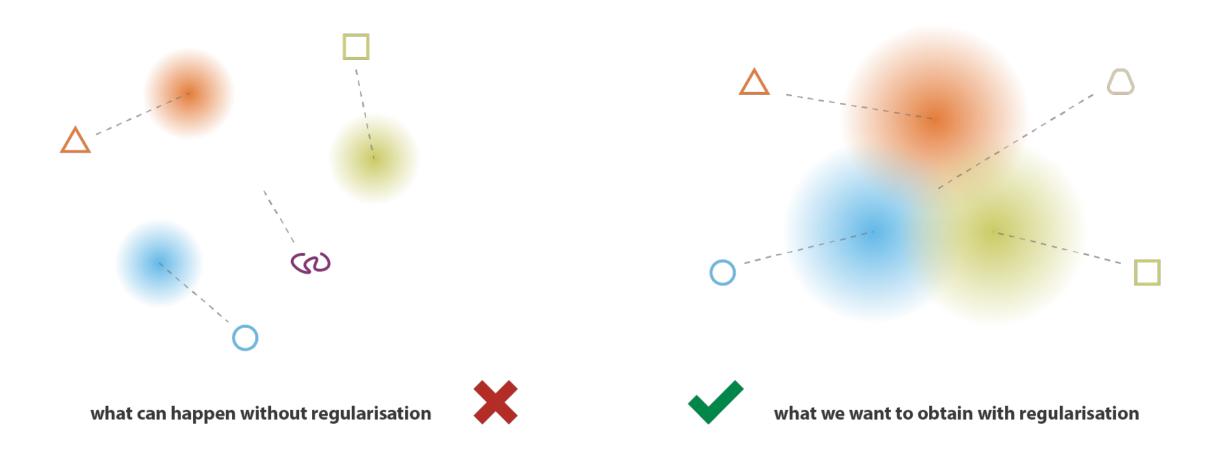


loss =
$$|| x - x^{\hat{}} ||^2 + KL[N(\mu_x, \sigma_x), N(0, I)] = || x - d(z)||^2 + KL[N(\mu_x, \sigma_x), N(0, I)]$$

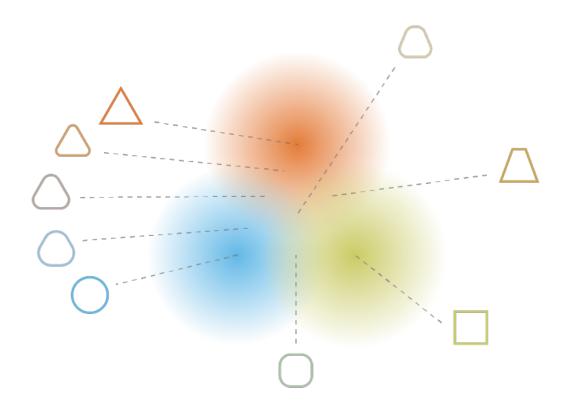
In variational autoencoders, the loss function is composed of a **reconstruction term** (that makes the encoding-decoding scheme efficient) and a **regularisation term** (that makes the latent space regular).



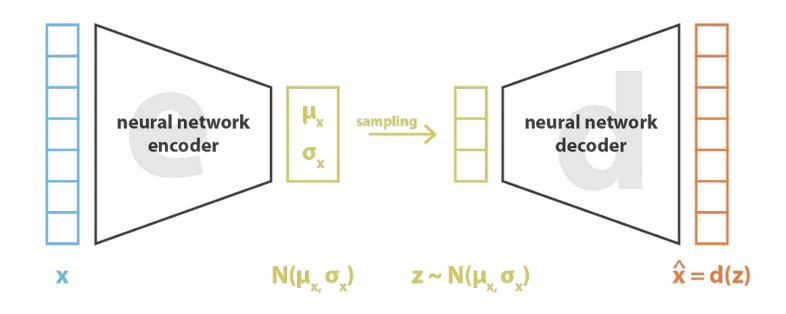
Difference between a "regular" and an "irregular" latent space.



