1. Introduction to Generative Modelling

M. Ravasi | AI Summer School @ KAUST

A short intro about myself

Assistant Professor of Applied Geophysics, ErSE, KAUST

Head of **Deep Imaging Group**

Co-PI of **DeepWave** consortium

Main developer of **PyLops**

Research Geophysicist – Statoil/Equinor

Intern – Schlumberger, WesternGeco

Phd, Geophysics – University of Edinburgh

Inverse Problems, Seismic Imaging,

Machine Learning, HPC, Open Software

A short intro about my group

Dig

Deep imaging group.

→ https://dig.kaust.edu.sa

→ http://github.com/dig-kaust

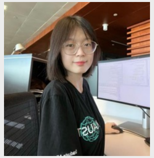
Deepen our understanding of the subsurface (possibly with the help of Deep Learning)

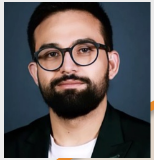
*Applications in **oil & gas**, **CCUS**, **geothermal**, **near surface***

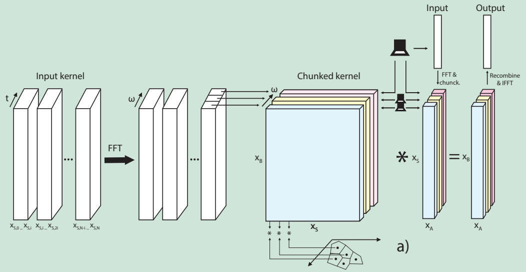
$$-g^{-}(x_R, x_{VS}, \omega) = f^{-}(x_R, x_{VS}, \omega) + \int_S R(x_R, x_S, \omega) f^{+}(x_S, x_{VS}, \omega) dx_S$$

Wave theory and inverse problems

- Marchenko-based processing and imaging
- Target-oriented full-wavefield inversion
- Proximal solvers for seismic inversion problems

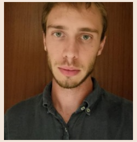


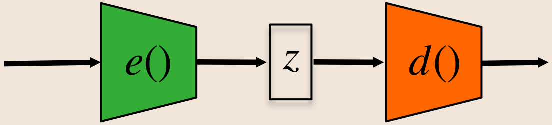




HPC for geoscience

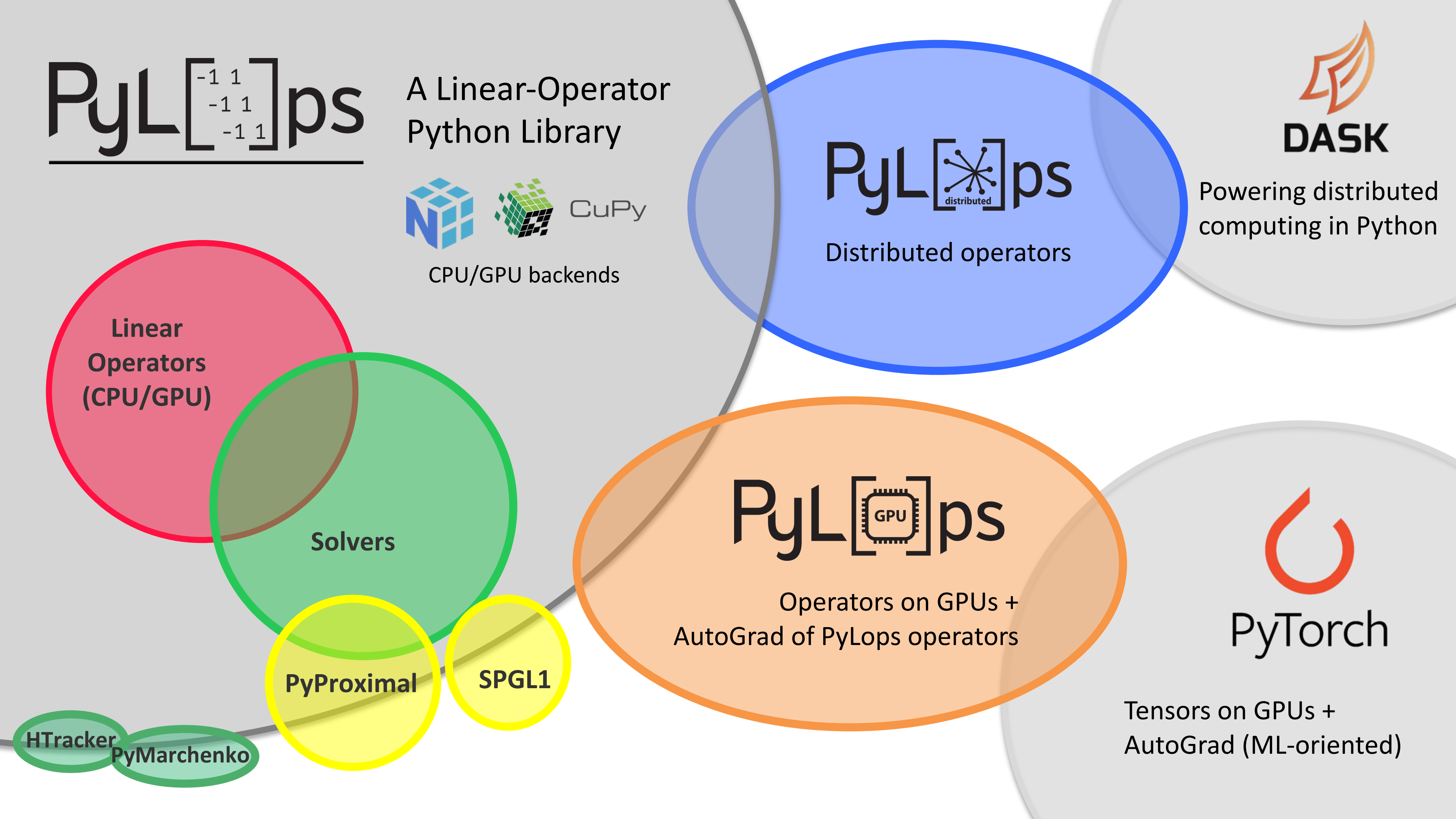
- Open-source software tools for large-scale inversion
- Seismic processing with SVD-based compression and mixed precision





ML-aided inverse problems

- Physics-Informed NN for geophysical applications
- Self-supervised learning
- Deep-learning assisted UQ


PyLops
A Linear-Operator Python Library
CuPy
CPU/GPU backends
Linear Operators (CPU/GPU)
Solvers
PyProximal
SPGL1
HTracker
PyMarchenko
PyLops distributed
Distributed operators
DASK
Powering distributed computing in Python
PyLops GPU
Operators on GPUs +
AutoGrad of PyLops operators
PyTorch
Tensors on GPUs +
AutoGrad (ML-oriented)

Generative Modelling: course material

All slides and codes available at:

https://github.com/DIG-Kaust/GenModelling

Generative Modelling: examples

- Can you imagine a **dog driving a car**?
- Can you imagine a **story of a young boy travelling to the moon**?
- Can you imagine a **soundtrack of a videogame**?
- Can you imagine a **panda surfing in the sea**?

