Lecture 11:

Convolution and Image Classification & Segmentation

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Bayesian Data Analysis and Machine Learning for Physical Sciences

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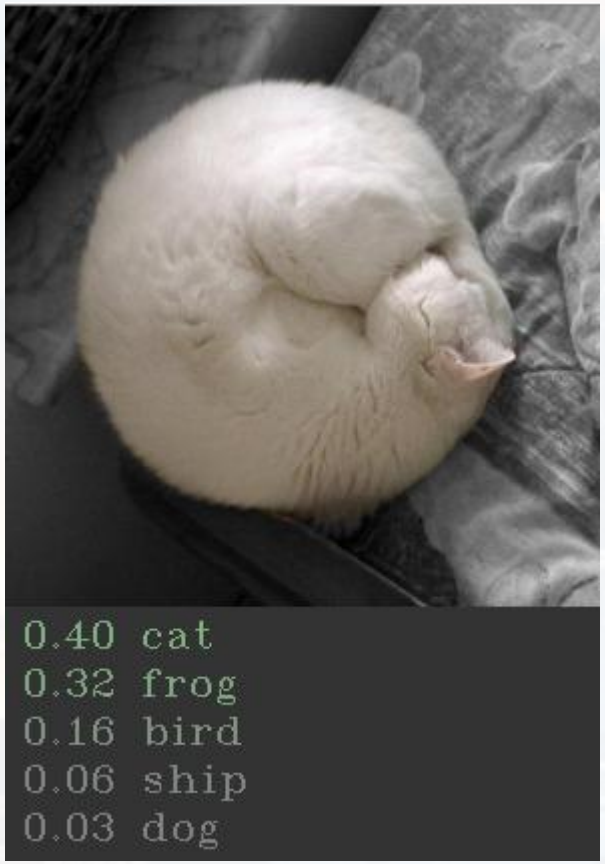
Course Map

Module 1	Maximum Entropy and Information, Bayes Theorem
Module 2	Naive Bayes, Bayesian Parameter Estimation, MAP
Module 3	MLE, Lin Regression
Module 4	Model selection I: Comparing Distributions
Module 5	Model Selection II: Bayesian Signal Detection
Module 6	Variational Bayes, Expectation Maximization
Module 7	Hidden Markov Models, Stochastic Processes
Module 8	Monte Carlo Methods
Module 9	Machine Learning Overview, Supervised Methods & Unsupervised Methods
Module 10	ANN: Perceptron, Backpropagation, SGD
Module 11	**Convolution and Image Classification and Segmentation**
Module 12	RNNs and LSTMs
Module 13	RNNs and LSTMs + CNNs
Module 14	Transformer and LLMs
Module 15	Graphs & GNNs

Part III

Convolution and Image Classification & Segmentation



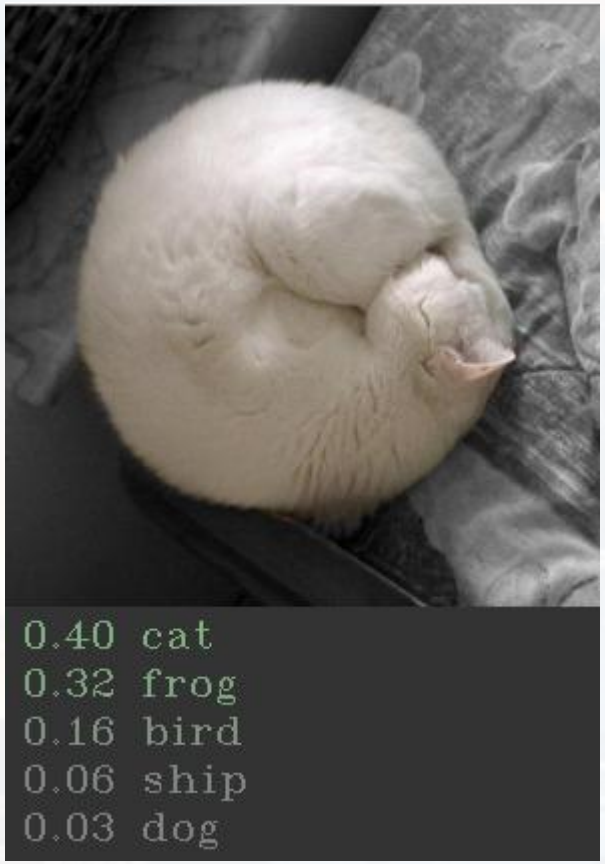
Outline

PyTorch & Cuda

Generative Adversarial Network (GAN)

Variational AutoEncoder (VAE)

Convolution and Image Classification & Segmentation



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problem: even for moderate setups, computational time becomes the limiting factor

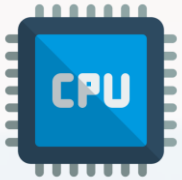
self made ANN `keras/tensor flow` `pytorch` `pytorch on GPU (Cuda)`

speed

```
512/512 [==============================] - 4072s 8s/step - loss: 3.4534 - accuracy: 0.3338
Epoch 4/5
512/512 [==============================] - ETA: 0s - loss: 3.1926 - accuracy: 0.3980     saved  ../data/segmentation
pics/checkpoints//.3
512/512 [==============================] - 3363s 7s/step - loss: 3.1926 - accuracy: 0.3980
Epoch 5/5
512/512 [==============================] - ETA: 0s - loss: 3.0071 - accuracy: 0.4318   saved  ../data/segmentation
pics/checkpoints//.4
512/512 [==============================] - 3616s 7s/step - loss: 3.0071 - accuracy: 0.4318
```

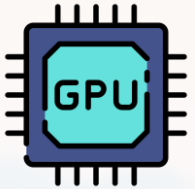
Lenovo T14, NVIDIA GeForce MX450: (simple LSTM)

Keras (CPU):	**300 sec**
PyTorch (CPU):	11 sec
PyTorch (GPU):	**3 sec**



training AI

→ mainly matrix operations
→ GPUs are a lot better at it!



