Computational Modeling for Materials Engineering

Deep Learning Application in Materials Engineering

HANDS-ON SESSION 4: Generative Models

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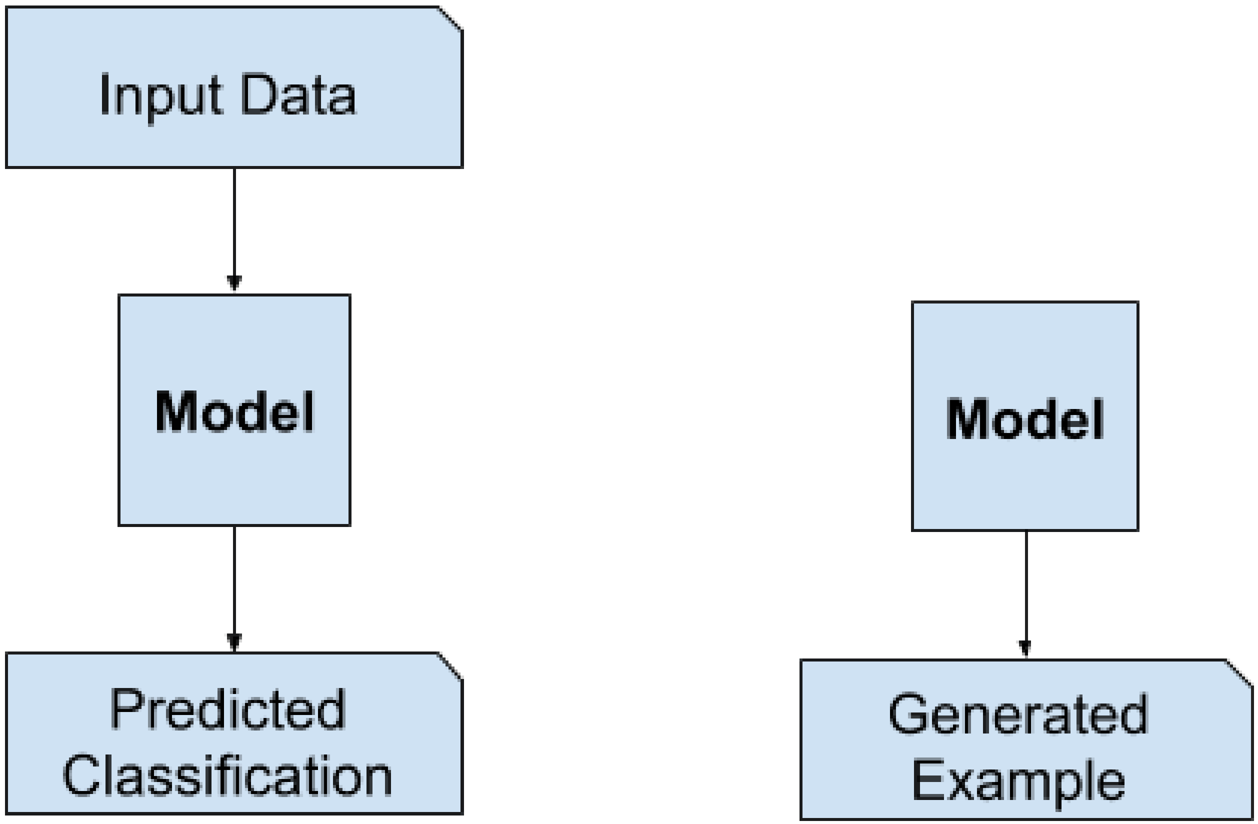
Agenda for today’s class:

1. Brief overview of Generative Models
2. Code implementation example.
3. Review of the Project.

Brief overview of Generative Models

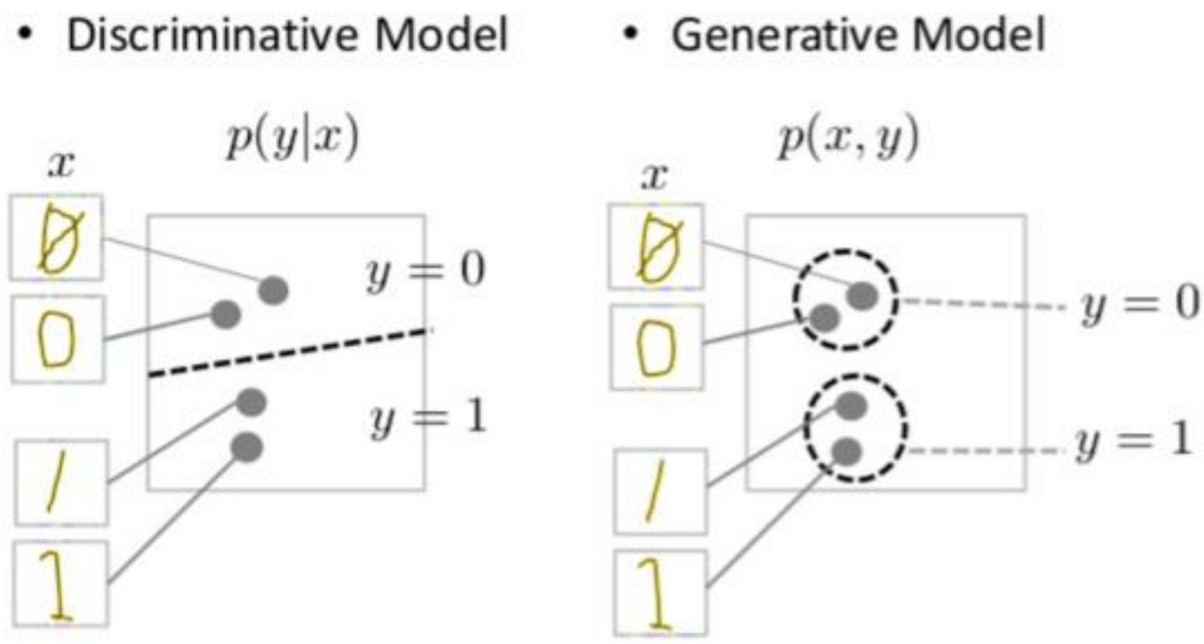
1

Discriminative vs. Generative Modeling



https://machinelearningmastery.com/what-are-generative-adversarial-networks-gans/

Background: What is a Generative Model?



•**Discriminative** models learn the boundary between classes

•**Generative** models model the distribution of individual classes

https://developers.google.com/machine-learning/gan/generative

Approaches to generative models

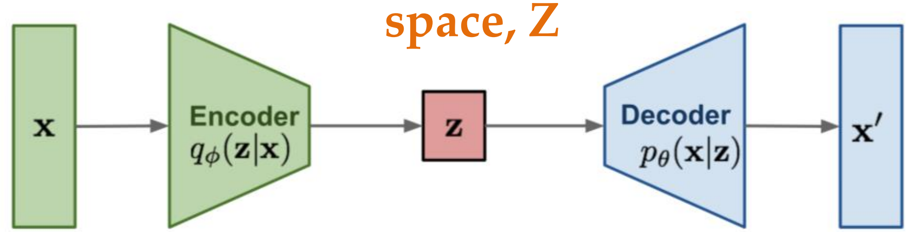
With the rise of deep learning, a new family of methods, called deep generative models (DGMs) is formed through the combination of **generative models** and **deep neural networks**. Popular DGMs include:

Variational autoencoders (VAEs)

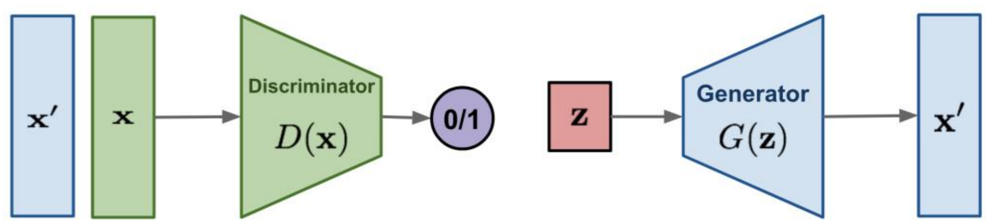
Sample x' from the modeled data distribution X'

Latent space, Z

Sample x from the true data distribution X



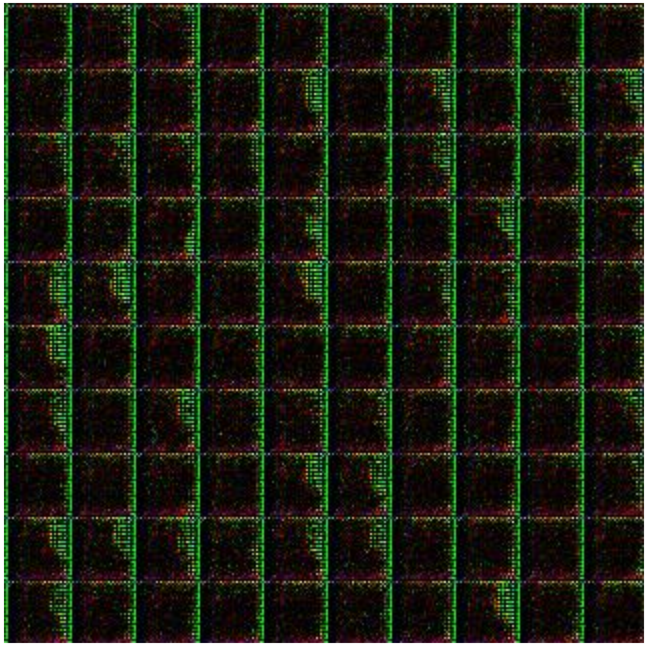
Generative adversarial networks (GANs)



