Introduction to diffusion models

Accelerate Programme for Scientific Discovery

Welcome!

About the course

- The history of generative AI
- Inspiration from physics
- Building blocks of diffusion
- Where can you get them from
- Code!

Code and slides available on:

Accelerate Science GitHub repo

Today's Schedule

- Introduction to the Accelerate Science Programme
- History of Generative AI
- Inspiration from Physics
- BREAK
- Building blocks
  - VAEs
  - U-Net
  - CLIP
- LUNCH
- DDPM Algorithm
- Applications
- Data Ethics
- BREAK
- Evaluation
- What’s out there?
- No code

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SCHMIDT FUTURES

Accelerate Science Programme

"Accelerate Science pursues research at the interface of AI and the sciences, generating new scientific insights and developing AI methods that can be deployed to advance scientific knowledge."

Accelerate Science Programme

Diffusion Workshop Goals

We want to:

- Support researchers across the university to use AI – that's diffusion models in this group.
- Better understand the challenges that researchers face.
- Identify what training courses or software resources we might want the Accelerate Science Programme to create.
  - Including shared code
- Start to build a community of like-minded researchers across the university.

What do you know…?

What do you know about Diffusion Models…?

What do you know…?

…about diffusion models?

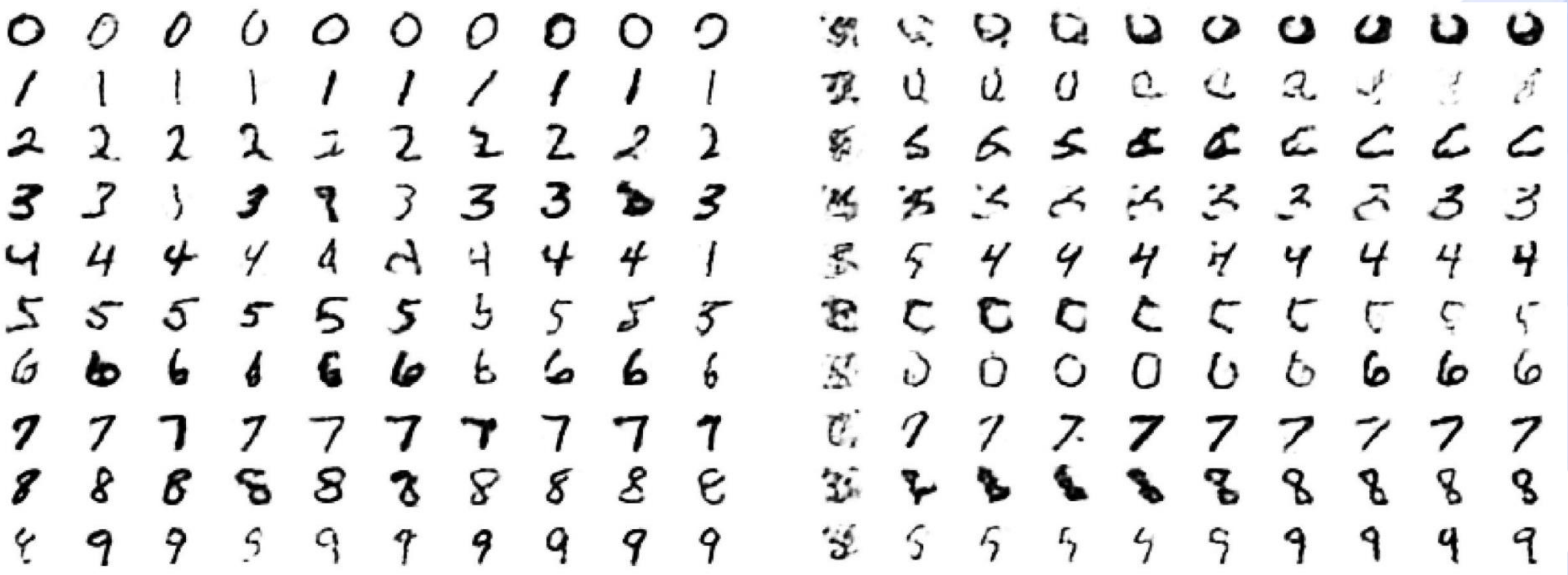
- How do they work?
- Can you name any?
- What can you use them for?
- What are potential problems?
- What do YOU intend to use them for?

