Deep Learning: advanced models

Generative models, Transformers, GNNs...

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ENSTA 2025

Pros and cons of deep learning

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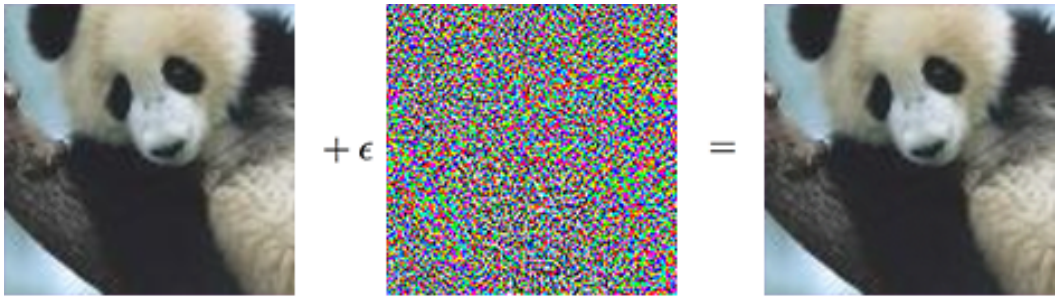

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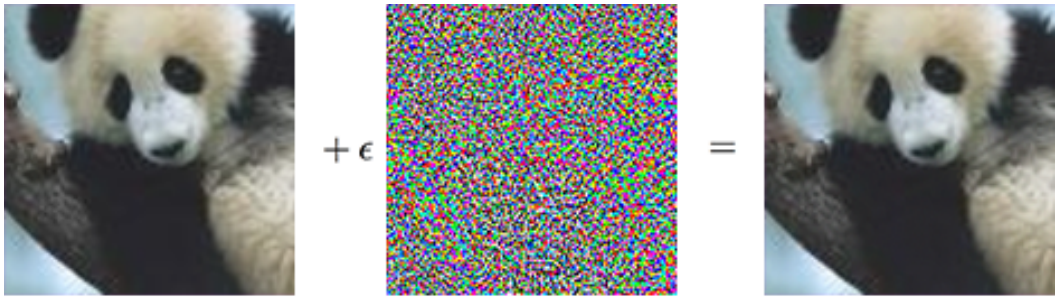

- A **bazooka**, when sometimes all you need to do is kill a fly ! In many real-life scenarii, linear models, PCA, k-means... work amazingly well

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But ! Deep Neural Nets :

- are easy to implement and optimize with modern libraries (Pytorch, JAX...), with automatic differenciation and GPU compatibility completely transparent
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- are amazingly flexible ! You can plug "anything anywhere", and it will almost always "work". Huge playground ! This can be dangerous ! Always be aware of what you do, or bugs will become impossible to fix.
- Today, we are going to see a few variants of DNNs, without going into details. Many ressources are available online.

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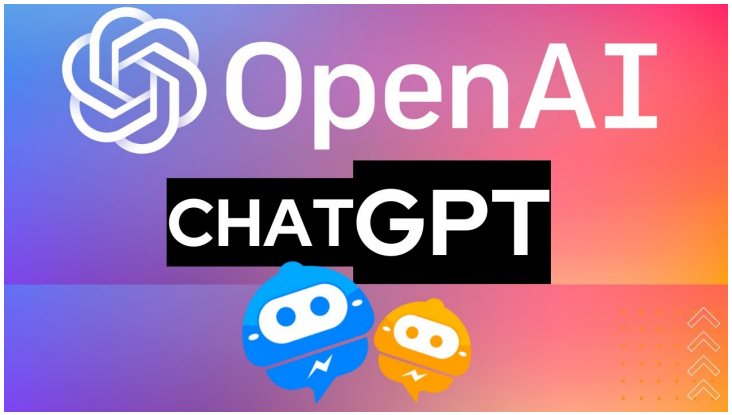
Some (subjective) non-technical considerations

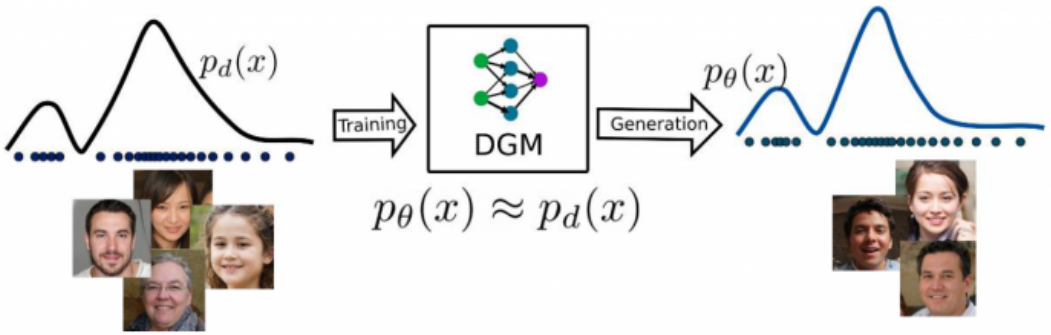
Generative model

- Goal : generate data ressembling other data.
- Have *de facto* become synonymous with “AI” for the mainstream audience



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)



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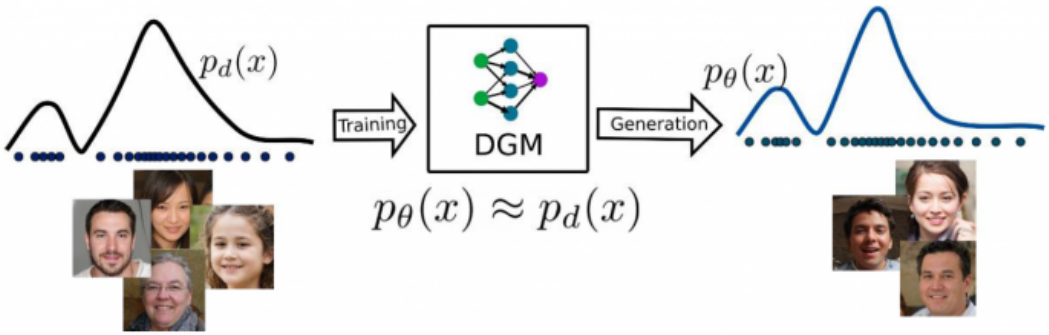
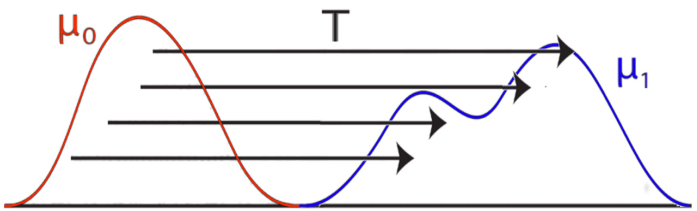


- Basic idea : take a very simple distribution in a latent space, eg $z \sim \mathcal{N}(0, Id)$, train a complicated function f_θ such that $f_\theta(z)$ are good samples.
  - This is an instantiation of a "transport" problem



N. Papadakis, Optimal Transport for Image Processing, habilitation à diriger des recherches, Université de Bordeaux, Dec. 2015

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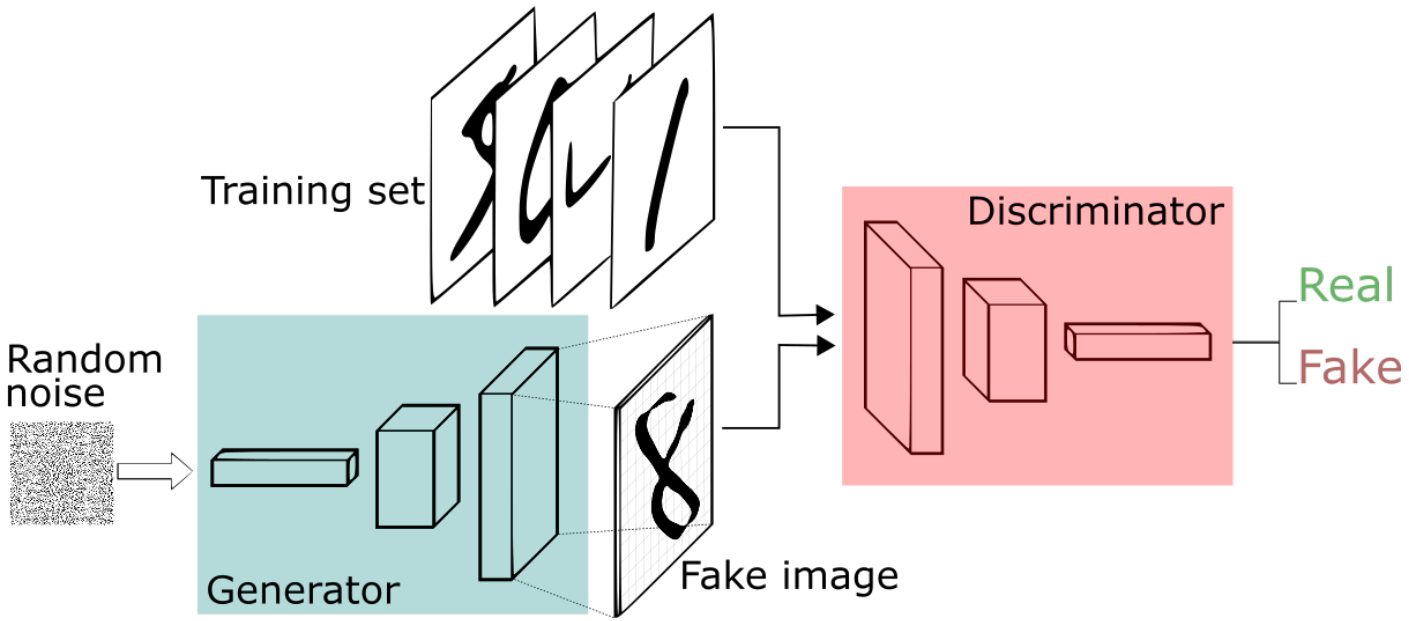
GAN description