CUDA is the link of your GPU to Python (PyTorch)
check, if graphic card is on list

check your graphics device:

→ Windows command shell prompt

→ type `nvidia-smi`

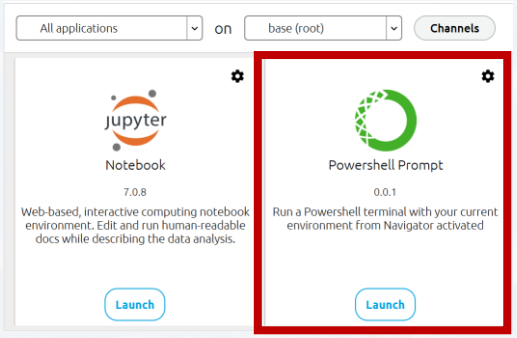
→ press *Enter*

```
(base) C:\Users\MMH_user>nvidia-smi
Tue Jan 16 20:09:26 2024
+---------------------------------------------------------------------------------------+
| NVIDIA-SMI 537.79                 Driver Version: 537.79       CUDA Version: 12.2     |
|-----------------------------------------+----------------------+----------------------+
| GPU  Name                     TCC/WDDM  | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |         Memory-Usage | GPU-Util  Compute M. |
|                                         |                      |               MIG M. |
|=========================================+======================+======================|
|   0  NVIDIA GeForce MX450         WDDM  | 00000000:01:00.0 Off |                  N/A |
| N/A   49C    P0              N/A /   9W |      0MiB /  2048MiB |      0%      Default |
|                                         |                      |                  N/A |
+-----------------------------------------+----------------------+----------------------+

+---------------------------------------------------------------------------------------+
| Processes:                                                                            |
|  GPU   GI   CI        PID   Type   Process name                            GPU Memory |
|        ID   ID                                                             Usage      |
|=======================================================================================|
|  No running processes found                                                           |
+---------------------------------------------------------------------------------------+
```

Installing CUDA

conda environment




```
C:\WINDOWS\System32\Win
(base) PS C:\Users\MMH_user>
```

```
C:\WINDOWS\System32\Win
(base) PS C:\Users\MMH_user> conda create --name CUDAenv
```

```
C:\WINDOWS\System32\Win
(base) PS C:\Users\MMH_user> conda activate CUDAenv
```

```
(base) PS C:\Users\MMH_user> conda activate CUDAenv
(CUDAenv) PS C:\Users\MMH_user> conda install -c pytorch pytorch
Channels:
 - pytorch
```

Installing CUDA

cuda toolkit

```
(CUDAenv) PS C:\Users\MMH_user> conda install -c anaconda cudatoolkit
```

check libraries

→ type: `conda list`

```
(CUDAenv) PS C:\Users\MMH_user> conda list
# packages in environment at C:\Users\MMH_user\anaconda3\envs\CUDAenv:
#
# Name                    Version                   Build  Channel
blas                      1.0                         mkl
bzip2                     1.0.8                h2bbff1b_6
ca-certificates           2024.7.2             haa95532_0
cudatoolkit               11.8.0               hd77b12b_0
expat                     2.6.2                hd77b12b_0
filelock                  3.13.1           py312haa95532_0
intel-openmp              2023.1.0          h59b6b97_46320
```

Installing CUDA

usually, a few libraries are missing

check again graphics card:	type in anaconda	**nvidia-smi**
check libraries:	type in anaconda	**conda list cudnn** **conda list cudatoolkit** **conda list torch**
	if not:	**conda install <library>**
check Python:	type in anaconda	**python** **import torch** **torch.cuda.is_available()**
open Spyder	run in Spyder	**pip install** (see the commented line in `CheckMyCuda.py`)

Installing CUDA

usually, a few libraries are missing

CheckMyCuda.py

```
import torch

def test_cuda():
    print("PyTorch version: ", torch.__version__)
    print("CUDA version: ", torch.version.cuda)
    print("CUDA Available: ", torch.cuda.is_available())
    if torch.cuda.is_available():
        print("Number of GPUs: ", torch.cuda.device_count())
        print("GPU Name: ", torch.cuda.get_device_name(0))

if __name__ == "__main__":
    test_cuda()
```

```
PyTorch version:  2.3.1+cu118
CUDA version:  11.8
CUDA Available:  True
Number of GPUs:  1
GPU Name:  NVIDIA GeForce MX450
```

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print("Using device:", device)
```

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

Congratulation! If you see this, you are ready to go!

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

Torch objects like **`model`** or **`torch.tensor`** have the property **`.to`**

```
TrainX = torch.tensor(TrainX, dtype = torch.float32)
TrainY = torch.tensor(TrainY, dtype = torch.float32)
```

turning numpy array into torch.tensor

```
TrainX = TrainX.to(device)
TrainY = TrainY.to(device)
```

allocating objects to the device

```
model  = model.to(device)
```

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

When running the training, we need to **synchronize** between GPU (for training the model) and CPU (for everything else)…

```
torch.cuda.synchronize()

        #training loop
        for epoch in range(n_epochs):
                outputs = model(TrainX)

                ... #do stuff...

