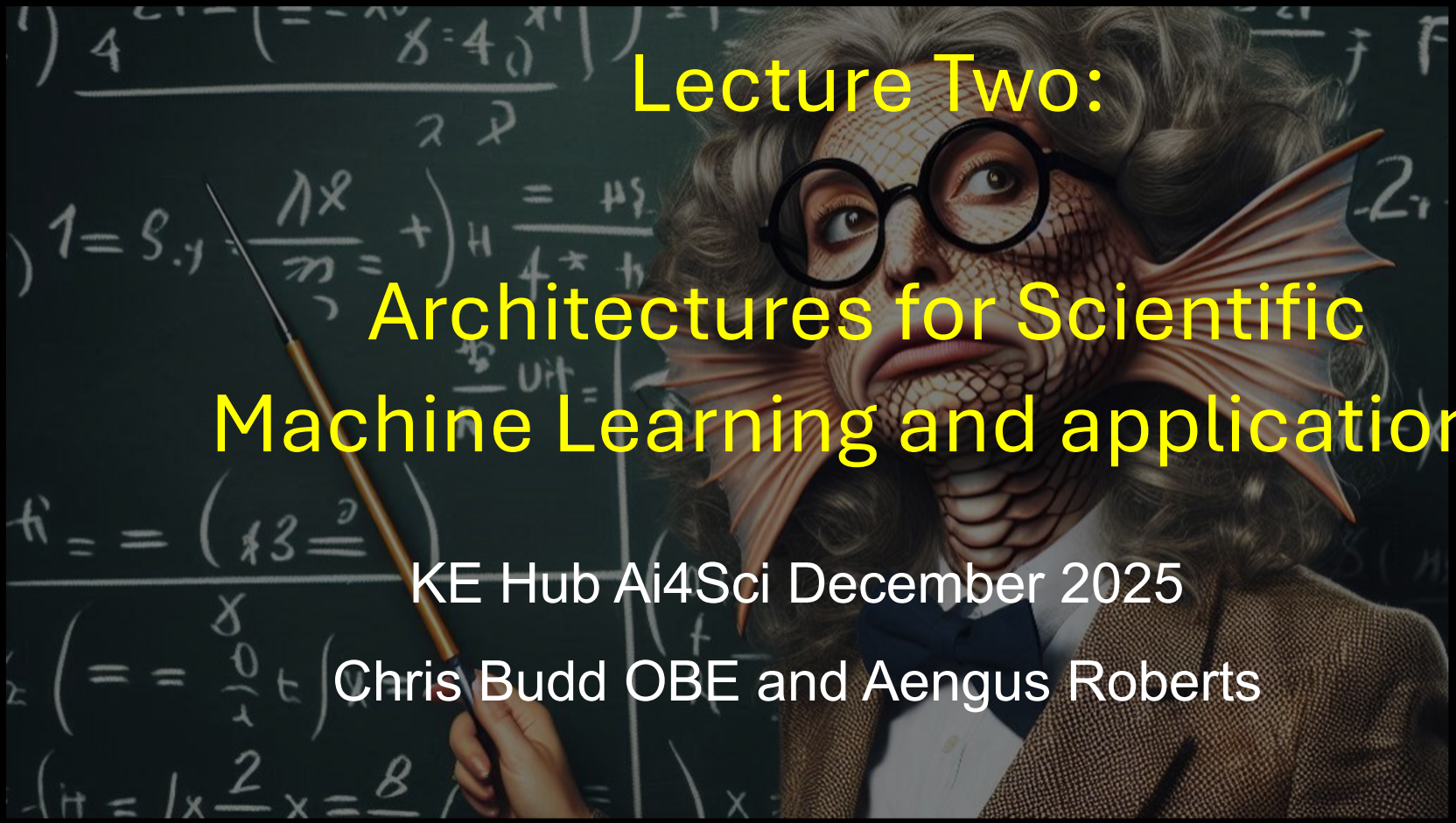


Lecture Two:

Architectures for Scientific Machine Learning and applications

KE Hub Ai4Sci December 2025

Chris Budd OBE and Aengus Roberts

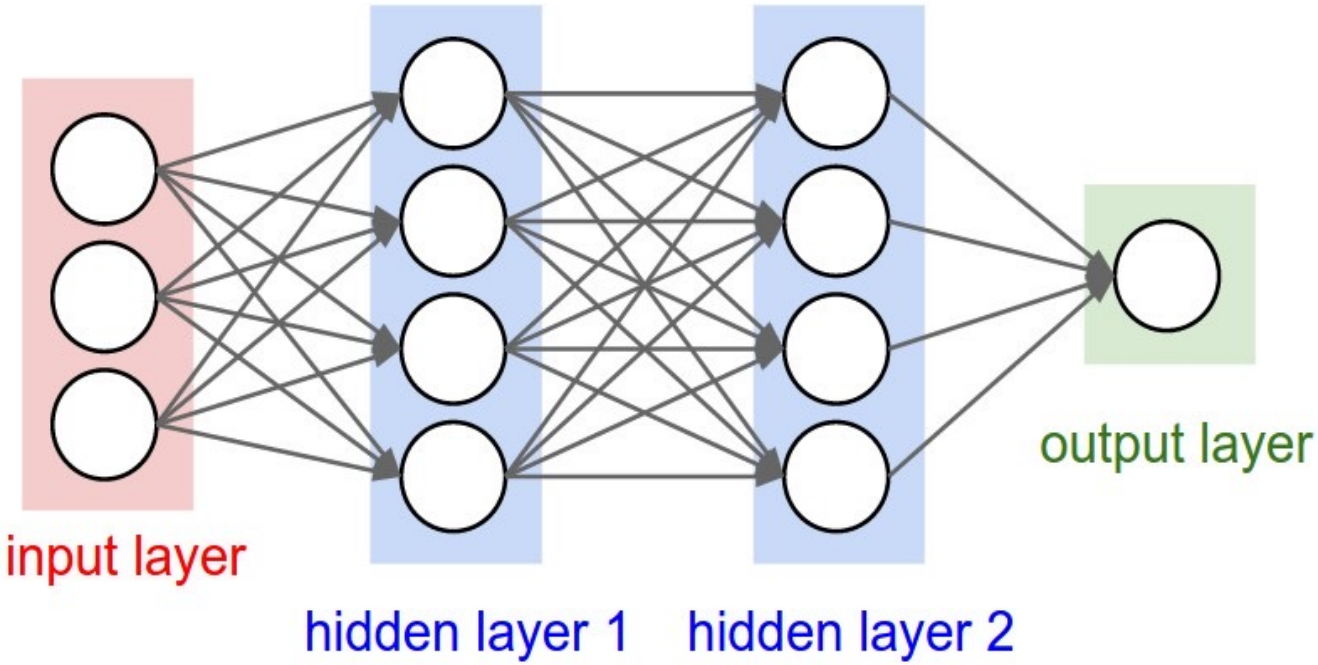
Knowledge Exchange Hub for Mathematical Sciences

m4DL

UNIVERSITY OF BATH

Multi-Layer Perceptron

Good for classification problems and general use

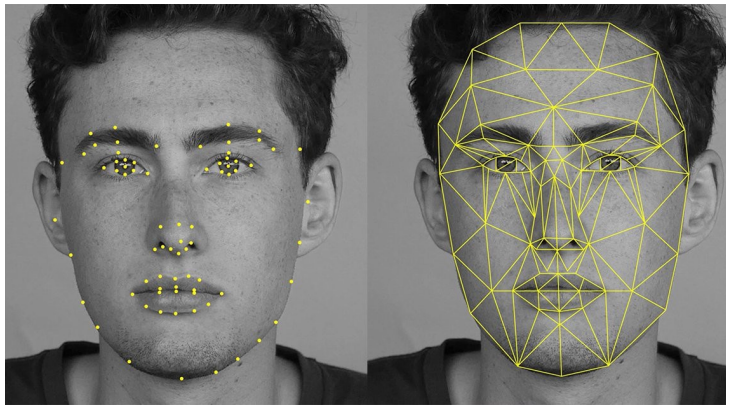


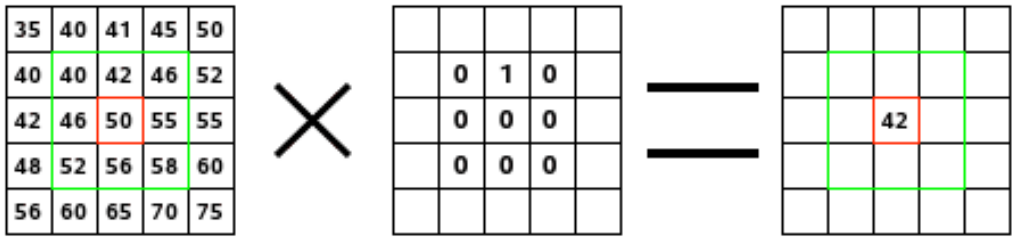
Special architectures:

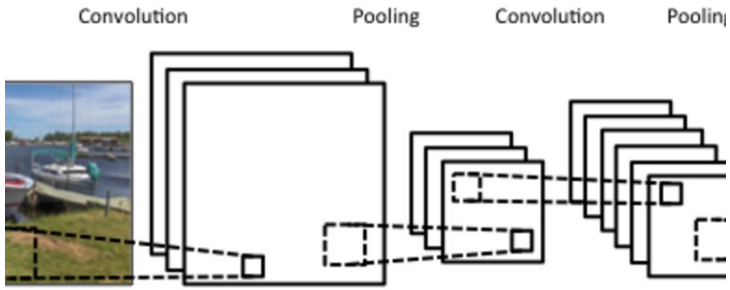
Convolutional Neural Network (CNN)