- 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



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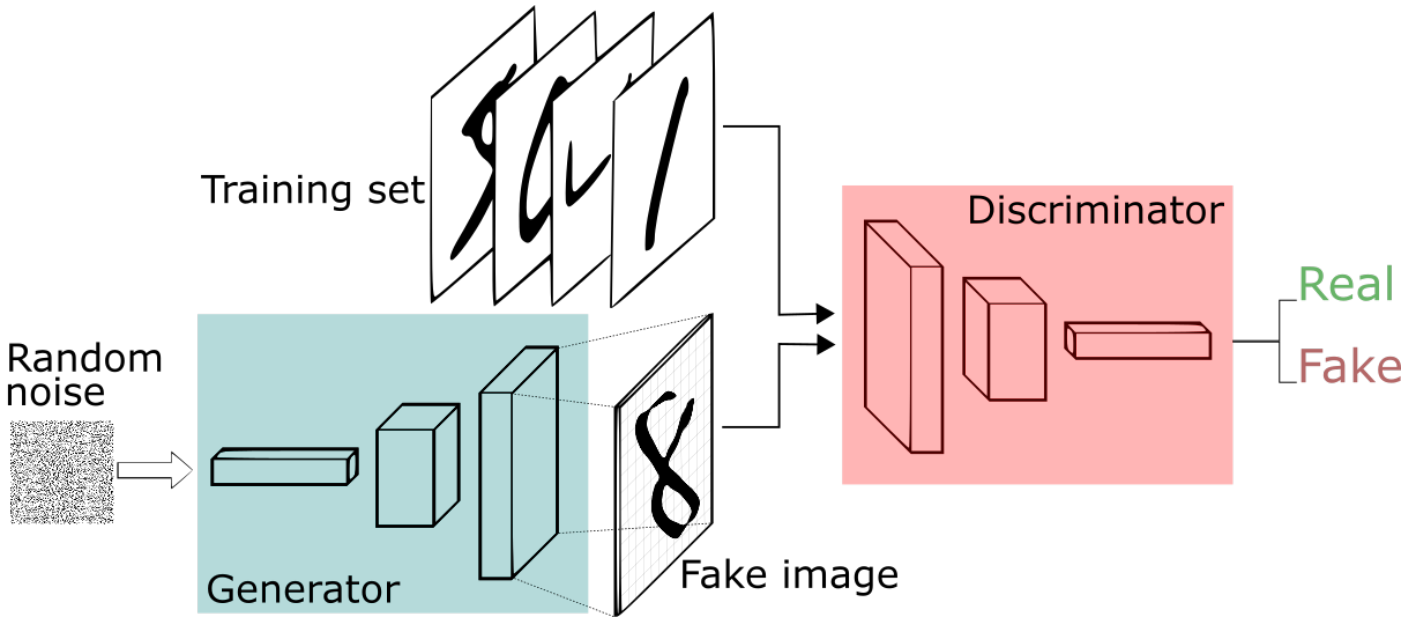
- Make them "compete" : the discriminator will become better at classifying the fake samples, the generator will become better at fooling the discriminator



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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  - they can loop
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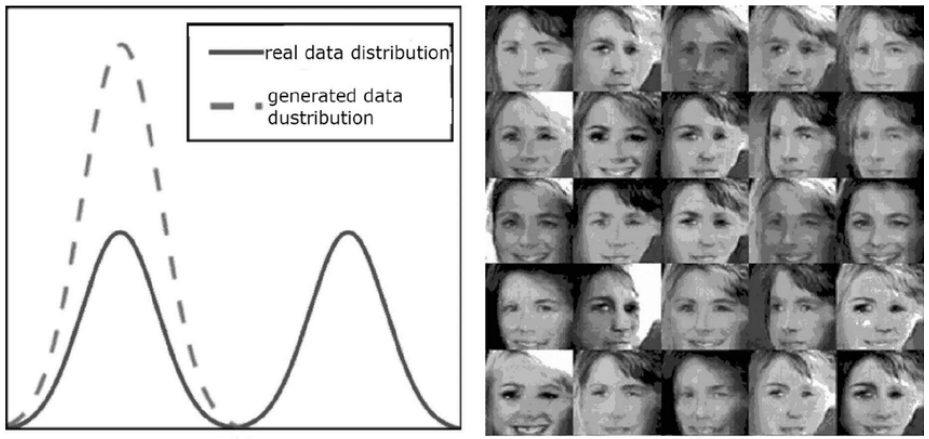
- Data-hungry : GANs require a **lot** of data to be trained properly
- Mode collapse : the generator produces limited diversity (eg, for a dataset with cats and dogs, produces only dogs)



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).

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

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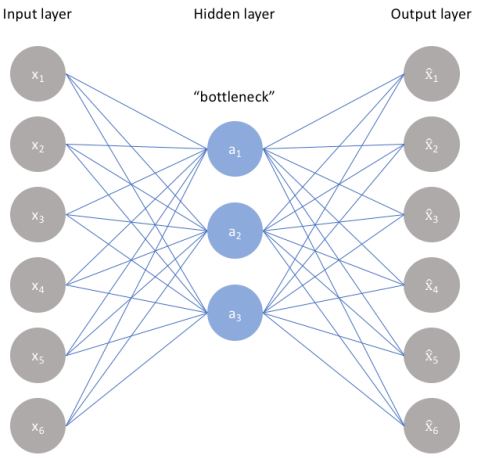
  - Encoder : images $\rightarrow$ compressed latent space
  - Decoder : latent space $\rightarrow$ image



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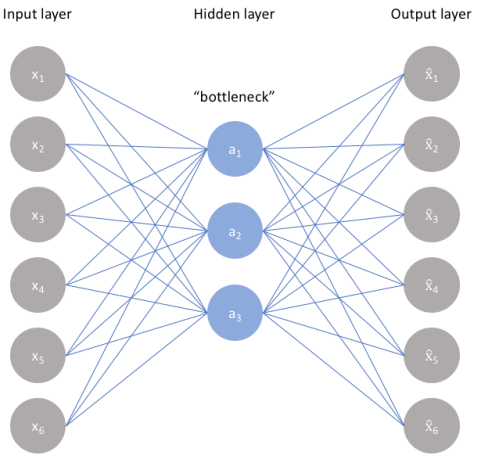

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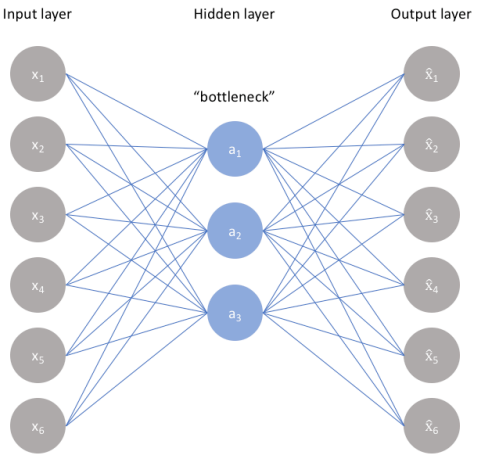

- Idea : by working directly in the latent space, the decoder is a generative model !
- Difficulty : sampling a random vector in the latent space might produce garbage. The latent space is highly irregular !

