

Deep Learning: advanced models

Generative models, Transformers, GNNs...

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ENSTA 2025

Pros and cons of deep learning

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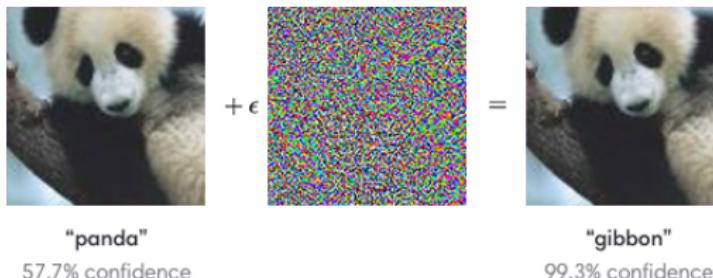
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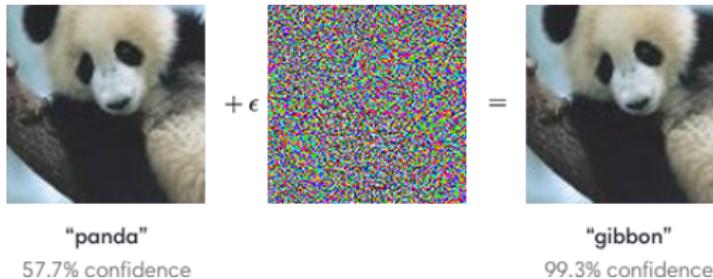
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- ▶ A **bazooka**, when sometimes all you need to do is kill a fly ! In many real-life scenarii, linear models, PCA, k -means... work amazingly well

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

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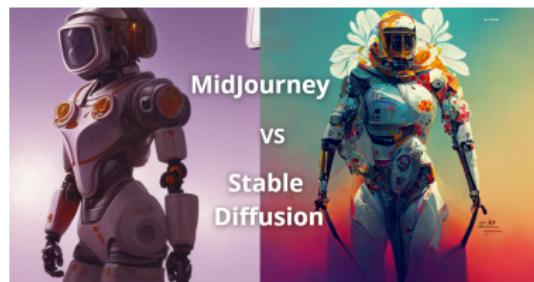
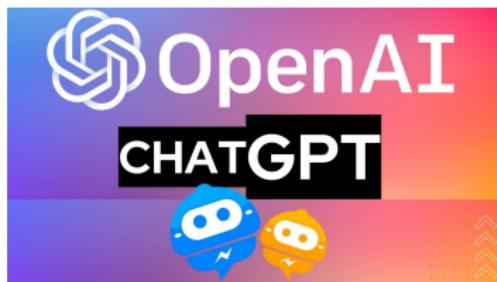
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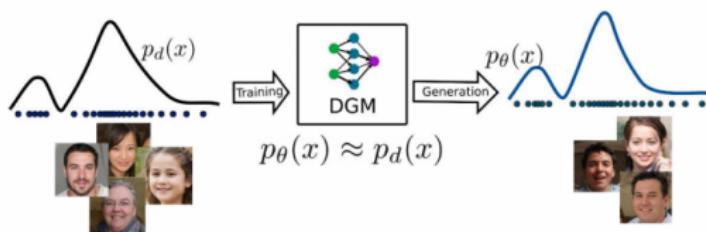
Generative model

- ▶ Goal : generate data resembling 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 explicitly (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.
 - ▶ This is an instantiation of a “transport” problem

