Deep Learning: advanced models

Generative models, Transformers, GNNs...

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Pros and cons of deep learning

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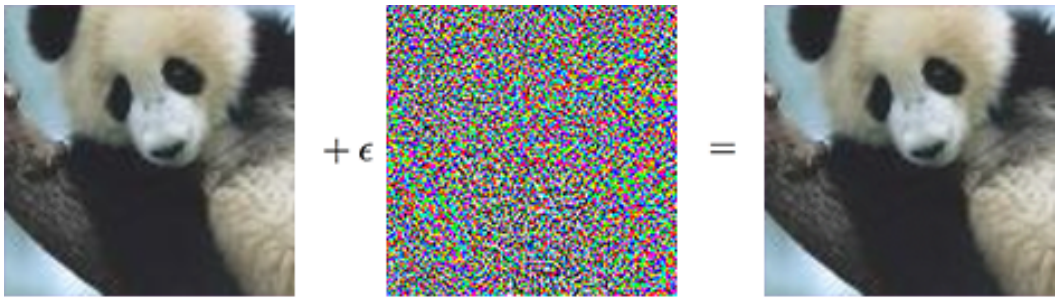

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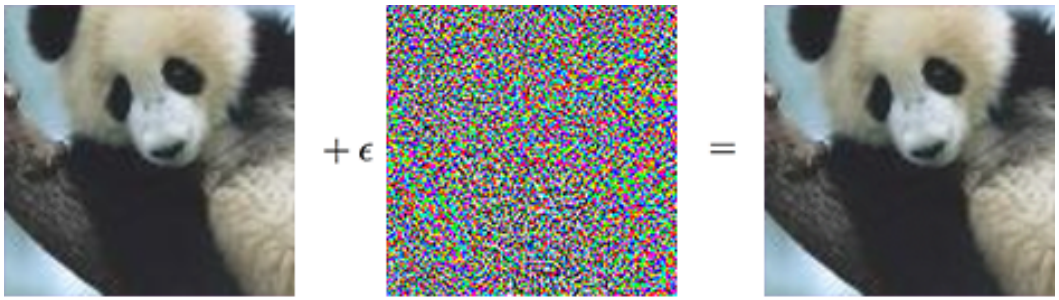

- A **bazooka**, when sometimes all you need to do is kill a fly ! In many real-life scenarii, linear models, PCA, k-means... work amazingly well

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- Today, we are going to see a few variants of DNNs, without going into details. Many ressources are available online.

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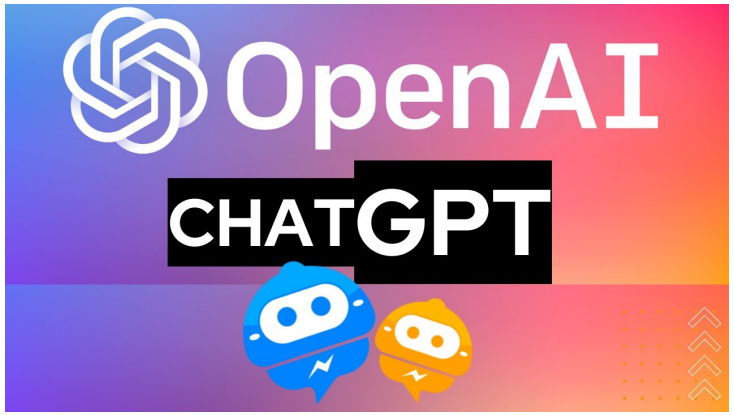
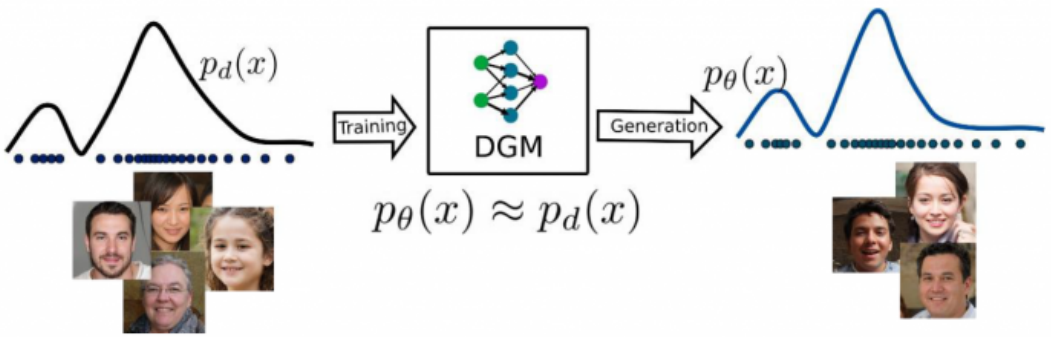
Generative model

- Goal : generate data ressembling other data.
- Extremely hot topic right now ! Text generation, image generation...



Basic generative model : density estimation !

- Most basic problem : observe samples from a distribution, generate new samples not observed before
- Just a *density estimation* problem ! But the probability distribution is far too complicated to be modelled explicitely (eg images)



- Basic idea : take a very simple distribution in a latent space, eg $z \sim \mathcal{N}(0, Id)$, train a complicated function f_θ such that $f_\theta(z)$ are good samples.

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GAN description

- Train a generator network G_{θ_g} such that $G_{\theta_g}(z)$, with z Gaussian, are good samples
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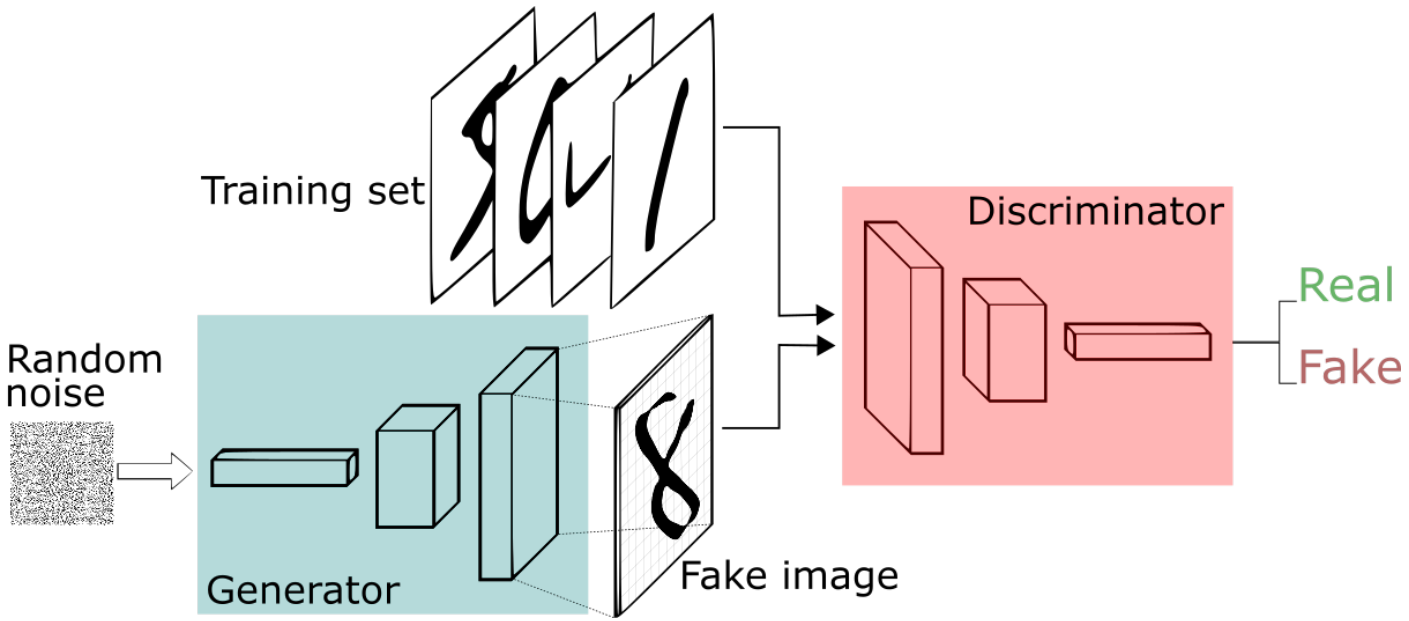