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

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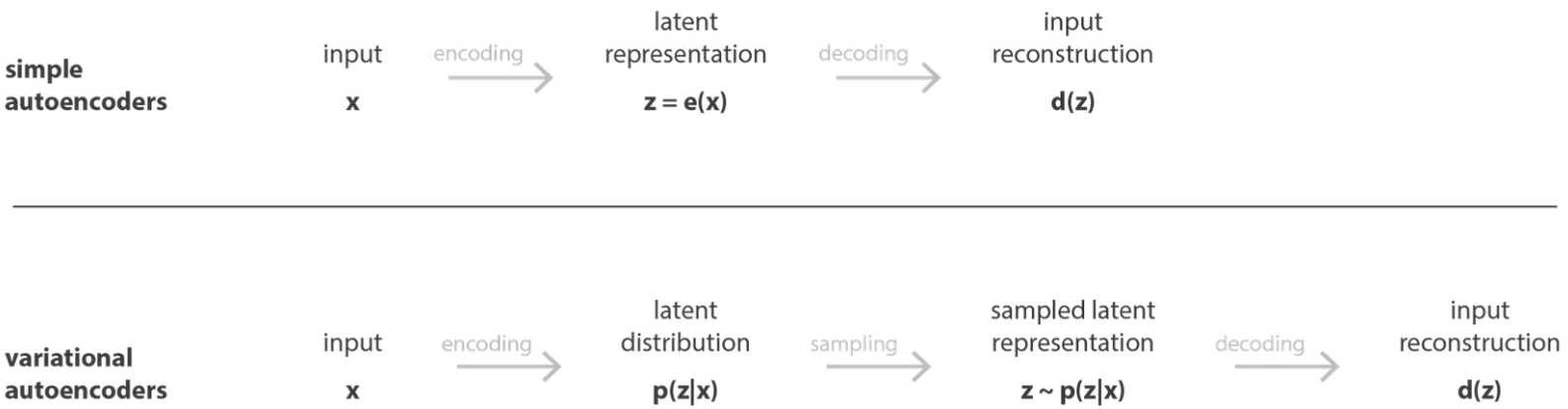

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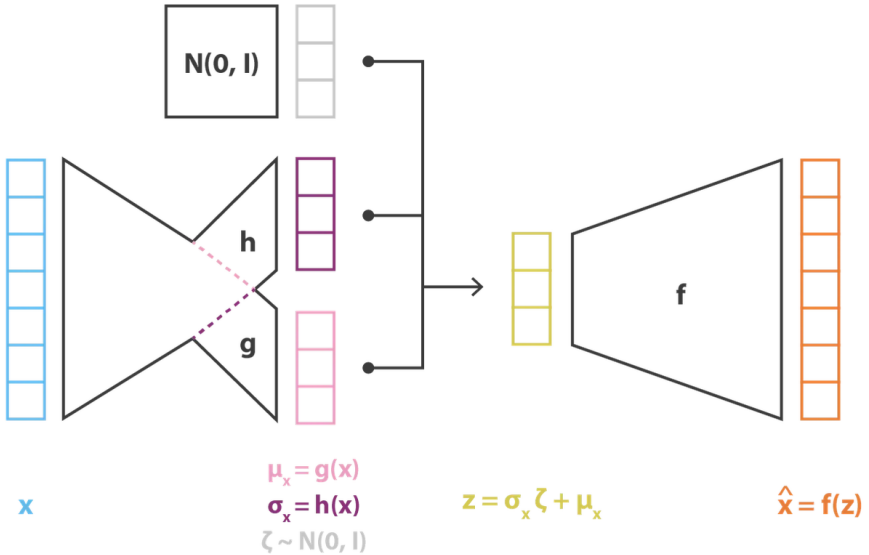
  - Add a regularizing term (Kullback-Leibler divergence) on these distributions.



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

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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)
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- Easier to train than GANs, but output might have less diversity

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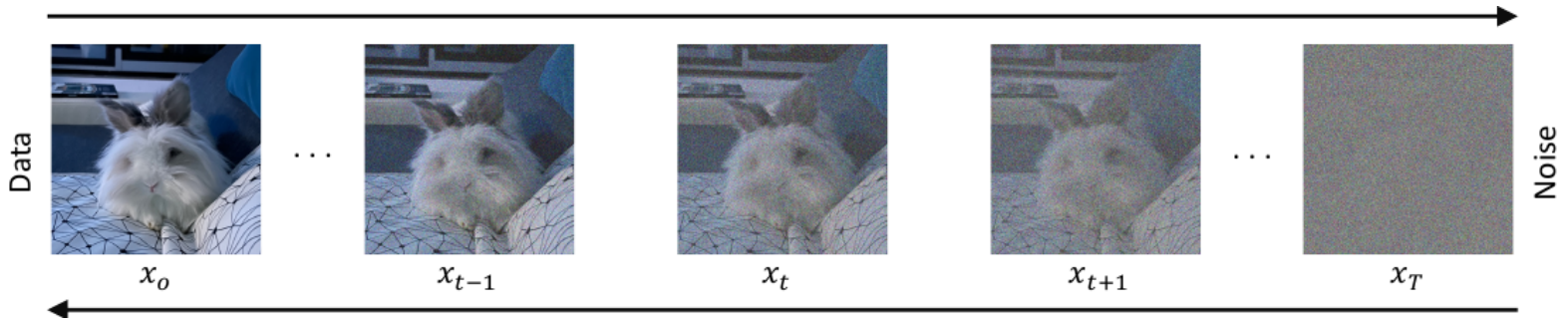
- Idea (roughly) : train a model to denoise an image, at many different noise levels. Then, start with random noise (!), and denoise it until an image is produced !
- Interpretation : we learn to "reverse" the diffusion process that gradually transforms an image into pure noise



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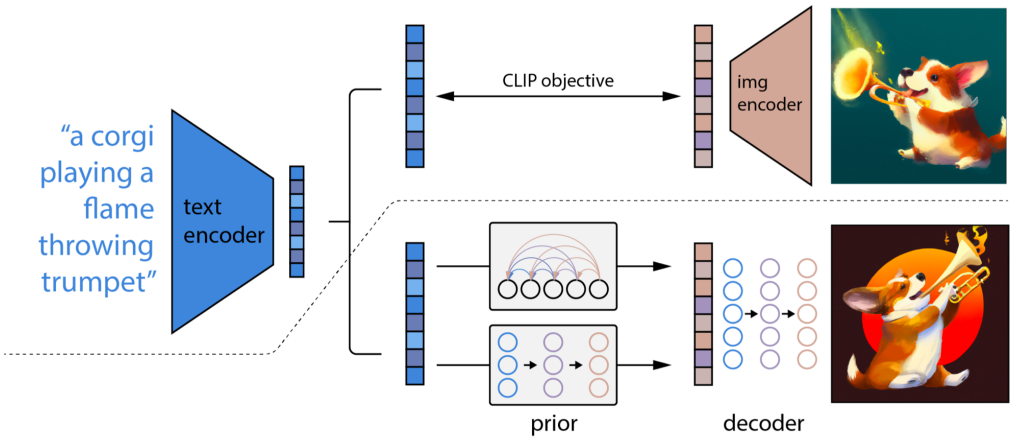

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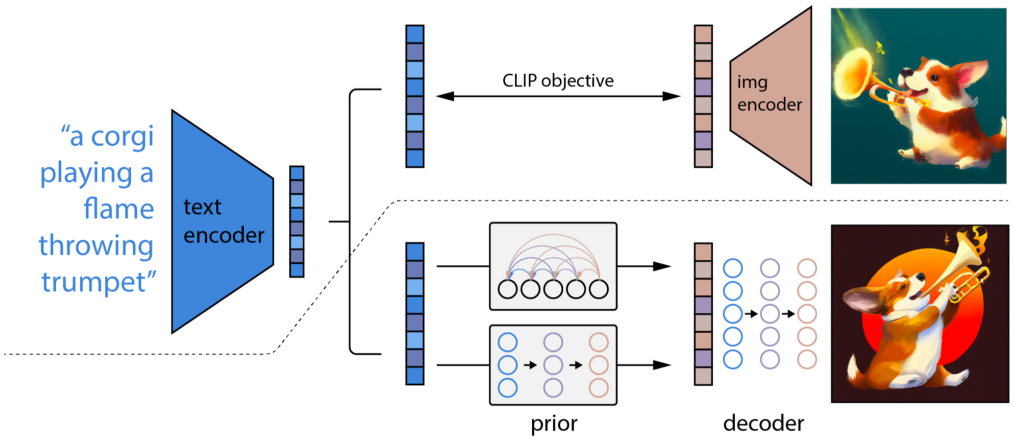

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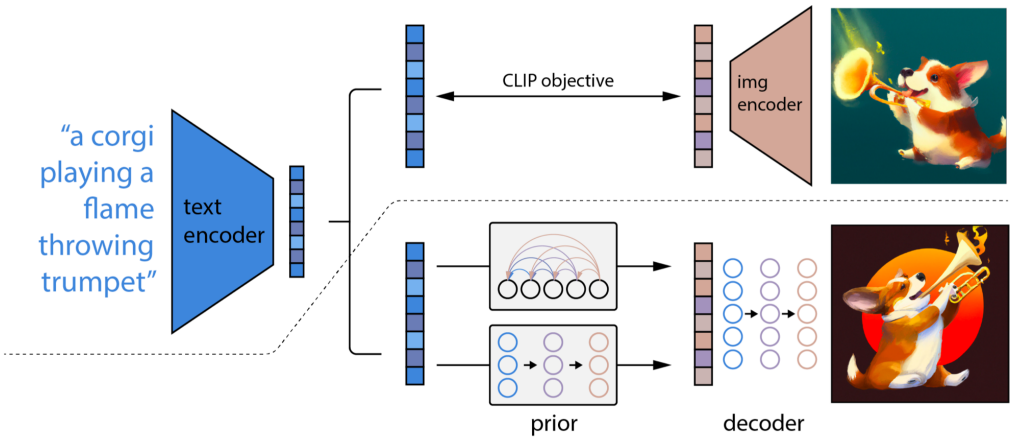