History of Generative AI

History of Generative AI

GenAI as we know it today really began in the mid 2000s

- “A fast learning algorithm for deep belief nets”, 2006, Hinton et al ~ 21k citations
- Restricted Boltzmann machines



Hinton, Geoffrey E., Simon Osindero, and Yee-Whye Teh. "A fast learning algorithm for deep belief nets." Neural computation 18.7 (2006): 1527-1554.

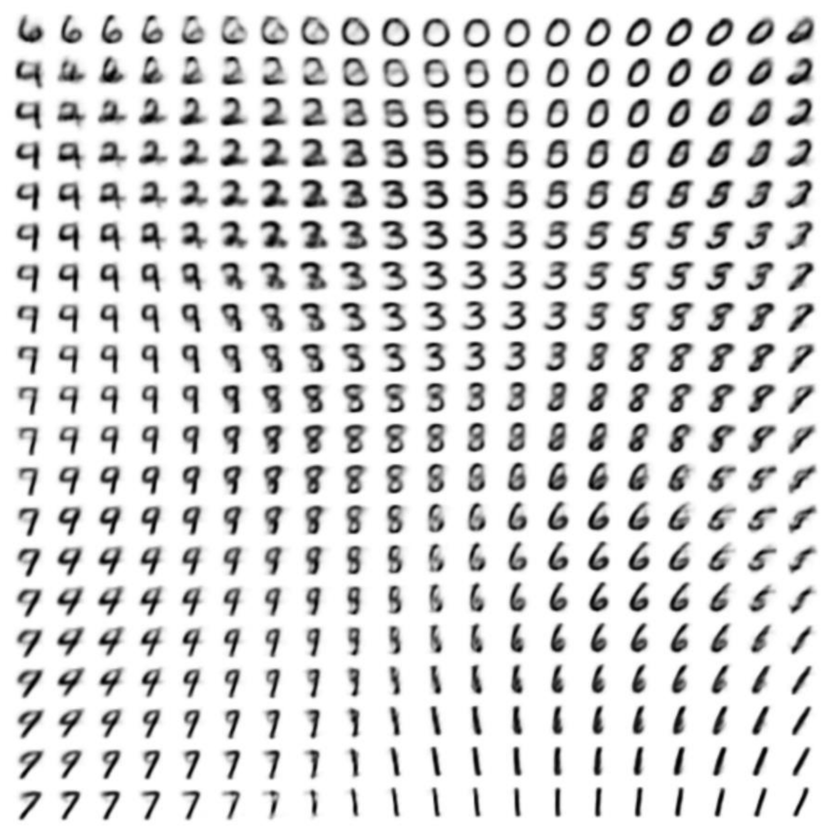
History of Generative AI

Variational Autoencoders

- “Auto-Encoding Variational Bayes” Kingma & Weilling, 2013, ~ 36k citations
- Connect an encoder and decoder via a probabilistic latent space
- We will talk more about this later…

(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Kingma, Diederik P., and Max Welling. "Auto-encoding variational bayes." arXiv preprint arXiv:1312.6114 (2013).