torch.cuda.synchronize()
```

The key part in PyTorch is to set all matrices and the model **to the device (CPU or GPU)**

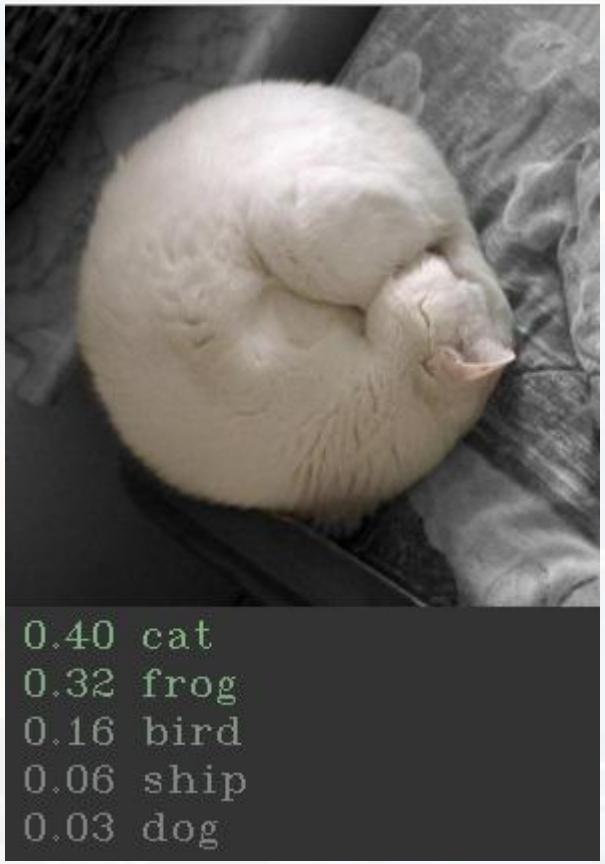
```
In [13]: device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
    ...: print("Using device:", device)
Using device: cuda
```

When running the training, we need to **synchronize** between GPU (for training the model) and CPU (for everything else)…

…and later allocate the model back to CPU

```
PredY = model(TestX).detach().to('cpu').numpy()
```

Convolution and Image Classification & Segmentation



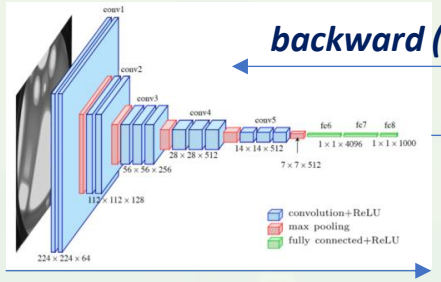
Outline

PyTorch & Cuda

Generative Adversarial Network (GAN)

Variational AutoEncoder (VAE)

set of real images

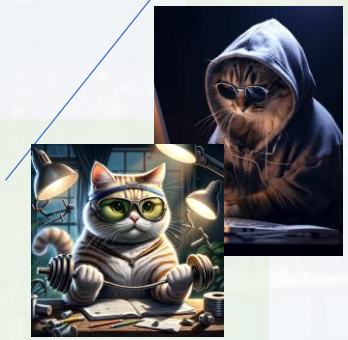


backward (up-sampling)

binary classification:
fake or real
(loss: cross entropy)

forward (down-sampling)

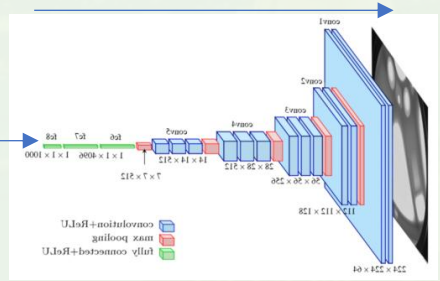
discriminator



set of fake images

forward (up-sampling)

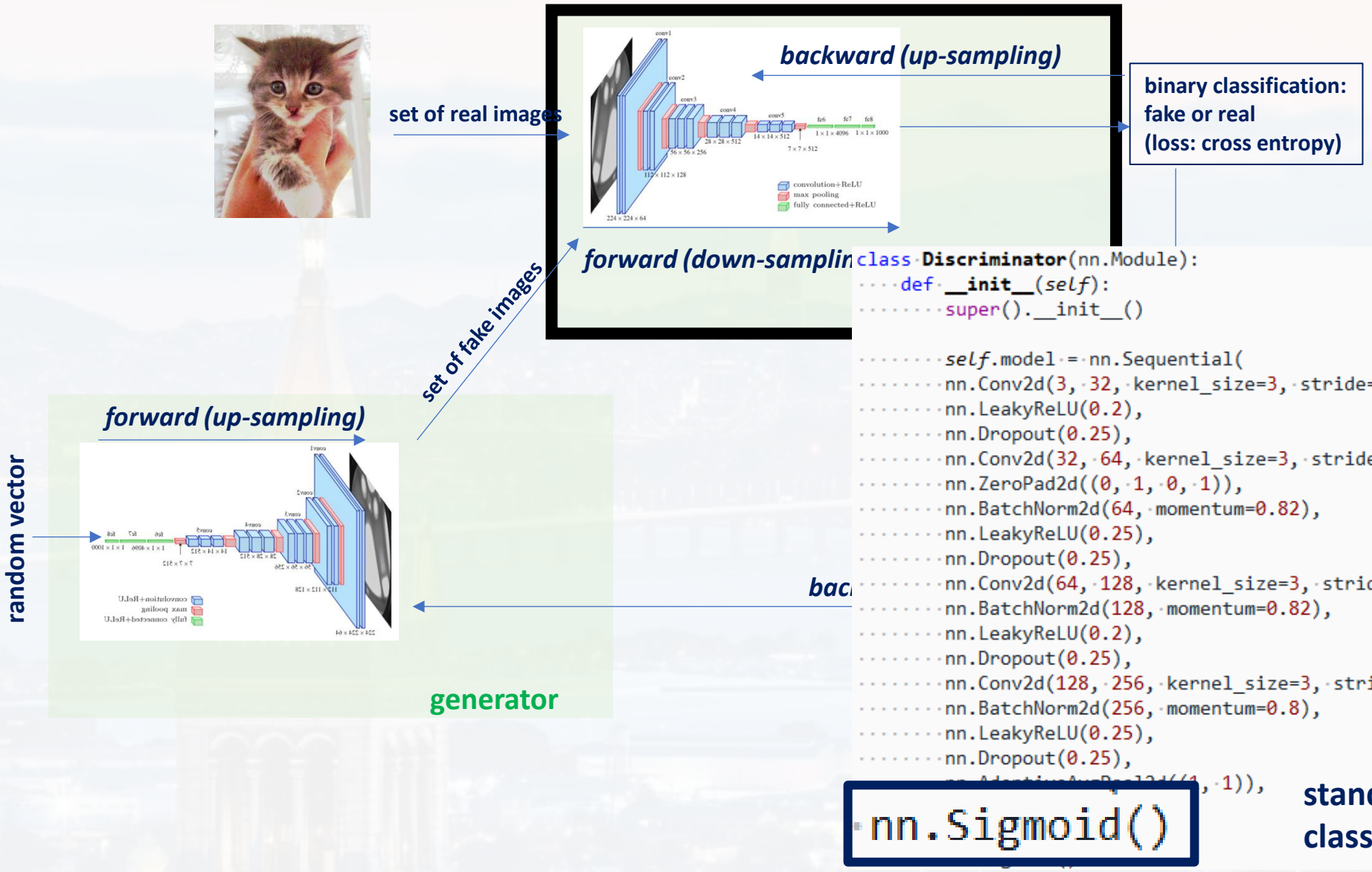
random vector



backward (down-sampling)

generator

Convolution, Image Classification & Segmentation

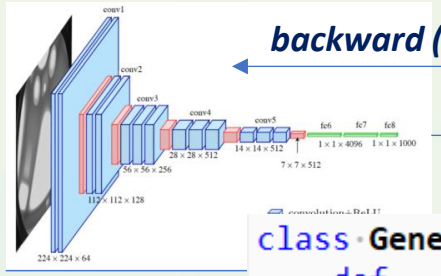