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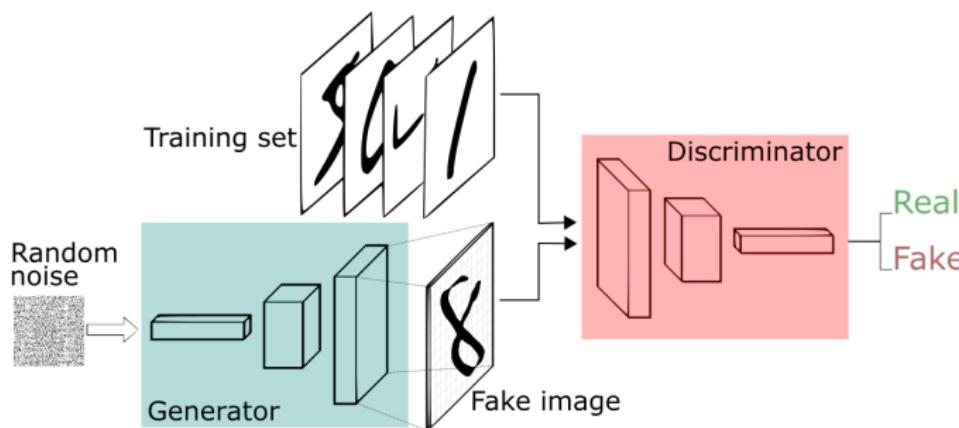
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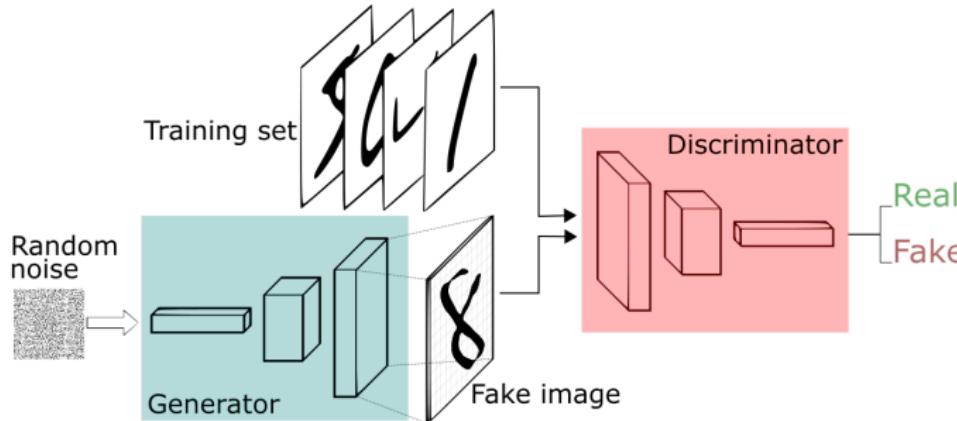
GAN description

- ▶ Train a **generator** network G_{θ_g} such that $G_{\theta_g}(z)$, with z Gaussian, are good samples
- ▶ Train a **discriminator** network D_{θ_d} to classify the samples as being from the training set or from the generator



GAN description

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- ▶ Train a **discriminator** network D_{θ_d} to classify the samples as being from the training set or from the generator
- ▶ 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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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 $\{z^{(1)}, \dots, z^{(m)}\}$ from noise prior $p_g(z)$.
- Sample minibatch of m examples $\{x^{(1)}, \dots, x^{(m)}\}$ from data generating distribution $p_{data}(x)$.
- Update the discriminator by ascending its stochastic gradient:

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

 end for

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

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

end for

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

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

GAN issues

- ▶ Hard to train : minimax problems are typically hard !

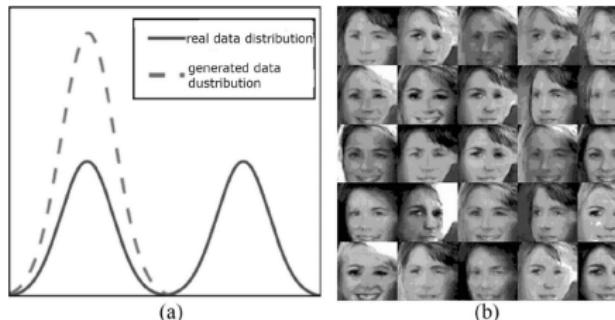
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GAN issues

- ▶ 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)



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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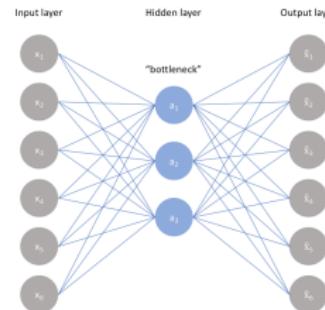
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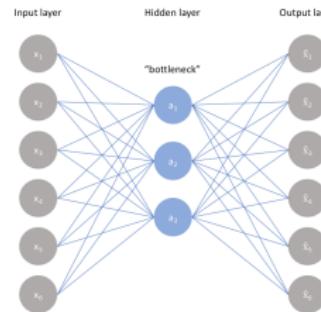
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 - ▶ Encoder : images → compressed **latent space**
 - ▶ Decoder : latent space → image



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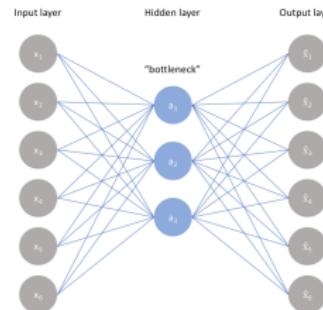
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- ▶ Idea : by working directly in the latent space, the decoder is a generative model !
- ▶ **Difficulty** : sampling a random vector in the latent space might produce garbage. The latent space is **highly irregular** !