DGMs: VAEs and GANs

ImageNet dataset

VAE learning to generate images

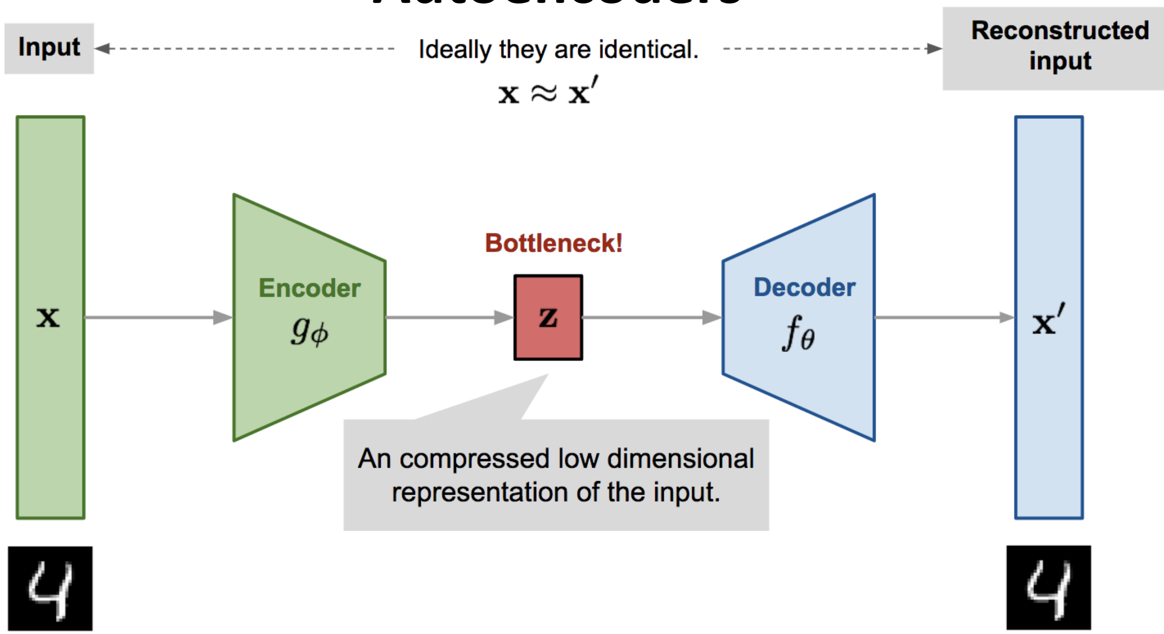


GAN learning to generate images

https://openai.com/blog/generative-models/

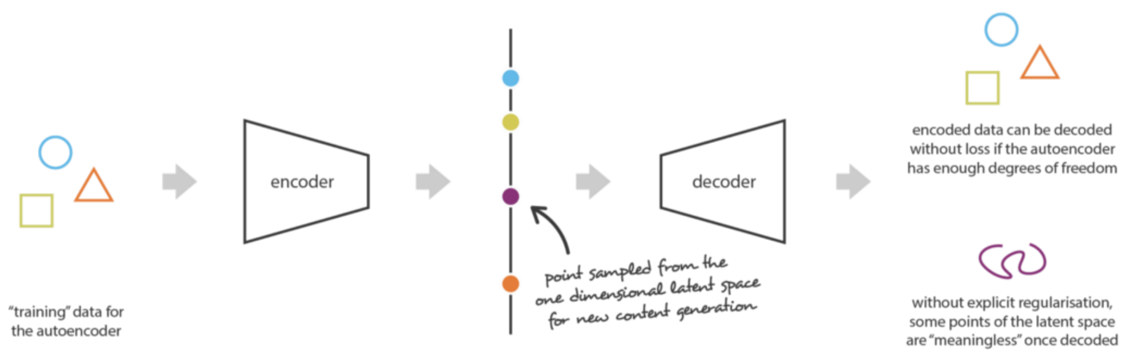
Autoencoders and Variational Autoencoders

Autoencoders



Generative ?