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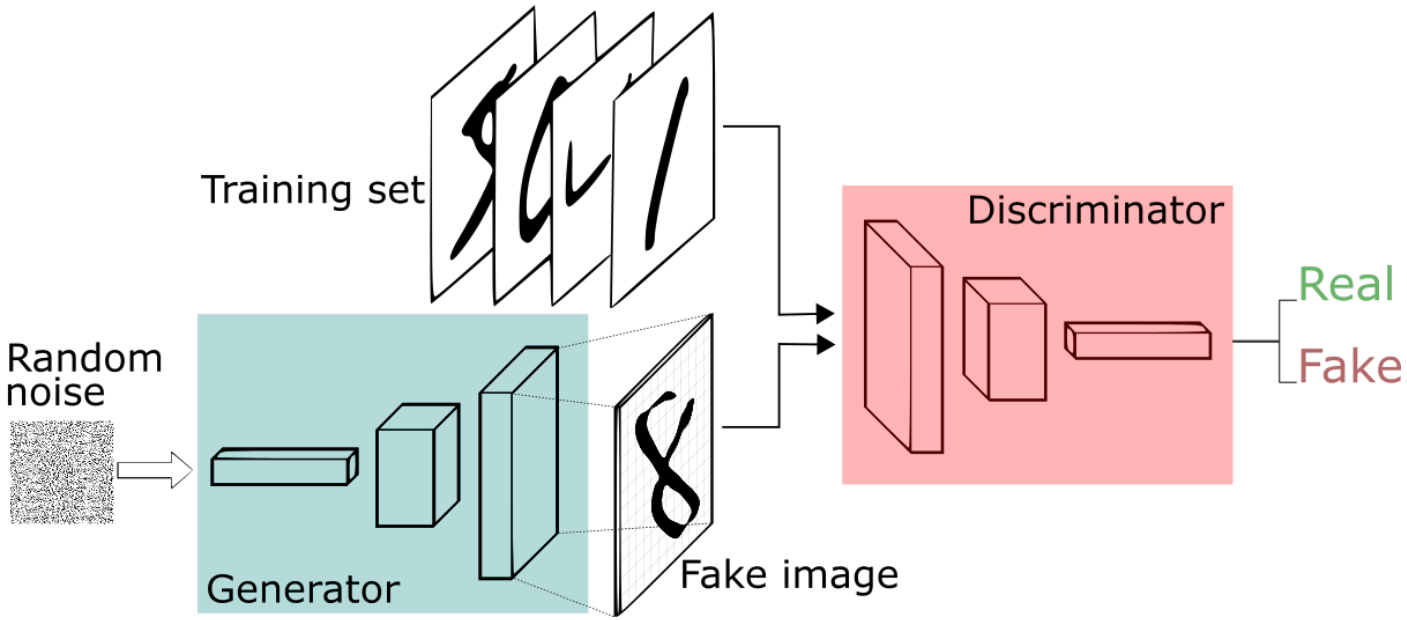
- Make them "compete" : the discriminator will become better at classifying the fake samples, the generator will become better at fooling the discriminator



GAN training

- The original GAN paper presents the problem as a two-players minimax game, based on the logistic regression loss :

$$\min_{\theta_g} \max_{\theta_d} \mathbb{E}_{x \sim p_{data}} [\log D_{\theta_d}(x)] + \mathbb{E}_{z \sim \mathcal{N}} [\log(1 - D_{\theta_d}(G_{\theta_g}(z)))]$$

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Original algo : alternate k steps of gradient ascent for D with one step of gradient descent for 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.

GAN issues

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- Hard to train : minimax problems are typically hard !
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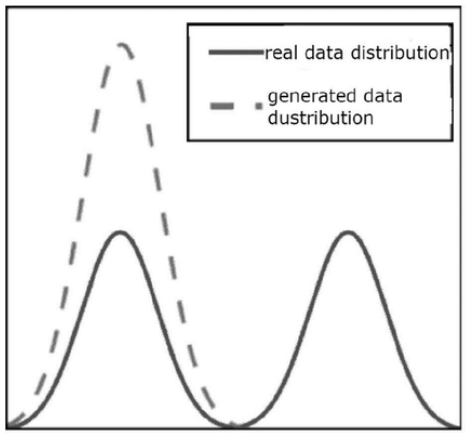
- Data-hungry : GANs require a **lot** of data to be trained properly
- Mode collapse : the generator produces limited diversity (eg, for a dataset with cats and dogs, produces only dogs)



(a)


(b)

Sota GANs

There are many (many!) tricks and variants to improve GANs. Mostly, bigger models with more data seem to be always better! (BigGAN below). Seemed a bit depressing for a time...

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But nowadays, they have been mostly replaced with more modern approaches like diffusion models.

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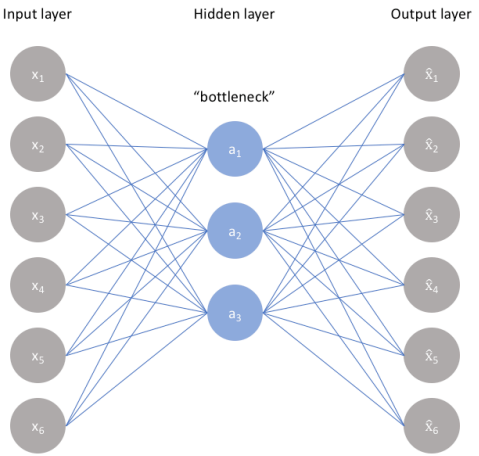
Auto-Encoder

- We have seen Auto-Encoder :
  - Encoder : images $\rightarrow$ compressed latent space
  - Decoder : latent space $\rightarrow$ image



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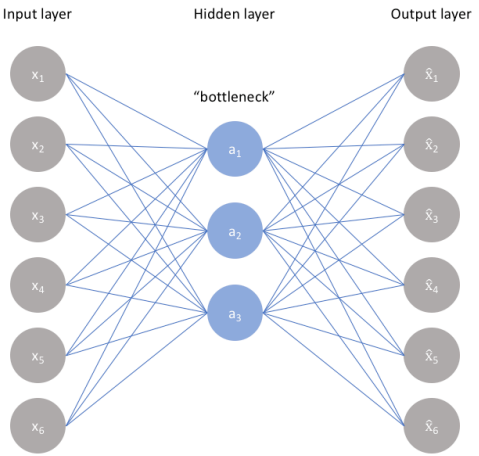