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

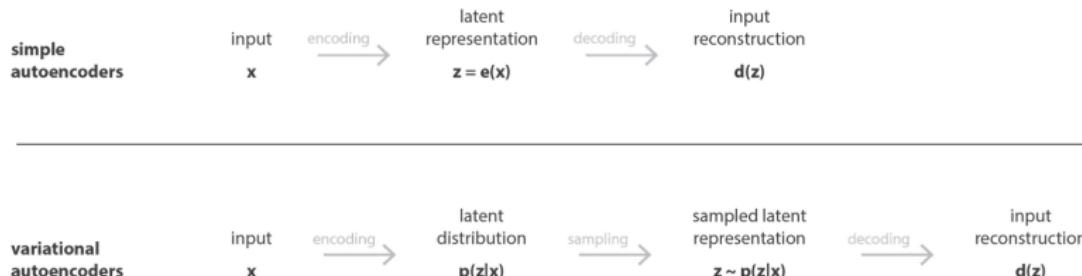
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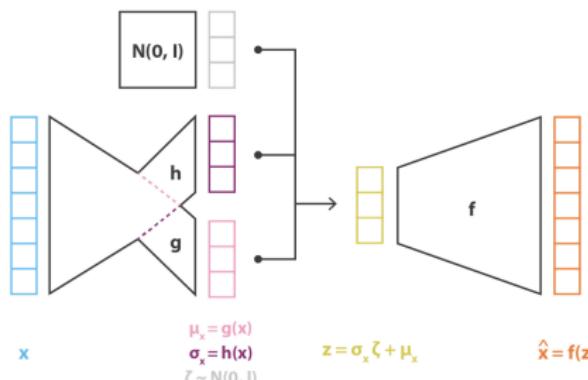
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 - ▶ encode inputs as distributions, and feed sample from these distributions to the decoder.
 - ▶ Add a regularizing term (Kullback-Leibler divergence) on these distributions.



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

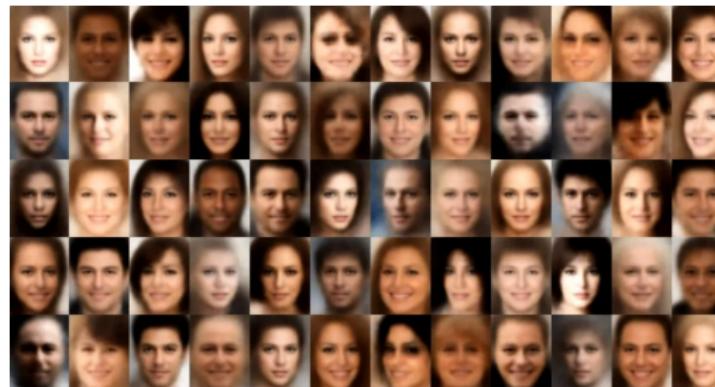
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- Desired properties : continuity (two close points in the latent space should give close outputs) and completeness (sampling any point should give a reasonable result)
- Connection with Variational Inference (hence the name)
- Easier to train than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



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

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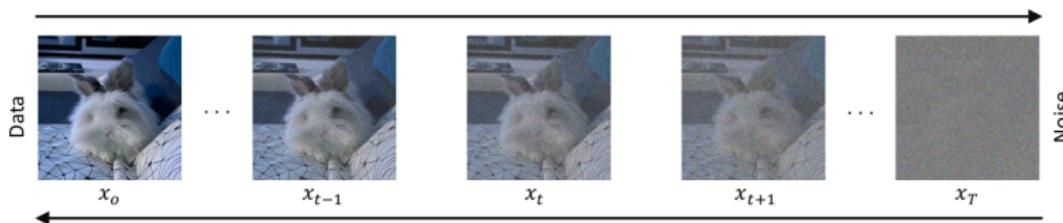
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- ▶ Idea (roughly) : train a model to **denoise** an image, at many different noise levels. Then, start with **random noise** (!), and denoise it until an image is produced !
- ▶ Interpretation : we learn to “reverse” the diffusion process that gradually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