```
class Discriminator(nn.Module):
    def __init__(self):
        super().__init__()

        self.model = nn.Sequential(
        nn.Conv2d(3, 32, kernel_size=3, stride=2, padding=1),
        nn.LeakyReLU(0.2),
        nn.Dropout(0.25),
        nn.Conv2d(32, 64, kernel_size=3, stride=2, padding=1),
        nn.ZeroPad2d((0, 1, 0, 1)),
        nn.BatchNorm2d(64, momentum=0.82),
        nn.LeakyReLU(0.25),
        nn.Dropout(0.25),
        nn.Conv2d(64, 128, kernel_size=3, stride=2, padding=1),
        nn.BatchNorm2d(128, momentum=0.82),
        nn.LeakyReLU(0.2),
        nn.Dropout(0.25),
        nn.Conv2d(128, 256, kernel_size=3, stride=1, padding=1),
        nn.BatchNorm2d(256, momentum=0.8),
        nn.LeakyReLU(0.25),
        nn.Dropout(0.25),
        nn.AdaptiveAvgPool2d((1, 1)),
```

Convolution, Image Classification & Segmentation

set of real images



backward (up-sampling)

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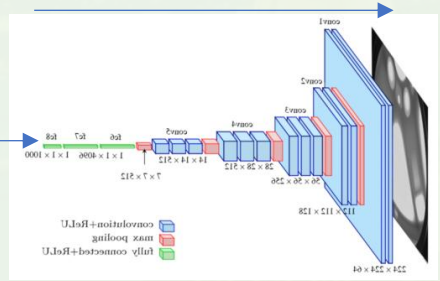
forward (down-

set of fake images

forward (up-sampling)



random vector

generator

```
class Generator(nn.Module):
    def __init__(self, latent_dim):
        super().__init__()

        self.model = nn.Sequential(
            nn.Linear(latent_dim, 128 * 8 * 8),
            nn.ReLU(),
            nn.Unflatten(1, (128, 8, 8)),
            nn.Upsample(scale_factor=2),
            nn.Conv2d(128, 128, kernel_size=3, padding=1),
            nn.BatchNorm2d(128, momentum=0.78),
            nn.ReLU(),
            nn.Upsample(scale_factor=2),
            nn.Conv2d(128, 64, kernel_size=3, padding=1),
            nn.BatchNorm2d(64, momentum=0.78),
            nn.ReLU(),
            nn.Conv2d(64, 3, kernel_size=3, padding=1),
            nn.Tanh()
        )