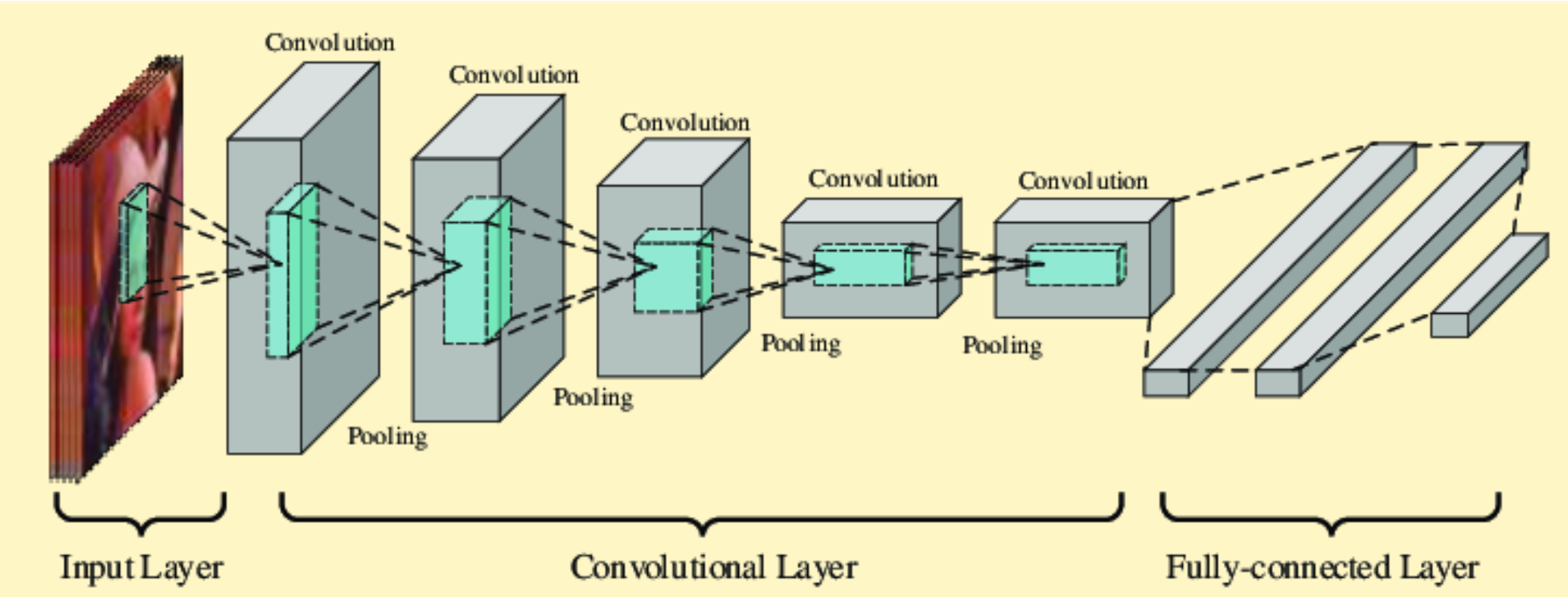
Uses structured sparse linear operators designed to take a convolution of an image.

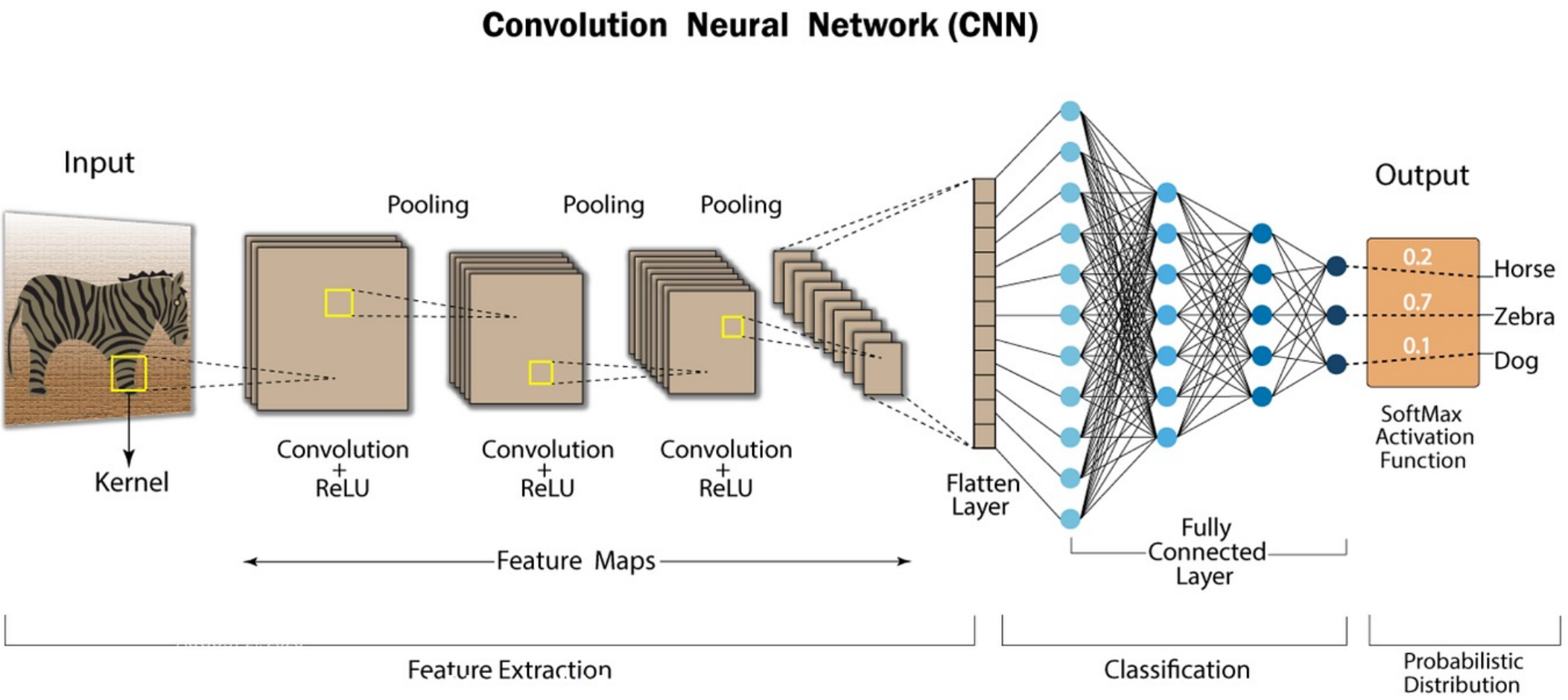
Excellent for feature extraction, image processing, etc.







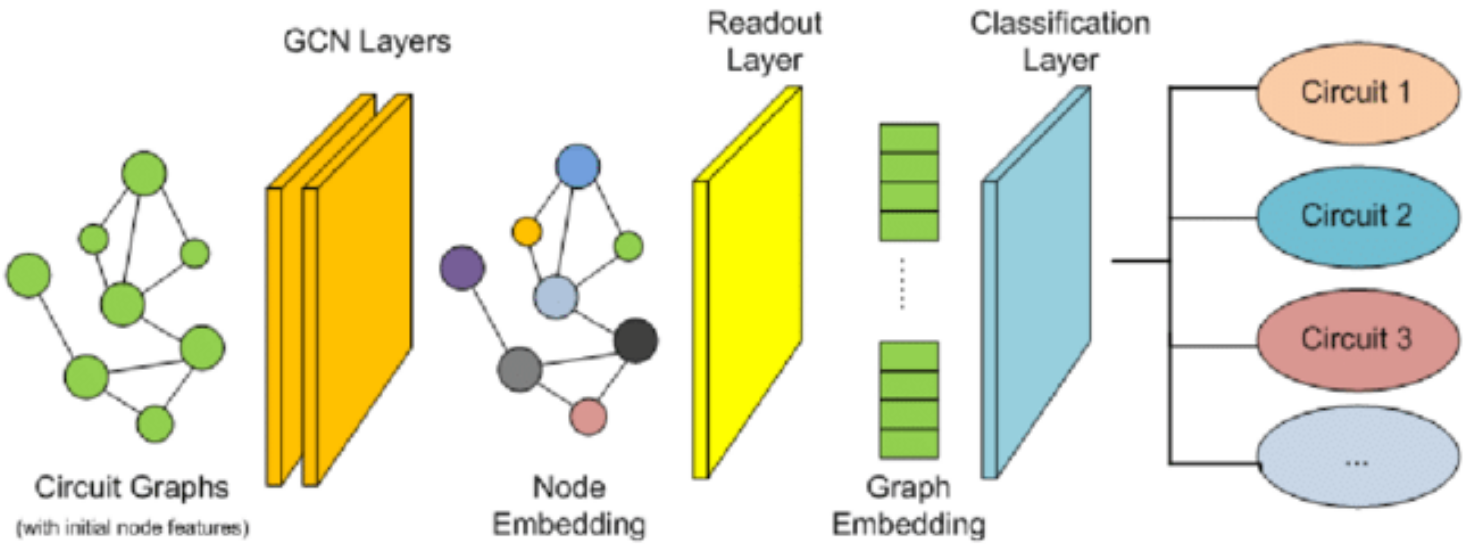

Convolution
Convolution
Convolution
Convolution
Convolution
Pooling
Pooling
Pooling
Pooling
Input Layer
Convolutional Layer
Fully-connected Layer


Convolution Neural Network (CNN)
Input
Pooling
Pooling
Pooling
Output
0.2
Horse
0.7
Zebra
0.1
Dog
Kernel
Convolution + ReLU
Convolution + ReLU
Convolution + ReLU
Flatten Layer
SoftMax Activation Function
Feature Maps
Fully Connected Layer
Feature Extraction
Classification
Probabilistic Distribution

Graph neural networks (GNN)

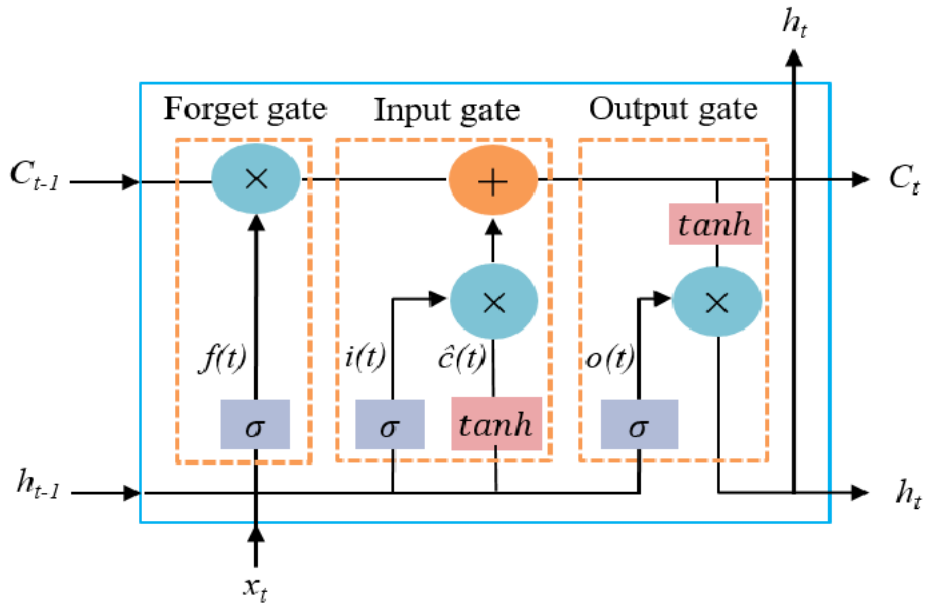
Specialized NNs that are designed for tasks whose inputs are graphs