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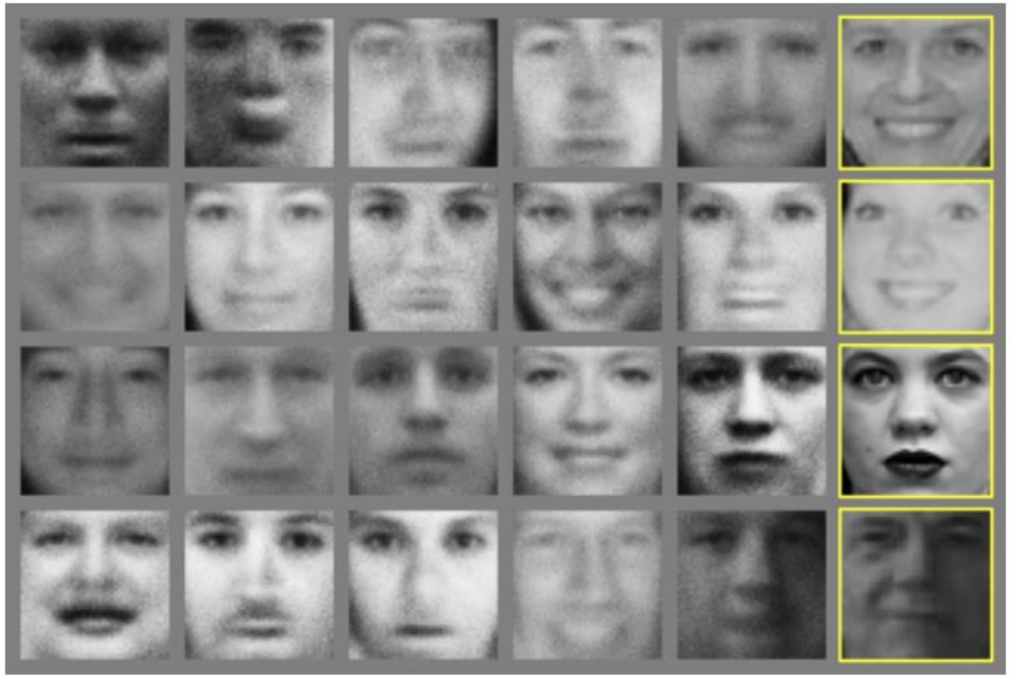
History of Generative AI

Generative Adversarial Networks (GANs)

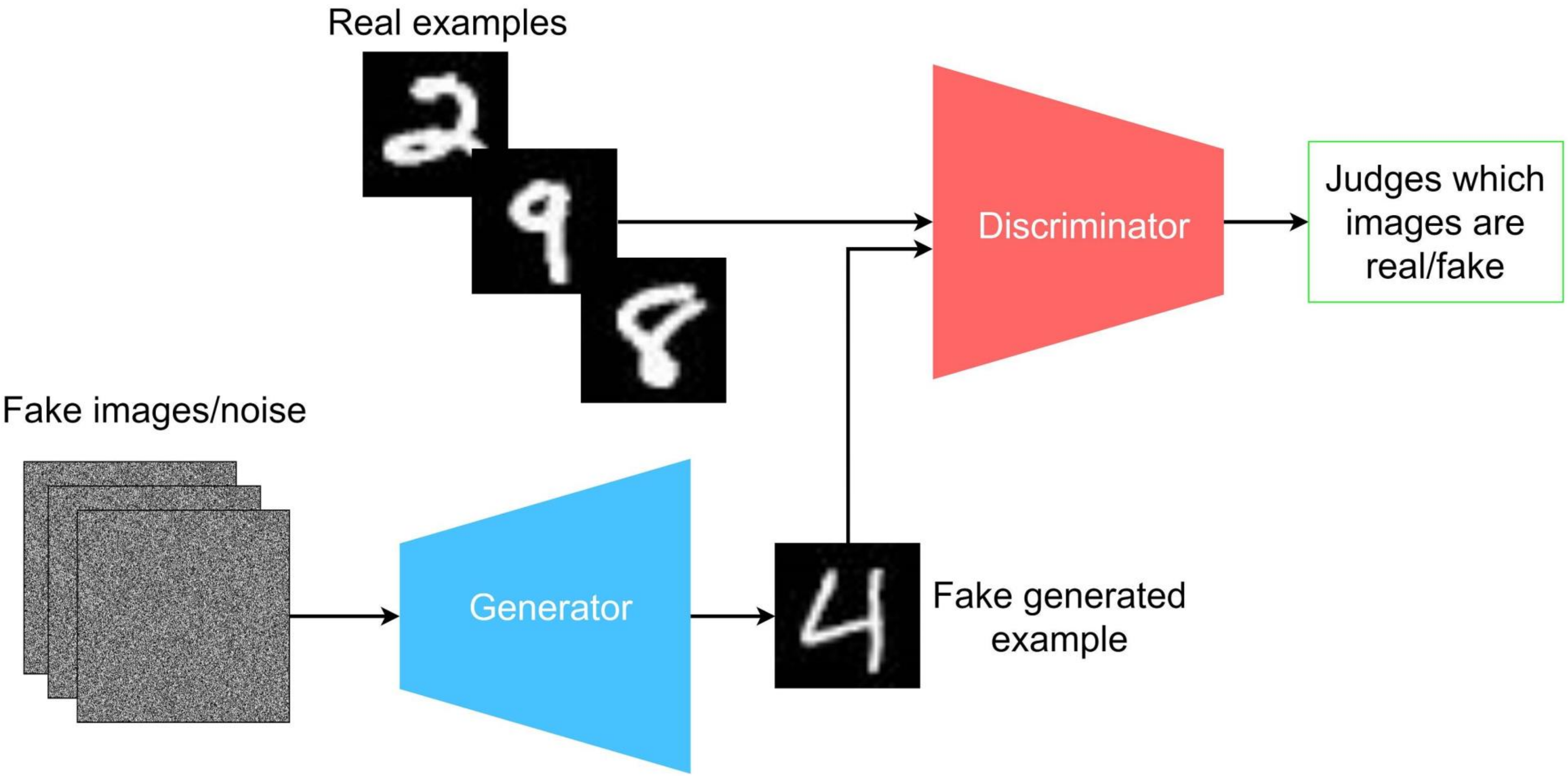
- Generative Adversarial Networks, 2014, Goodfellow et al, ~67k citations