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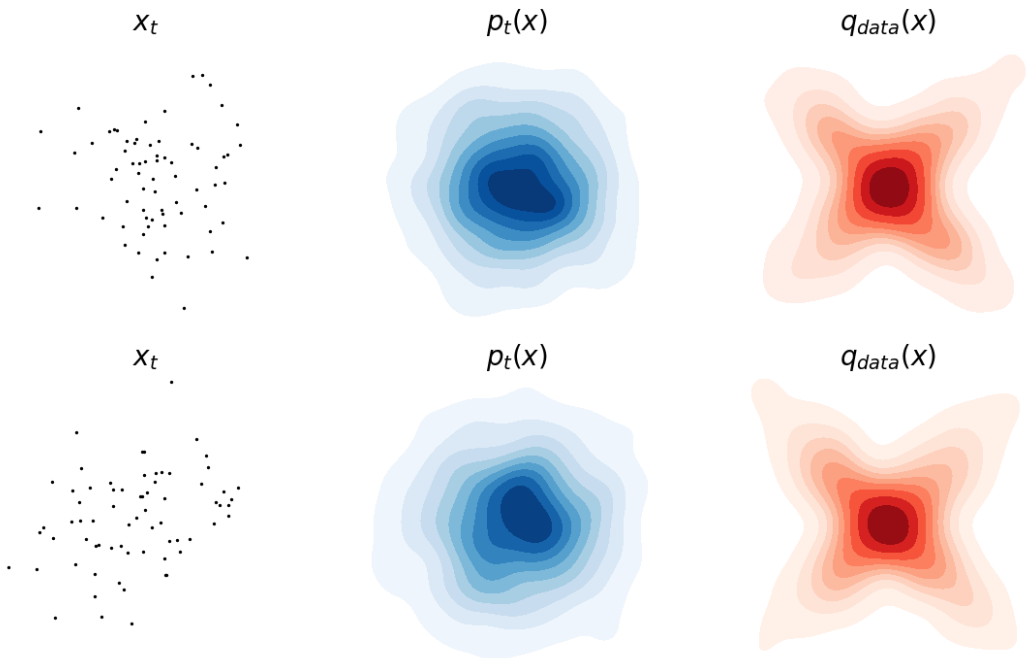
- Con : slow sampling. The sampling process is slower, we must perform many steps of denoising.

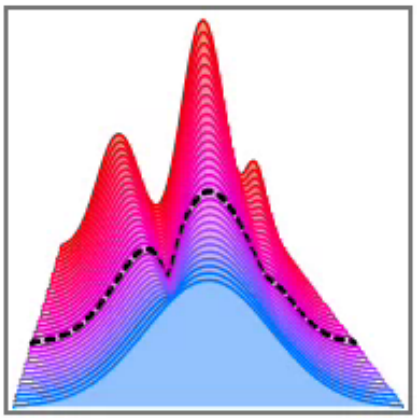
Diffusion models : the maths ?

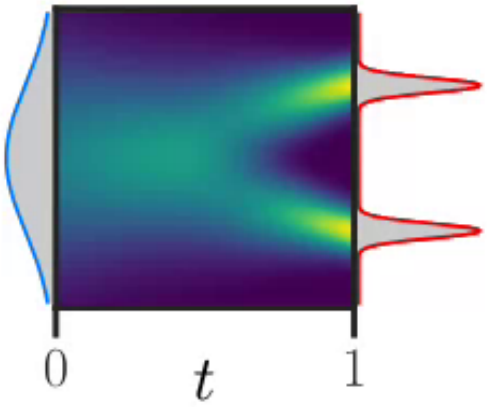
- Diffusion models have renewed the interest in classical ODEs theory (w/ a lot of tool from physics), with an ML flavor
  - probability path, brownian motion, Fokker-Planck/Langevin equation...
  - see `https://iclr-blogposts.github.io/2024/blog/diffusion-theory-from-scratch/`

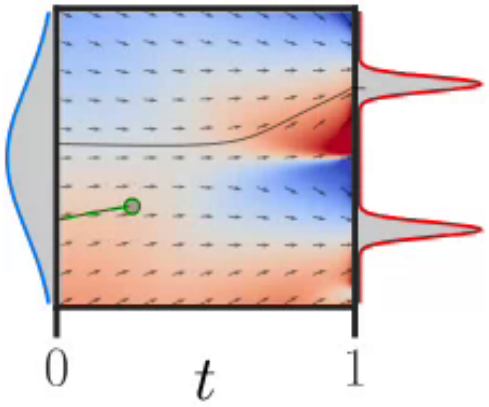


Diffusion : flow

- 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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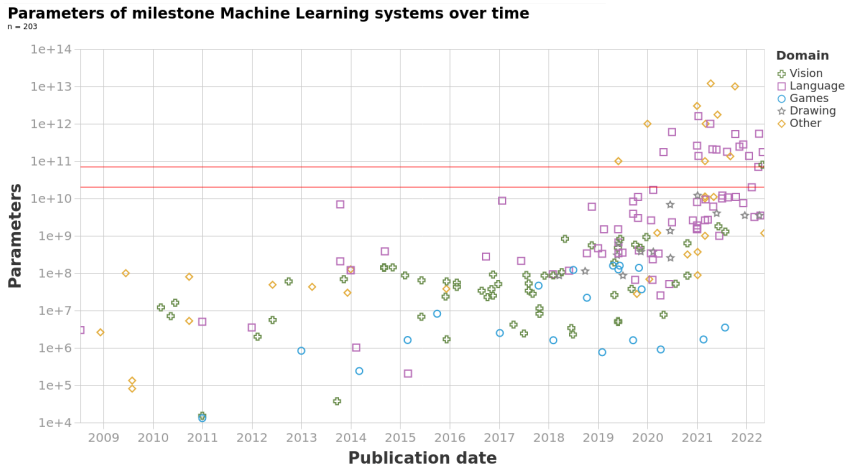
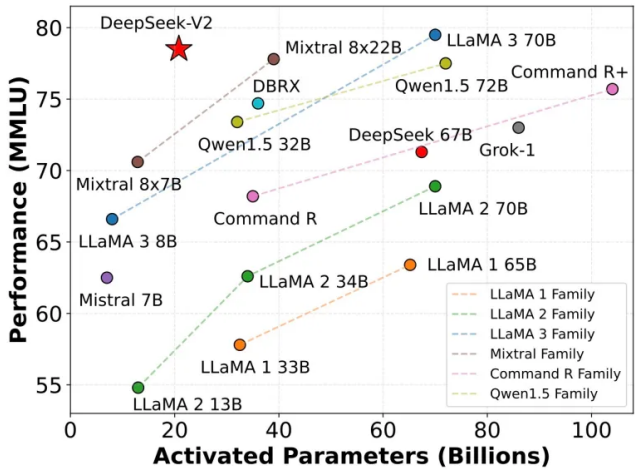
Transformers : what

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 !)



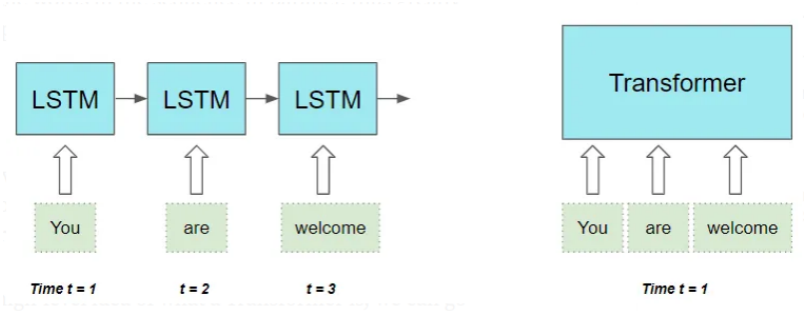


https://epoch.ai/blog/machine-learning-model-sizes-and-the-parameter-gap

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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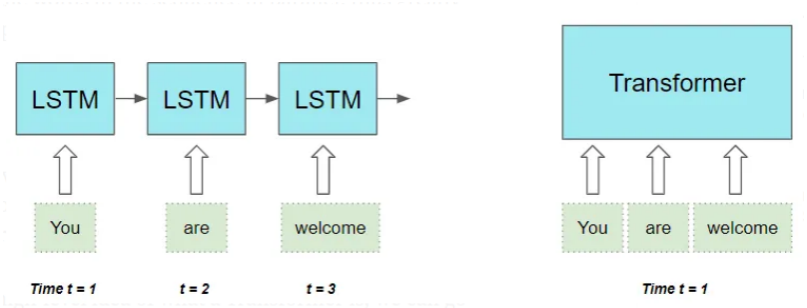

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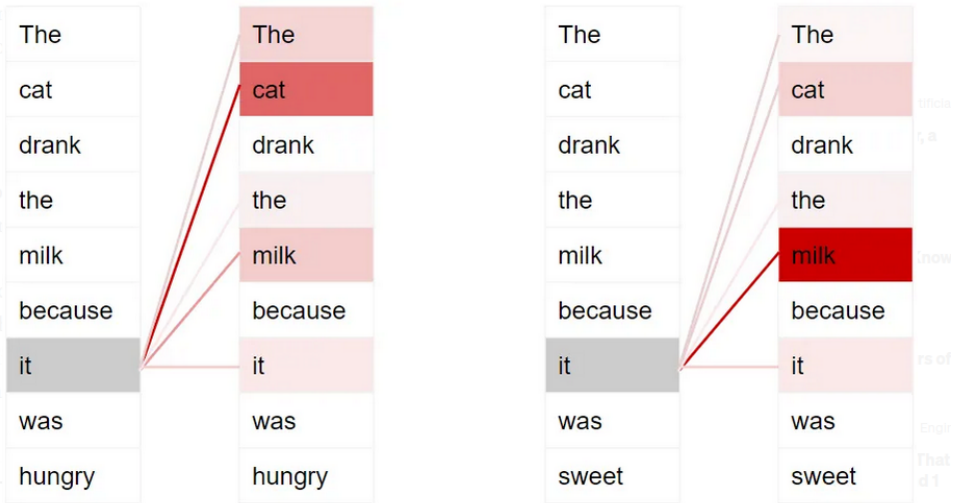
The key to Transformers is **attention** : a (deceptively) simple mechanism to model dependencies between words/objects



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.