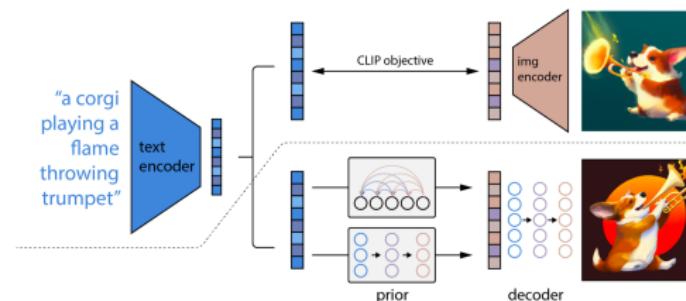
Diffusion models : pros

- ▶ Pro : Flexibility
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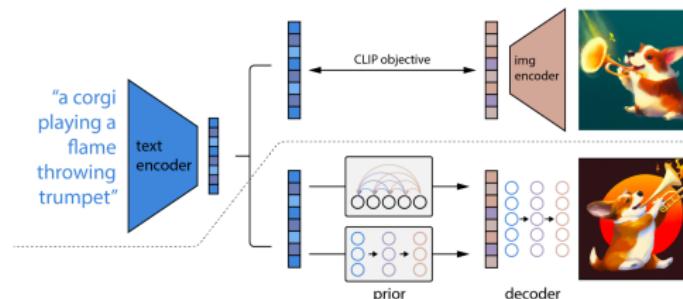
- denoising can happen **in the latent space**; somehow, learn to “project” random noise to a point in the latent space that makes sense
- possible to incorporate additional information/embedding at various stages before **conditional** diffusion happens : basis for all modern **text-to-image** systems ! (DALL-E, Stable Diffusion, Midjourney...)
- see eg <https://www.assemblyai.com/blog/how-dall-e-2-actually-works/>



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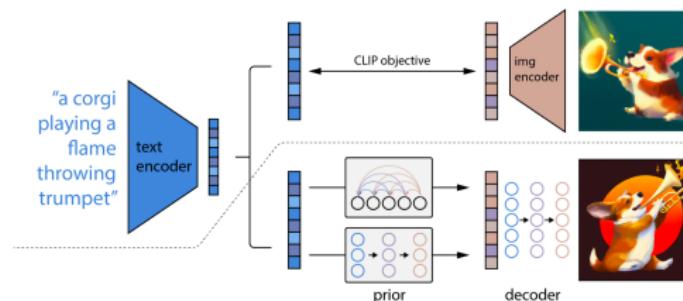


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- Pro : **Tractability and performance.** Every step is analytically tractable, thus improving stability and interpretability. Images are generally more realistic than GANs or VAEs
- Con : **slow sampling.** The sampling process is slower, we must perform many steps of denoising.

Diffusion models : the maths ?

- ▶ Diffusion models have renewed the interest in classical ODEs theory (w/ a lot of tool from physics), with an ML flavor
 - ▶ probability path, brownian motion, Fokker-Planck/Langevin equation...
 - ▶ see <https://iclr-blogposts.github.io/2024/blog/diffusion-theory-from-scratch/>

Diffusion : flow

- ▶ Variants/generalization are nowadays referred to as **flows** (matching flows, normalizing flows, conditional flow...)
 - ▶ see <https://dl.heeere.com/conditional-flow-matching/blog/conditional-flow-matching/>

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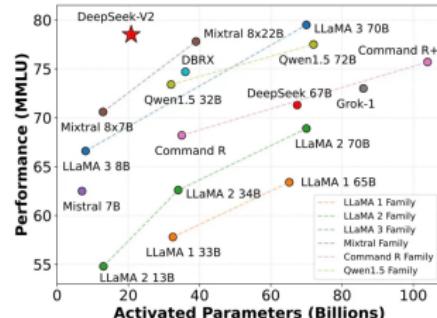
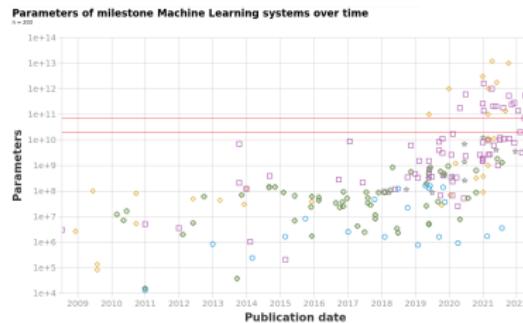
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Transformers : what

<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, historically from Google/Meta/OpenAI, now from everyone and their neighbors (go explore HuggingFace !)