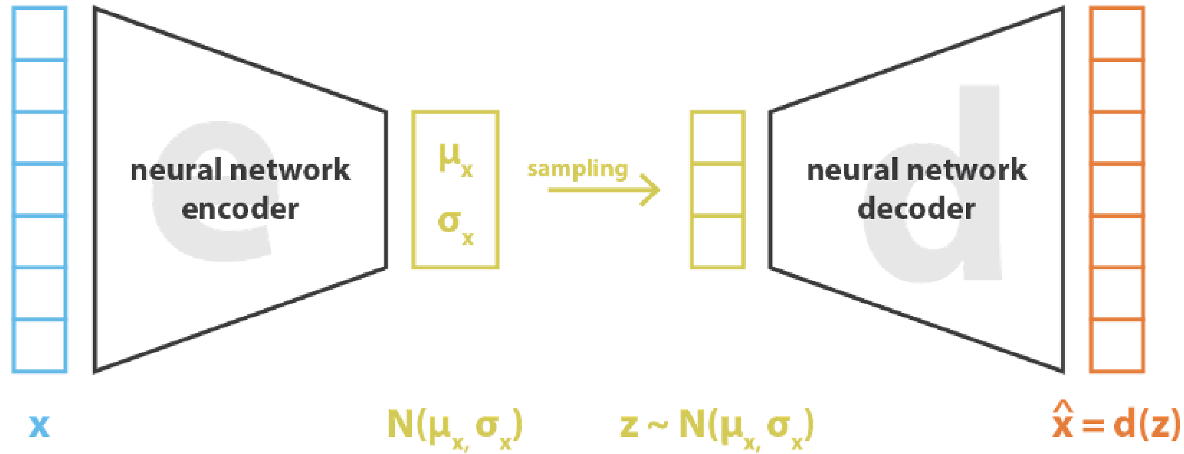
Irregular latent space !



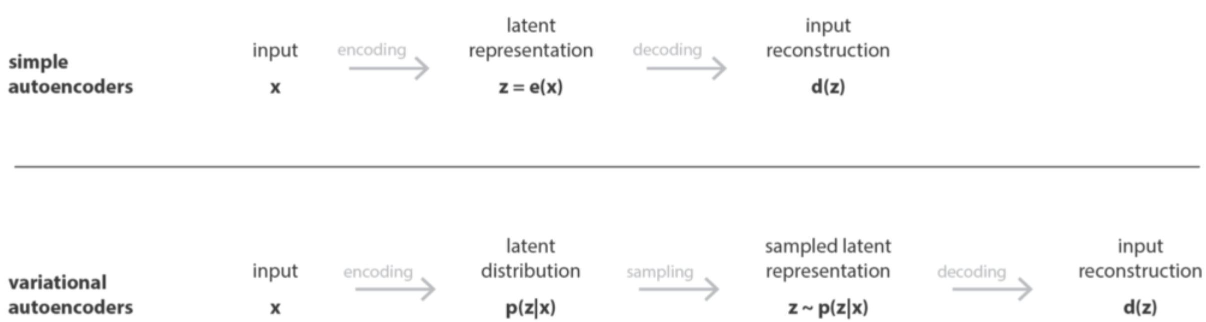
https://lilianweng.github.io/posts/2018-08-12-vae/
https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

Autoencoders and Variational Autoencoders

Variational autoencoder



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



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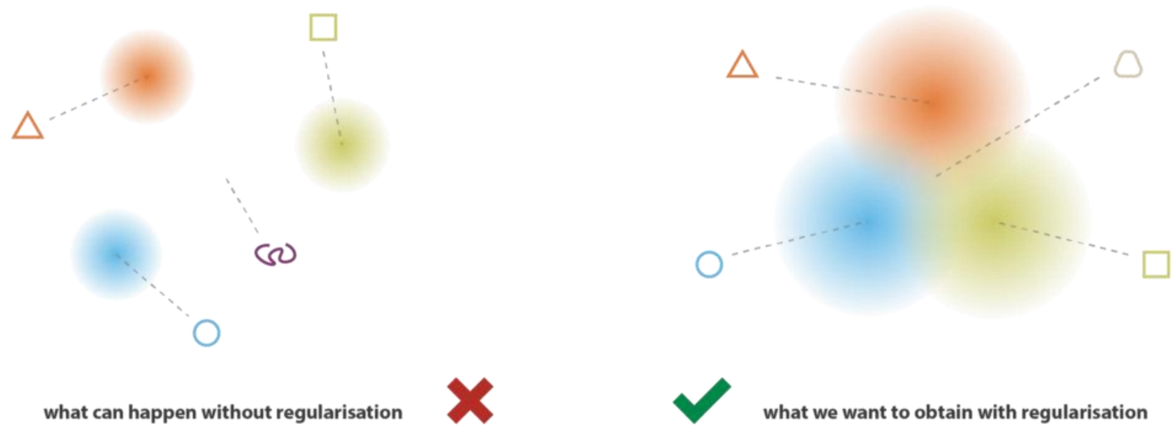
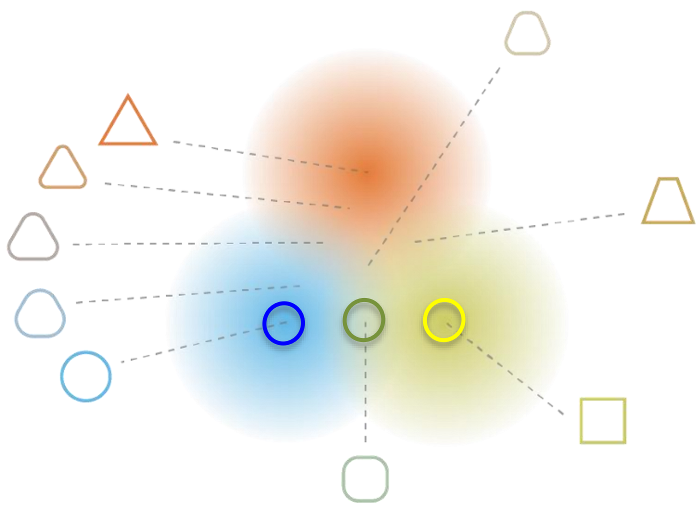
Autoencoders and Variational Autoencoders