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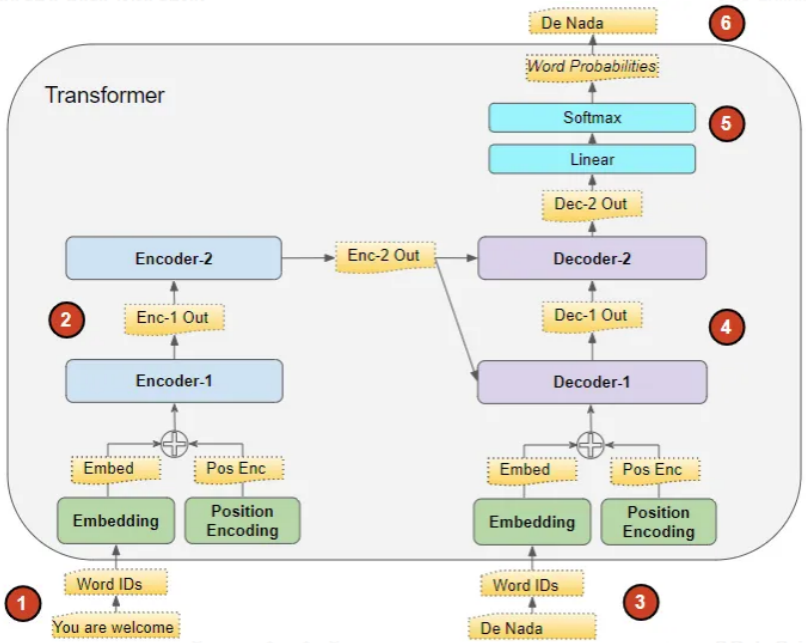
Transformer : example of a (high-level) seq2seq architecture

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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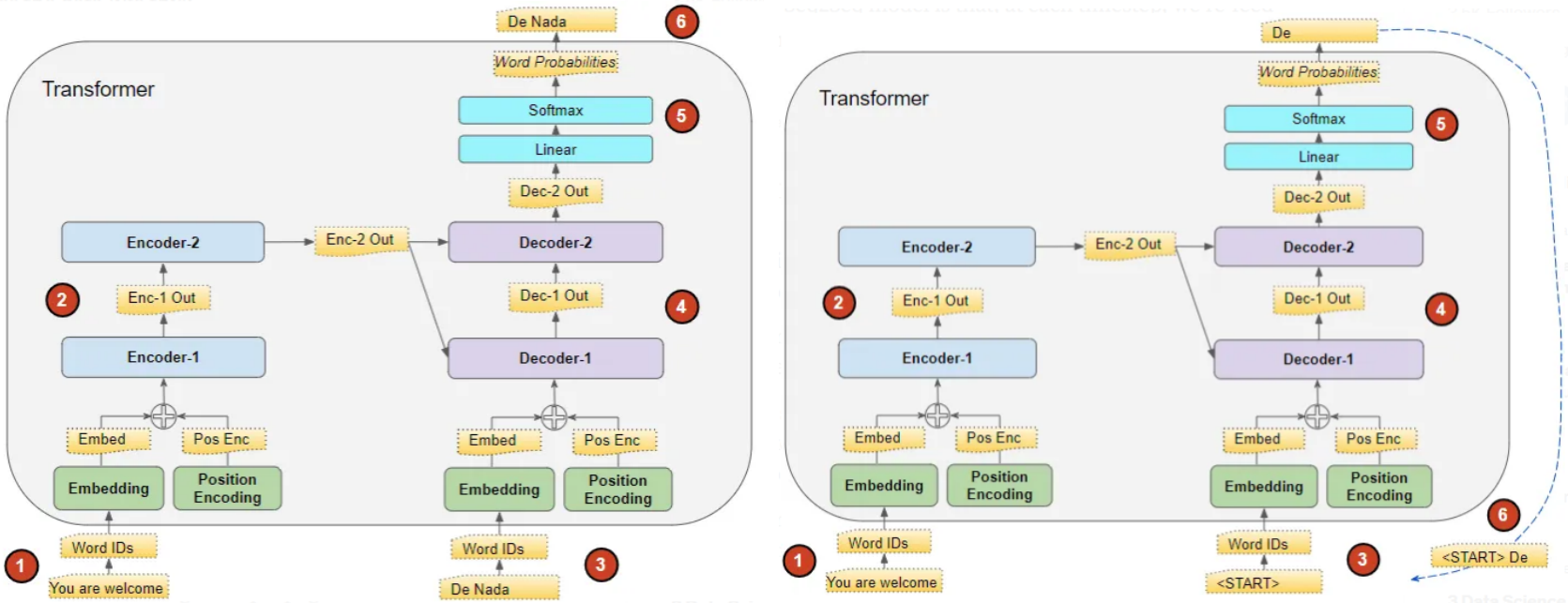

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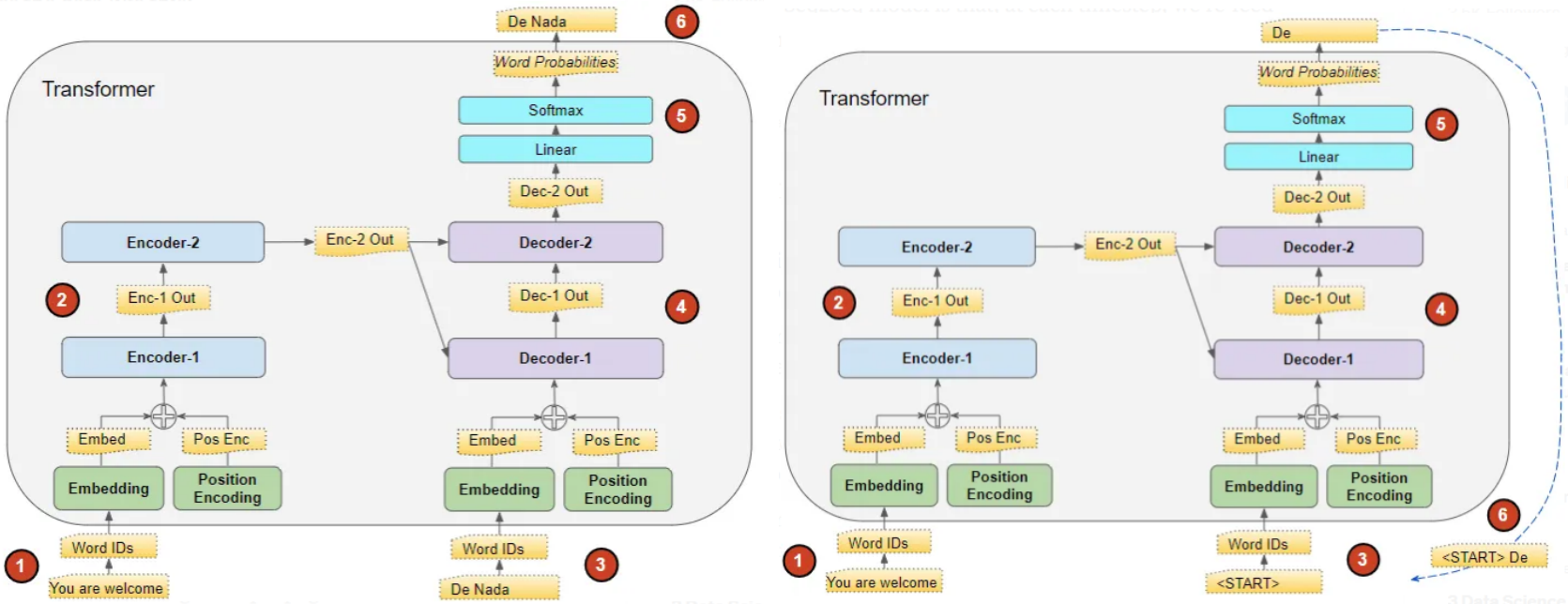
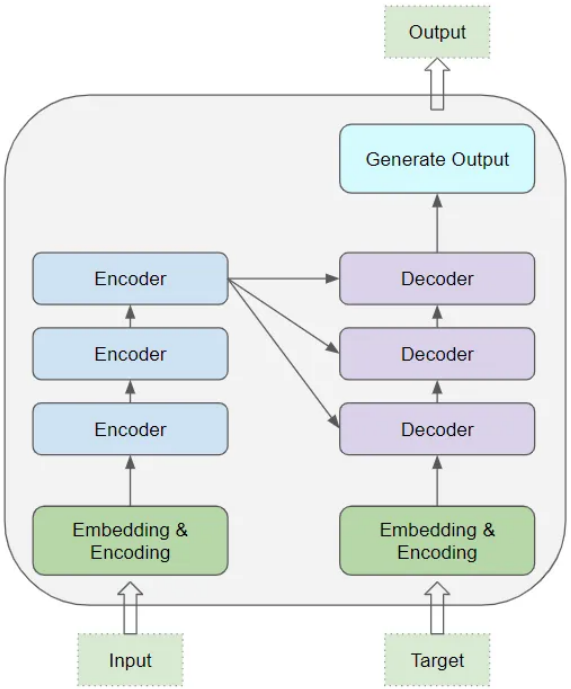
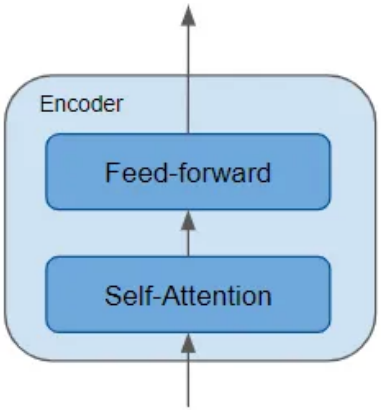
- Inference : takes a query x, start with an empty target, generate words one by one, by feeding the sequence generated until now as the target ("next word prediction")
- Unlike RNNs/LSTMs, the next word generated directly depends on everything else (through attention and self-attention), not just by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