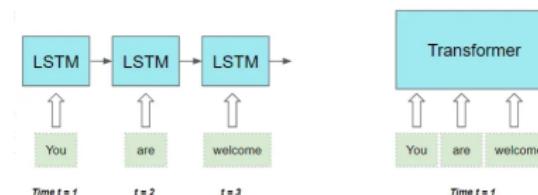


<https://epoch.ai/blog/machine-learning-model-sizes-and-the-parameter-gap>

<https://gradientflow.com/deepseek-v2-unpacked/>

Transformers : how ?

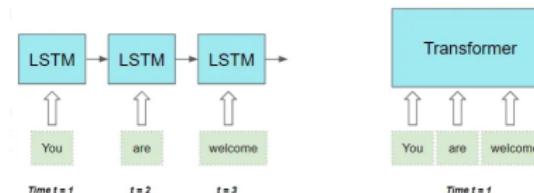
- ▶ Unlike RNNs, Transformers almost totally discard the “sequential” nature of texts : everything depends on everything !



- ▶ far, **far** more parameters ! (usually in the billions) : **huge training data, pre-trained components**. Modern Transformers can almost only be trained by companies with massive funding and resources. Ethical problems...

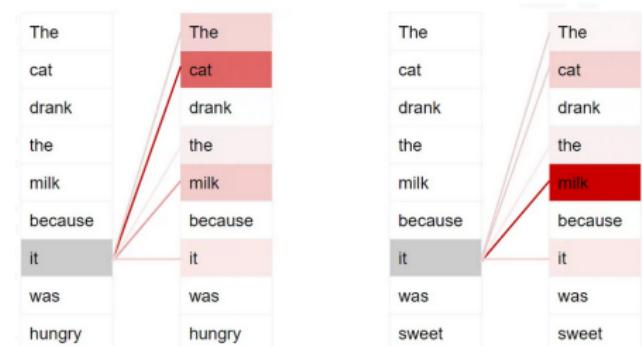
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The key to Transformers is **attention** : a (deceptively) simple mechanism to **model dependencies** between words/objects



Attention : equations

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

Algorithm 3: Basic single-query attention.

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

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

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

Parameters: $W_q, W_k \in \mathbb{R}^{d_{\text{attn}} \times d_{\text{in}}}$,
 $b_q, b_k \in \mathbb{R}^{d_{\text{attn}}}$, the query and key linear projections.

Parameters: $W_v \in \mathbb{R}^{d_{\text{out}} \times d_{\text{in}}}$, $b_v \in \mathbb{R}^{d_{\text{out}}}$, the value linear projection.

- 1 $q \leftarrow W_q e + b_q$
 - 2 $\forall t : k_t \leftarrow W_k e_t + b_k$
 - 3 $\forall t : v_t \leftarrow W_v e_t + b_v$
 - 4 $\forall t : \alpha_t = \frac{\exp(q^\top k_t / \sqrt{d_{\text{attn}}})}{\sum_u \exp(q^\top k_u / \sqrt{d_{\text{attn}}})}$
 - 5 **return** $\tilde{v} = \sum_{t=1}^T \alpha_t v_t$
-

Attention : equations

- ▶ In NLP, words (or subwords) are *token*, embedded using a [tokenizer](#).
- ▶ Given a token e , and **context tokens** e_t , **attention coefficients** are computed to relate e to the context

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

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 $b_q, b_k \in \mathbb{R}^{d_{\text{attn}}}$, the query and key linear projections.

Parameters: $W_v \in \mathbb{R}^{d_{\text{out}} \times d_{\text{in}}}$, $b_v \in \mathbb{R}^{d_{\text{out}}}$, the value linear projection.

- 1 $q \leftarrow W_q e + b_q$
 - 2 $\forall t : k_t \leftarrow W_k e_t + b_k$
 - 3 $\forall t : v_t \leftarrow W_v e_t + b_v$
 - 4 $\forall t : \alpha_t = \frac{\exp(q^\top k_t / \sqrt{d_{\text{attn}}})}{\sum_u \exp(q^\top k_u / \sqrt{d_{\text{attn}}})}$
 - 5 **return** $\tilde{v} = \sum_{t=1}^T \alpha_t v_t$
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Attention : equations

- ▶ In NLP, words (or subwords) are *token*, embedded using a [tokenizer](#).
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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 than common linear operations with learned parameters, [with proper normalization](#).