Similar to CNNs. Can be used for structured images, or PDES



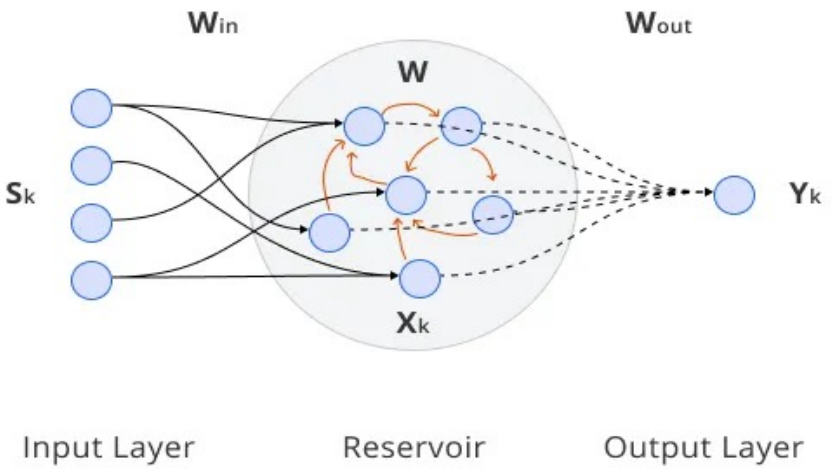
LSTM (Long, Short, Term Memory)

The Long Short-Term Memory (LSTM) architecture is a type of recurrent neural network (RNN) designed to overcome the vanishing gradient problem and effectively model long-term dependencies in sequential data. Eg. short term predition