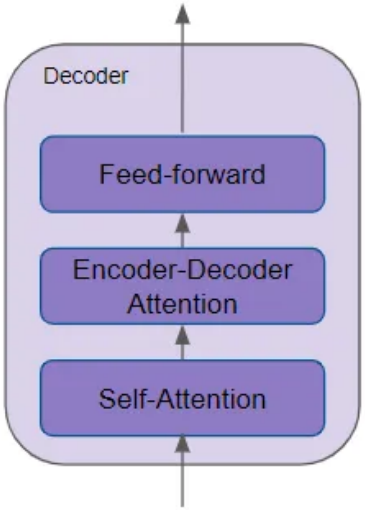


Transformer : example of a (high-level) seq2seq architecture

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







Transformers + RL

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

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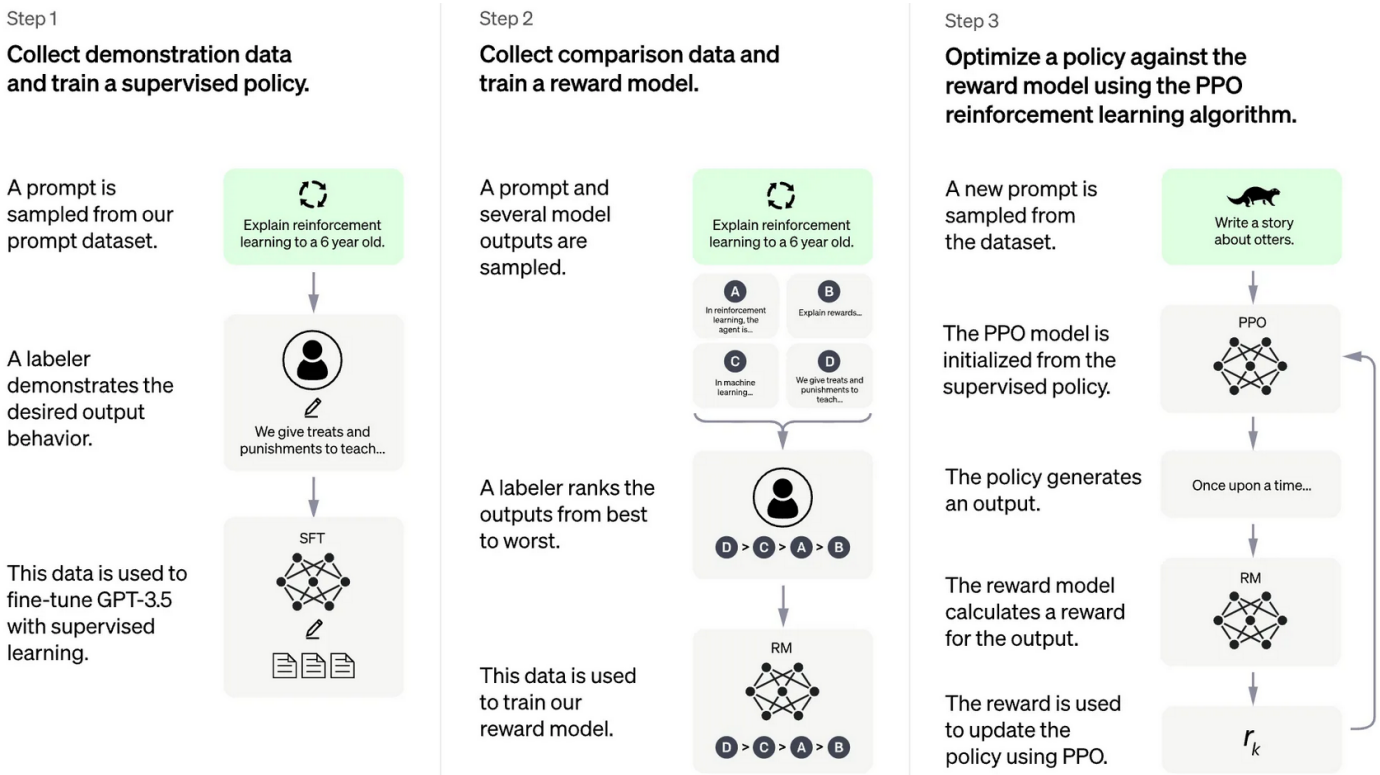
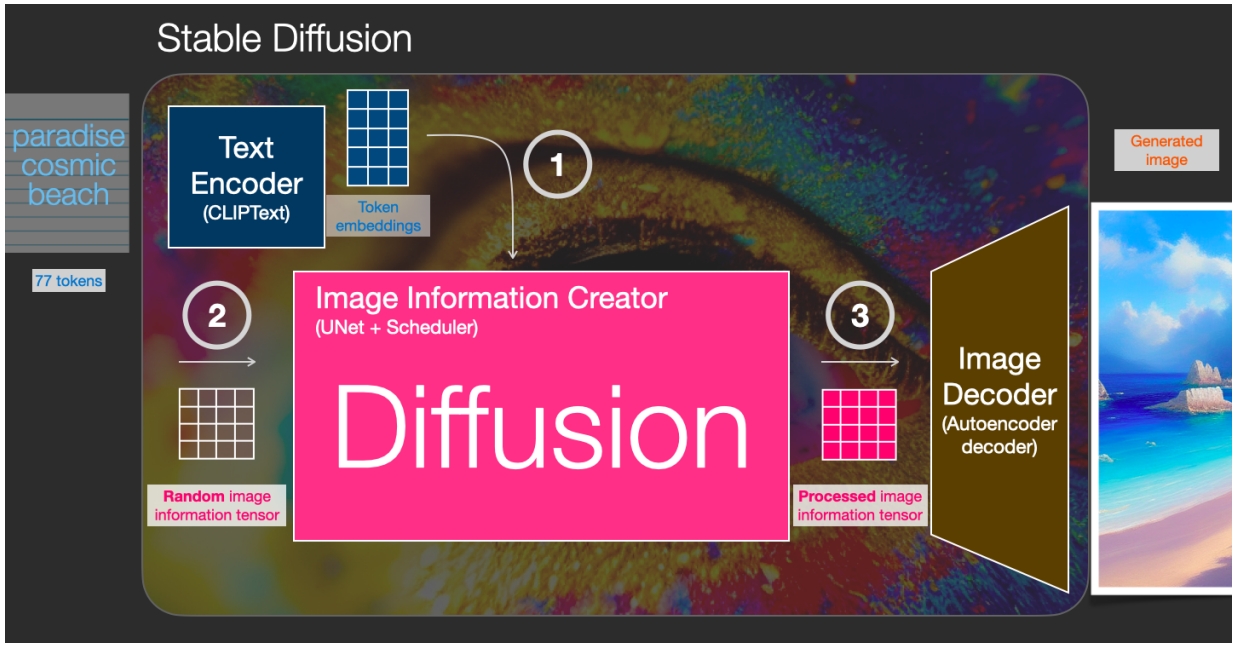
- ChatGPT is based on the GPT3 model (Generative Pre-trained Transformer), trained with complex RL strategies and HUGE amount of data.