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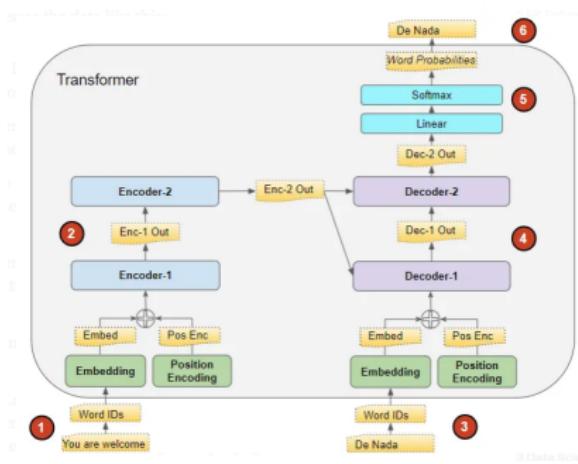
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Transformer : example of a (high-level) seq2seq architecture

https:

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

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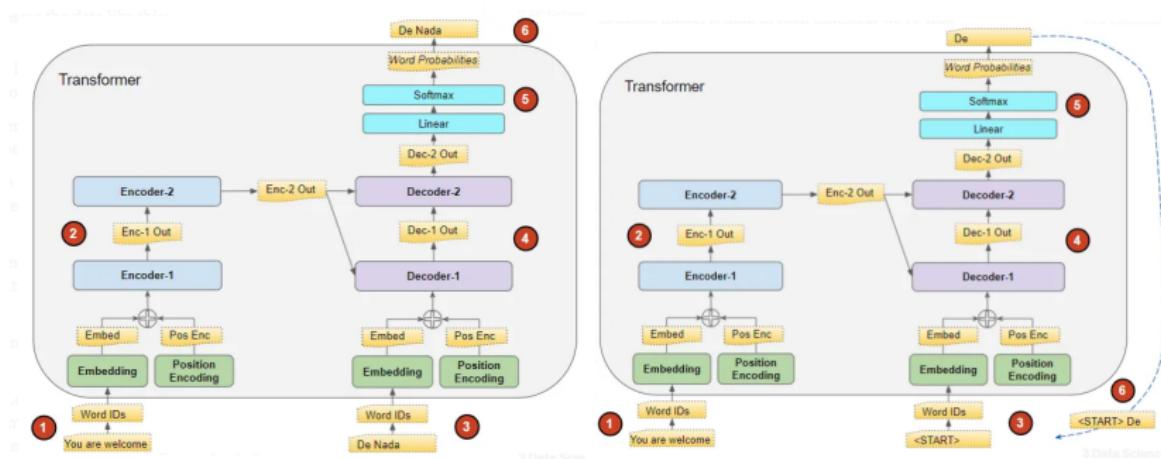


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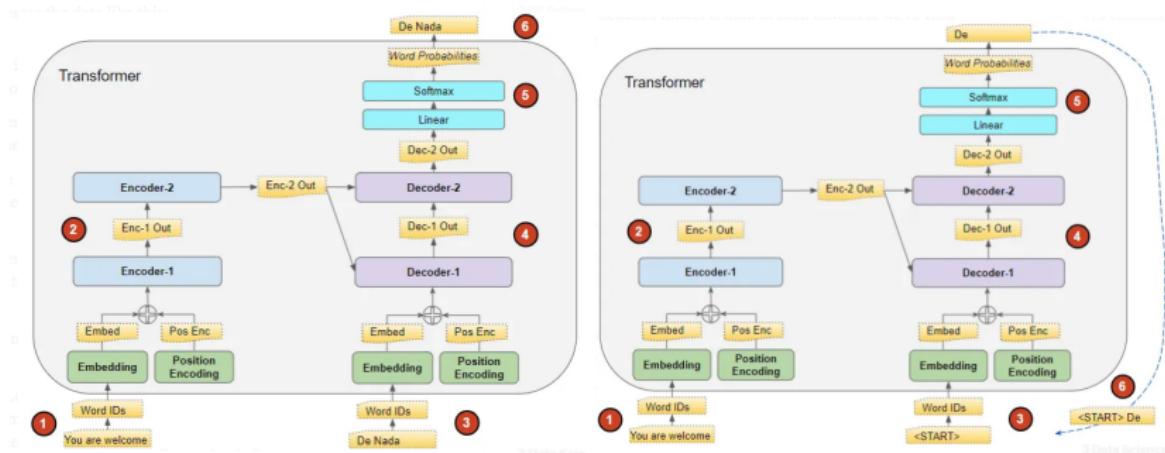