Generative ?
Regular
latent space !



https://lilianweng.github.io/posts/2018-08-12-vae/
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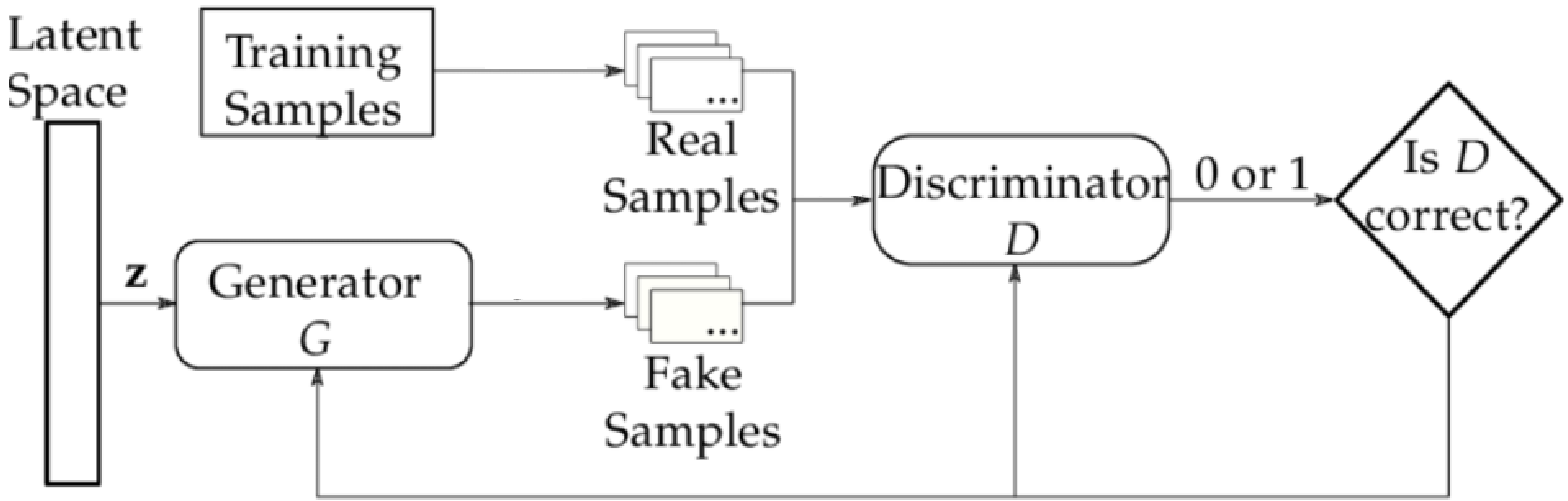
Generative Adversarial Network (GAN)