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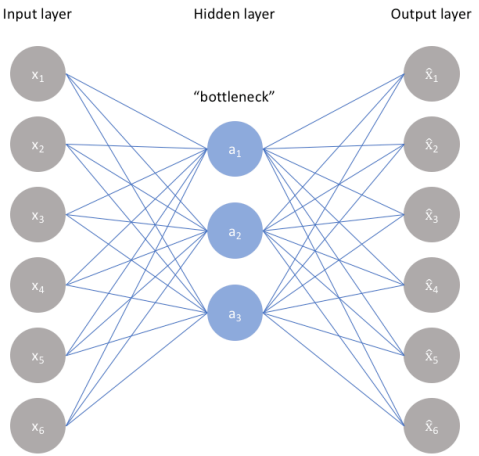

- Idea : by working directly in the latent space, the decoder is a generative model !
- Difficulty : sampling a random vector in the latent space might produce garbage. The latent space is highly irregular !

Variation Auto-Encoder (VAE) Kingma and Welling, 2014

https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

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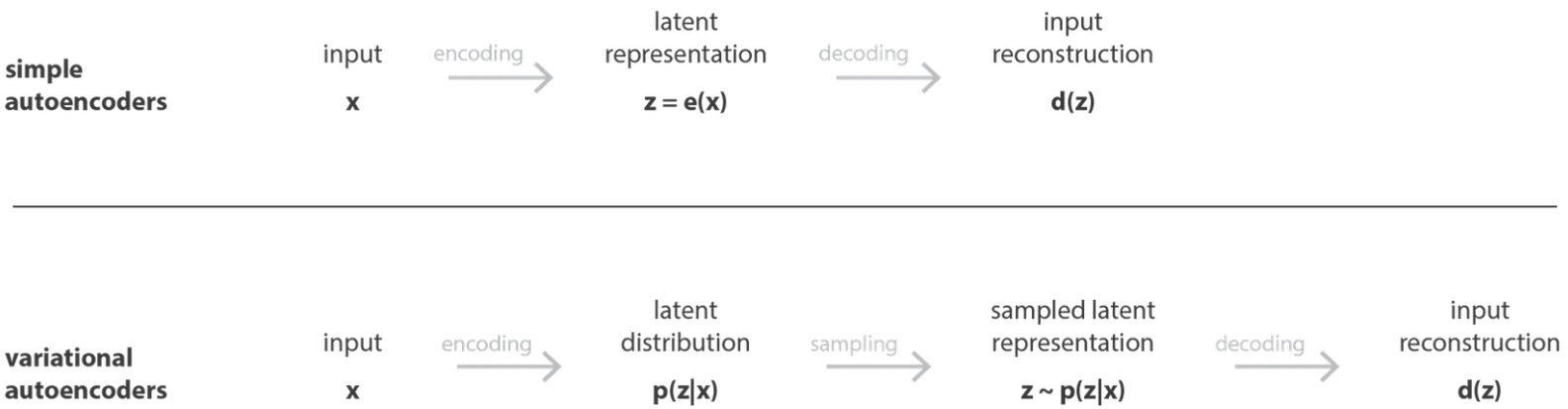

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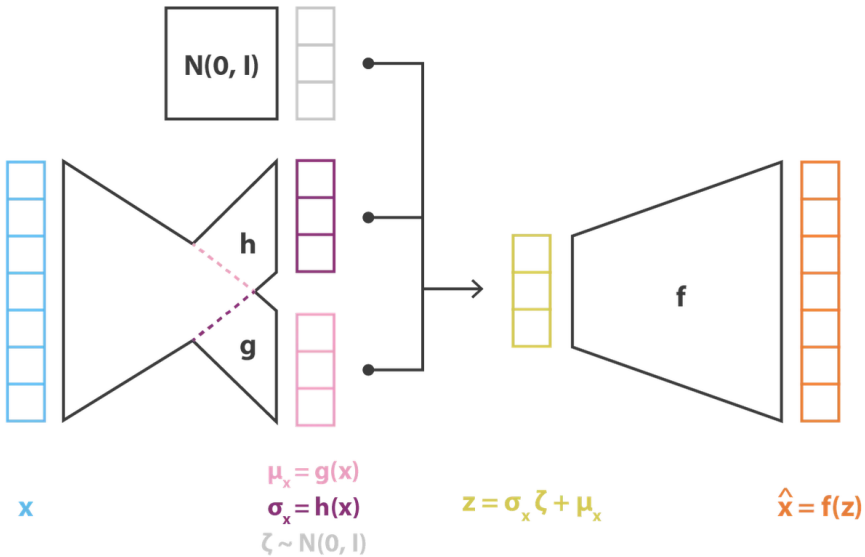

$$\text{loss} = C \,||\, x - \hat{x} \,||^2 + KL[\, N(\mu_x, \sigma_x), N(0, I)\,] = C \,||\, x - f(z) \,||^2 + KL[\, N(g(x), h(x)), N(0, I)\,]$$

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- Desired properties : continuity (two close points in the latent space should give close outputs) and completeness (sampling any point should give a reasonable result)
- Connection with Variational Inference (hence the name)
- Easier to train than GANs, but output might have less diversity

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Diffusion models

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

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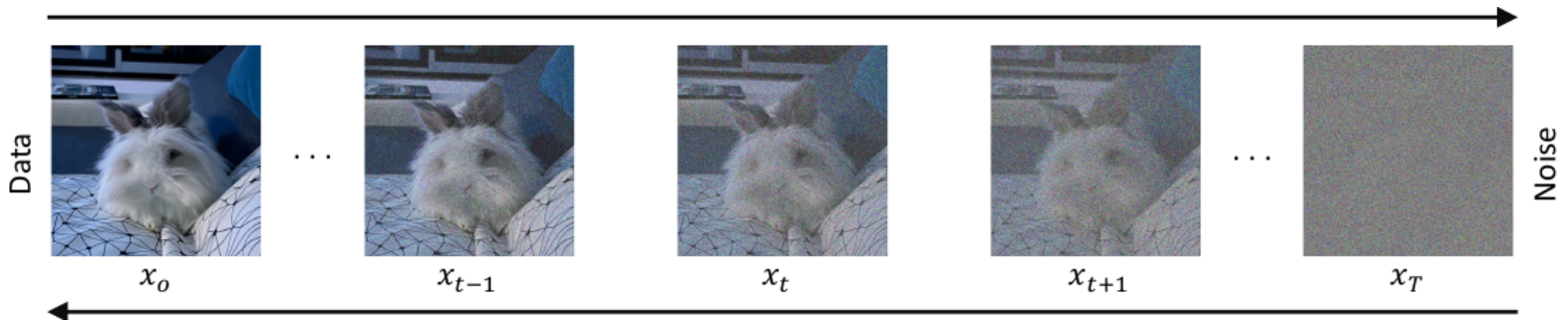
- Idea (roughly) : train a model to denoise an image, at many different noise levels. Then, start with random noise (!), and denoise it until an image is produced !
- Interpretation : we learn to "reverse" the diffusion process that gradually transforms an image into pure noise