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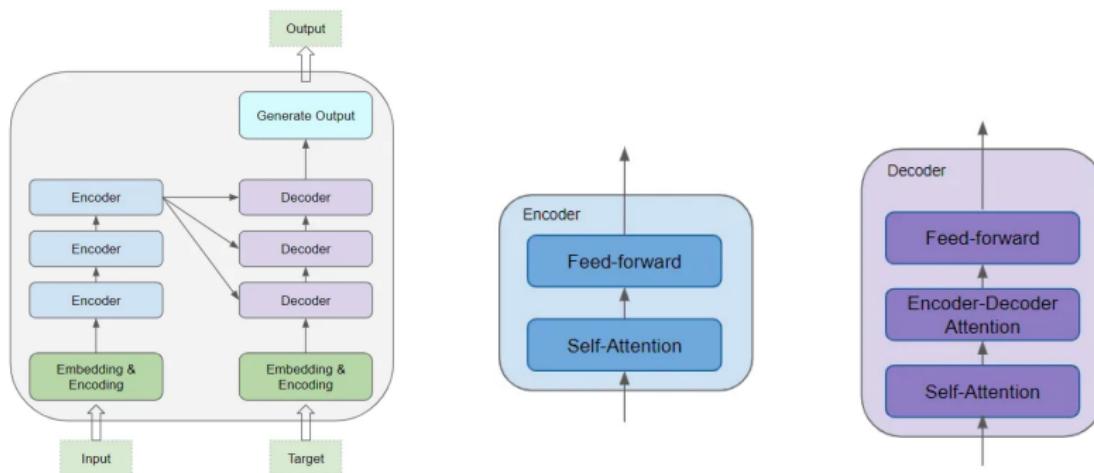
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- ▶ Training : takes a query x , a target y , produces an output
- ▶ Inference : takes a query x , start with an empty target, generate words one by one, by feeding the sequence generated until now as the target ("next word prediction")
- ▶ Unlike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