Prediction
Real
45.0
42.5
40.0
37.5
35.0
32.5
30.0
Price

Echo State Networks



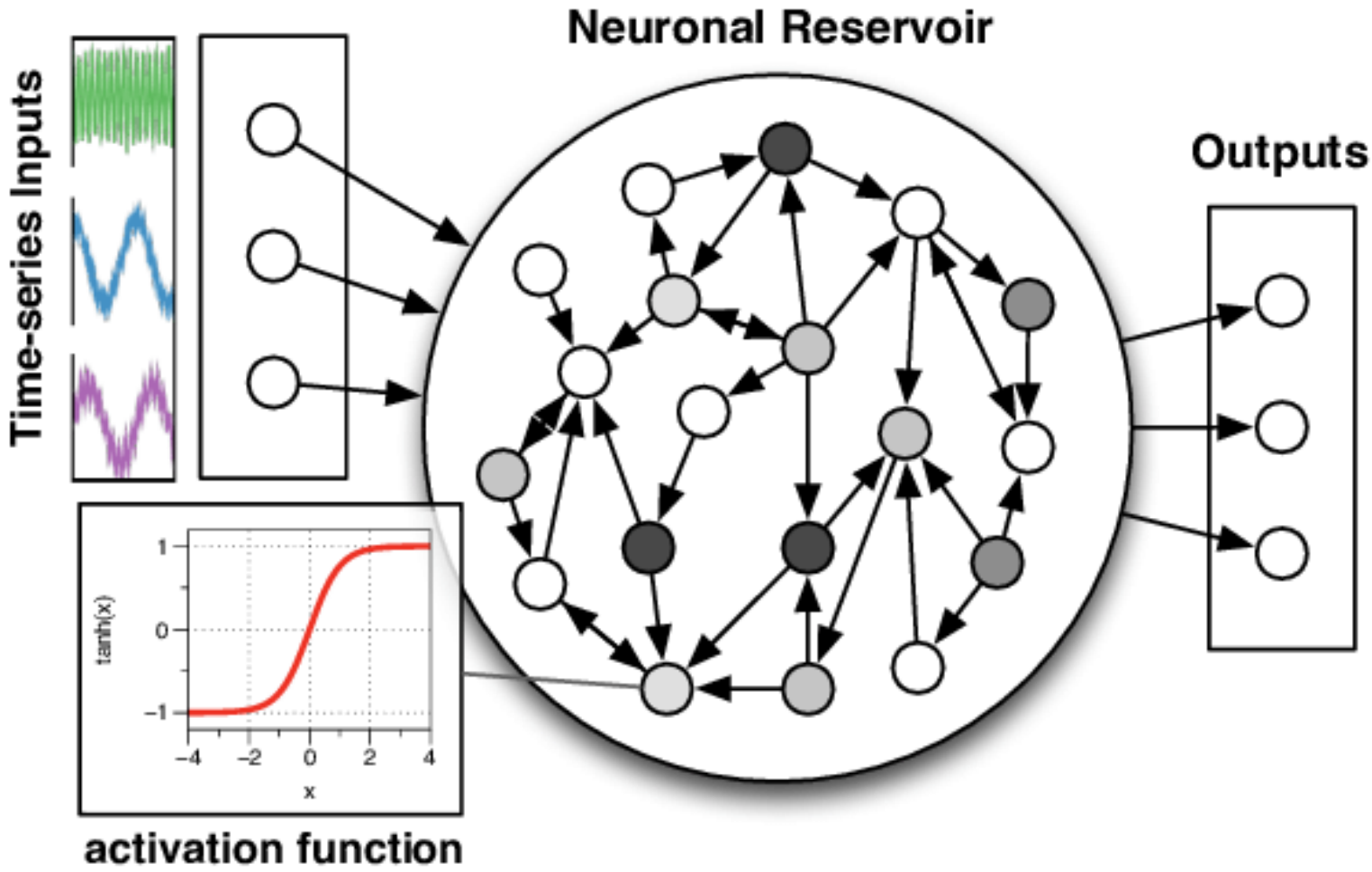
Random (fixed) interior layers

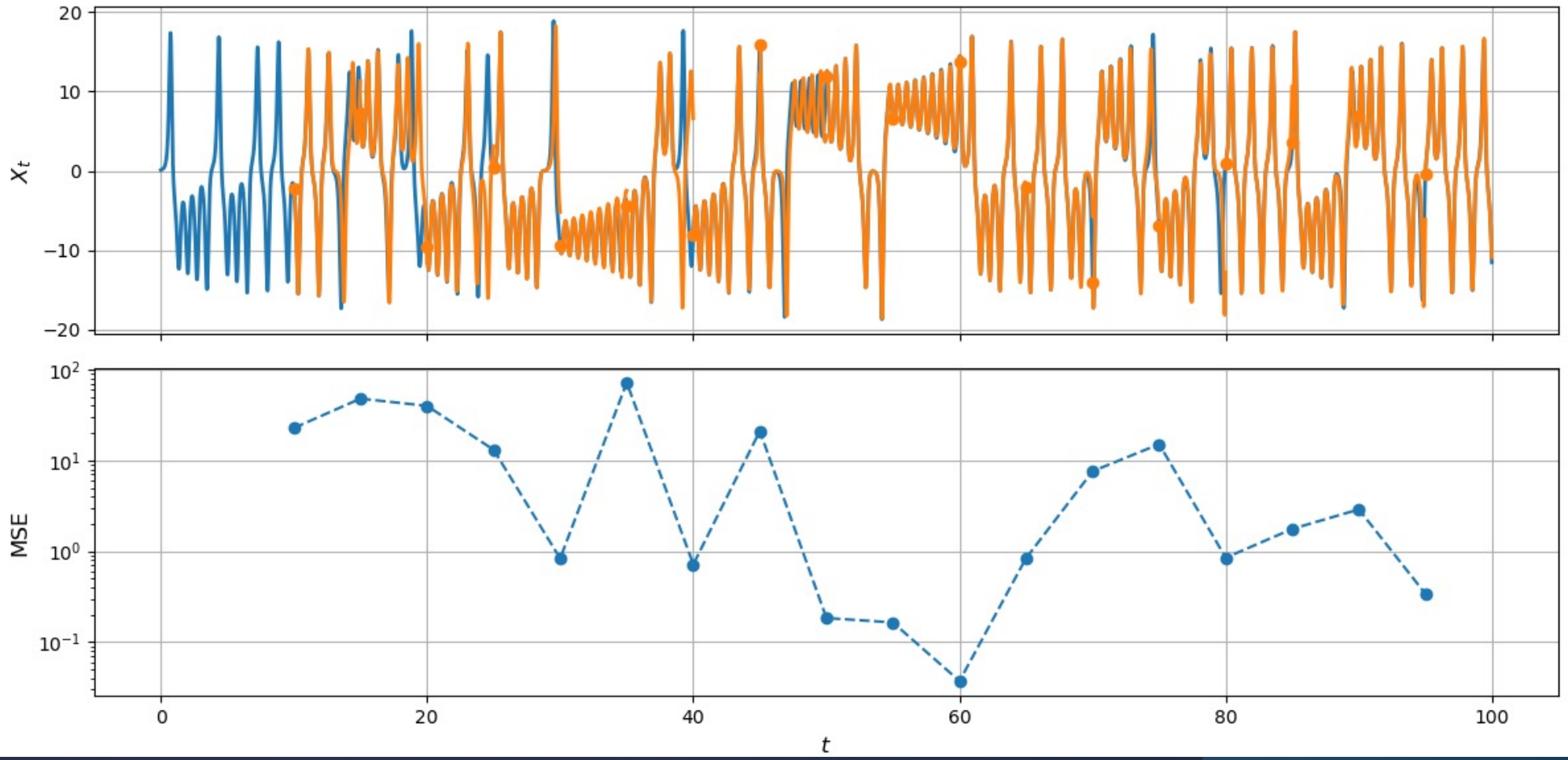
Trainable (linear) OUTPUT layer

Used to make predictions on chaotic systems

Large Language Models/Transformers

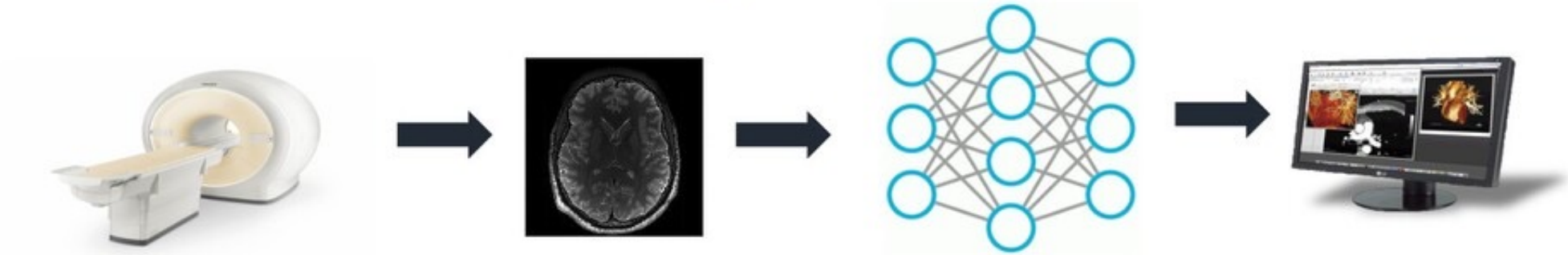
Very powerful .. But not on the course!


Neuronal Reservoir
Time-series Inputs
Outputs
tanh(x)
1
0
−1
−4
−2
0
2
4
x
activation function

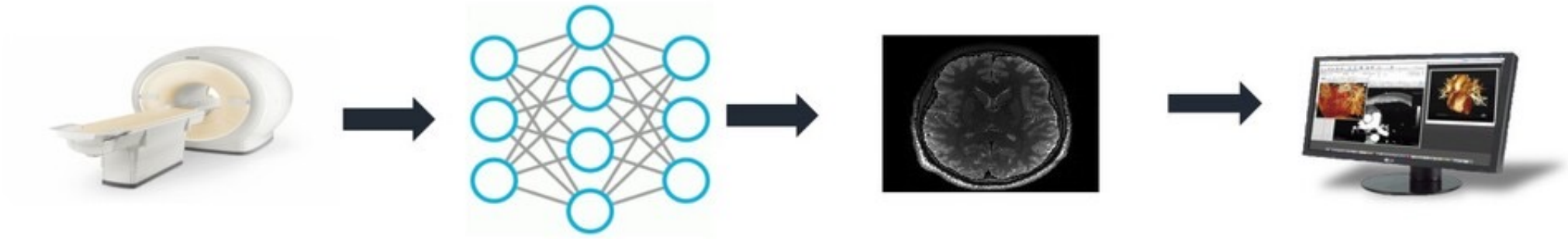

20
10
0
−10
−20
X_t
10^2
10^1
10^0
10^{-1}
MSE
0
20
40
60
80
100
t

Deep Learning for Inverse Problems

Diagnosis & analysis

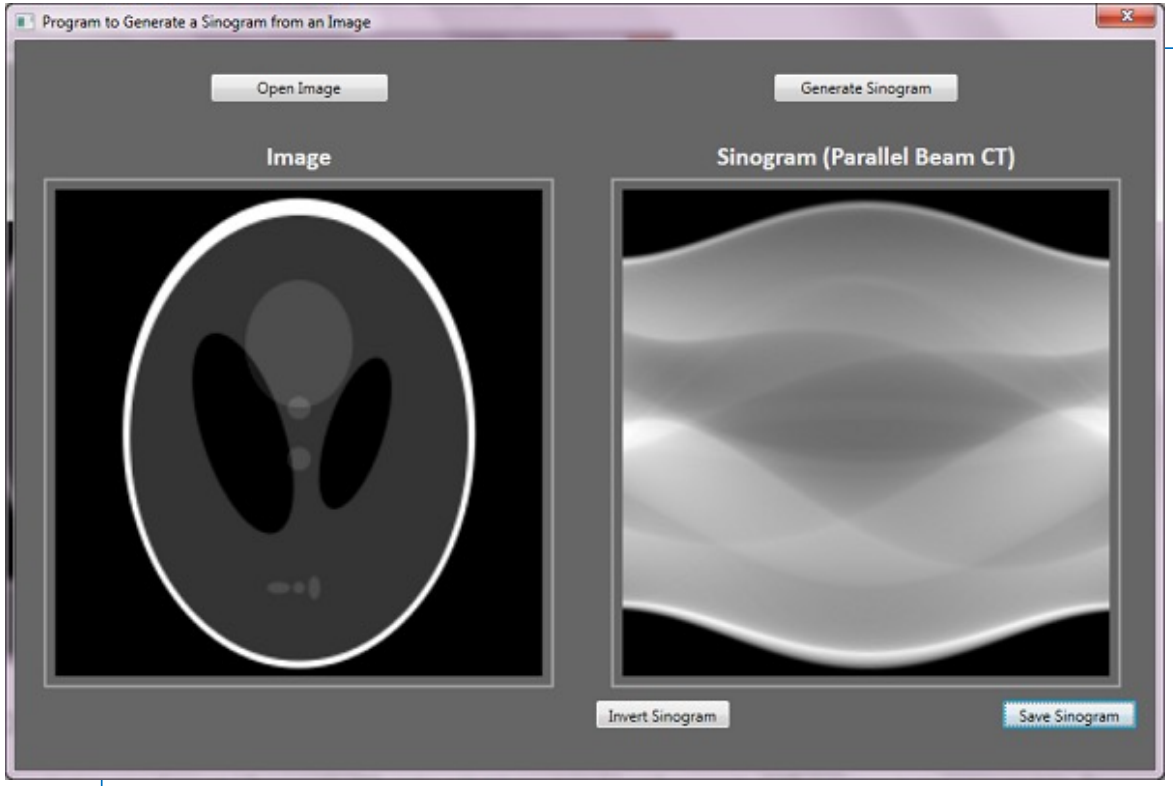


New trend of deep learning: inverse problems



$$A\,x = y + \text{noise}$$

A: ill-conditioned



Use

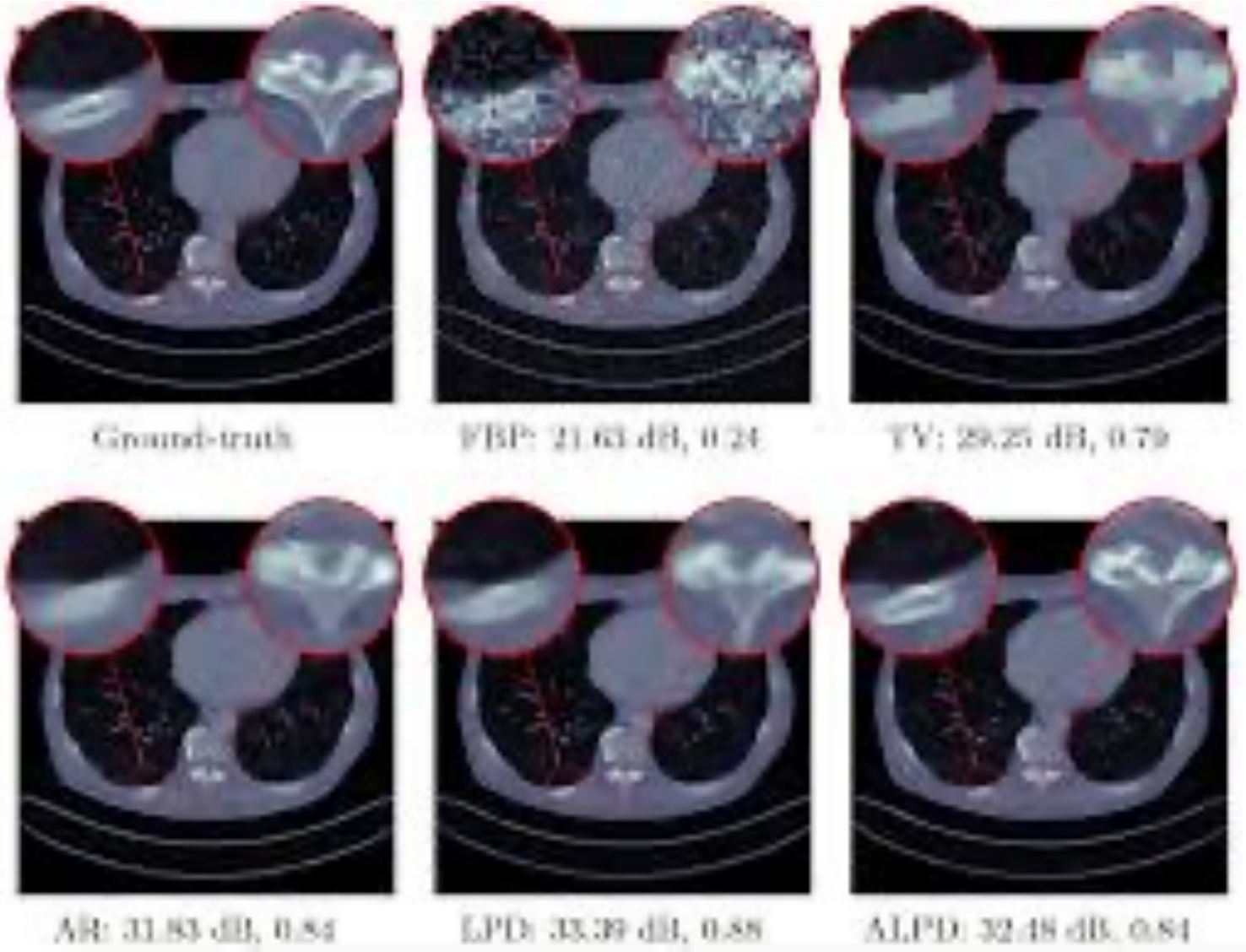
$$x = argmin_x |A\,x - y|^2 + \mathrm{R(x)}$$: Data error + Regulariser