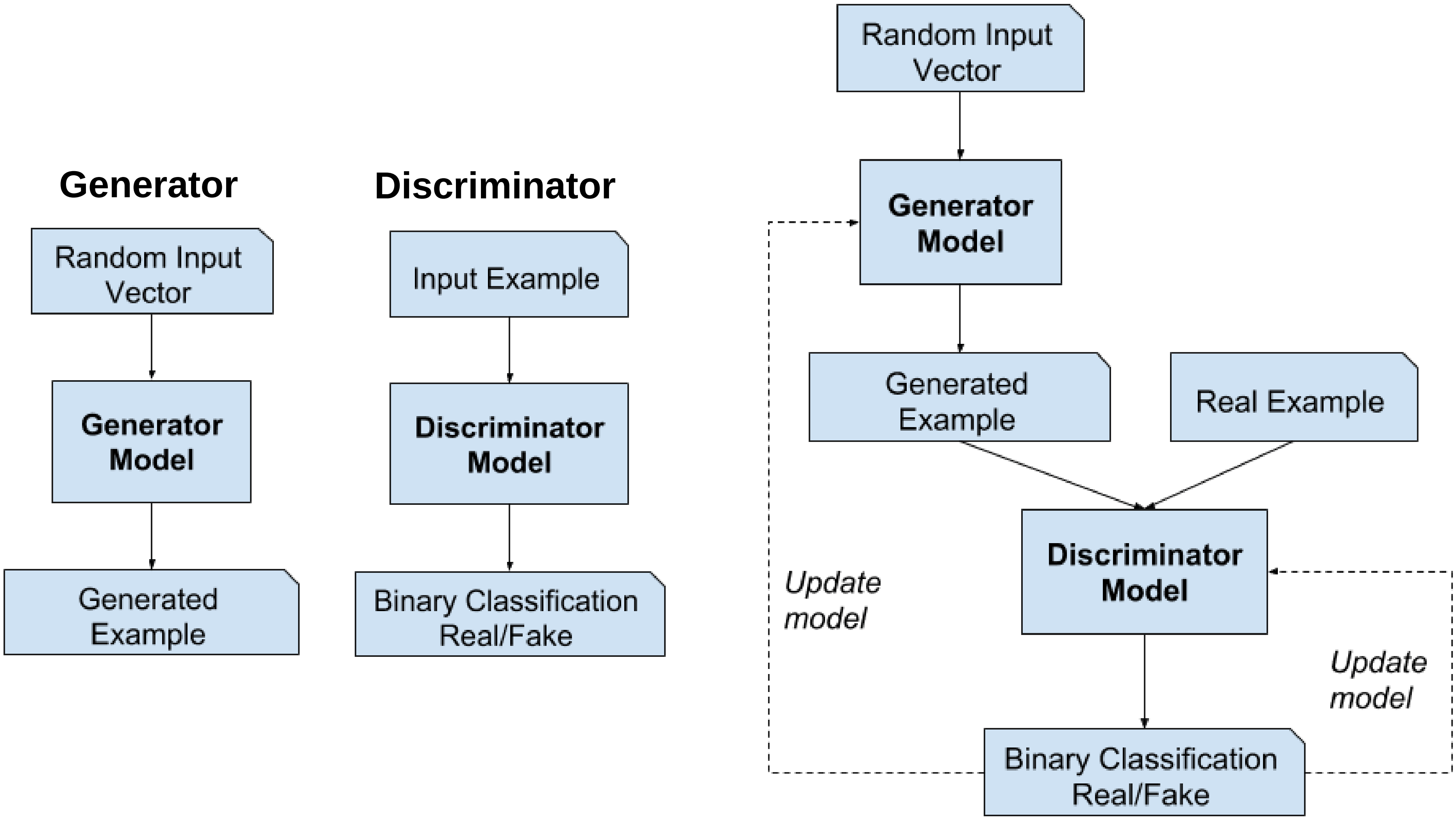


D: real | real

D: fake | real

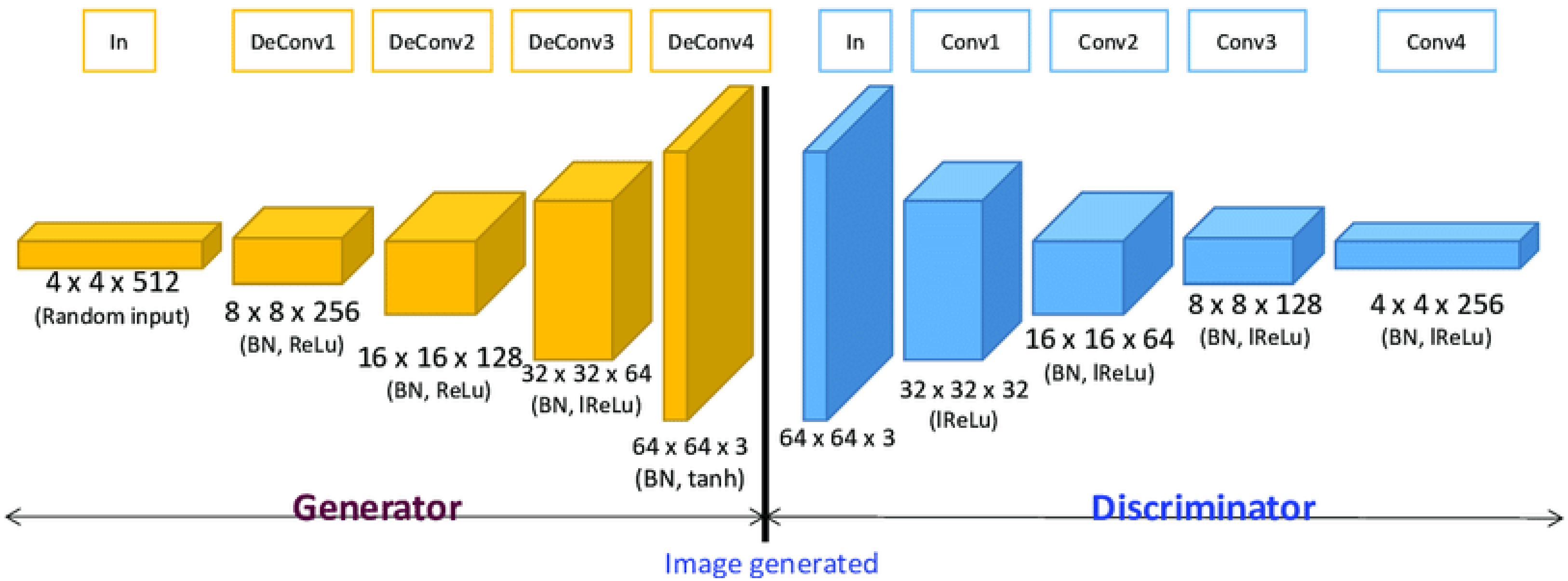
$$\min_G \max_D L(D,G) = \underbrace{\mathbb{E}_{x\sim p_r(x)}[\log D(x)] + \mathbb{E}_{z\sim p_z(z)}[\log(1 - D(G(z)))]}_{\text{max}}$$