Goodfellow, Ian, et al. "Generative adversarial nets." Advances in neural information processing systems 27 (2014).

History of Generative AI

GANs



https://developer.ibm.com/articles/generative-adversarial-networks-explained/

History of Generative AI

GANs

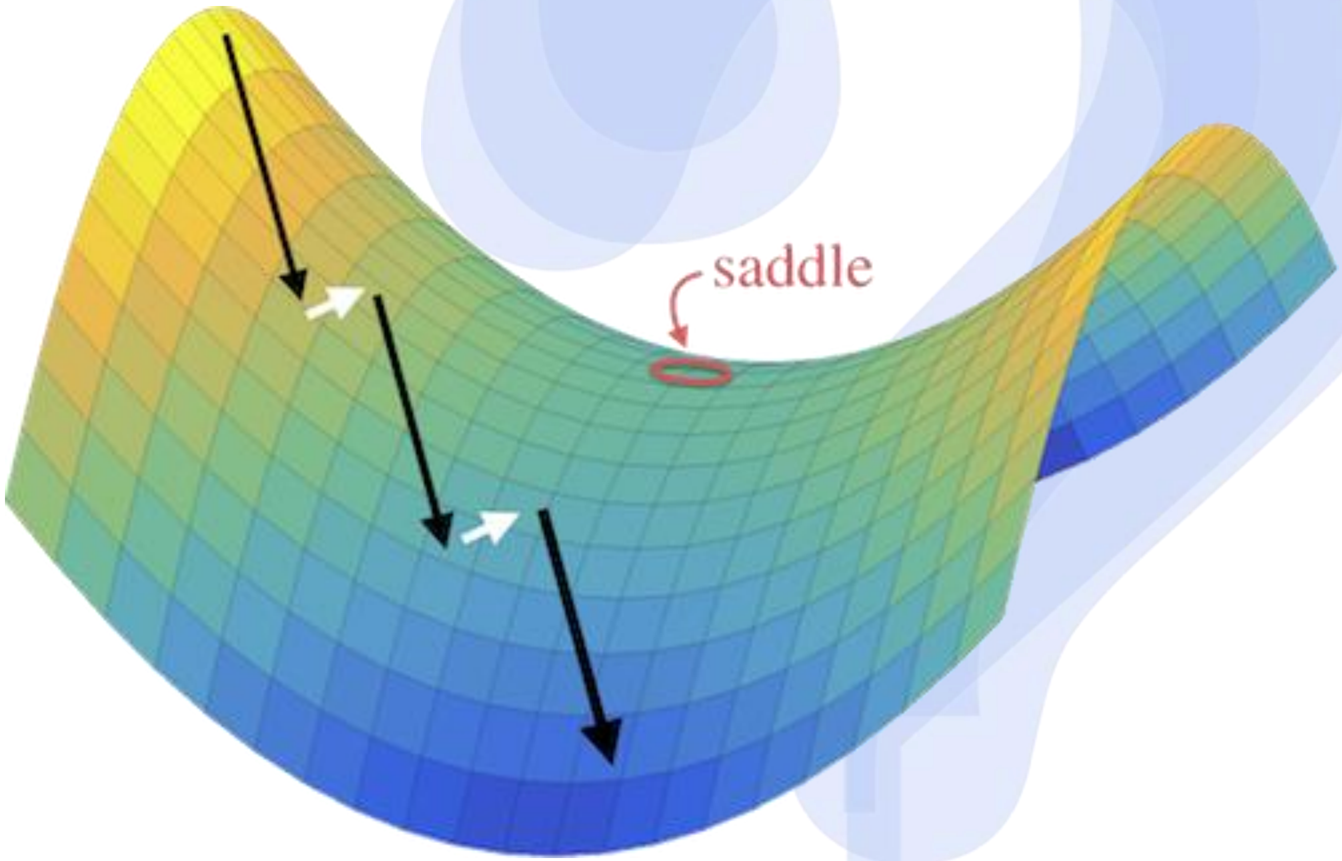
- They quickly advanced…

Karras, Tero, Samuli Laine, and Timo Aila. "A style-based generator architecture for generative adversarial networks." Proceedings of the IEEE/CVF conference on computer vision and pattern recognition. 2019.