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

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

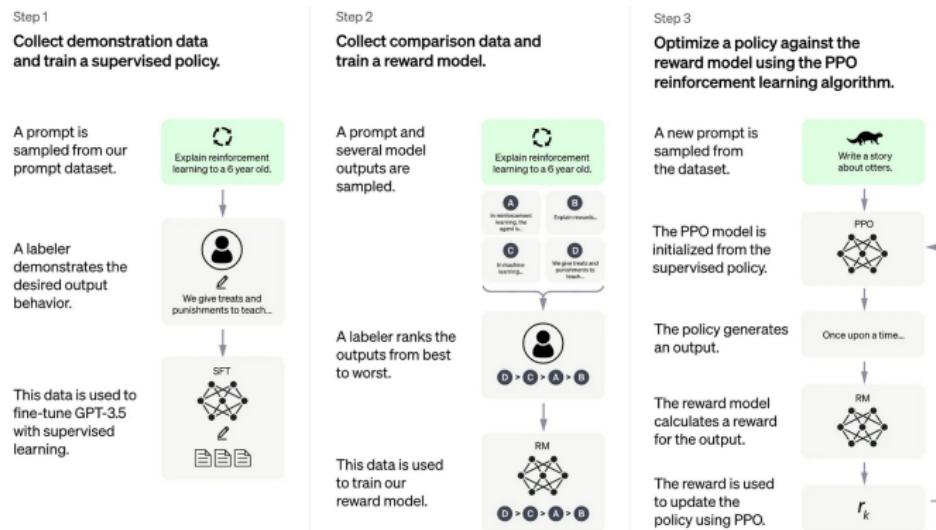


Transformers + RL

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

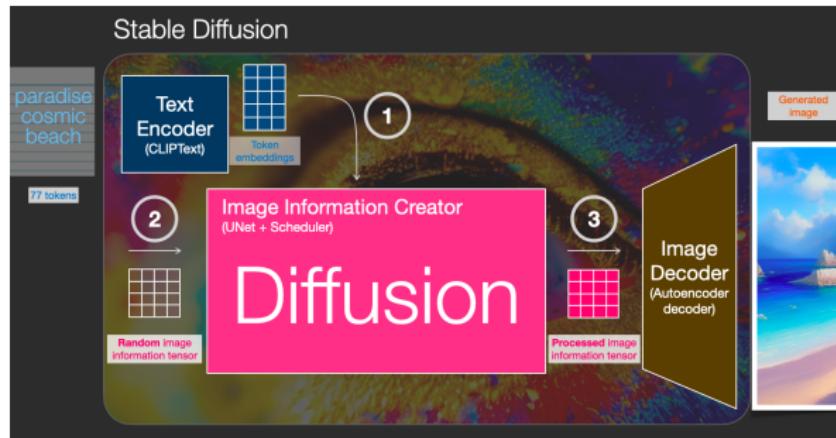
Transformers + RL

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



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

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Generative Models

Generative Adversarial Networks

Variational Auto-encoder

Diffusion models

Attention, Transformers

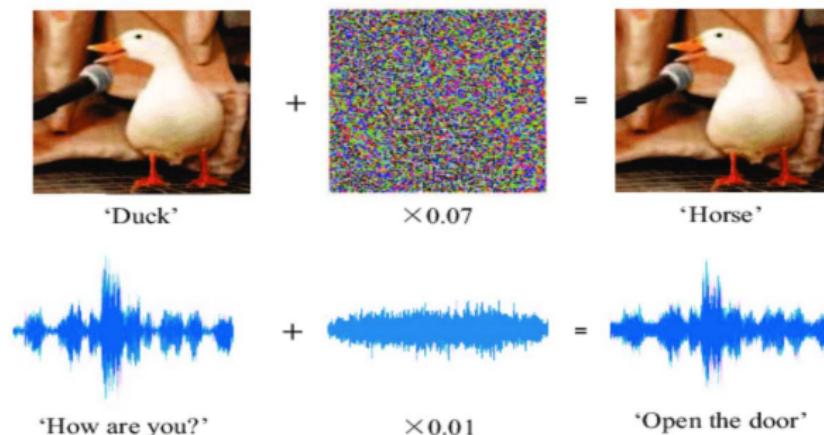
Conclusions and open questions

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 libraries make them easy to build, easy to train...
- ▶ ... but they are useful for non-deep stuff too !

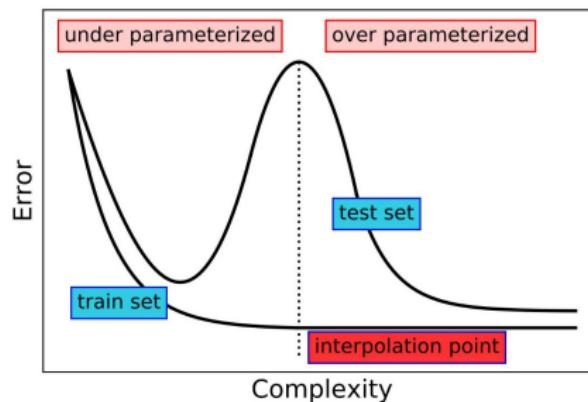
Hot question : adversarial attack

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 !



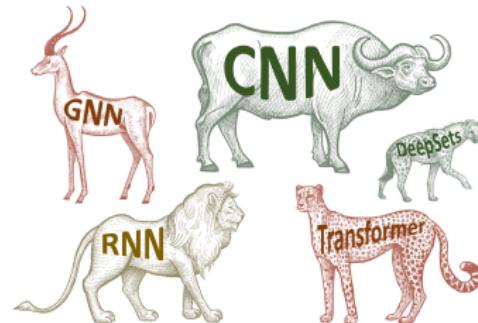
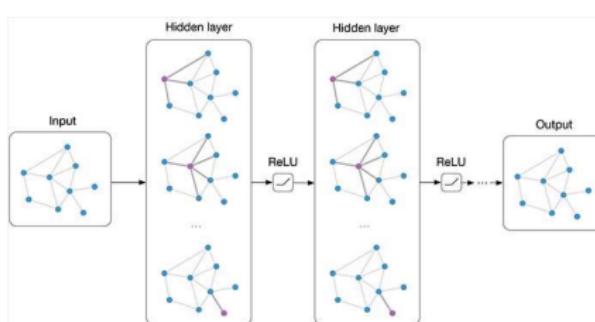
Hot question : generalization and double descent

- ▶ 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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- ▶ The **economic model** of a **chatbot** is discutable
- ▶ "A4Science" (healthcare, biology...) is promising, but has been for a long time
- ▶ A single "super-intelligent" entity is probably
 - ▶ unreachable
 - ▶ essentially useless
 - ▶ a fantasy from the 60s
- ▶ **Multiple systems** interacting for a better (?) society is probably what we should aim at
- ▶ M. Jordan at AI summit : "Beyond the hype, AI might simply be a **new engineering field**, one in which human is in the loop"
 - ▶ <https://www.youtube.com/live/W0QLq4qEmKg?si=umJjs-o3JTZqPDF5&t=3811>

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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 ?