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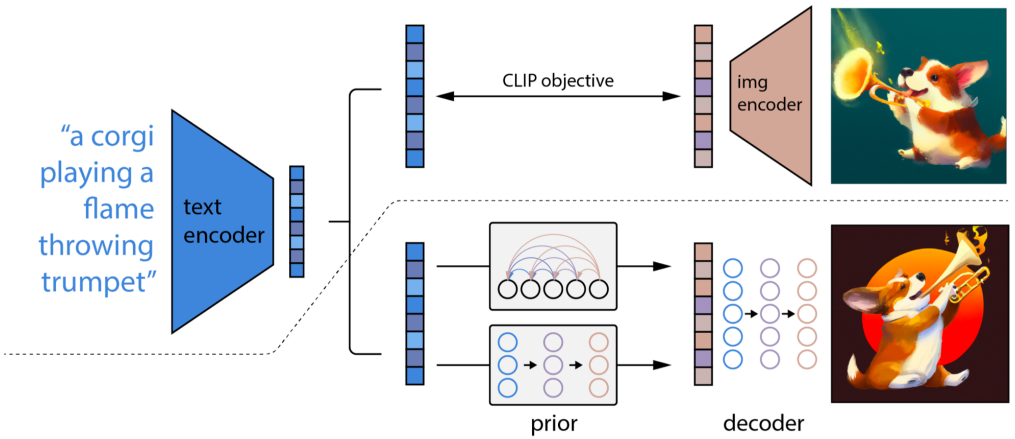

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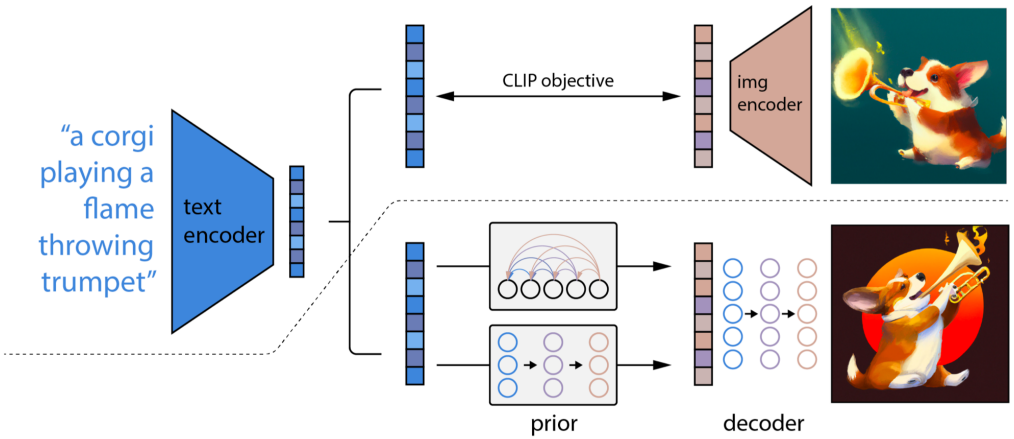

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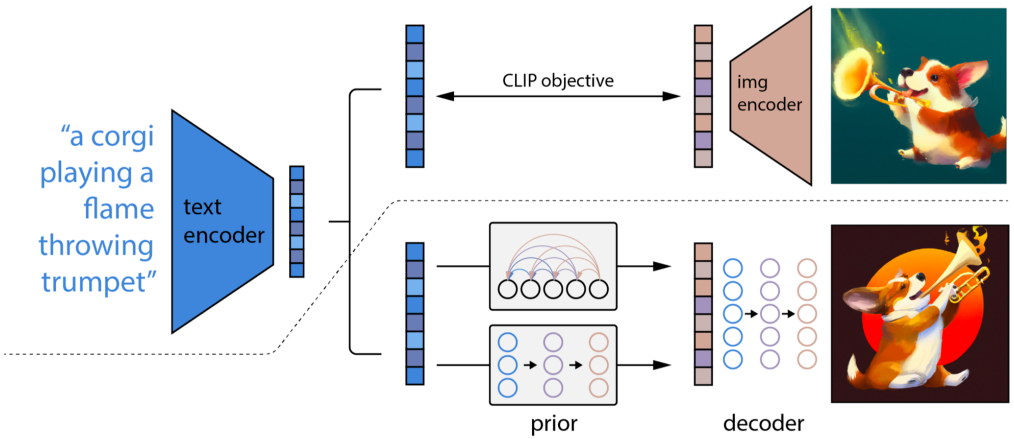

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- Con : slow sampling. The sampling process is slower, we must perform many steps of denoising.

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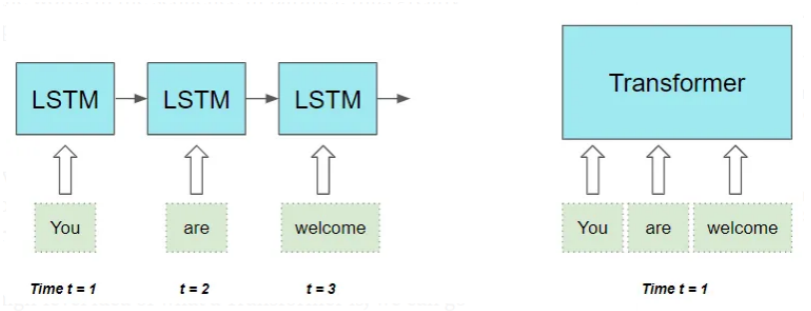
Transformers : what

https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

- Transformers (Vaswani et al.), introduced by Google in 2017, have revolutionized first Natural Language Processing (NLP), then many other domains
- Documents classification, translation, text generation, text-to-image, image-to-text, chatbots...
- Well-known models, mostly from two companies :
  - Google : BERT, and successors : RoBERTa, ALBERT... (for French language : CamemBERT model !). Also T5, PaLM, etc.
  - OpenAI : GPT, and successors : GPT-2, GPT-3, ChatGPT...

Transformers : how ?

- Unlike RNNs, Transformers almost totally discard the "sequential" nature of texts : everything depends on everything !



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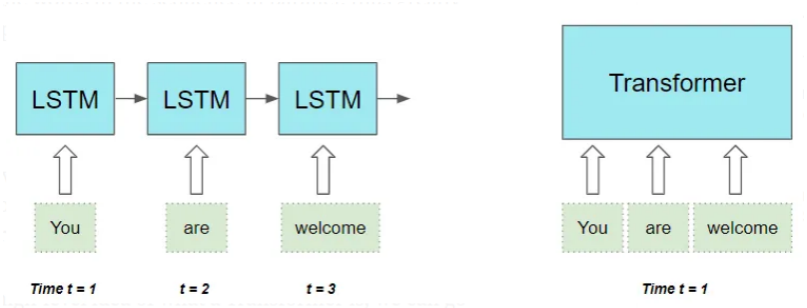