R(x)

Q: Best regulariser

Tychonov: R(x) = $|B(x)|^2$. TV: R(x) = $|\nabla x|$

Learned: Train the regulariser on a set of problems


Ground-truth
FBP: 21.63 dB, 0.24
TV: 29.25 dB, 0.79
AR: 31.83 dB, 0.84
LPD: 33.39 dB, 0.88
ALPD: 32.48 dB, 0.84

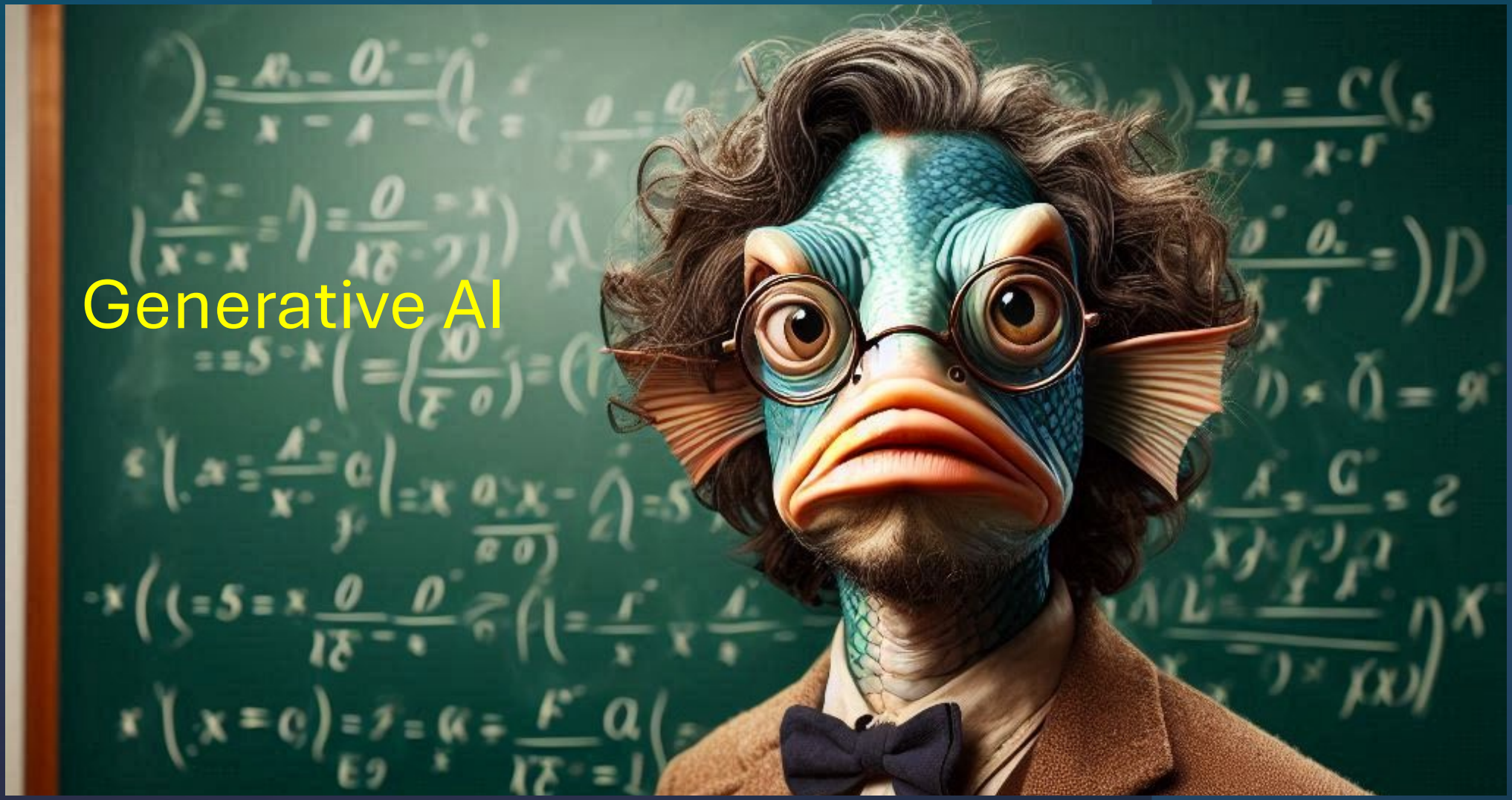
AI and Cultural Heritage: Investigating Artworks and Manuscripts

The Adoration of the Kings (NG592), tempera on wood, about 1472, at the National Gallery, London. Attributed to Sandro Botticelli and Fillipino Lippi. Image © The National Gallery, London.

Left: Punch marks (from [2]). Right: *St Augustine* (accession number 552) attributed to Simone Martini at The Fitzwilliam Museum, Cambridge; Image © The Fitzwilliam Museum, University of Cambridge.

[1] W. Peaslee, L. Wrapson, C.-B. Schönlieb, "Domain generalization and punch mark classification," *Journal of Cultural Heritage*, vol. 72, 2025

[2] M. Zullich, et al., "An Artificial Intelligence System for Automatic Recognition of Punches in Fourteenth-Century Panel Painting," *IEEE Access*, vol. 11, 2023.


Generative AI

Generative AI: Image creation

Probability distribution of images and classifiers

Take samples from this

Generate samples that are similar to training examples

Image label/Partial Image

Eg. Fishy mathematician

Trained NN

Generate new samples conditional on the text prompt

Problems with averaging if not done carefully

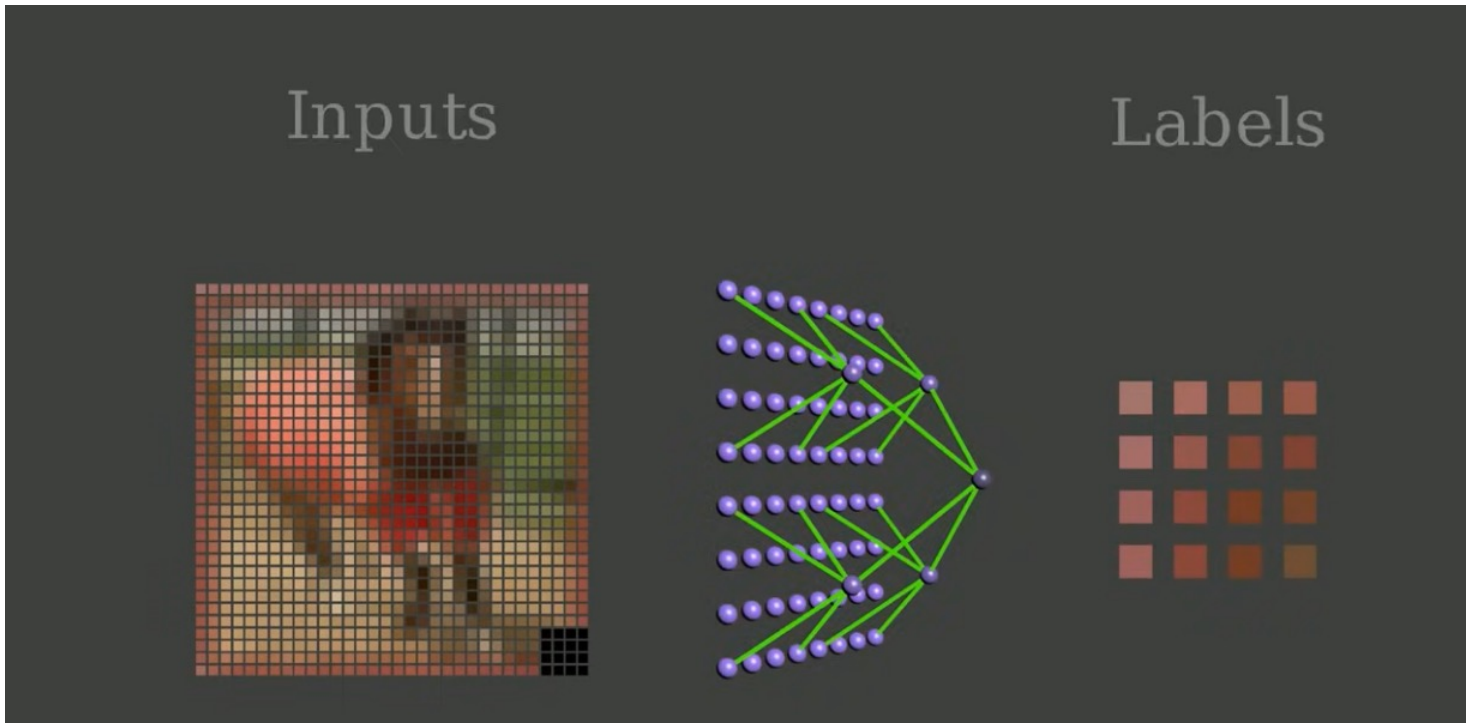
https://en.wikipedia.org/wiki/Stable_Diffusion

Applications

- Inpainting
- Image reconstruction
- Down scaling
- Fake image creation (random)
- Fake image creation (labled by text prompt)
- Protein synthesis
- Climate prediction