The returned distributions of VAEs have to be regularised to obtain a latent space with good properties.

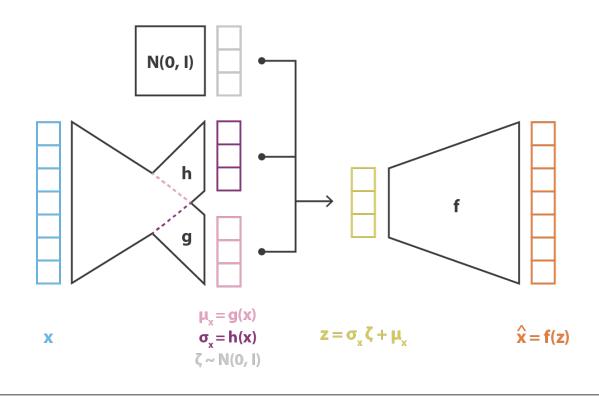


Regularisation tends to create a "gradient" over the information encoded in the latent space.



loss =
$$|| x - x^{\hat{}} ||^2 + KL[N(\mu_x, \sigma_x), N(0, I)] = || x - d(z)||^2 + KL[N(\mu_x, \sigma_x), N(0, I)]$$

In variational autoencoders, the loss function is composed of a **reconstruction term** (that makes the encoding-decoding scheme efficient) and a **regularisation term** (that makes the latent space regular).



loss =
$$C || x - \hat{x} ||^2 + KL[N(\mu_x, \sigma_x), N(0, I)] = C || x - f(z) ||^2 + KL[N(g(x), h(x)), N(0, I)]$$

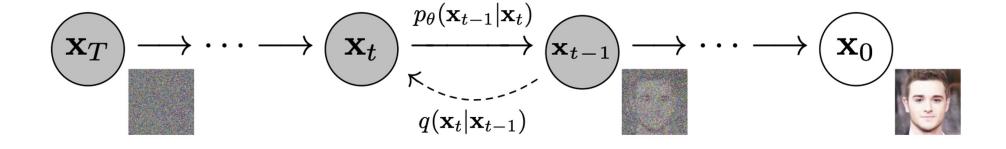


Figure 1: Class-conditional 256x256 image samples from a two-level model trained on ImageNet.

Agenda for today

- 1. VAEs
- 2. Diffusion

The principle of diffusion



Schedulers

Schedulers define the methodology for iteratively adding noise to an image or for updating a sample based on model outputs.

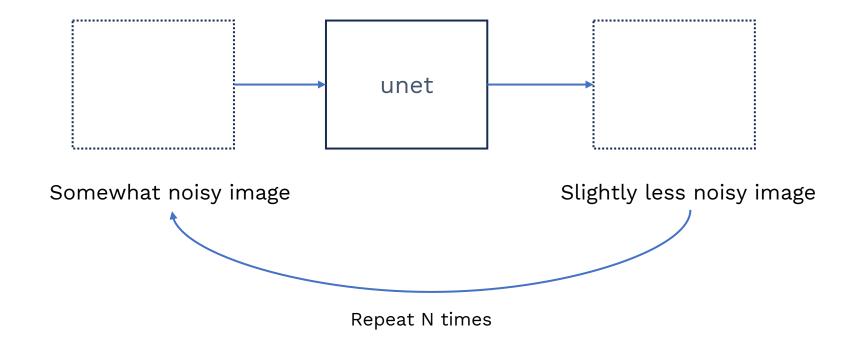
- How to add noise for training
- How to update a sample based on an output from a pretrained model for inference

Schedulers are often defined by a noise schedule and an update rule to solve the differential equation solution.