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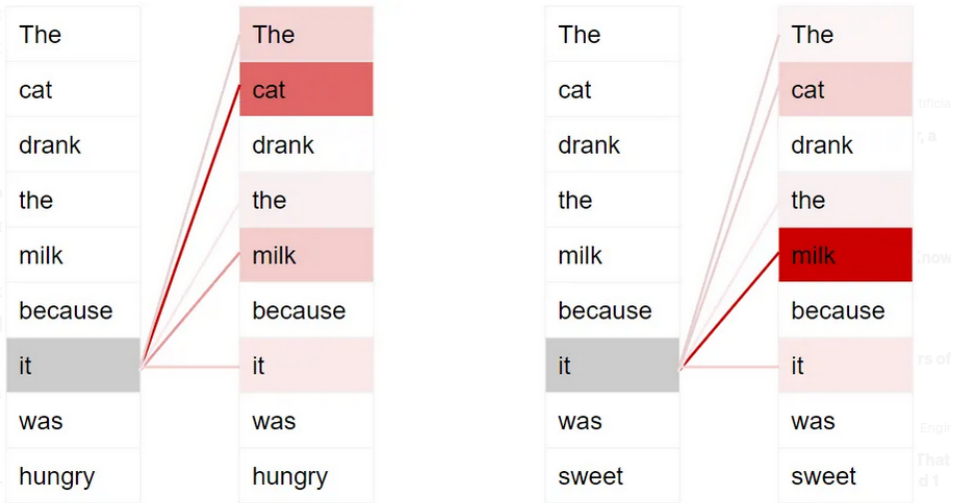
The key to Transformers is **attention** : a (deceptively) simple mechanism to model dependencies between words/objects



Attention : equations

- In NLP, words (or subwords) are *token*, embedded using a tokenizer.

Algorithm 3: Basic single-query attention.

Input: $\boldsymbol{e} \in \mathbb{R}^{d_{\text{in}}}$, vector representation of the current token

Input: $\boldsymbol{e}_t \in \mathbb{R}^{d_{\text{in}}}$, vector representations of context tokens $t \in [T]$.

Output: $\tilde{\boldsymbol{v}} \in \mathbb{R}^{d_{\text{out}}}$, vector representation of the token and context combined.

Parameters: $\boldsymbol{W}_q, \boldsymbol{W}_k \in \mathbb{R}^{d_{\text{attn}} \times d_{\text{in}}}$, $\boldsymbol{b}_q, \boldsymbol{b}_k \in \mathbb{R}^{d_{\text{attn}}}$, the query and key linear projections.

Parameters: $\boldsymbol{W}_v \in \mathbb{R}^{d_{\text{out}} \times d_{\text{in}}}$, $\boldsymbol{b}_v \in \mathbb{R}^{d_{\text{out}}}$, the value linear projection.

$\boldsymbol{q} \leftarrow \boldsymbol{W}_q \boldsymbol{e} + \boldsymbol{b}_q$

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Phuong and Hutter. Formal Algorithms for Transformers. 2022

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- The key operation is softmax $a_k : x \mapsto \frac{e^{x_k}}{\sum_i e^{x_i}}$. Attention is nothing else that common linear operations with learned parameters, with proper normalization.

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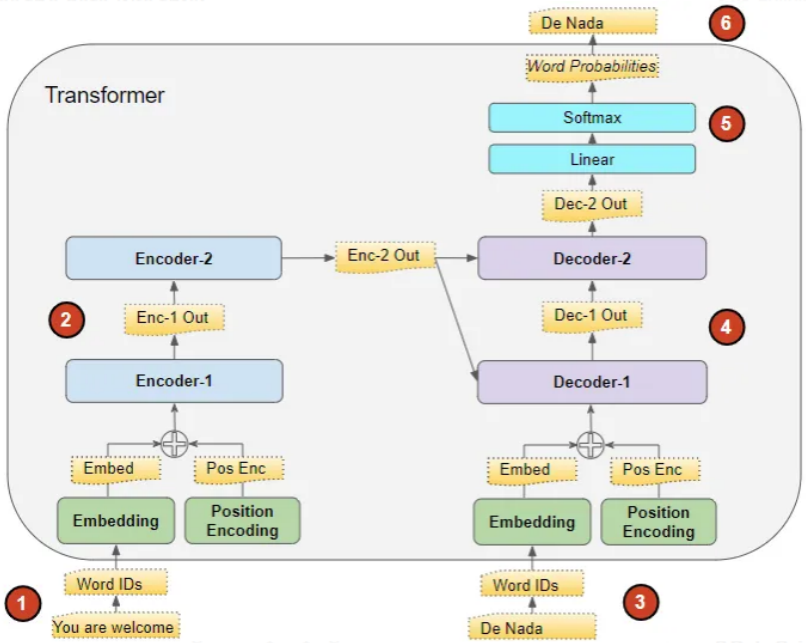
Transformer : example of a (high-level) seq2seq architecture

https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

- Training : takes a query x, a target y, produces an output



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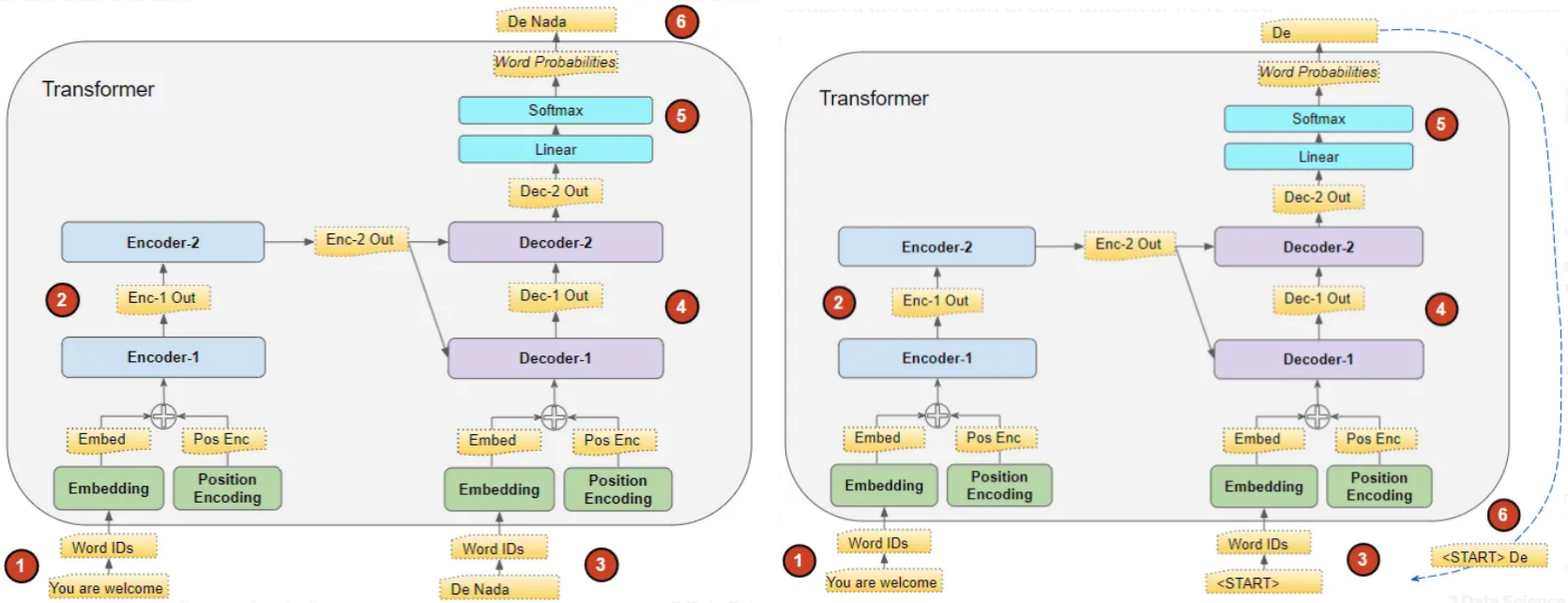