GAN Architecture



https://machinelearningmastery.com/what-are-generative-adversarial-networks-gans/

1. Deep Convolutional GAN (DCGAN)

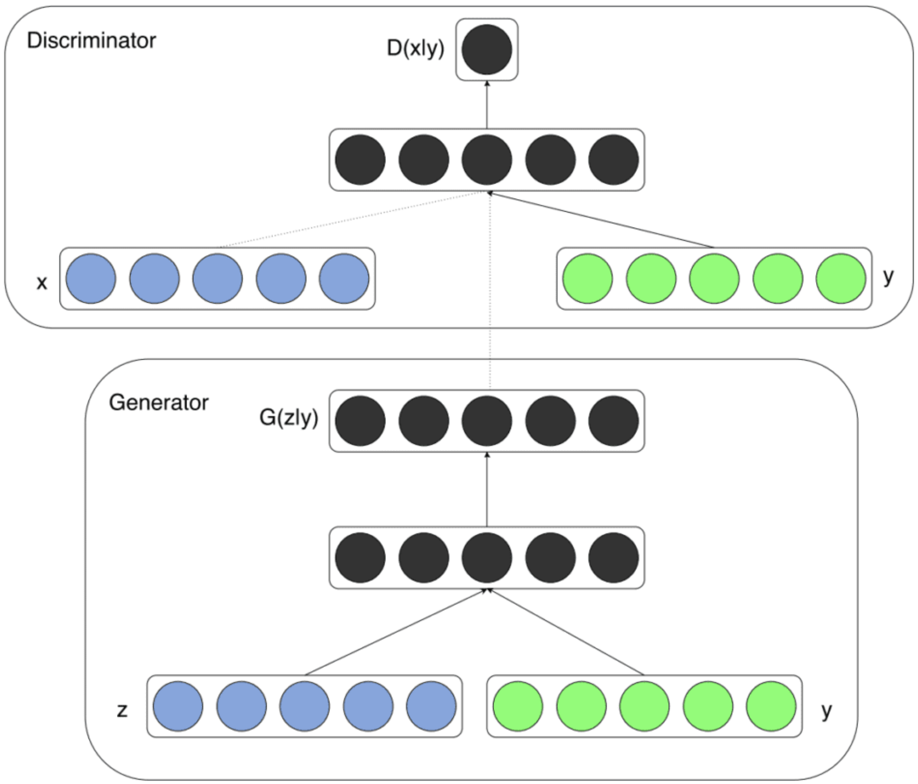


Uses convolutional and convolutional-transpose (sometimes called Deconvolution) layers in the discriminator and generator, respectively

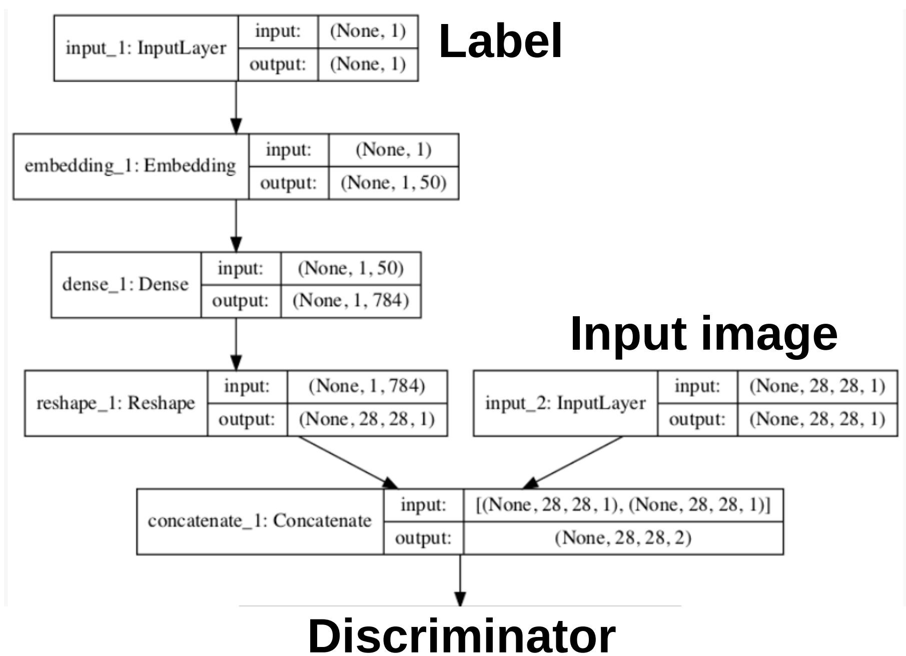
https://machinelearningmastery.com/how-to-develop-a-conditional-generative-adversarial-network-from-scratch/