Linear



Cosine



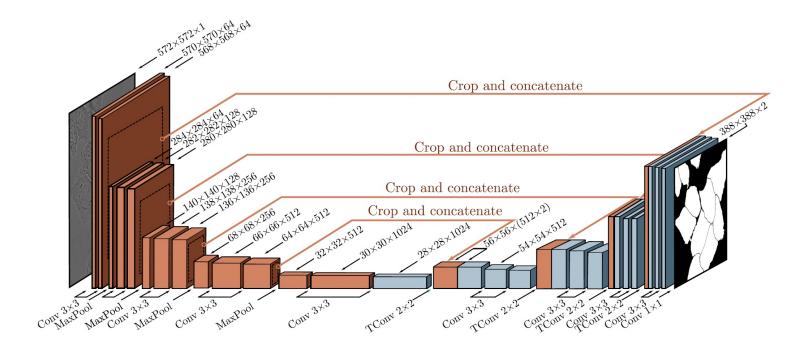
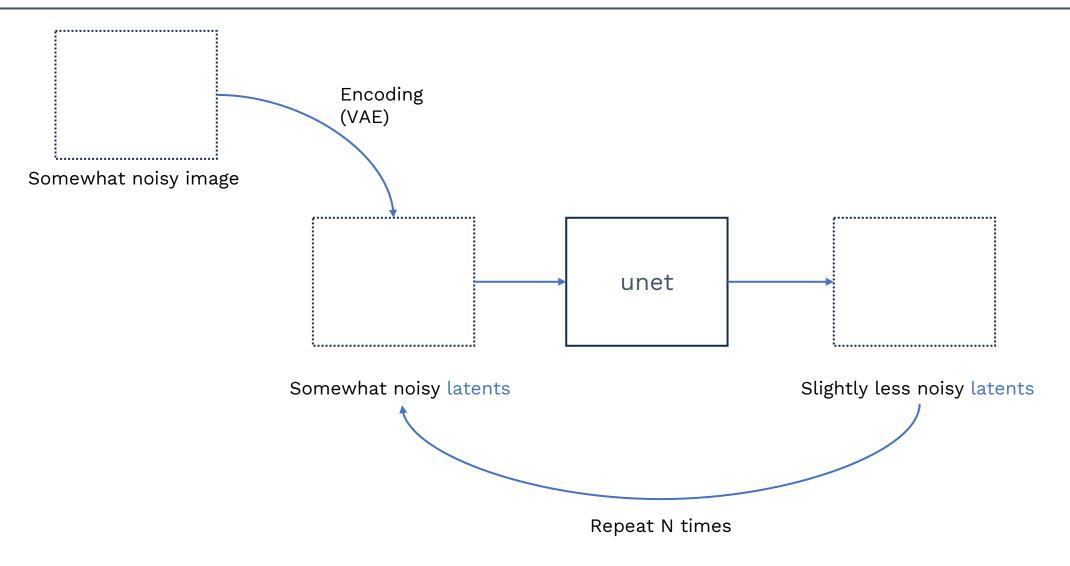
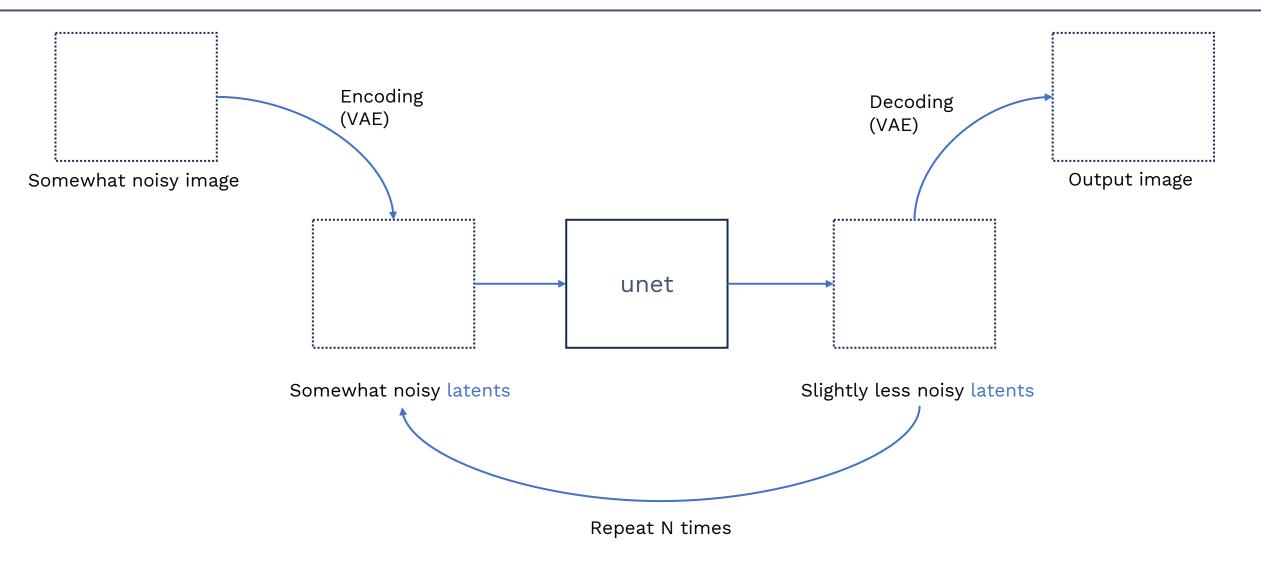