    def forward(self, z):
        img = self.model(z)
        return img
```

up-sampling:
like in standard segmentation CNN

x: real image
z: latent vector (random numbers)

$p_D(x)$: probability that discriminator *D* classifies *x* as real image
$G(z)$: fake image generated from generator *G*

$\mathcal{L}_D$: loss function of discriminator *D*
$\mathcal{L}_G$: loss function of generator *G*

(mean) binary cross entropy (BCE): $\mathcal{L}_D = -\frac{1}{N}\sum_{i=1}^{N} \log[p_D(x_i)] + \log[1 - p_D(G(z_i))]$

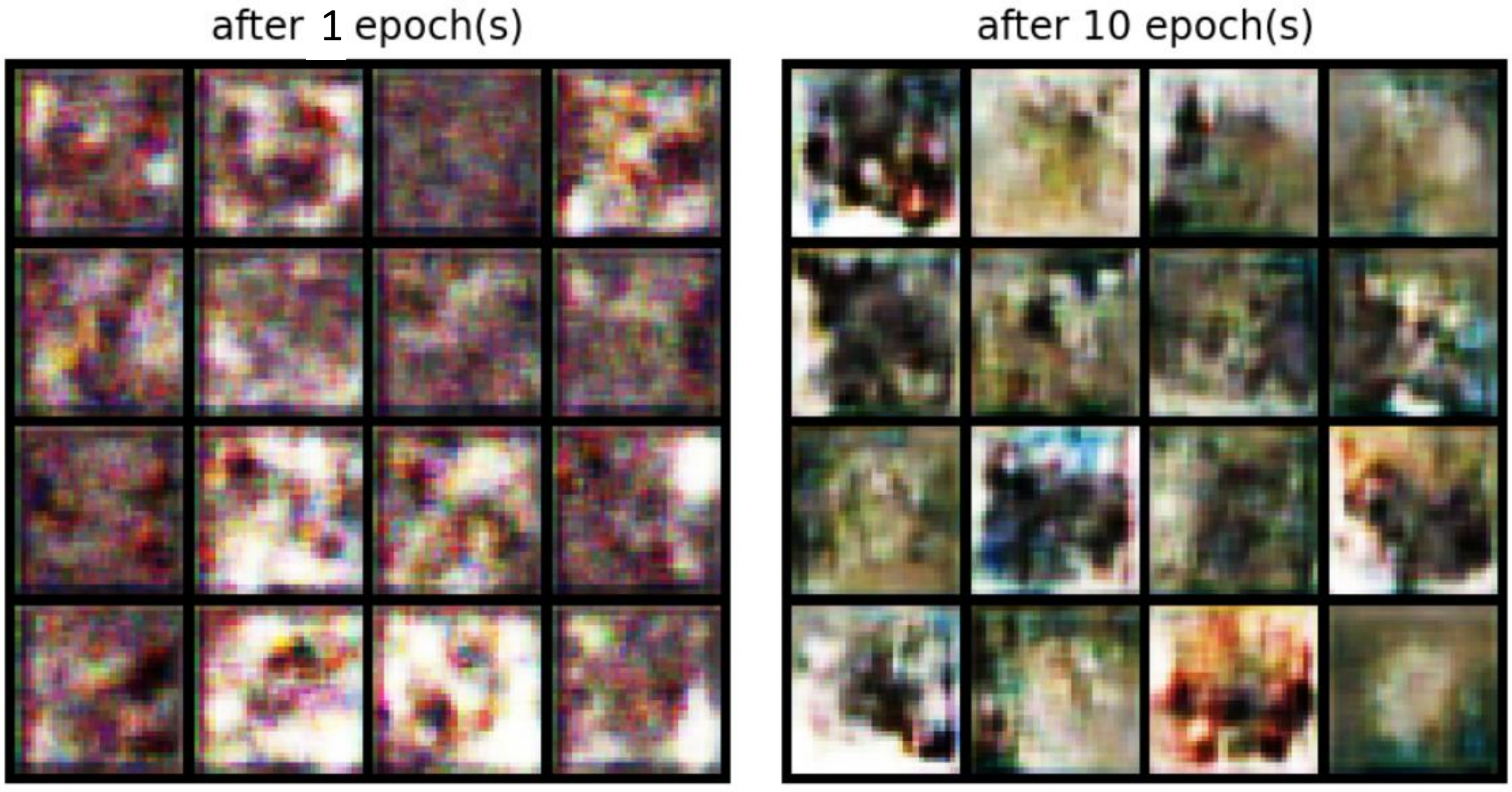
over all *N* images $\mathcal{L}_G = \frac{1}{N}\sum_{i=1}^{N} \log[1 - p_D(G(z_i))]$

ideal case for *D*: $\mathcal{L}_D = -\log[1] - \log[1 - 0] = 0$
worst case for *D*: $\mathcal{L}_D = -\log[1] - \log[1 - \mathbf{0.5}] = \mathbf{0.69}$

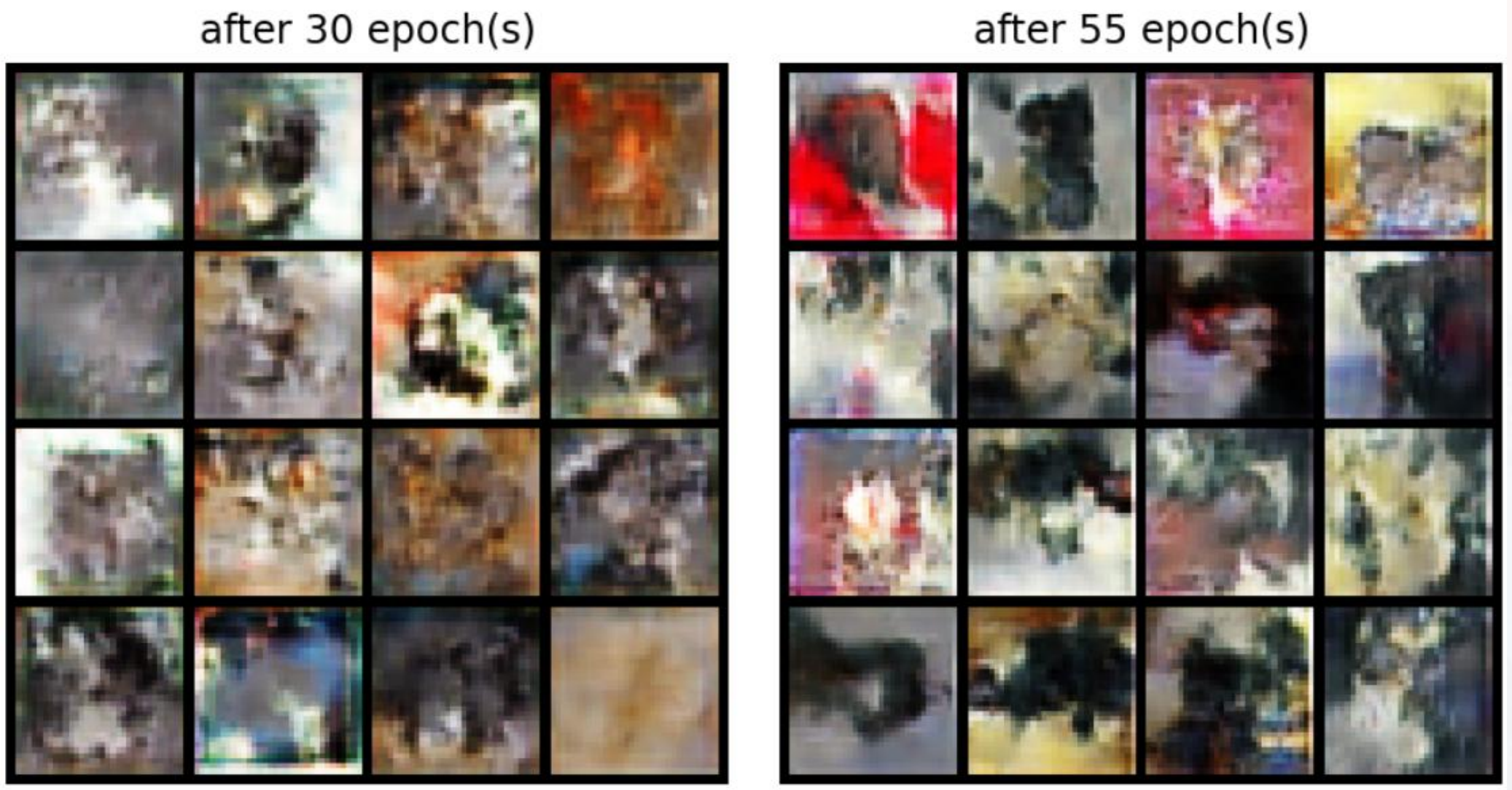
ideal case for *G*: $\mathcal{L}_G = \log[1 - \mathbf{0.5}] = \mathbf{-0.69}$
worst case for *G*: $\mathcal{L}_G = \log[1 - 0] = 0$