*As humans, we have **great imagination** -> and sometimes can put it into practice…*

Generative Modelling: examples

- Can you imagine a **dog driving a car**?

Adobe Firefly (Beta)

Generative Modelling: examples

- Can you imagine a **story of a young boy travelling to the moon**?

Once upon a time, in a small town, there lived a curious and imaginative young boy named Tommy. Tommy loved to explore and dream of distant places, but his greatest fascination was the moon. Every night, he would gaze up at the sky, wondering what it would be like to visit that silver, glowing orb.

One evening, as Tommy sat outside, gazing at the moon, a shooting star streaked across the sky. In that moment, he made a wish with all his might. "I wish I could go to the moon and see it up close!" he whispered.

To his astonishment, a small, shimmering figure appeared before him. It was a moon fairy, with sparkling wings and a smile that lit up the night. "Tommy, your wish has been heard," she said in a gentle voice. "I can take you on a grand adventure to the moon."

Excitement bubbled inside Tommy's heart as he followed the moon fairy. She waved her wand, and suddenly, a magnificent rocket stood before them. It was painted with bright colors and had the words "Dream Express" written on its side.

Tommy climbed aboard the rocket, and the moon fairy joined him. "Hold on tight!" she exclaimed, as the rocket's engines roared to life. With a thunderous blast, the Dream Express soared into the sky, leaving a trail of stardust in its wake.

ChatGPT

Generative Modelling: examples

- Can you imagine a **soundtrack of a videogame**?

The main soundtrack of an arcade game. It is fast-paced and upbeat, with a catchy electric guitar riff. The music is repetitive and easy to remember, but with unexpected sounds, like cymbal crashes or drum rolls.

Google MusicLM

Generative Modelling: examples

- Can you imagine a **panda surfing in the sea**?

NVIDIA
Toronto AI Lab

Generative Modelling: what and how?

Generative modelling is a subset of artificial intelligence that aims to ***create new and original content*** *(images, text, music, videos, etc.)* ***using machine learning tools.***

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- Some training data: $\mathbb{X} = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N_s)}\}$
- A model with learnable parameters (which learns the data): f_θ

Generative Modelling: what and how?

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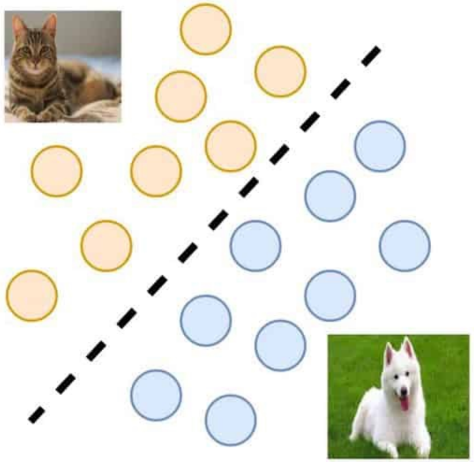
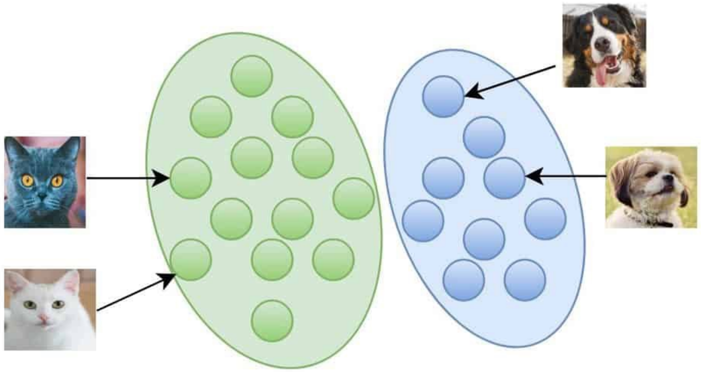
- Some training data: $\mathbb{X} = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N_s)}\}$
- A model with learnable parameters (which learns the data): f_θ
- A procedure for the model to learn: $\mathbf{x}^{(i)} \longrightarrow f_\theta$
- A procedure to generate data (or evaluate prob): $f_\theta \longrightarrow \mathbf{x}^{(new)} / p(\mathbf{x}^{(new)})$

Generative Modelling: what’s new?

Two types of Machine Learning models:



Discriminative

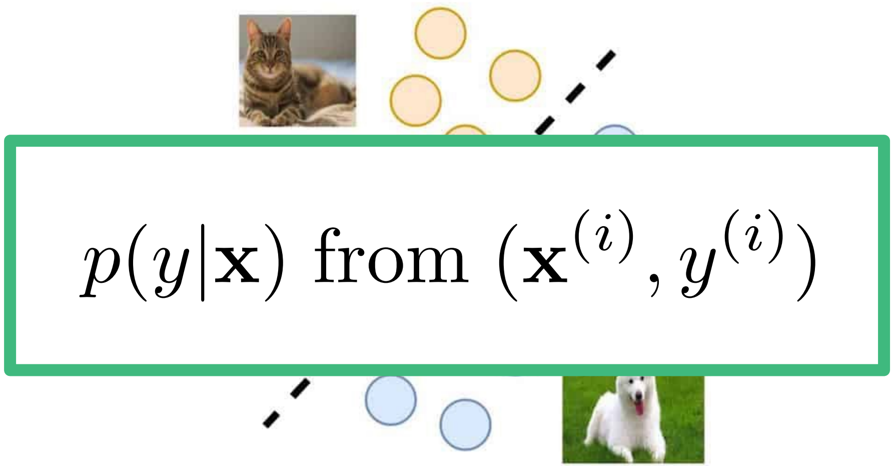


Generative

Source: https://learnopencv.com/generative-and-discriminative-models/

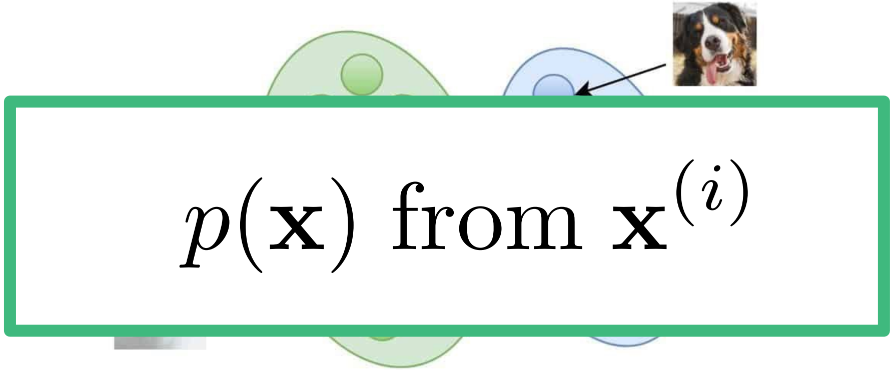
Generative Modelling: what's new?

Two types of Machine Learning models:



$$p(y|\mathbf{x}) \text{ from } (\mathbf{x}^{(i)}, y^{(i)})$$

Discriminative



$$p(\mathbf{x}) \text{ from } \mathbf{x}^{(i)}$$

Generative

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Generative Modelling: what's new?

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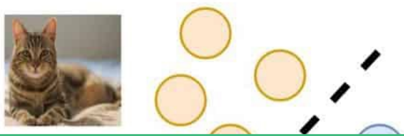
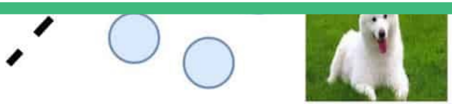


$$p(y|\mathbf{x}) \text{ from } (\mathbf{x}^{(i)}, y^{(i)})$$



$$p(\mathbf{x}) \text{ from } \mathbf{x}^{(i)}$$

or $p(\mathbf{x}|y)$ from $(\mathbf{x}^{(i)}, y^{(i)})$

Discriminative

Generative

Source: https://learnopencv.com/generative-and-discriminative-models/

Generative Modelling: what's new?

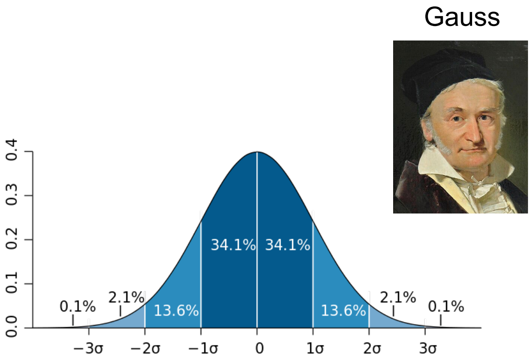
Ideally a generative modelling is a model solving the following problem

$$\underset{\theta}{\operatorname{argmax}}\, p(\mathbf{x}) \text{ from } \mathbf{x}^{(i)}$$

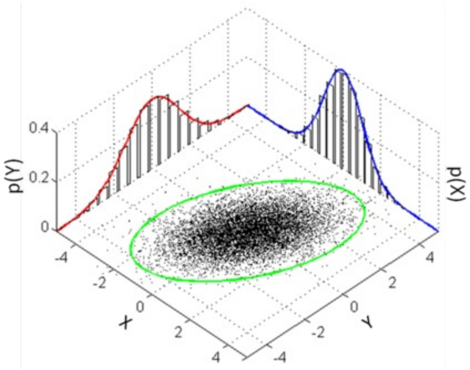
Maximum-likelihood estimator

We will see that this is not easy to do, usually approximations are required.

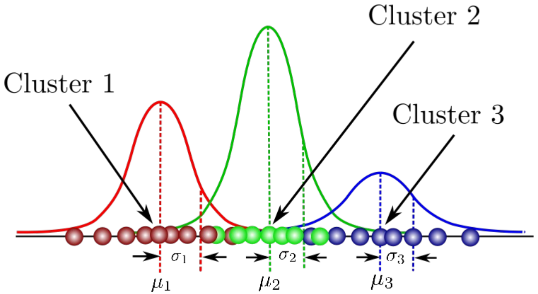
History of Generative Modelling



1809: Gaussian distribution

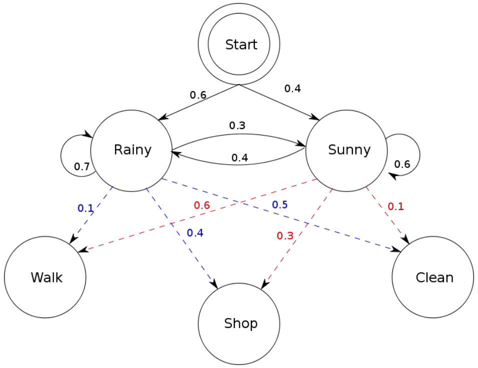


Multi-variate Gaussian distribution

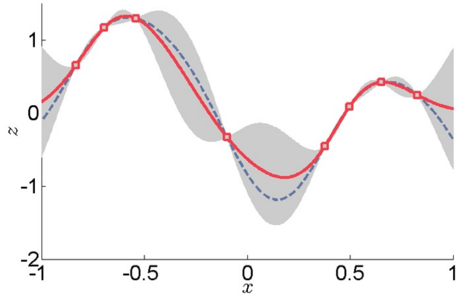


50’/60’: Gaussian Mixture Models (GGMs)

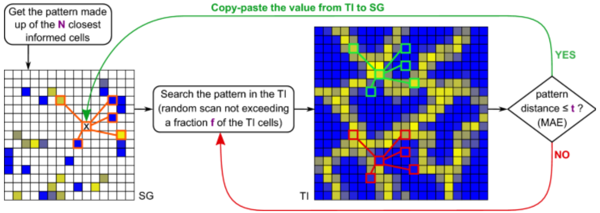
History of Generative Modelling



60’: Hidden Markov Models (HMMs)