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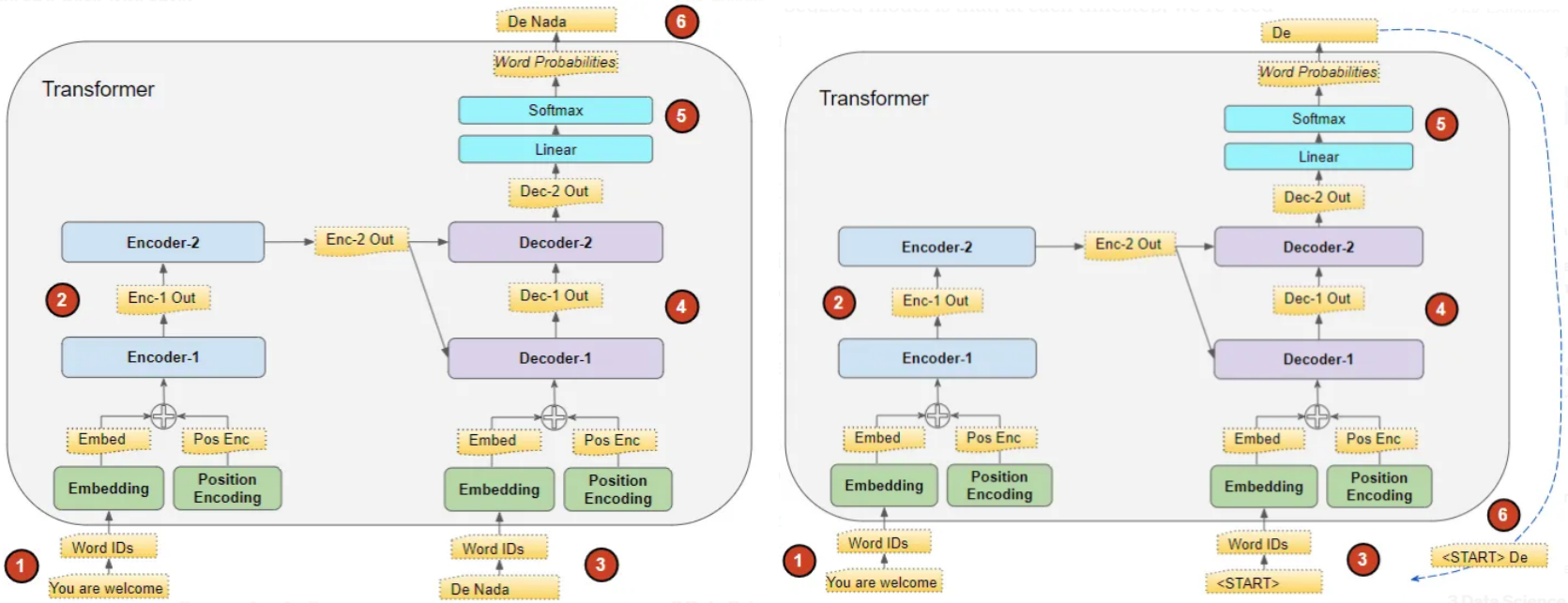
- Inference : takes a query x, start with an empty target, generate words one by one, by feeding the sequence generated until now as the target ("next word prediction")
- Unlike RNNs/LSTMs, the next word generated directly depends on everything else (through attention and self-attention), not just by recurrent mechanisms



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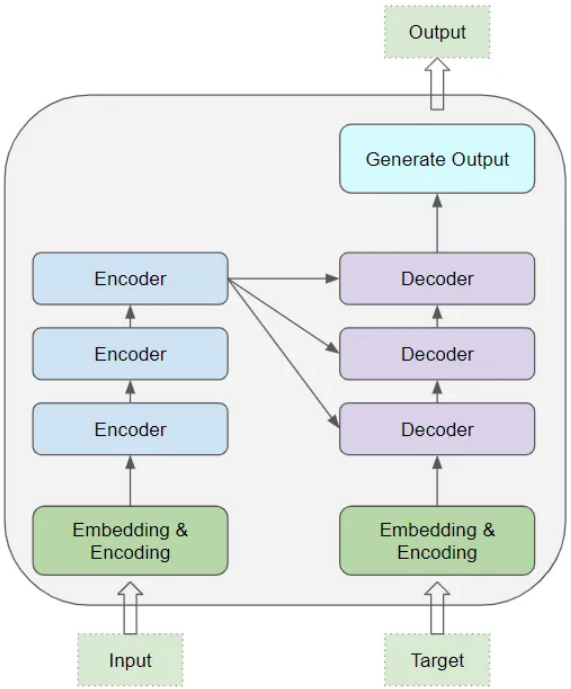
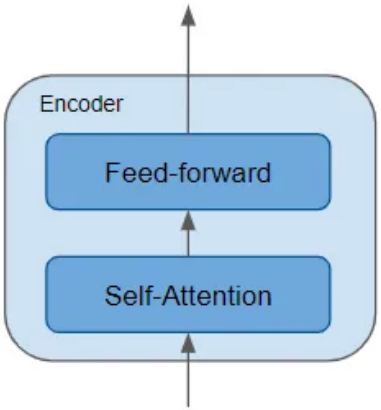
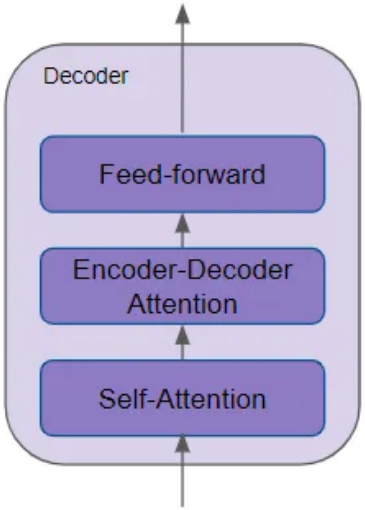
- Familiar concepts : encoding/decoding, latent space... but with attention layers !







Transformers + RL

- Combined with RL strategies (action/rewards), Transformers become incredible chatbots.