Convolution, Image Classification & Segmentation

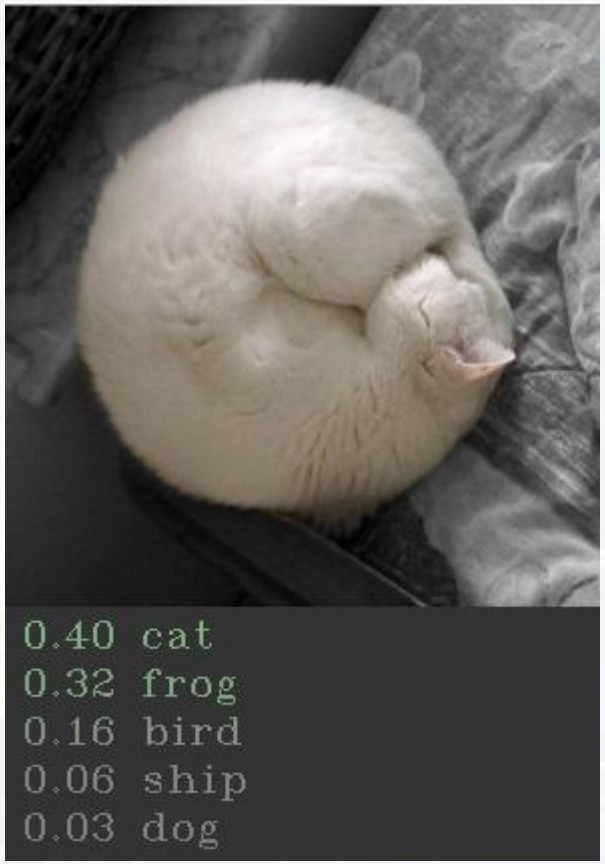
check out `GAN architecture.ipynb`



check out `GAN architecture.ipynb`



Convolution and Image Classification & Segmentation



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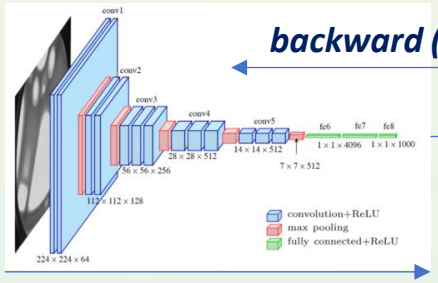
GAN:

set of real images



backward (up-sampling)

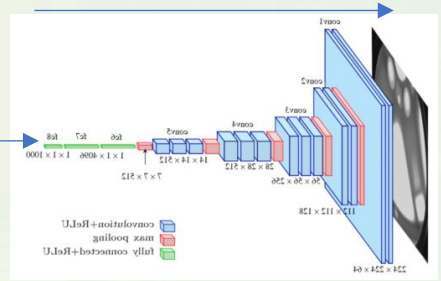
binary classification:
fake or real
(loss: cross entropy)

forward (down-sampling)

discriminator

set of fake images

forward (up-sampling)



random vector

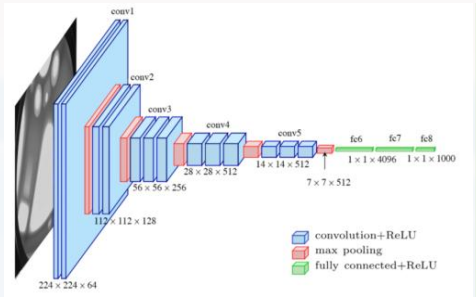
backward (down-sampling)

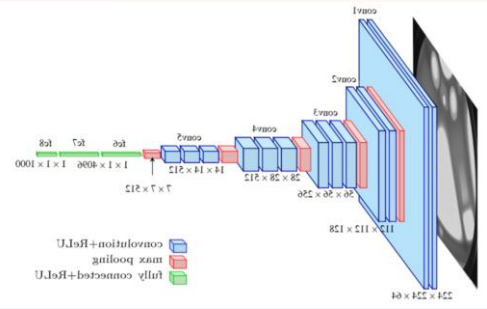
generator

each image x is represented by **one single** vector z

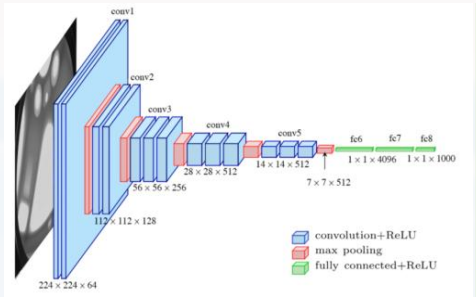
Convolution, Image Classification & Segmentation

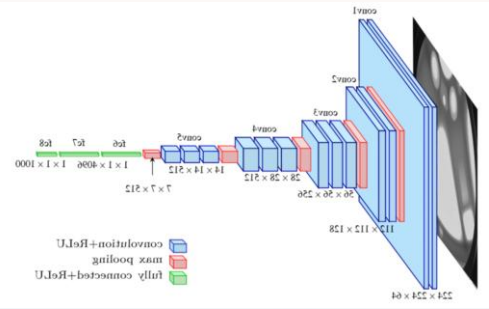
now:





now:





GAN: each image x is represented by **one single** vector z