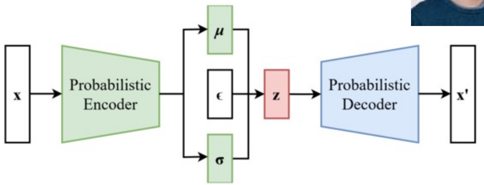
70’: Kriging – later popularized as Gaussian Process regression (GP)



90’: Geostatistics – two-point and multiple-point statistics

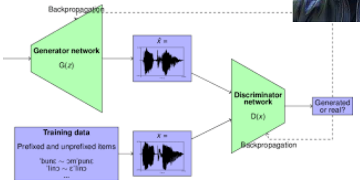
History of Generative Modelling

Kingma



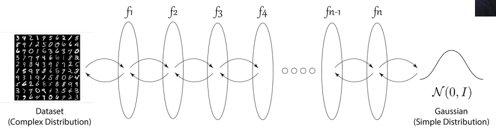
2014: Variational AutoEncoders

Goodfellow



2014: Generative Adversarial Networks (GANs)

Rezende

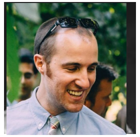


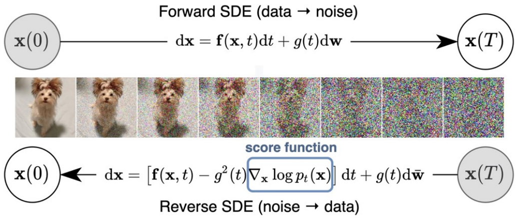
2015: Normalizing flows

....

History of Generative Modelling

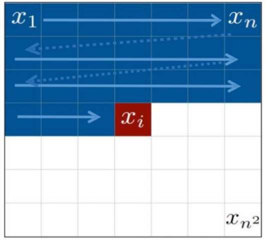
Sohl-Dickstein





2015: Diffusion models

Aaron van den Oord



2015: Autoregressive (image) models

Bahdanau

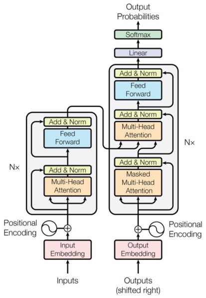
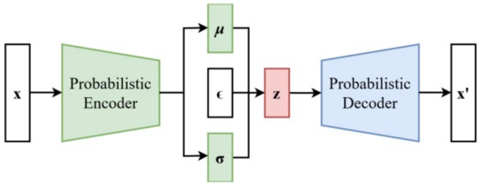


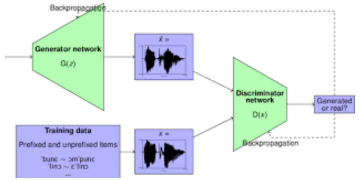
Figure 1: The Transformer - model architecture.

2015/7: Attention mechanism and Transformers

Generative Modelling in this week



2014: Variational AutoEncoders



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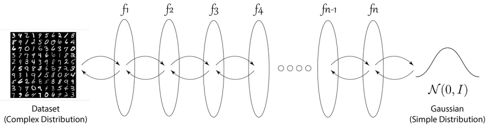
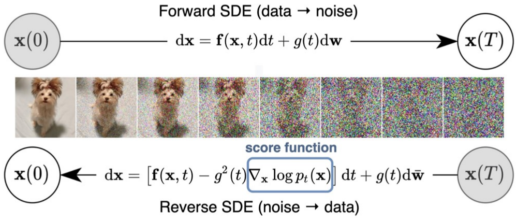


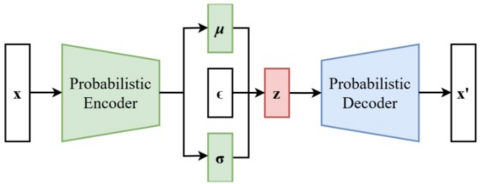
2015: Normalizing flows



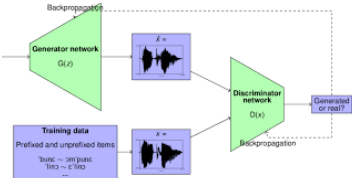
2015: Diffusion models

Generative Modelling in this week

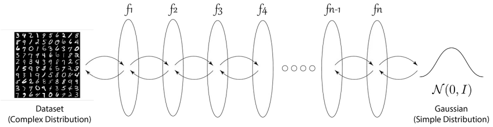
Implicit models: distribution is implicitely represented by a model of its sampling process



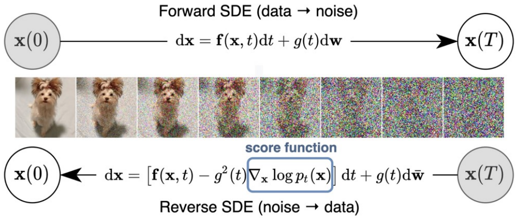
2014: Variational AutoEncoders



2014: Generative Adversarial Networks (GANs)