History of Generative AI

GANs

- Training GANs is hard
- We want to find a point on a saddle that is a minimum about the generator, and a maximum about the discriminator.
- We can inject noise into the discriminator using a noise schedule determined by a diffusion model.
- Subject to mode collapse



Min, Zhiyu. “Generative adversarial networks, Wasserstein distance and adversarial loss.” Alibaba AliMe X-Lab

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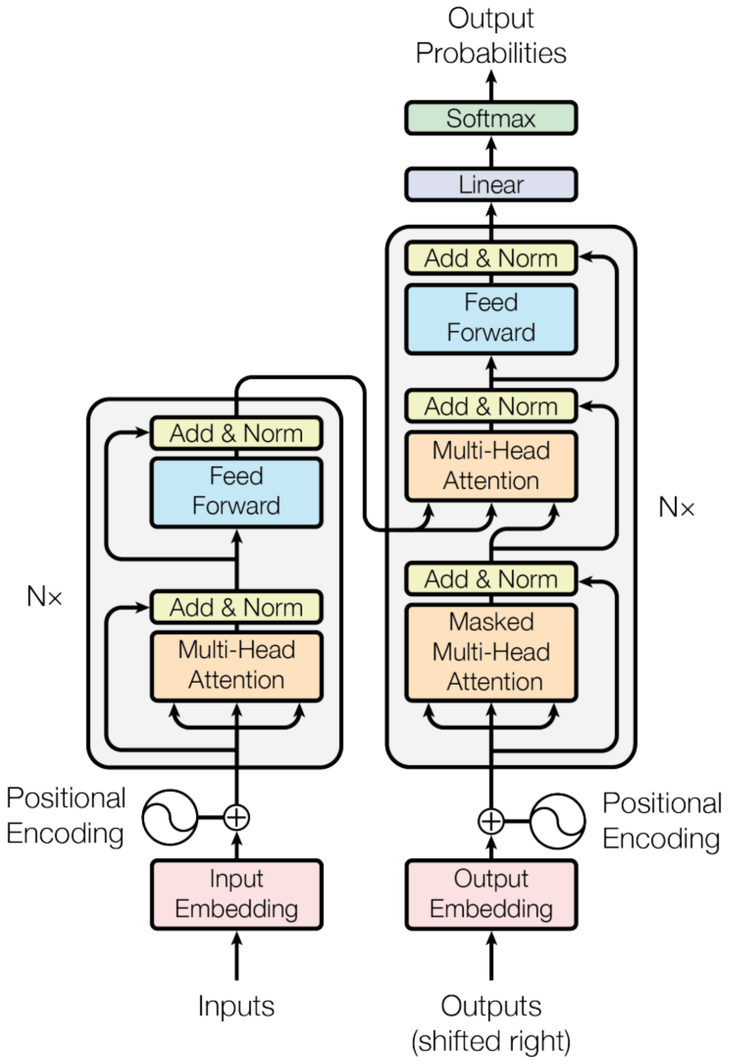
History of Generative AI