VAE: each image x is represented by **a distribution** we sample from in order **to get z**

i: index over dimensions of z

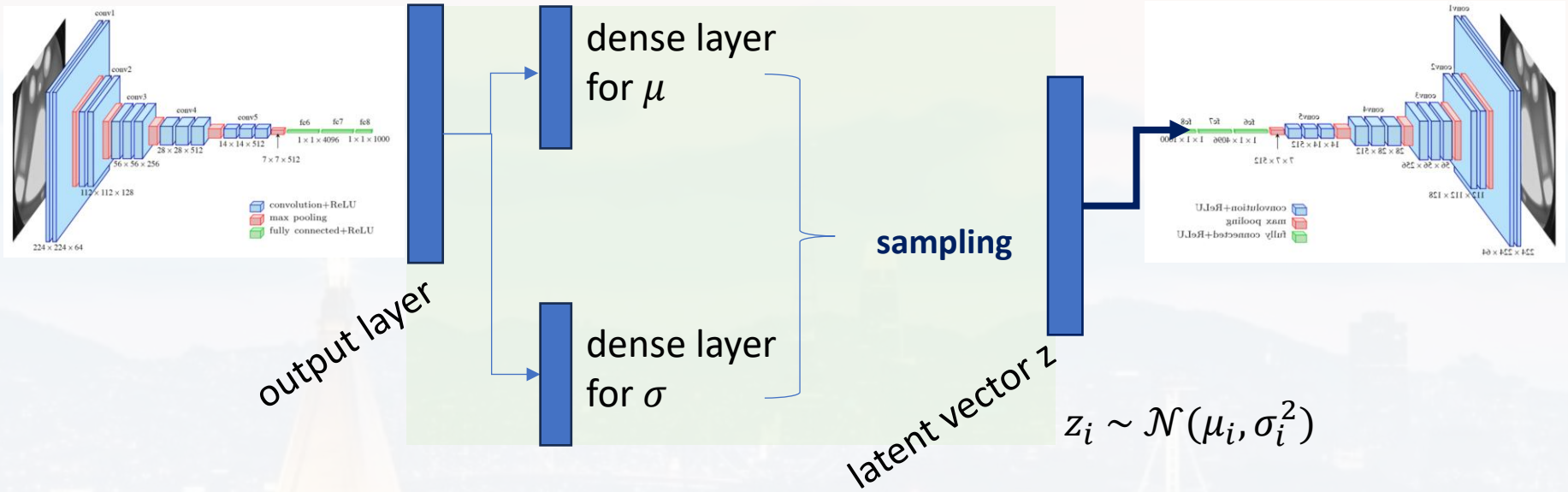
$z_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$ (max entropy!)

→ generate image from up-sampling as before

→ randomnes accounts for diverisity in generated data

Convolution, Image Classification & Segmentation

now:



example:

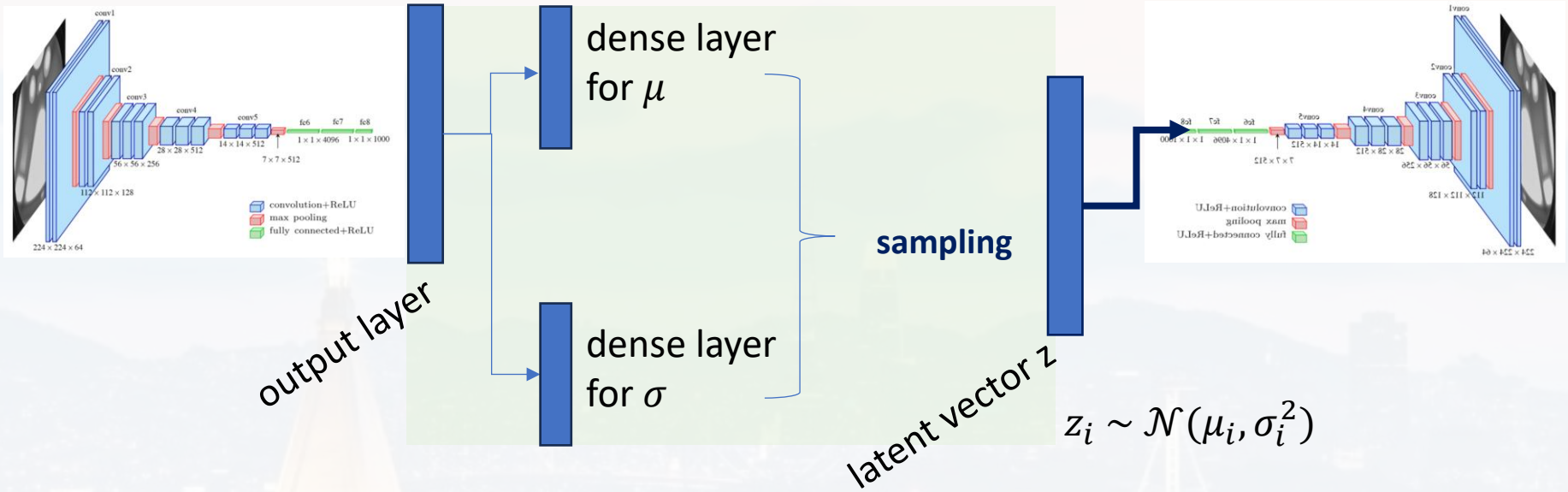
output layer has shape (None, N)

we want M dimensional encoding for z

→ weights in dense layer for σ and μ have shape (N, M)

→ latent vector has length M

now:

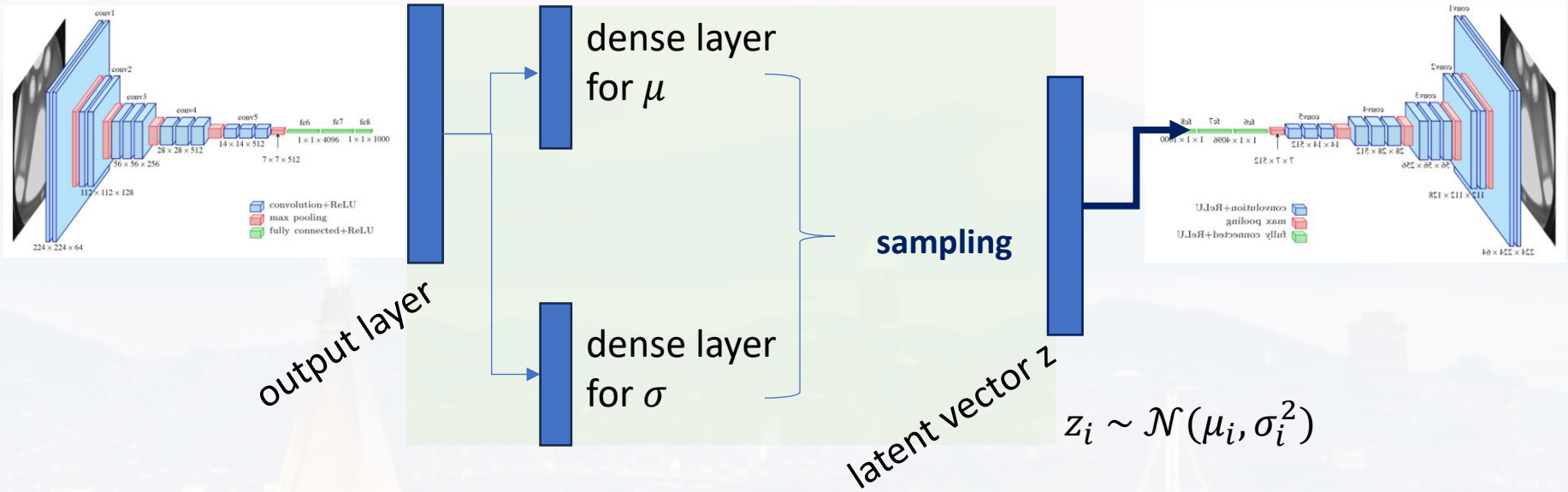


backprop:

- μ_i and σ_i^2 have been generated deterministically from a dense layer
- we need to run backpropagation through μ_i and σ_i^2 in order to adjust the weights/biases
- in order to keep randomness, we actually sample via