2015: Normalizing flows



2015: Diffusion models

Likelihood-based models: learn $p(\mathbf{x})$ via (approx.) Max-Likelihood

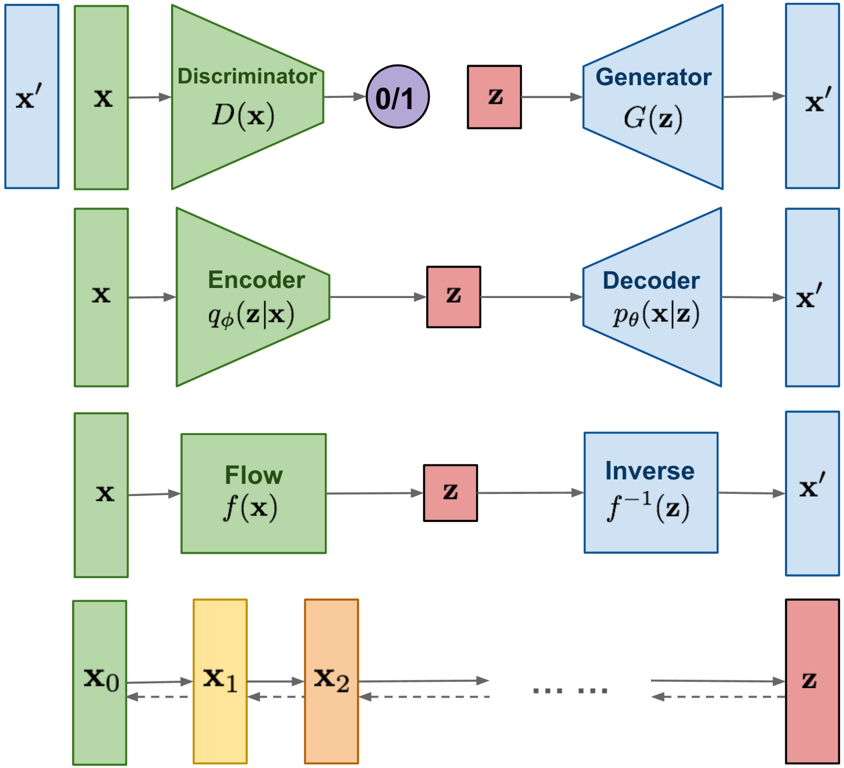
Generative Modelling in this week

GAN: Adversarial training

VAE: maximize variational lower bound

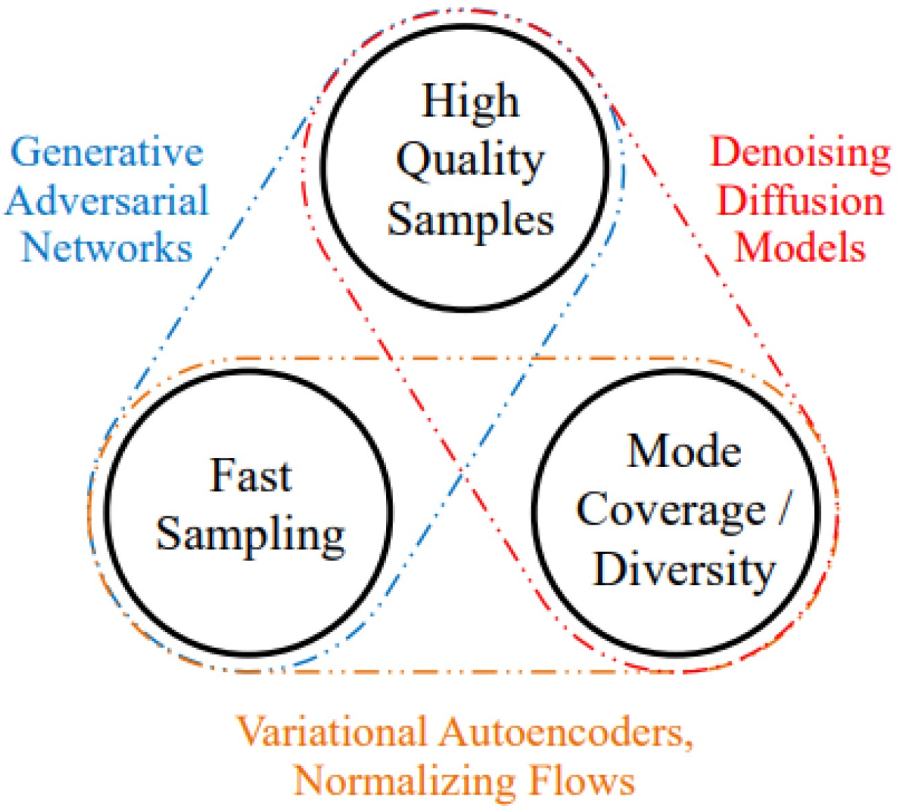
Flow-based models: Invertible transform of distributions