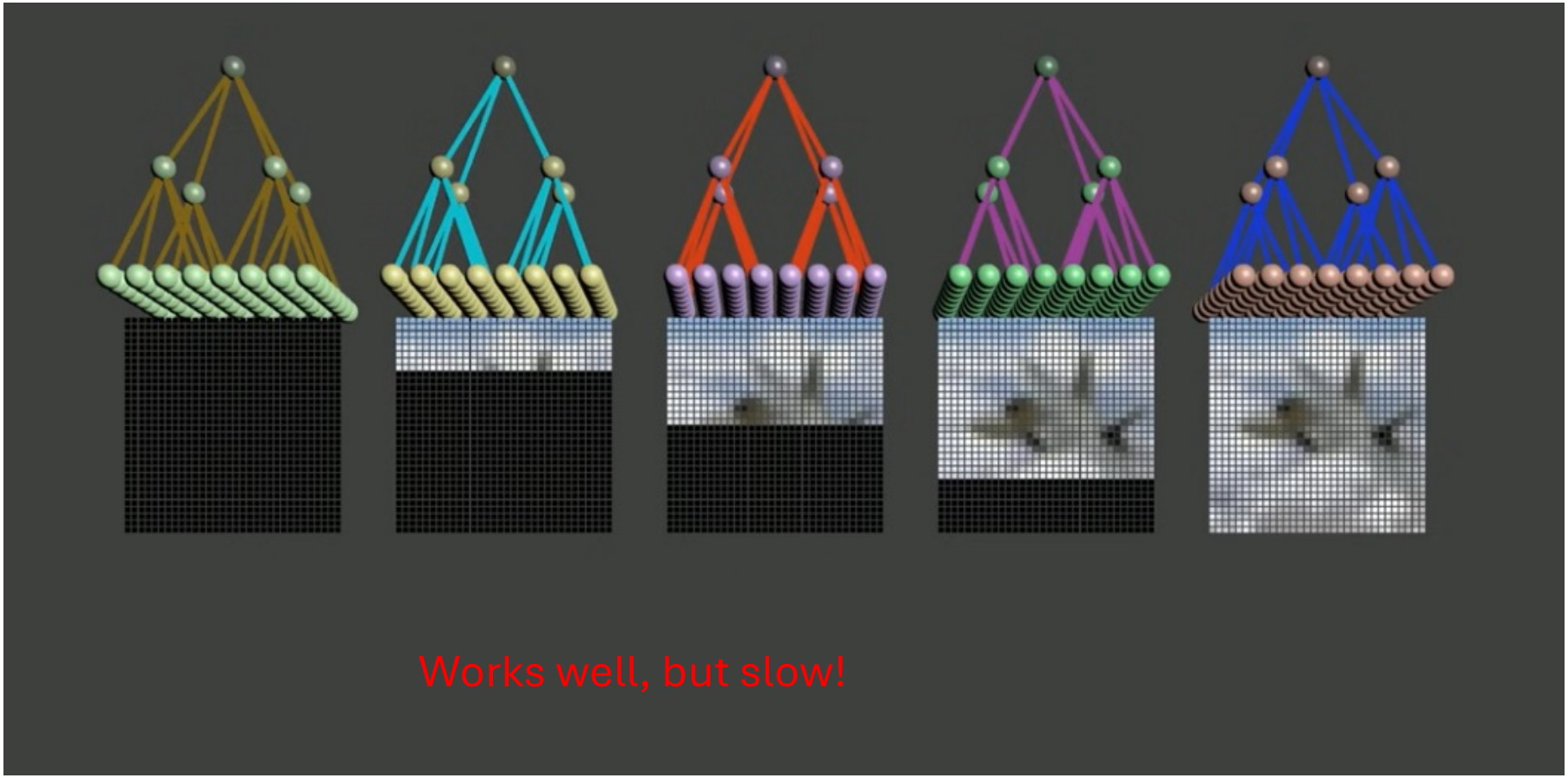
Generative AI Methods I : Auto Regressive Methods [1927!]

(used for example in Chat GPT)



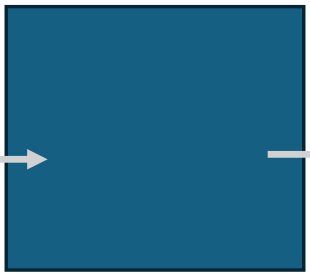
- Given an image with some Pixels missing,
- Train a NN to fill in the missing Pixels (as a probability distribution)

- Do this repeatedly to build up a whole image from an initially blank screen



Generative AI Methods II: GANs

Trained Generator (NN)



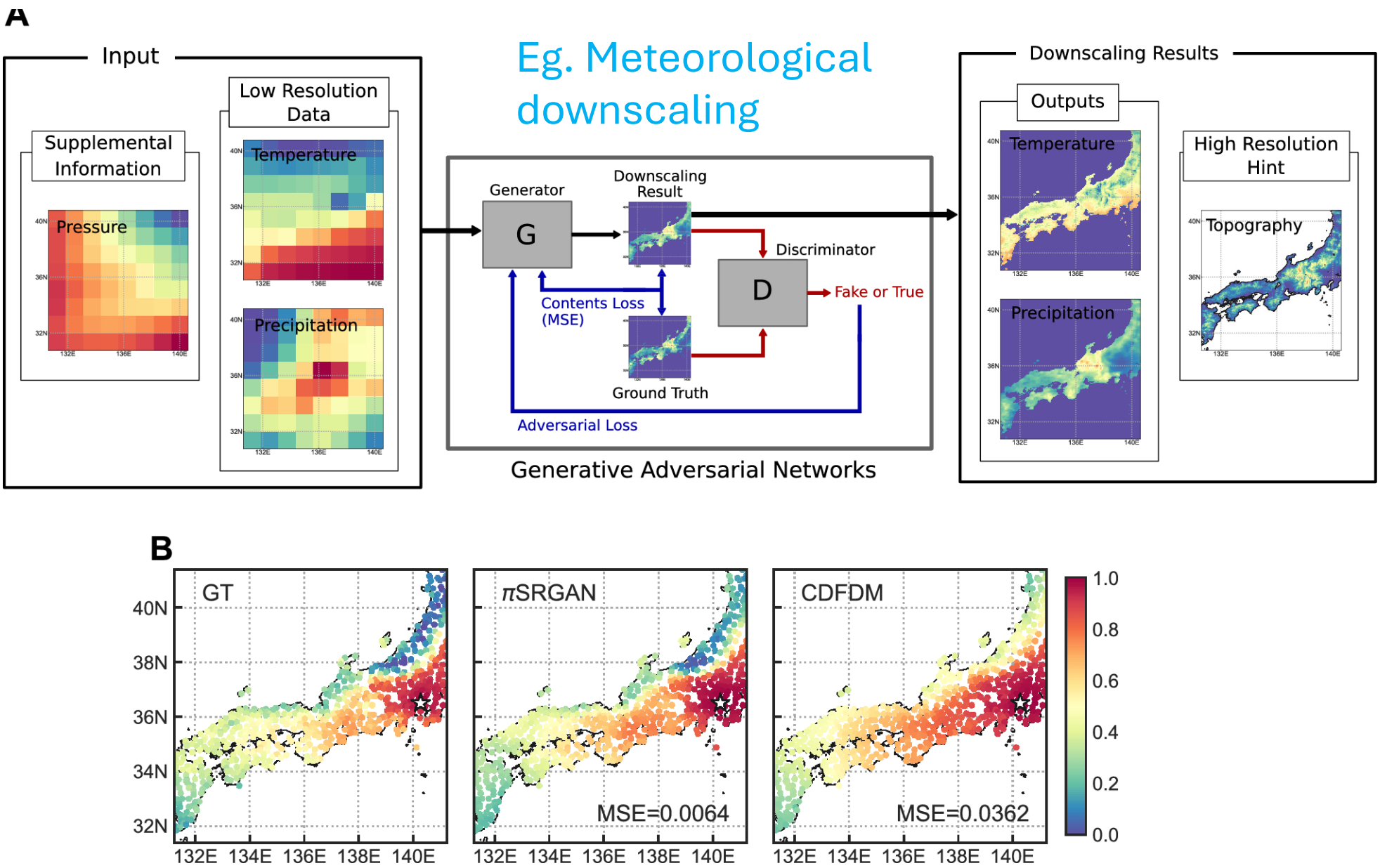
Random noise z

Fake image G(z)