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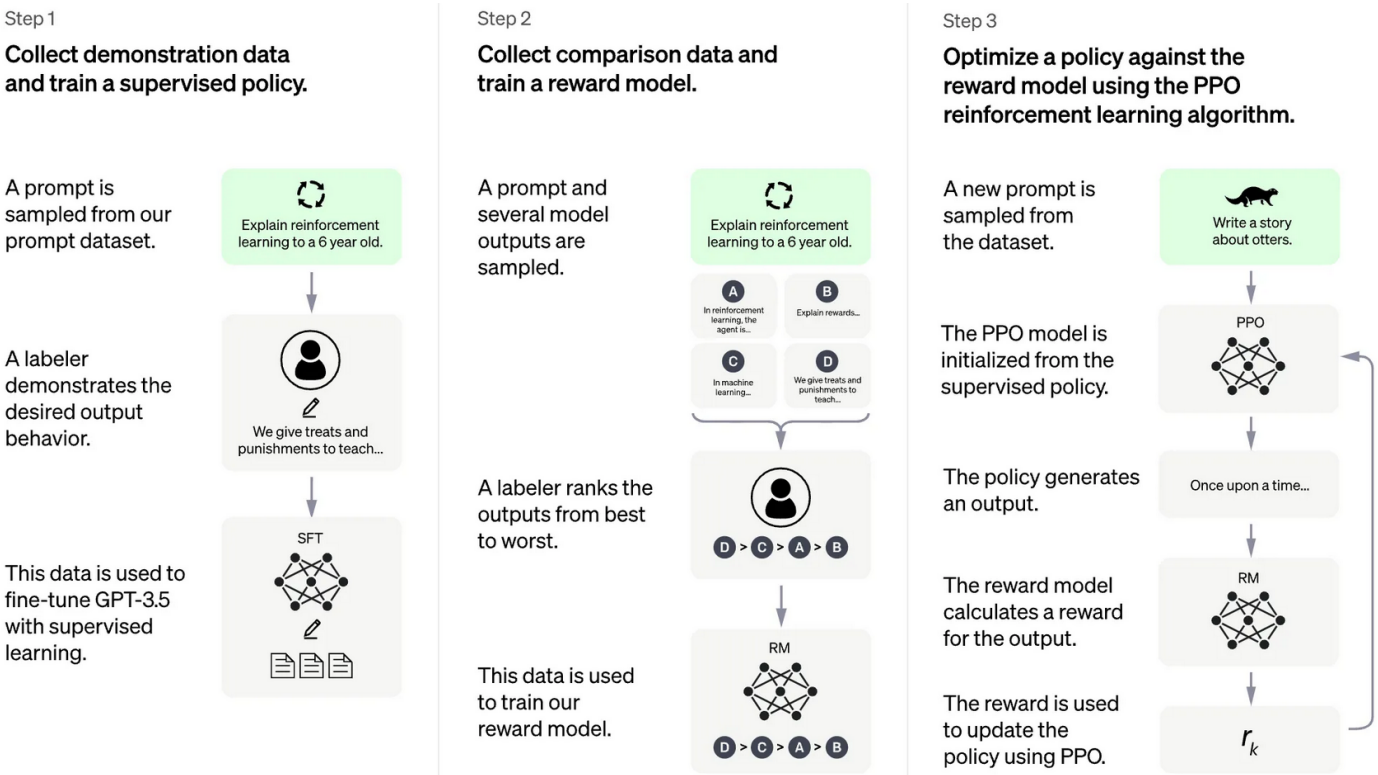
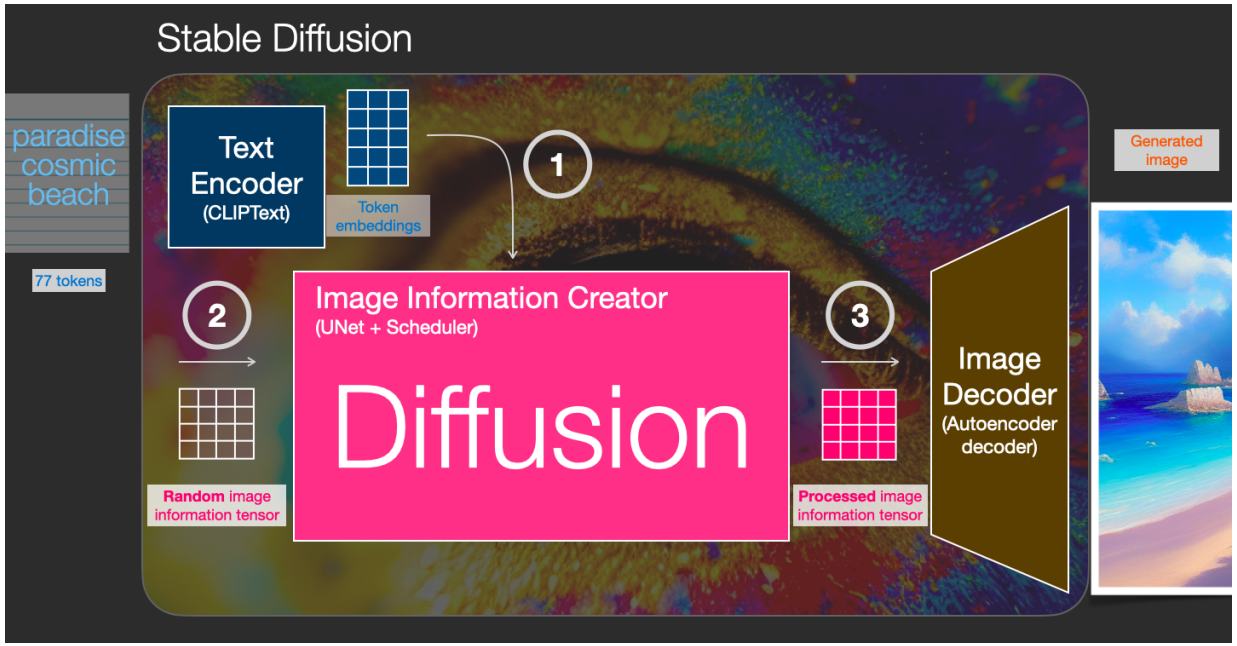
- ChatGPT is based on the GPT3 model (Generative Pre-trained Transformer), trained with complex RL strategies and HUGE amount of data.



Transformers + diffusion models

- Transformers are great at computing embeddings for text, that can be used for other tasks. The BERT model is only an embedding model !
- These embeddings can be fed to other generative models. For instance, all the modern text-to-images models (Stable Diffusion, Midjourney, Imagen, DALL-E 2...) are based on Transformers + diffusion models.
- All these components are pretrained ! And then fine-tuned once put together.
- Many models/datasets are open-source ! See HuggingFace 🤗 and eg `https://www.assemblyai.com/blog/build-a-free-stable-diffusion-app-with-a-gpu-backend/`



Transformers + language models + diffusion models + time series analysis + CNN + massive training data + immense computing power + ...