Diffusion models: Gradually add Gaussian noise and then reverse



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

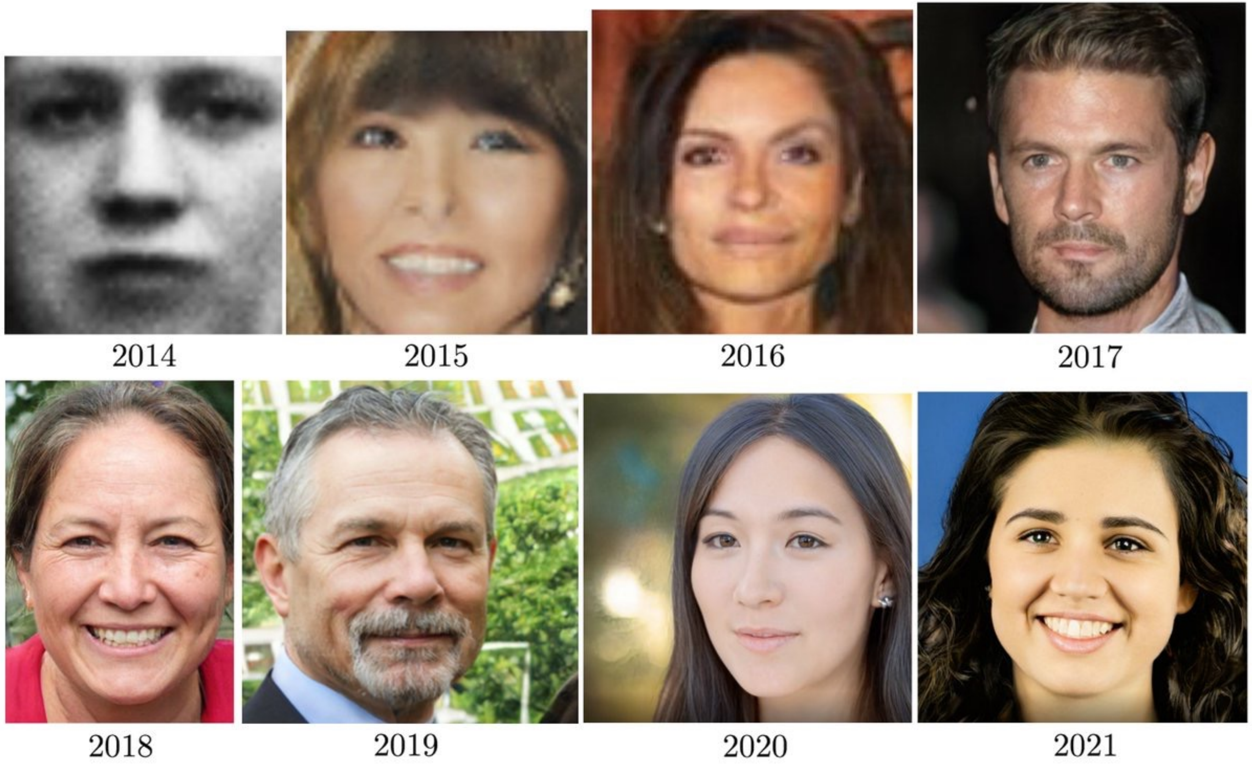
Generative Modelling in this week



Generative learning trilemma

From: Tackling the Generative Learning Trilemma with Denoising Diffusion GANs

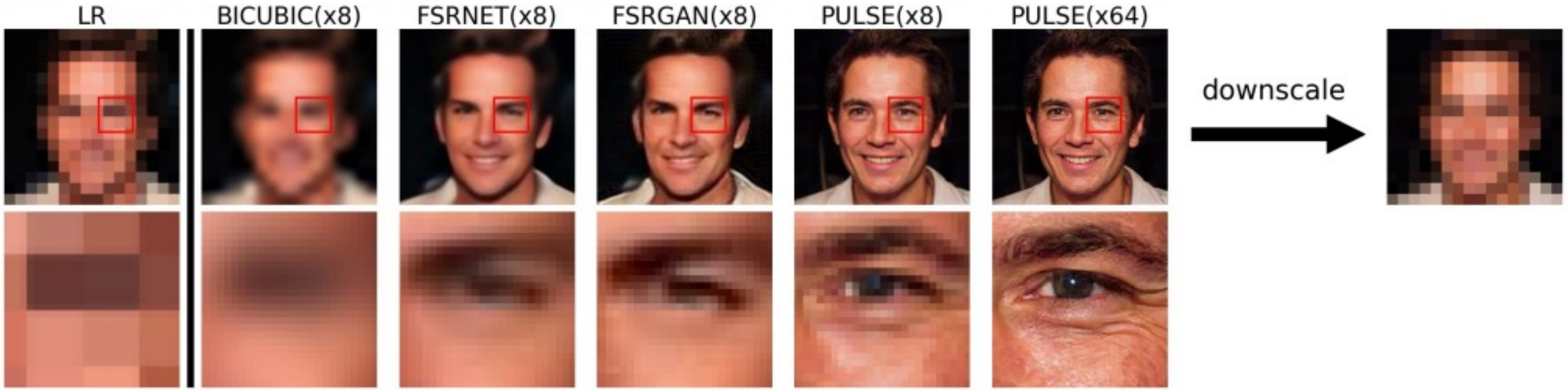
Success stories of GM: Face generation



Source: https://twitter.com/tamaybes/status/1450873331054383104

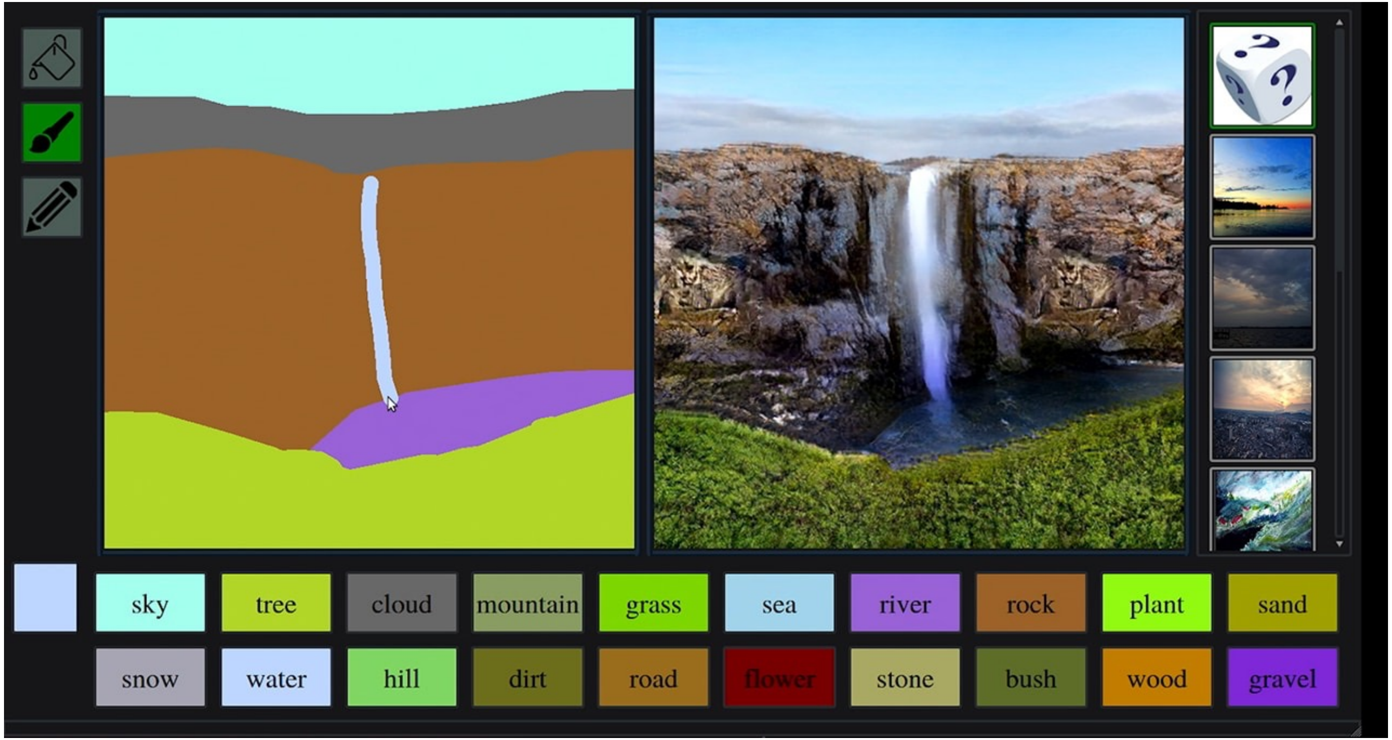
Success stories of GM: Inpainting

Success stories of GM: Super-resolution



Source: https://openaccess.thecvf.com/content_CVPR_2020/papers/Menon_PULSE_Self-Supervised_Photo_Upsampling_via_Latent_Space_Exploration_of_Generative_CVPR_2020_paper.pdf