Figure 11.10 U-Net for segmenting HeLa cells. The U-Net has an encoder-decoder structure, in which the representation is downsampled (orange blocks) and then re-upsampled (blue blocks). The encoder uses regular convolutions, and the decoder uses transposed convolutions. Residual connections append the last representation at each scale in the encoder to the first representation at the same scale in the decoder (orange arrows). The original U-Net used "valid" convolutions, so the size decreased slightly with each layer, even without downsampling. Hence, the representations from the encoder were cropped (dashed squares) before appending to the decoder. Adapted from Ronneberger et al. (2015).

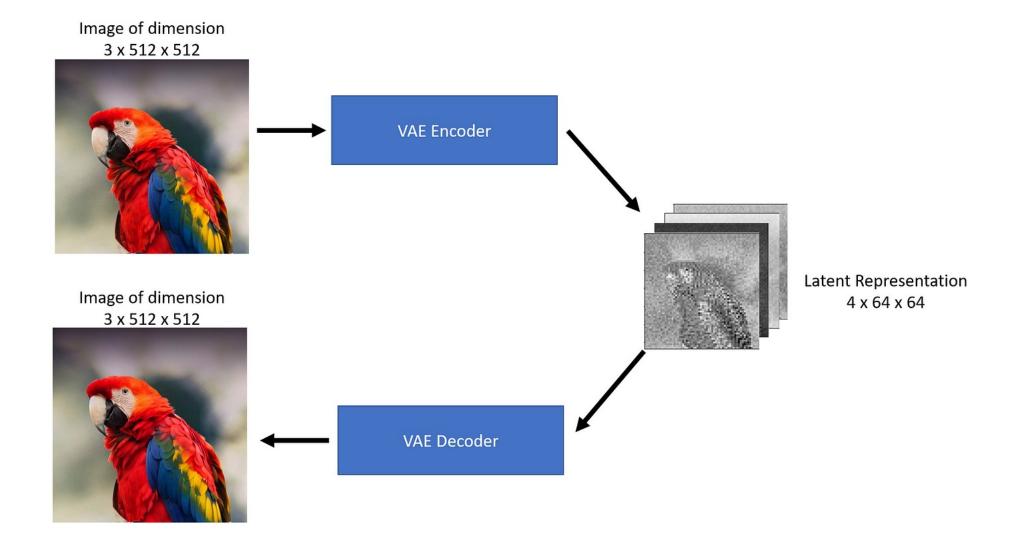
Stable Diffusion



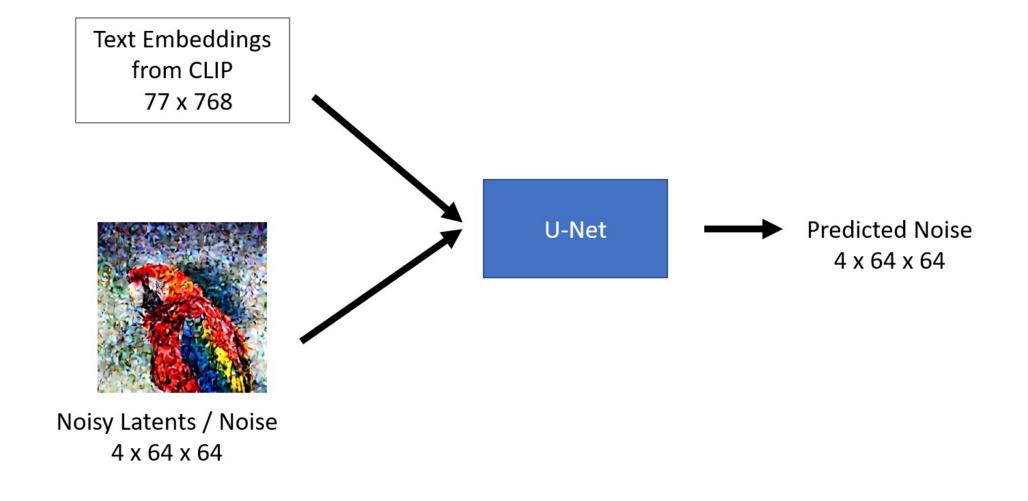
Stable Diffusion



VAE Encoder

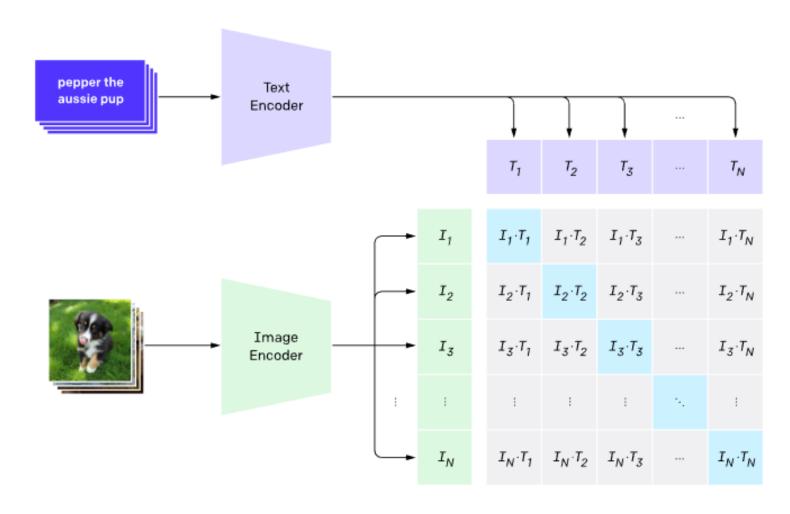


Guiding the diffusion with CLIP text encoding

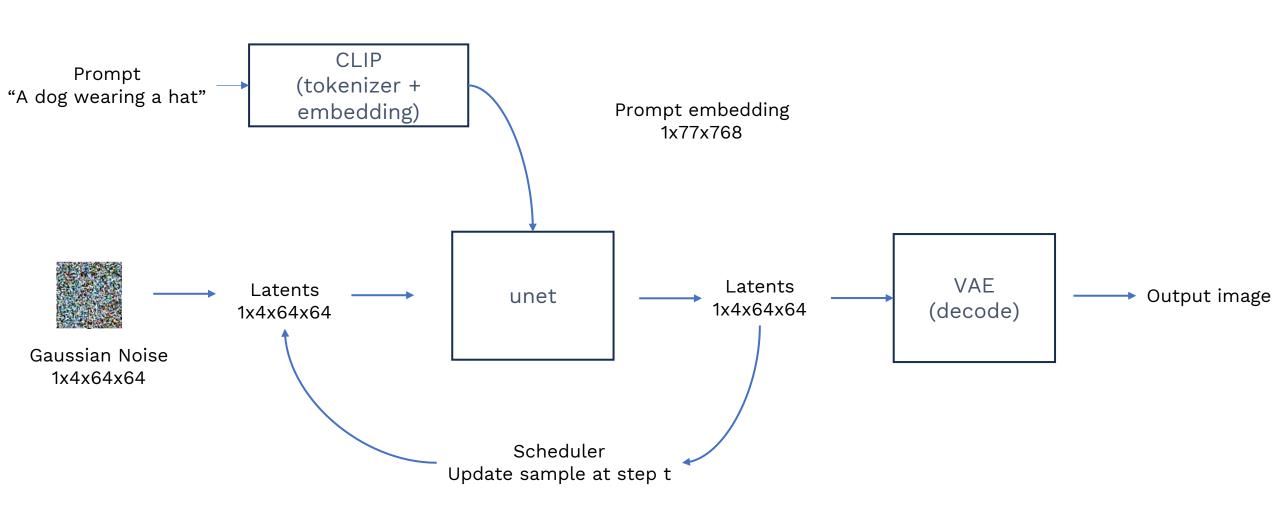