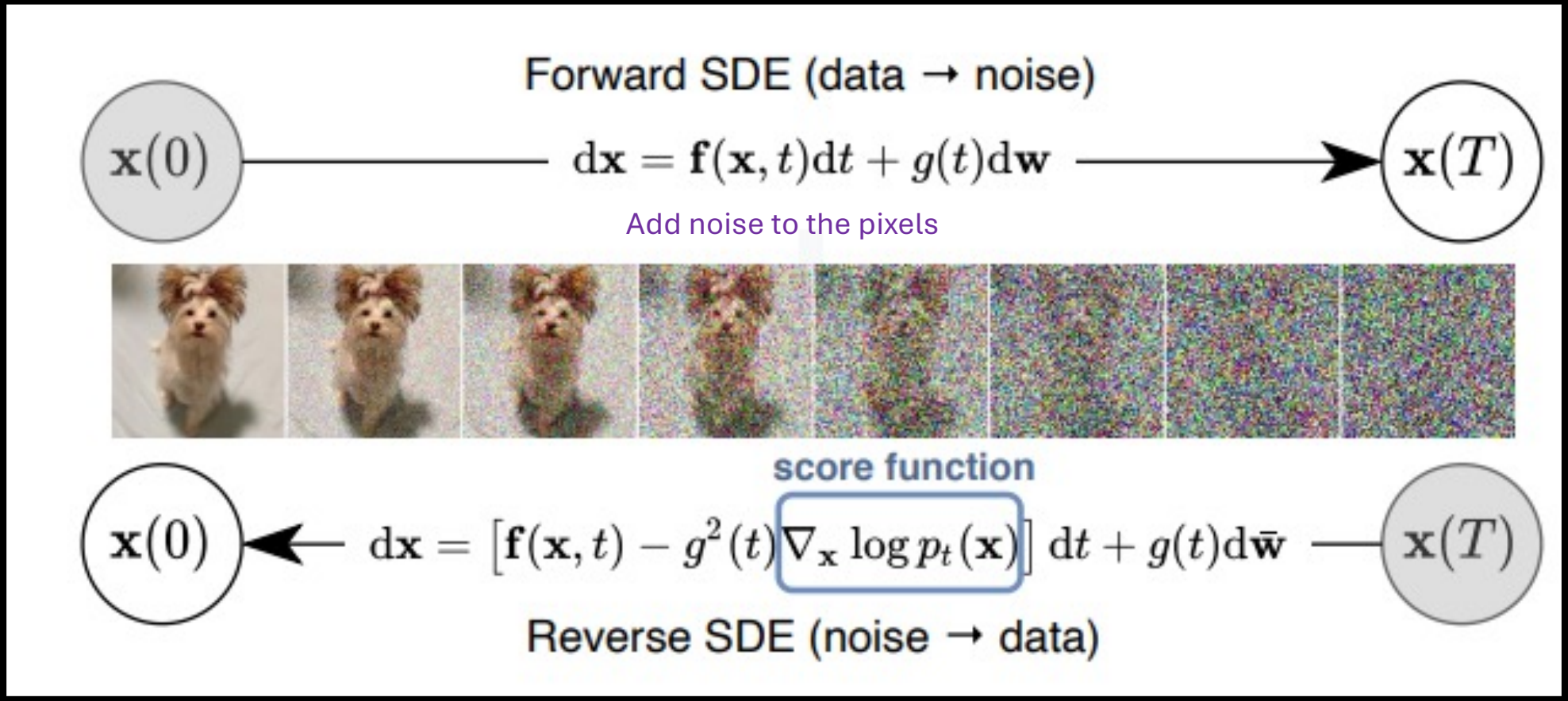
Trained Discriminator D

Training set: Real image x

Optimise G and D via: $\min_G \max_D E_x(\log(D)) + E_z(\log(1 - D(G(z))$

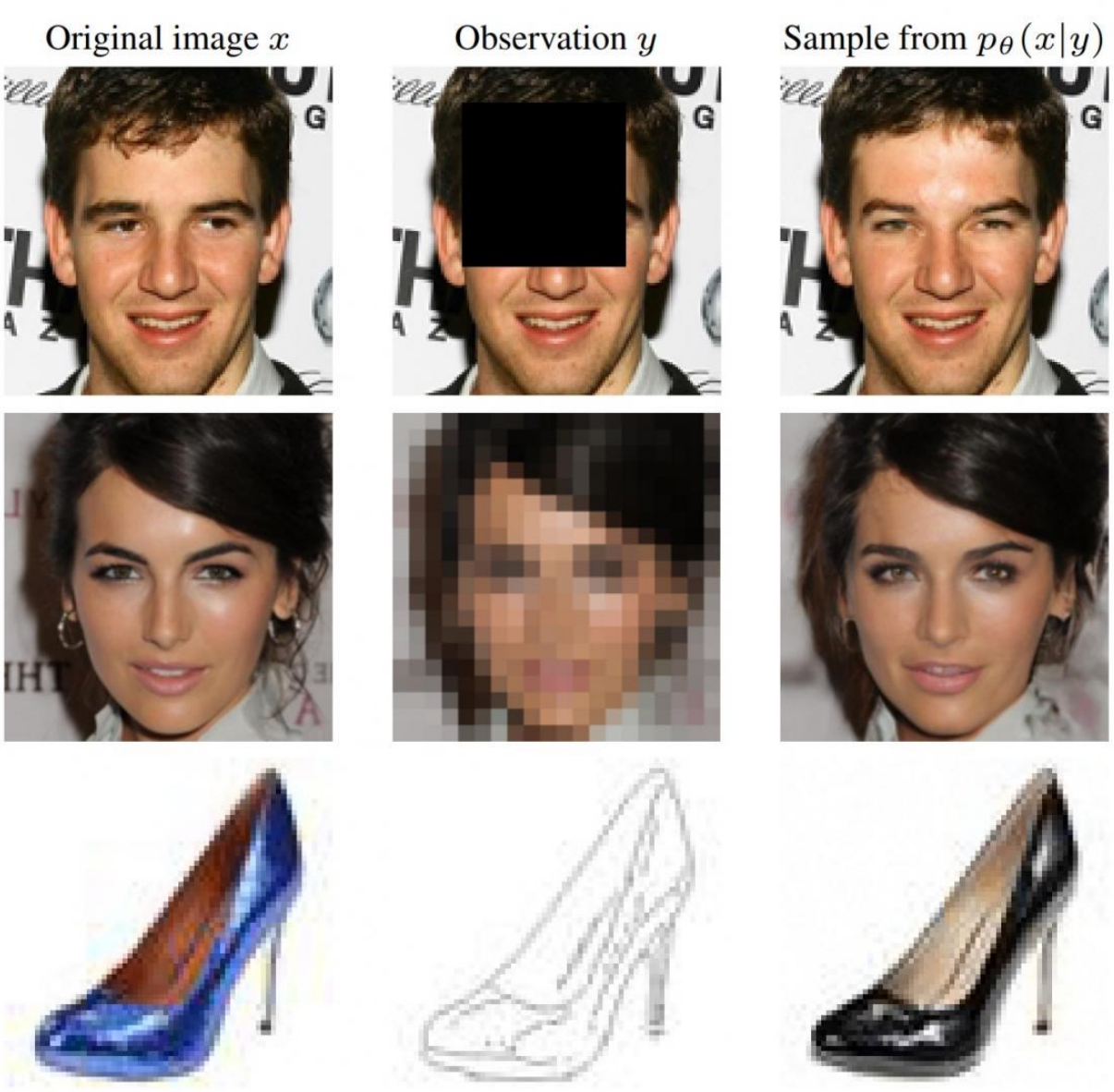

A
Input
Supplemental Information
Pressure
Low Resolution Data
Temperature
Precipitation
Eg. Meteorological downscaling
Generator
G
Downscaling Result
Discriminator
D
Fake or True
Contents Loss (MSE)
Ground Truth
Adversarial Loss
Generative Adversarial Networks
Downscaling Results
Outputs
Temperature
Precipitation
High Resolution Hint
Topography
B
GT
πSRGAN
MSE=0.0064
CDFDM
MSE=0.0362
40N
38N
36N
34N
32N
132E 134E 136E 138E 140E
1.0
0.8
0.6
0.4
0.2
0.0

Generative AI Methods III: Diffusion methods (SBD)



MUCH FASTER!!

Eg. Stable diffusion to generate image from a label



[Schoenlieb et al]

Can produce photo-realistic images .. How can we tell whether they are faked?

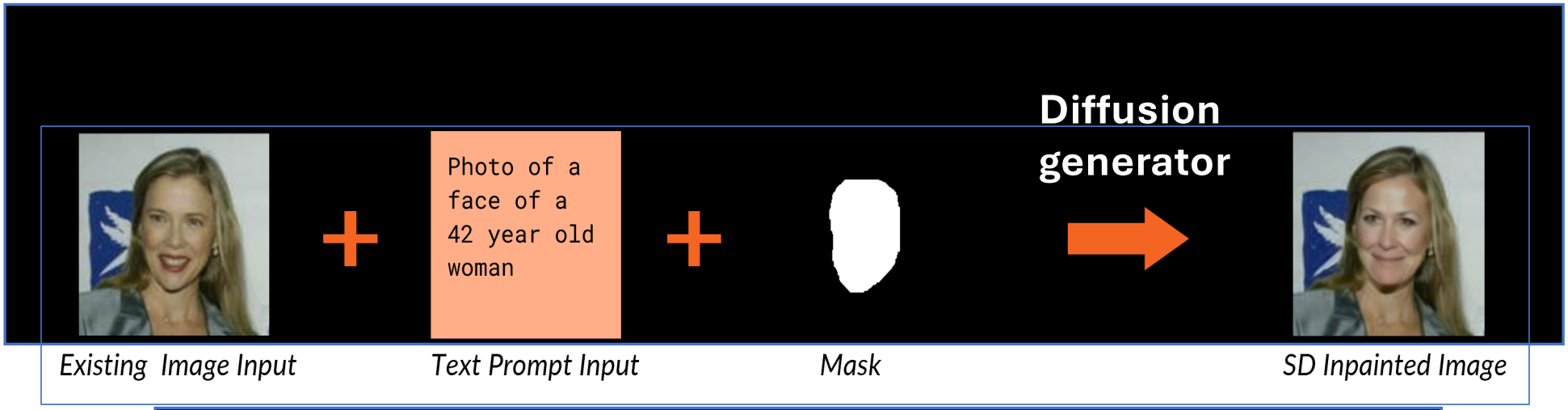
Stable diffusion inpainting: analysing image authenticity