Success stories of GM: Sketch-to-image



Source: https://blogs.nvidia.com/blog/2019/03/18/gaugan-photorealistic-landscapes-nvidia-research/

Success stories of GM: Text generation

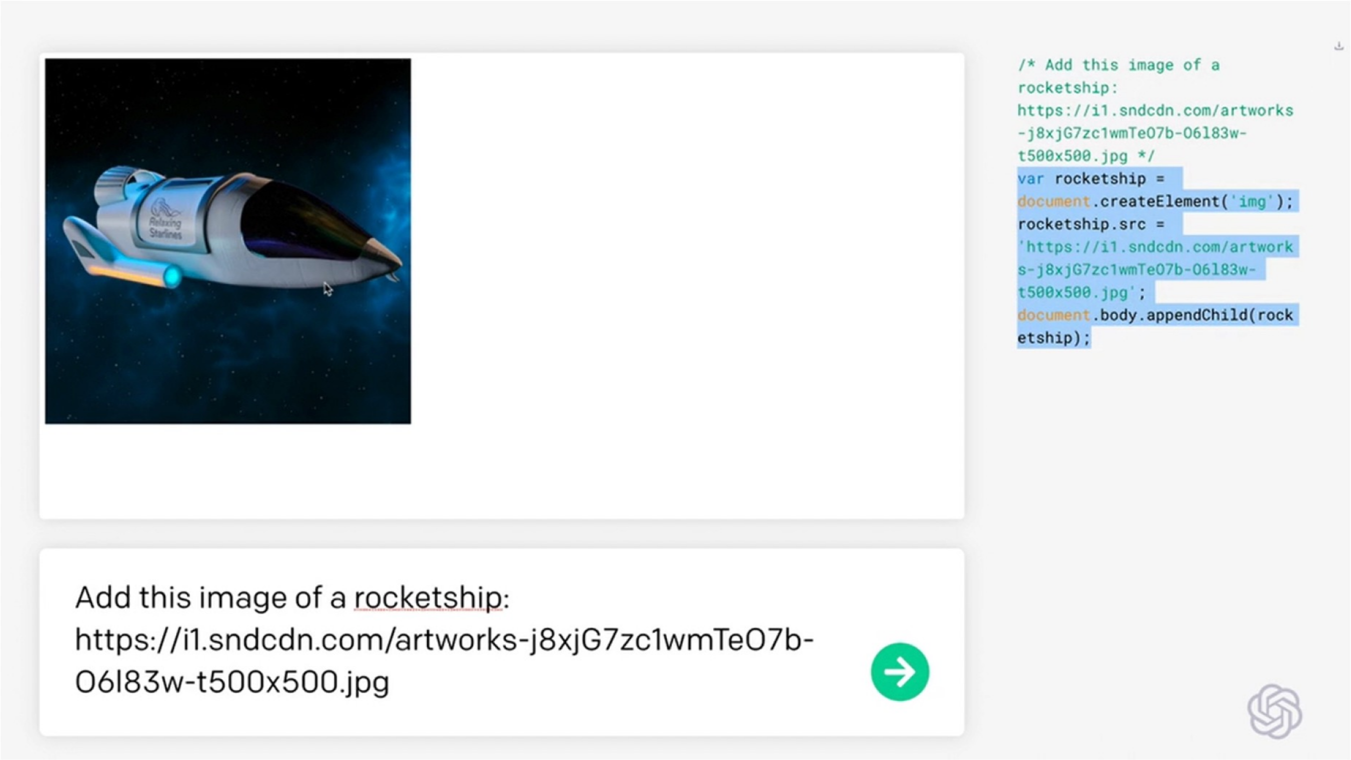
MA

Write a short description of the AI Summer School to be held in KAUST in June

Join us at the AI Summer School, hosted by KAUST (King Abdullah University of Science and Technology), a renowned research university located on the shores of the Red Sea in Saudi Arabia. Taking place in June, this immersive educational event offers a unique opportunity to dive deep into the world of Artificial Intelligence.

Designed for students, researchers, and professionals interested in AI, the AI Summer School at KAUST brings together experts, industry leaders, and passionate individuals to explore the latest advancements, applications, and challenges in the field of AI. Whether you're a beginner or an experienced practitioner, this program caters to a wide range of backgrounds and skill levels.

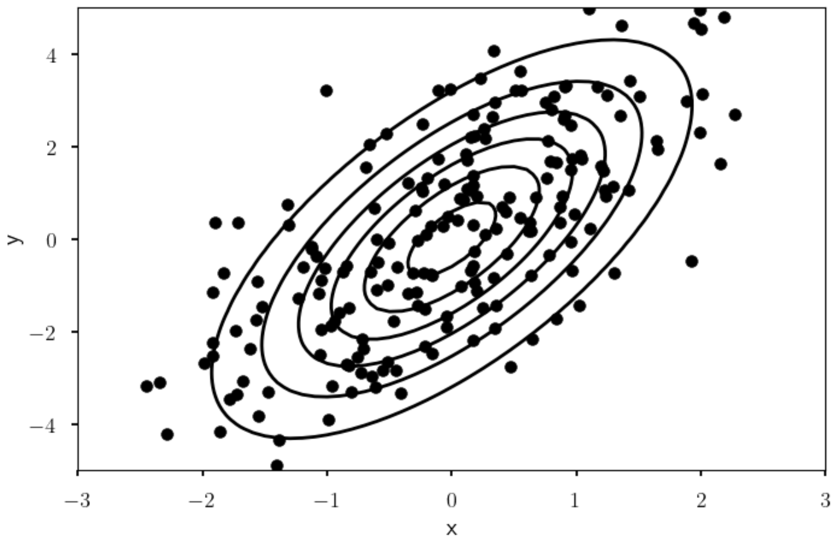
Success stories of GM: Code generation



Source: https://openai.com/blog/openai-codex/

Generative Modelling: Gauss's legacy

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \rightarrow \qquad p(\mathbf{x}) = \frac{1}{(2\pi)^{k/2} det(\boldsymbol{\Sigma})^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$