Text-to-video : OpenAI's Sora (from last week)

https://cdn.openai.com/sora/videos/tokyo-walk.mp4

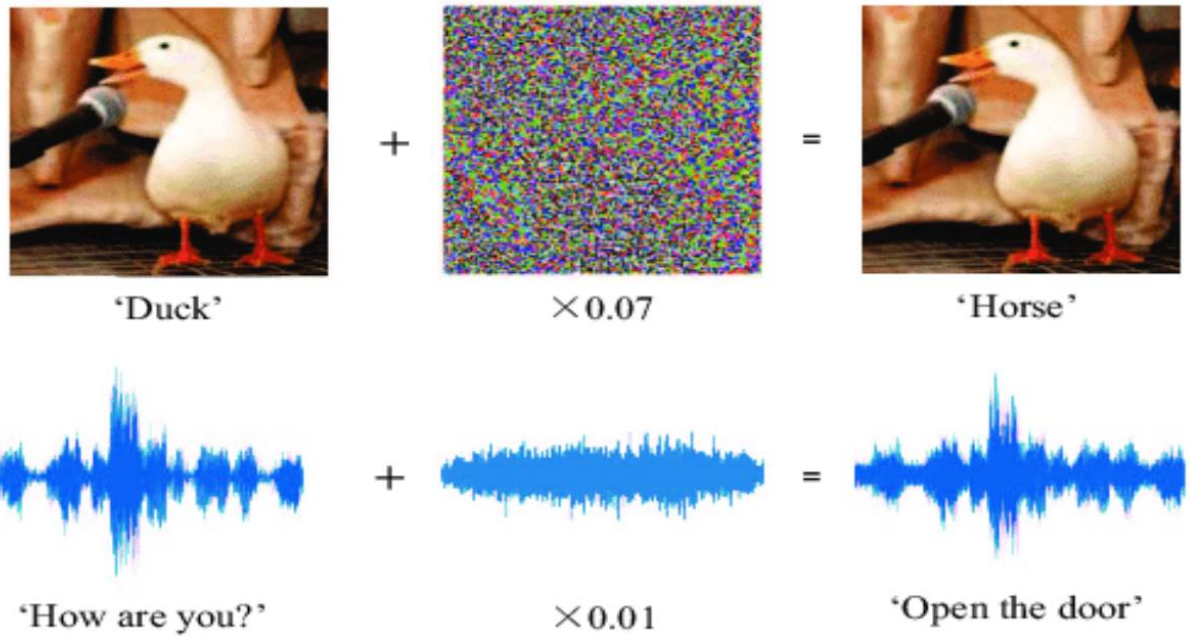
Table of Contents

Conclusion

- Deep learning is still mysterious and frustrating for many reasons
- They work incredibly well in some situations...
- ...but don't kill flies with bazookas, and always remember the basic principles ! (which are useful in deep learning too !)
- Modern librairies make them easy to build, easy to train...
- ... but they are useful for non-deep stuff too !

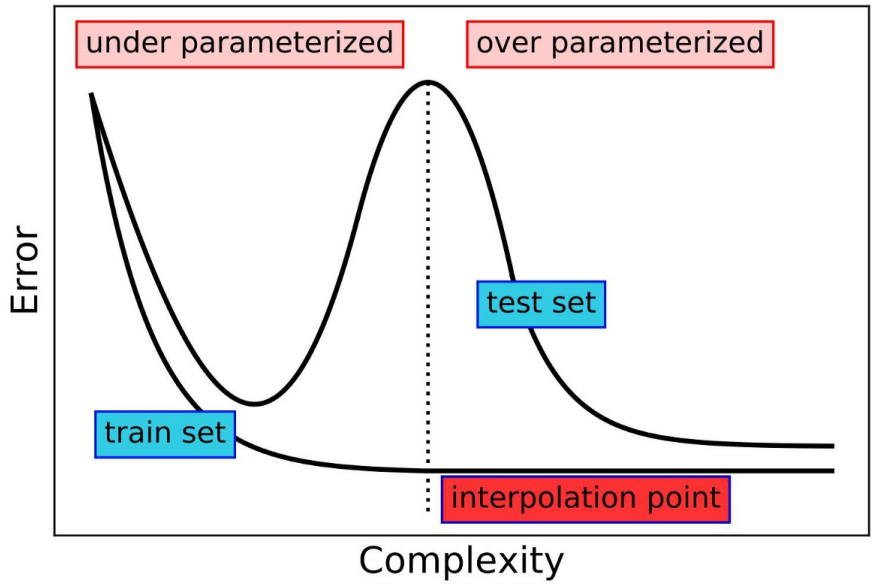
Hot question : adversarial attack

Once trained, a deep NN usually can be fooled easily, by designing an attack specifically for this NN. This unstability seems to be an integral part of high-performance NNs !



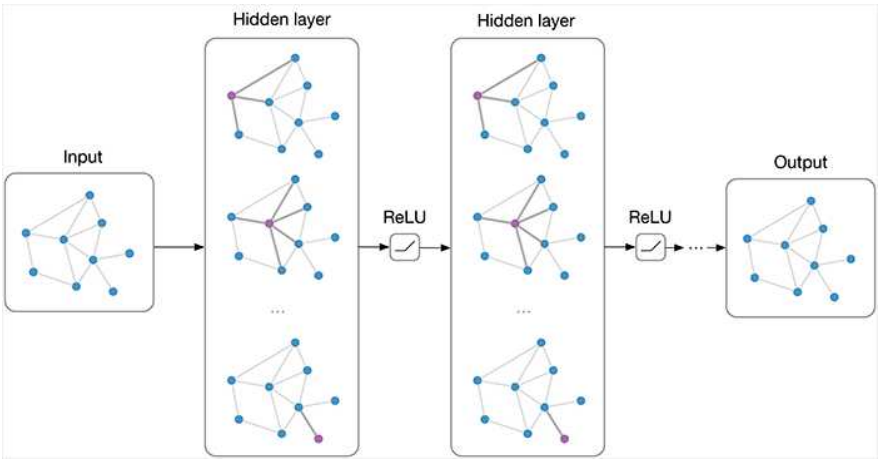
Hot question : generalization and double descent

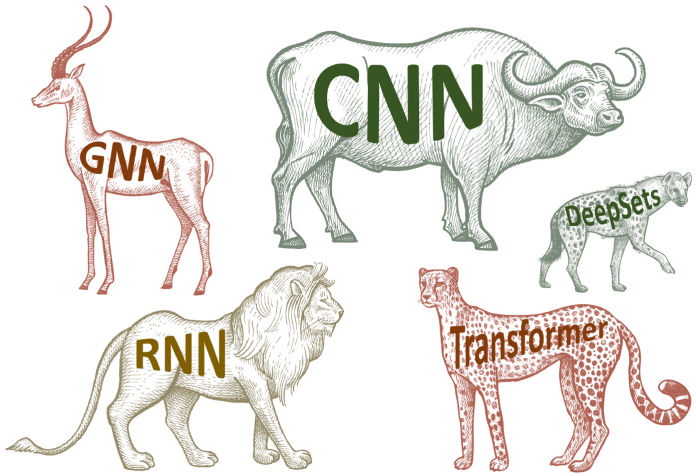
- Modern Deep NN are wildly overparametrized, and do interpolate the training data ! !
- But they still generatlize well !
- There is a double descent phenomenon : by increasing the complexity of the model past the interpolation point, among *all* interpolating models, it seems DNN+SGD favors models that generalize well. Still very much an open topic.



Hot topic : GNN, Geometric Deep Learning

- Graph Neural Networks (GNNs) work on irregular data that lives on network : molecules, proteins, social networks, computer networks, meshes, etc. They use "convolution" in this irregular space
- Most importantly, they are permutation-invariant : their output are left unchanged by a relabelling of nodes of the graph (graph isomorphism)
- They gave rise to geometric deep learning, which is the study of symmetries and invariances in DNNs : translation for CNN, permutation for GNN, but also rotation, gauge, etc. Much inspired by physics !





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AI is *not* gonna "destroy" the world, at least not Terminator-style. But... have we just destroyed / altered fundamentally crucial common goods ? Like the Internet ? Are we the last generation to "mostly" trust what we see online ?