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 year)

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

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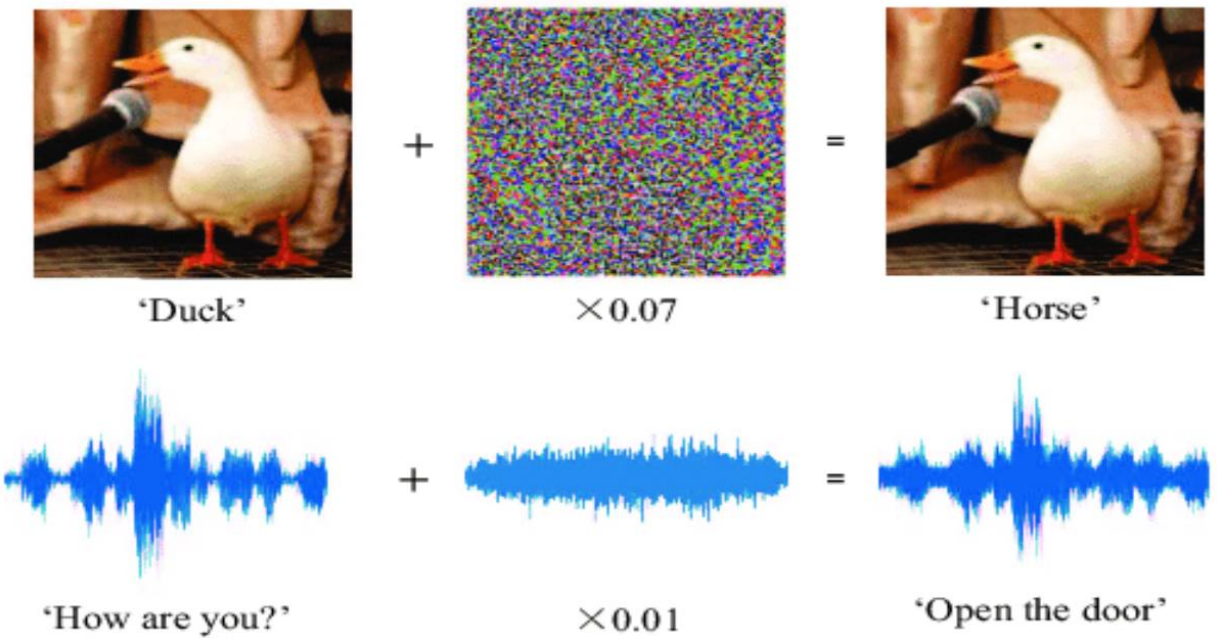
Conclusion

- 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 !

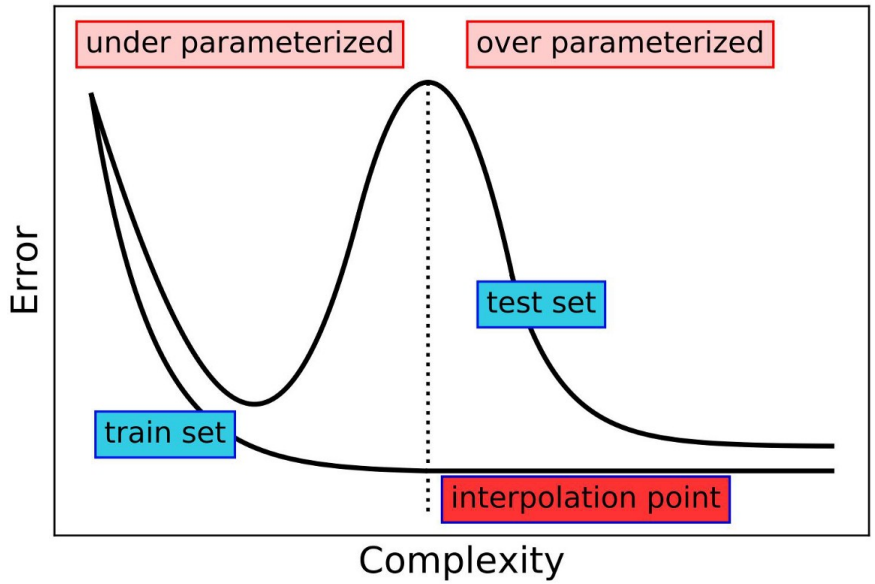
Hot question : adversarial attack

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 !



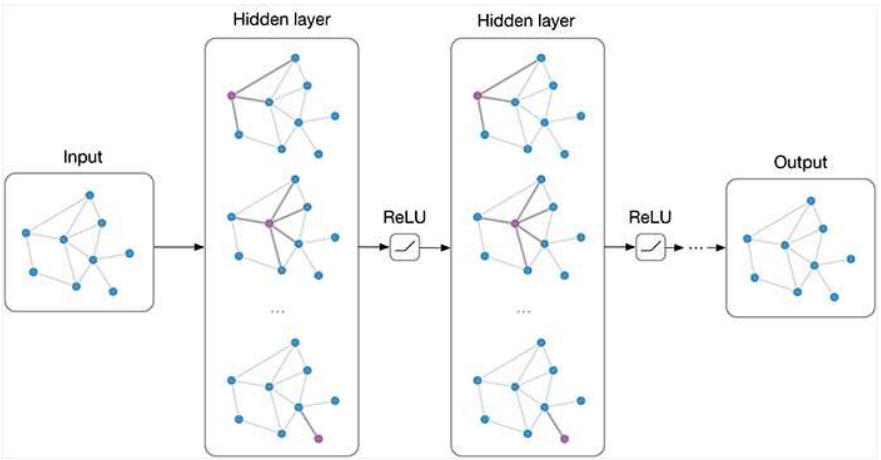
Hot question : generalization and double descent

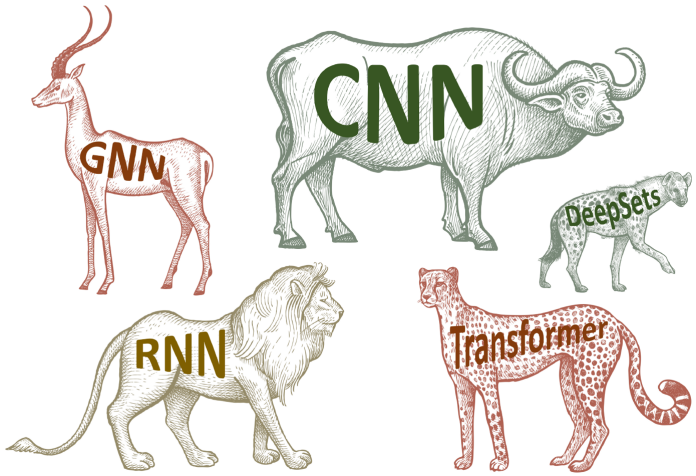
- Modern Deep NN are wildly overparametrized, and do interpolate the training data ! !
- But they still generatlize well !
- There is a double descent phenomenon : by increasing the complexity of the model past the interpolation point, among *all* interpolating models, it seems DNN+SGD favors models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

Hot topic : what about the scientific discipline ?

- Interpretability : Large (Language) Models are increasingly mysterious, people probe them as if they were natural phenomenon, and not human-made
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  - were kernel methods really more interpretable... ?
- Already a few years ago, deep learning was accused of being "alchemy" (and things were *incomparable* with today)
- Fundamental/academic research *somewhat* lack the ressources (compute, man-power) to compete with large companies, but
  - it has (or must redefine) its place ! Many fields besides "training the biggest models" : privacy, efficiency, fairness, fundamentally new ideas, etc.
  - Likeness : companies are building skyscrapers, fundamental research establish the law of physics and the physics of materials.
  - Right now, the problem is that we overlap too much the two...

Hot topic : privacy

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- Model privacy
  - keep sensitive algorithms private/secure
  - but open-sourceness is the only guarantee of transparency

Ethics and Justice, Law, Regulation, and Policy

Privacy in an AI Era: How Do We Protect Our Personal Information?

A new report analyzes the risks of AI and offers potential solutions.

Mar 18, 2024 | Katharine Miller

Hot topic : fairness

- By default, a model reproduce the biases in its training data (it's not inherently good or bad, it just is)
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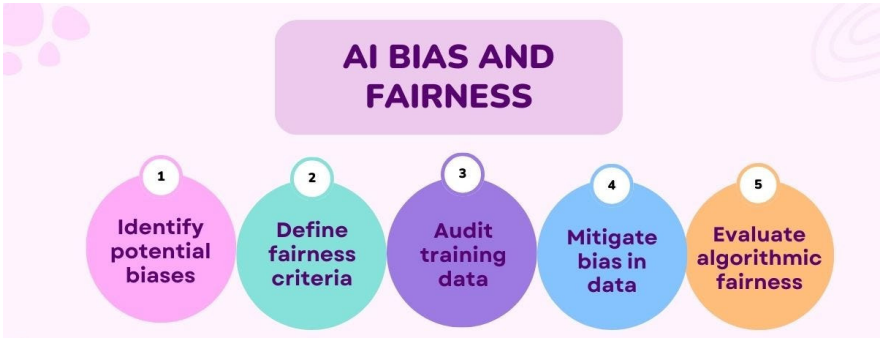