CLIP (Contrastive Language-Image Pretraining)

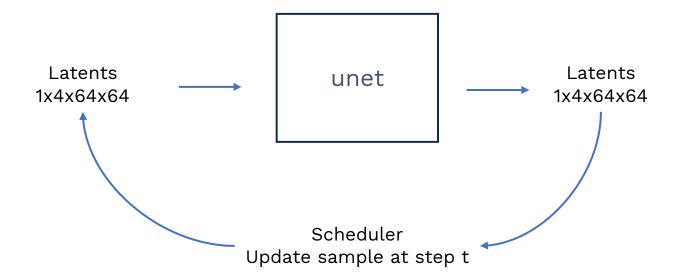
1. Contrastive pre-training



Stable Diffusion - Putting it all together



Repeat N times



The U-Net does not predict noise between step t-1 and step t

The U-Net predicts the *entire* noise

The scheduler takes care of removing part of the noise

See <u>demo</u>

Stable Diffusion in 15 lines of code

```
tokenizer = CLIPTokenizer.from_pretrained("openai/clip-vit-large-patch14",
torch_dtype=torch.float16)
text_encoder = CLIPTextModel.from_pretrained("openai/clip-vit-large-patch14",
torch dtype=torch.float16).to("cuda")
vae = AutoencoderKL.from_pretrained("stabilityai/sd-vae-ft-ema",
torch_dtype=torch.float16).to("cuda")
unet = UNet2DConditionModel.from_pretrained("CompVis/stable-diffusion-v1-4",
subfolder="unet", torch_dtype=torch.float16).to("cuda")
beta start, beta end = 0.00085, 0.012
scheduler = LMSDiscreteScheduler(beta_start=beta_start, beta_end=beta_end,
beta_schedule="scaled_linear", num_train_timesteps=1000)
```

```
bs = len(prompts)
text = text_enc(prompts)
uncond = text_enc([""] * bs, text.shape[1])
emb = torch.cat([uncond, text])
latents = torch.randn((bs, unet.in_channels, height//8, width//8))
scheduler.set_timesteps(steps)
latents = latents.to("cuda").half() * scheduler.init_noise_sigma
for i,ts in enumerate(tqdm(scheduler.timesteps)):
    inp = scheduler.scale_model_input(torch.cat([latents] * 2), ts)
    with torch.no_grad():
        u,t = unet(inp, ts, encoder_hidden_states=emb).sample.chunk(2)
    pred = u + q*(t-u)
    latents = scheduler.step(pred, ts, latents).prev_sample
with torch.no_grad():
    return vae.decode(1 / 0.18215 * latents).sample
```

Going deeper

The <u>maths of diffusion</u> by Lilian Weng

Classifier-free guidance (CFG)

Denoising Diffusion Implicit Models (DDIM)

Diffusion Models for Text Generation (AR-Diffusion)

Diffusion Models in Reinforcement Learning (DDPO)

Applications in Molecular Design (GaUDI)