We know what has been dominating this space…

- "Attention is all you need", Vaswani et al, 2017, ~ 125k citations
- Introduced scaled dot-produce attention and the transformer architecture



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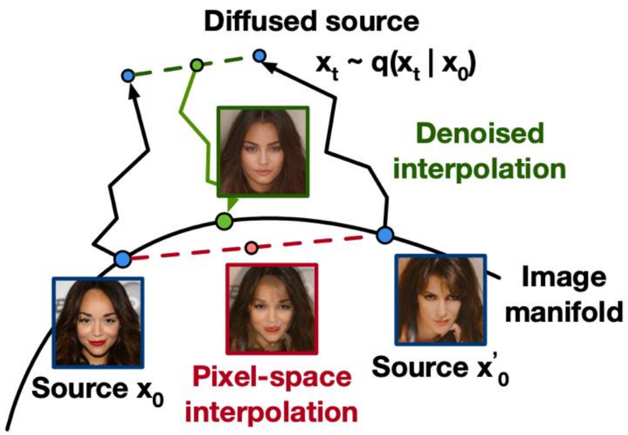
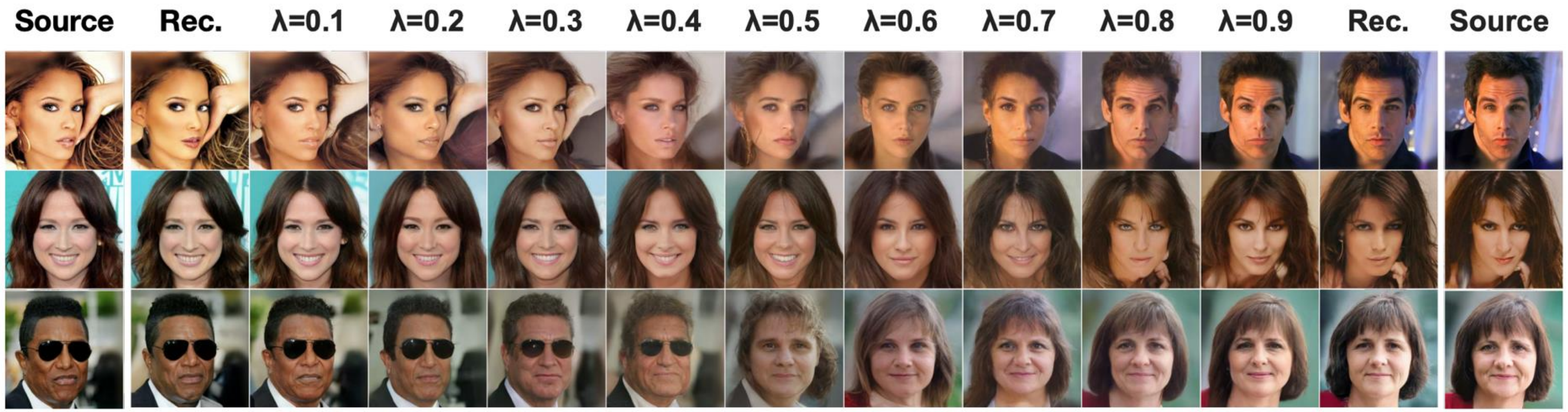
History of Generative AI

Diffusion

- Deep unsupervised learning using nonequilibrium thermodynamics, Sohl-Dickstein et al, 2015, ~ 5k citations
- Denoising diffusion probabilistic models (DDPM), Ho et al, 2020 ~ 10k citations
- High-resolution image synthesis with latent diffusion models, Rombach et al 2022, ~ 8k citations





History of Generative AI

Midjourney

OpenAI

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