$$\boldsymbol{\mu} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \boldsymbol{\Sigma} = \begin{bmatrix} 5 & 1.5 \\ 1.5 & 1 \end{bmatrix}$$

$$\theta = \{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$$

Generative Modelling: Gauss's legacy

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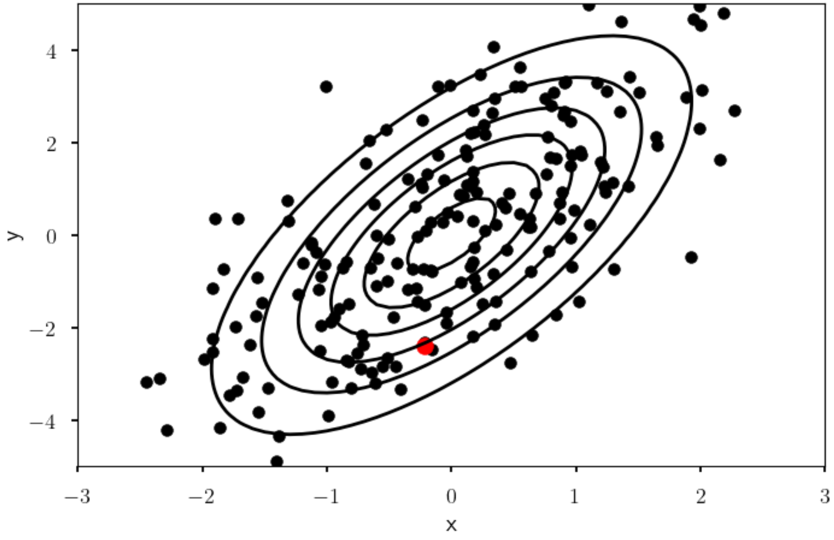

Sample distribution:

Being able to draw a sample from the distribution (red dot)

If we sample many points (e.g., 1000), we can then estimate sample statistics - mean, cov

Generative Modelling: Gauss's legacy

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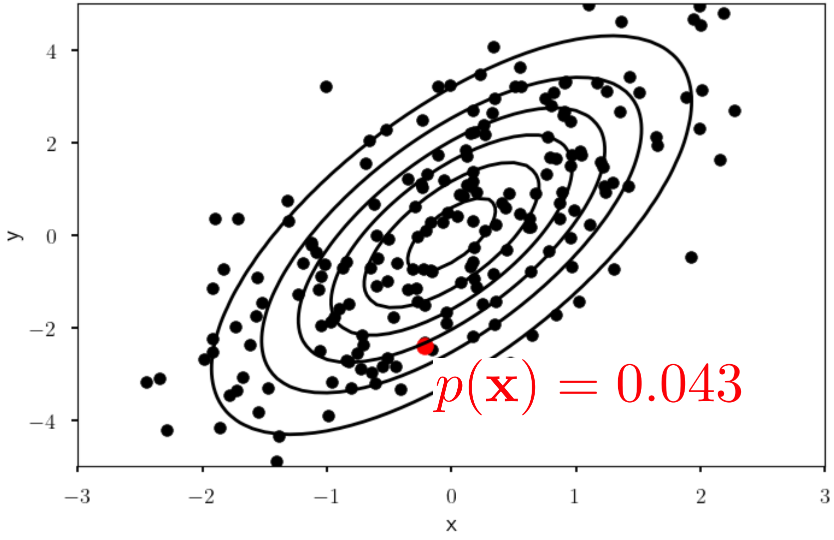

Evaluate distribution:

Being able to insert **x** in the probability density function and get the probability of occurrence of that sample

Generative Modelling: Gauss's legacy

Sample a Gaussian distribution:

Training

1. Compute the sample mean and covariance from the training samples: $\boldsymbol{\mu}, \boldsymbol{\Sigma}$
2. Apply Cholesky decomposition of the covariance matrix: $\boldsymbol{\Sigma} = \mathbf{L}^T \mathbf{L}$

Inference/generation

1. Sample a vector from normal distribution: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2. Create new sample from true distribution by scaling and shifting: $\mathbf{x}^{(new)} = \mathbf{L}\mathbf{z} + \boldsymbol{\mu}$

Generative Modelling: Gauss's legacy

Operations on Gaussian distributions:

<u>Sum and multiplication *with 'scalars'*</u>

Univariate: $z \sim \mathcal{N}(0, 1),\qquad x = az + b \sim \mathcal{N}(b, a^2)$

Multivariate: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}),\qquad \mathbf{x} = \mathbf{L}\mathbf{z} + \boldsymbol{\mu} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma} = \mathbf{L}^T\mathbf{L})$

<u>Sum *of variables*</u>

$$x \sim \mathcal{N}(b, a^2), y \sim \mathcal{N}(c, d^2) \rightarrow z = x + y \sim \mathcal{N}(a + c, b^2 + d^2)$$

Convolution

$$p(z) = p(x) * p(y)$$

Generative Modelling: Gauss's legacy

Operations on Gaussian distributions:

Sum of distributions

Gaussian mixture: $p_1(x) \sim \mathcal{N}(b, a^2), p_2(x) \sim \mathcal{N}(c, d^2) \rightarrow p(x) = w_1 p_1(x) + w_2 p_2(x) (w_1 + w_2 = 1)$

Product of distributions

$$p_1(x) \sim \mathcal{N}(a, b^2), p_2(x) \sim \mathcal{N}(c, d^2) \rightarrow p_1(x) p_2(x) \sim \mathcal{N}\left(\frac{b^2 c + d^2 a}{b^2 + d^2}, \frac{1}{1/b^2 + 1/d^2}\right)$$

Generative Modelling: Gauss's legacy

There is a bit of Gauss in every modern generative model:

- **VAEs:** latent code distribution
- **GANs:** noise input to generator
- **Normalizing flows:** basic distribution (to be warped into $p(x)$)
- **Diffusion models:** noise added at every step

My specific interest in Generative modelling

Solving physics-driven inverse problems:

$$\mathcal{L}(\mathbf{d} - g(\mathbf{x})) + \mathcal{R}(\mathbf{x})$$

… leveraging powerful learned priors:

$$\mathcal{L}(\mathbf{d} - g(\mathbf{x})) + f_\theta(\mathbf{x})$$

or

$$\mathcal{L}(\mathbf{d} - g(f_\theta(\mathbf{z})))$$