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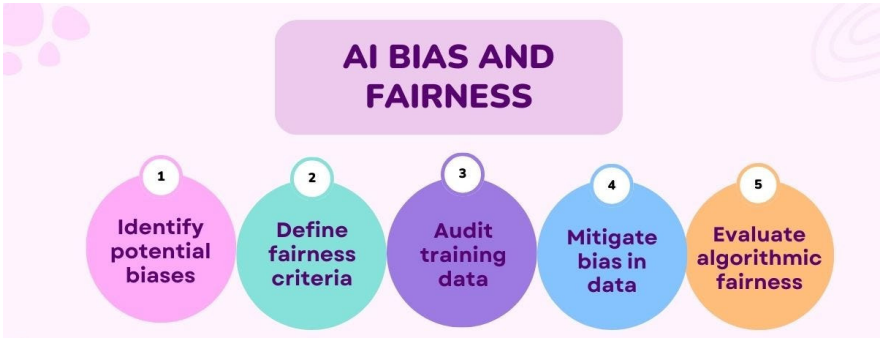
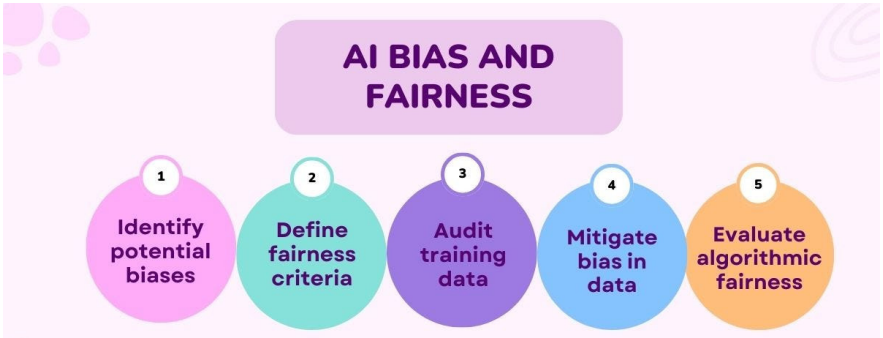


- Mathematical models : unbalanced classes, conditional probabilities...

Hot topic : fairness

- By default, a model reproduce the biases in its training data (it's not inherently good or bad, it just is)
  - some sensitive data are not collected, so cannot be used to compensate for bias



- Mathematical models : unbalanced classes, conditional probabilities...
- Non-open-source models can be *volontarily* biased !
  - even open-source models are so complicated that bias can be hard to detect
  - from ads on the internet to democratic threat... 𝕏


FEBRUARY 4, 2025 | 5 MIN READ

Inside the NSF's Effort to Scour Research Grants for Violations of Trump's Orders

The U.S. National Science Foundation has unfrozen grant funding, but it continues to scrutinize research projects, sowing turmoil

BY DAN GARISTO, MAX KOZLOV & NATURE MAGAZINE

Hot topic : sovereignty

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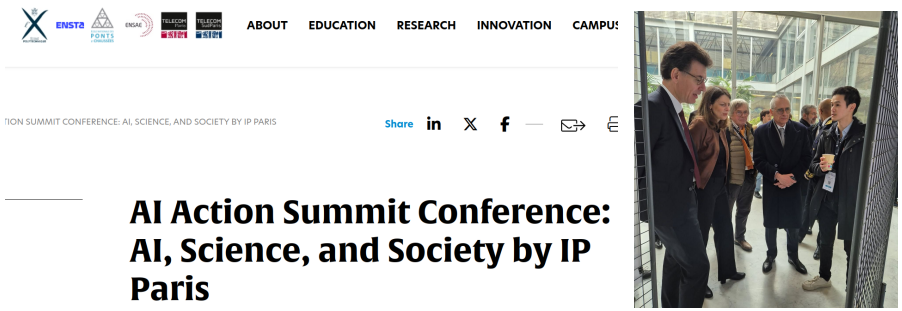
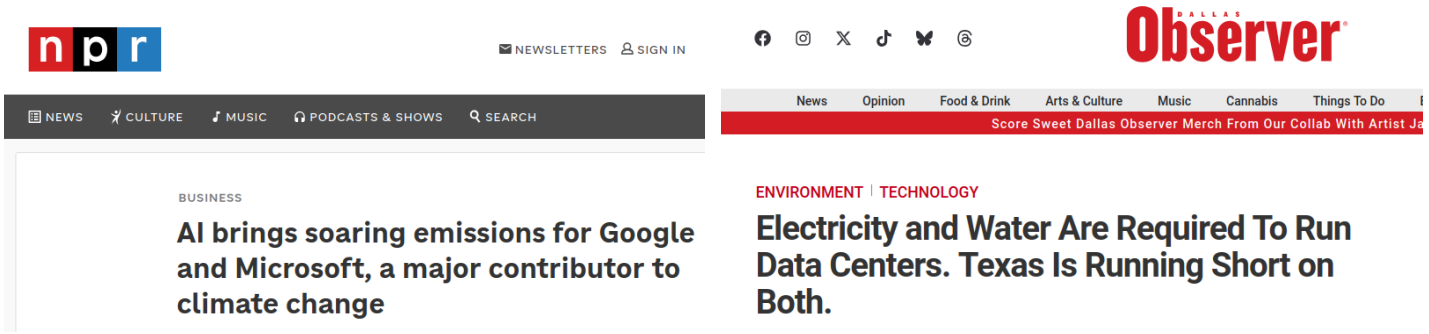
- until now, the community was still very "*academic*" : open-source, international, everyone is nice and sharing. Recent events indicate that that may change...
- What about France/Europe ? For now, policy-makers have decided to focus on "ethical" AI (open-source, fair, frugal, **useful** etc.), while still investing in local infrastructures.



Hot topic : environmental cost

- AI/ML requires large amount of resources : water, electricity, rare earths and metals...



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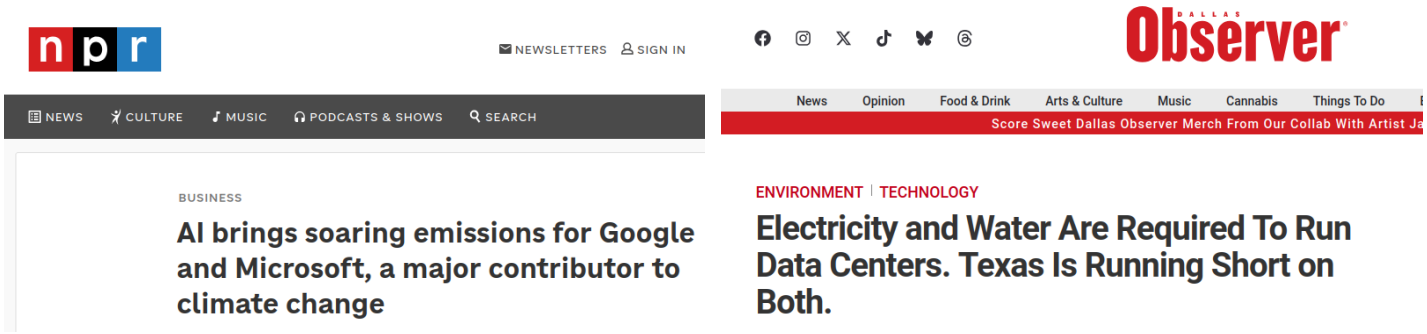
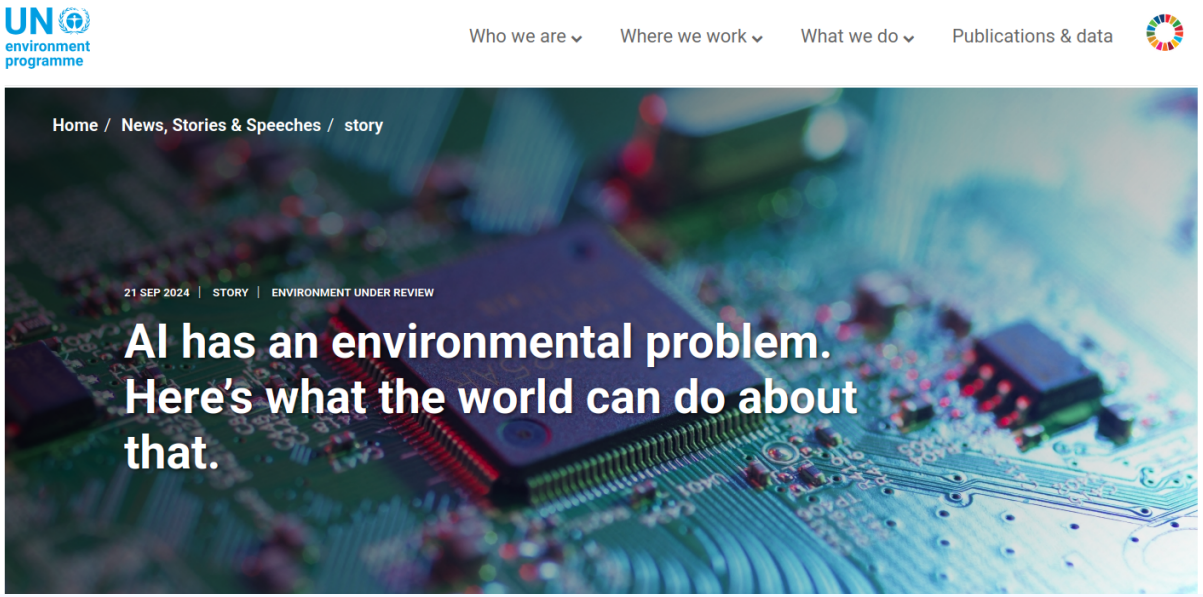


- AI may help "tackle climate change"... but beware the rebound effect !
  - `https://www.climatechange.ai/`



Hot topic : creativity and ethics

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AI is *not* gonna "destroy" the world, at least not Terminator-style (humans are far more dangerous). 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 ?