2. Conditional Deep Convolutional GAN (cDCGAN)

Both the generator and discriminator are **conditioned** on some extra information i.e. labels.



Example to encode and incorporate the class labels into the discriminator input



https://machinelearningmastery.com/how-to-develop-a-conditional-generative-adversarial-network-from-scratch/

(some) Types of GAN

Deep Convolutional GAN (DCGAN)

Conditional Deep Convolutional GAN (cDCGAN)

https://machinelearningmastery.com/how-to-develop-a-conditional-generative-adversarial-network-from-scratch/

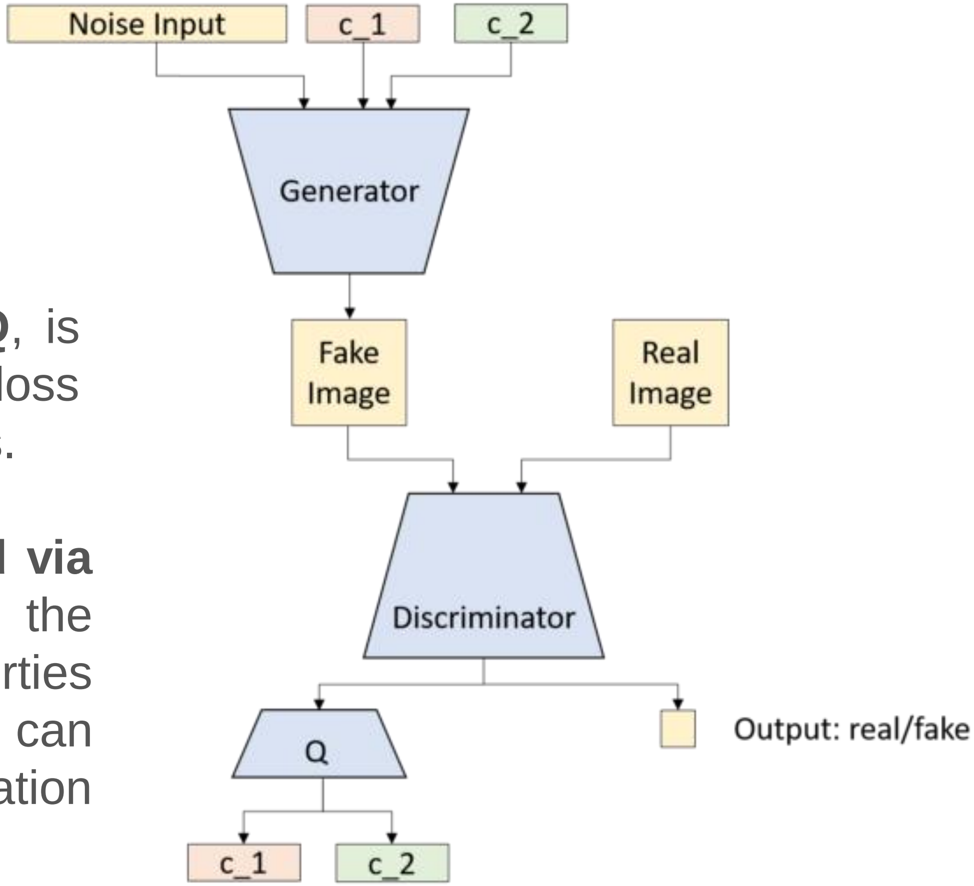
(some) Types of GAN

3. Information Maximizing GAN (InfoGAN)

- **Control variables** (categorical and continuous) are added as input to the generator, along with the point in latent space

- **An auxiliary network denoted as Q**, is trained via Mutual Information loss function to predict the control variables.

- **The generator model is regularized via mutual information loss** such that the control variables capture salient properties of the generated images and, in turn, can be used to control the image generation process



https://towardsdatascience.com/build-infogan-from-scratch-f20ee85cba03
https://machinelearningmastery.com/how-to-develop-an-information-maximizing-generative-adversarial-network-infogan-in-keras/

Code implementation example

2

https://github.com/josepabloquesadamolina/CMME2022/tree/main/Session%204

Review of the Project.

3

https://github.com/josepabloquesadamolina/CMME2022/tree/main/Project