Bitdefender et. al

https://arxiv.org/pdf/2311.04584

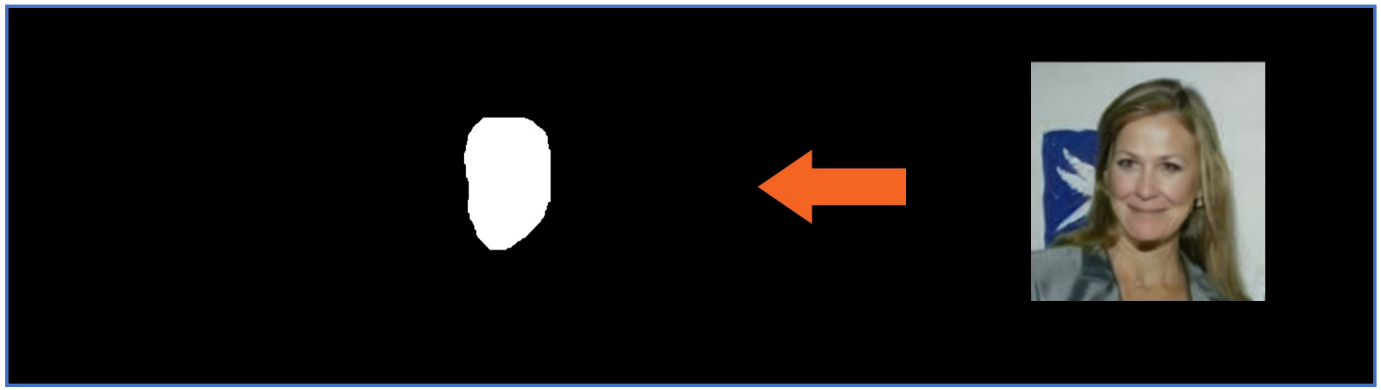
Daire O'Kane,
PhD student

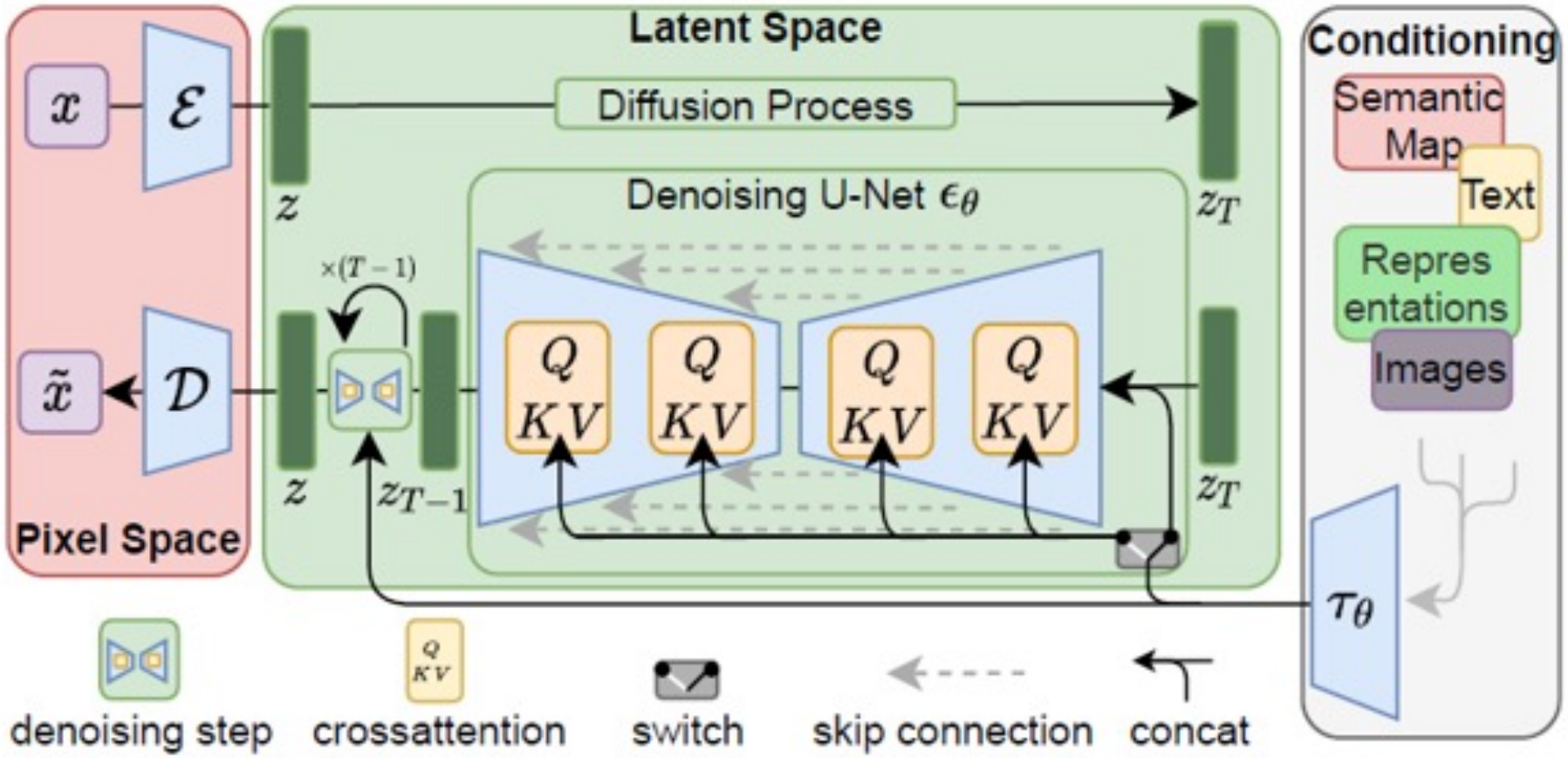
Using Maths to Detect Inpainted AI Images



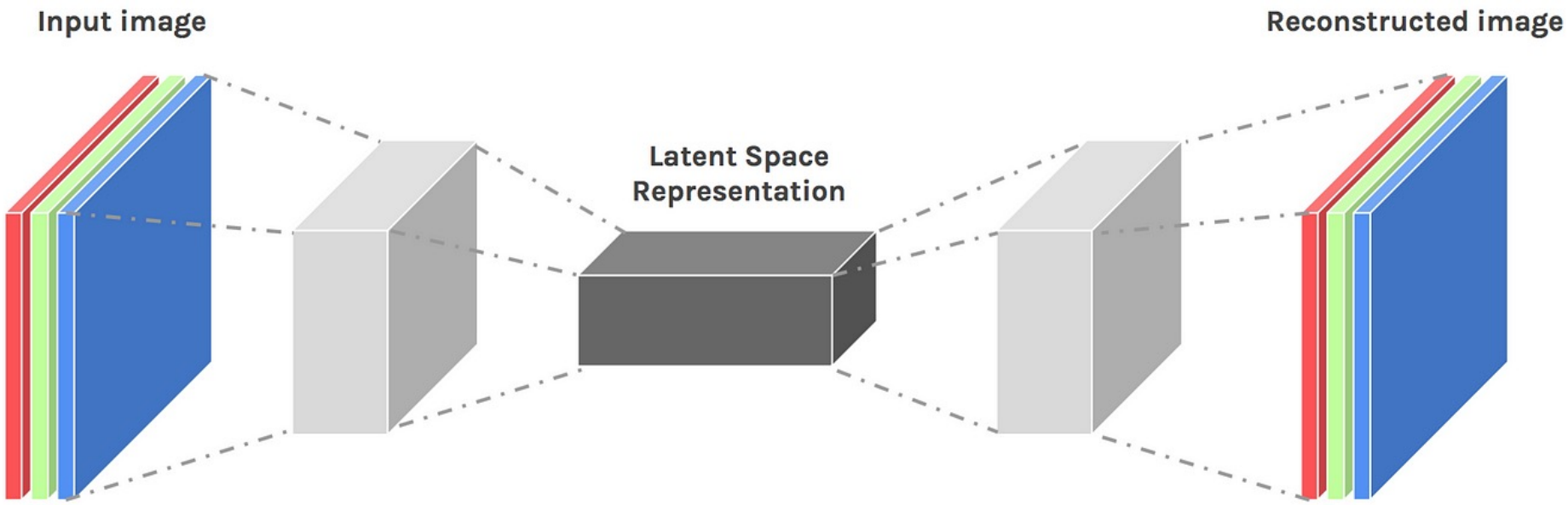
Goal: Identify in-painting and obtain the mask applied

This is a current research area in maths involving **diffusion models**, **deep learning** ad **image analysis**




Latent Space
Diffusion Process
Denoising U-Net ϵ_θ
$\times(T-1)$
x
$\mathcal{E}$
z
z_T
$\tilde{x}$
$\mathcal{D}$
z_{T-1}
Q
K V
Pixel Space
Conditioning
Semantic Map
Text
Repres entations
Images
τ_θ
denoising step
crossattention
switch
skip connection
concat

- Inpainting mask is applied in the latent space
- ”decoding step hides the traces of the latent manipulation”



U-Net architecture

Using Maths to Detect Inpainted AI Images

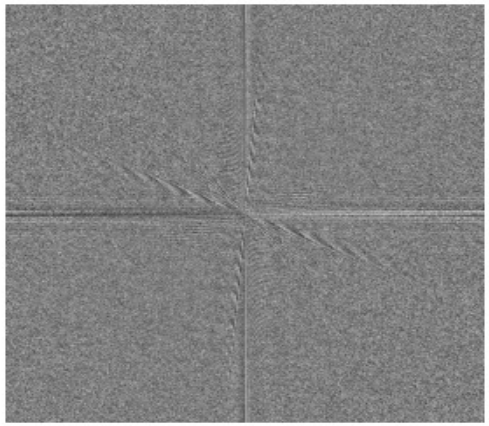
Original Image

Inpainted Image

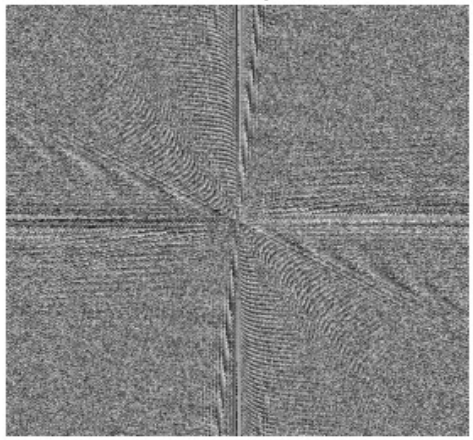
Fast Fourier Transform Algorithm

Identifies changes in frequency at each image pixel

FFT Phase Spectrum



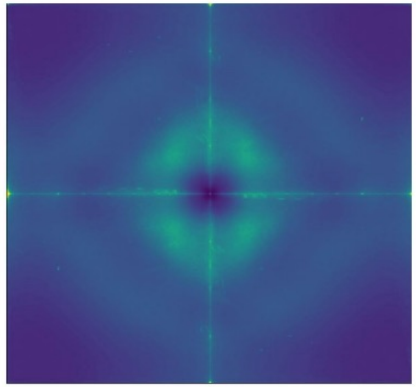
FFT Phase Spectrum



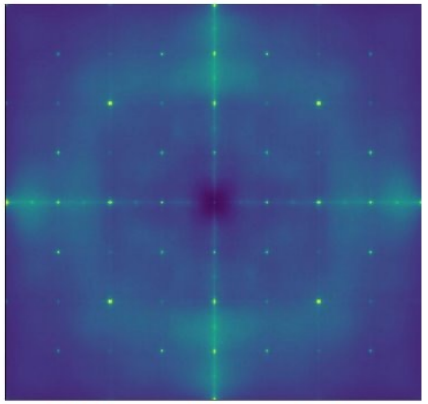
Smooth textures; no in-painting

Rough textures due to mask applied; indicate in-painting

Artefacts to identify an AI-generated image



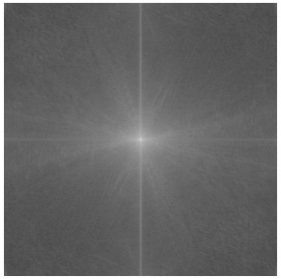
Real Image Fingerprint



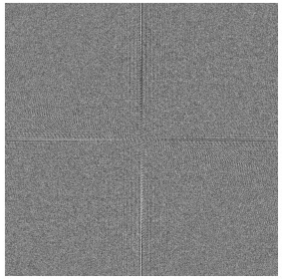
SD Image Fingerprint

SD Generated Image

FFT Magnitude Spectrum

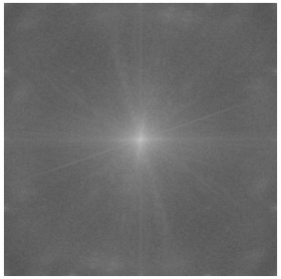


FFT Phase Spectrum



SD Generated Image

FFT Magnitude Spectrum



FFT Phase Spectrum