$z_i = \mu_i + \sigma_i \cdot \epsilon$ where $\epsilon \sim \mathcal{N}(0,1)$ is not affected by backpropagation

now:



loss: 1) **reconstruction loss L_R**, i. e. the difference between input image x and reconstructed image $p(x|z)$. Note: L_R alone would **lead to overfitting**, exact image gets reproduced!

2) we need a **regularization term** that counteracts L_R:

KL-divergence $L_{KL} = KL[q(z|x)|p(z)]$, which increases if learned distribution $q(z|x)$ gets too far from prior $p(z) \sim \mathcal{N}(0,1)$

loss: 1) **reconstruction loss L_R**, i. e. the difference between input image x and reconstructed image $p(x|z)$. Note: L_R alone would **lead to overfitting**, exact image gets reproduced!

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see here and **module 6 (variational Bayes)**

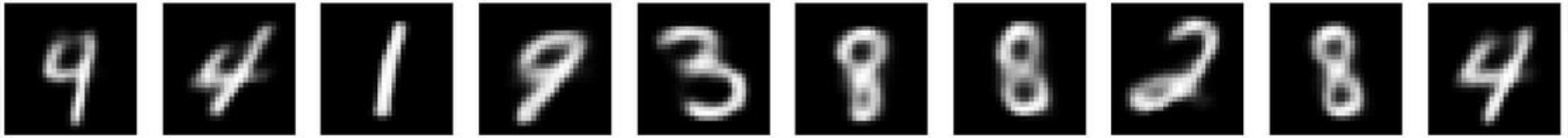
check out `VAR architecture.ipynb`

Convolution, Image Classification & Segmentation

check out `VAR architecture.ipynb`

original

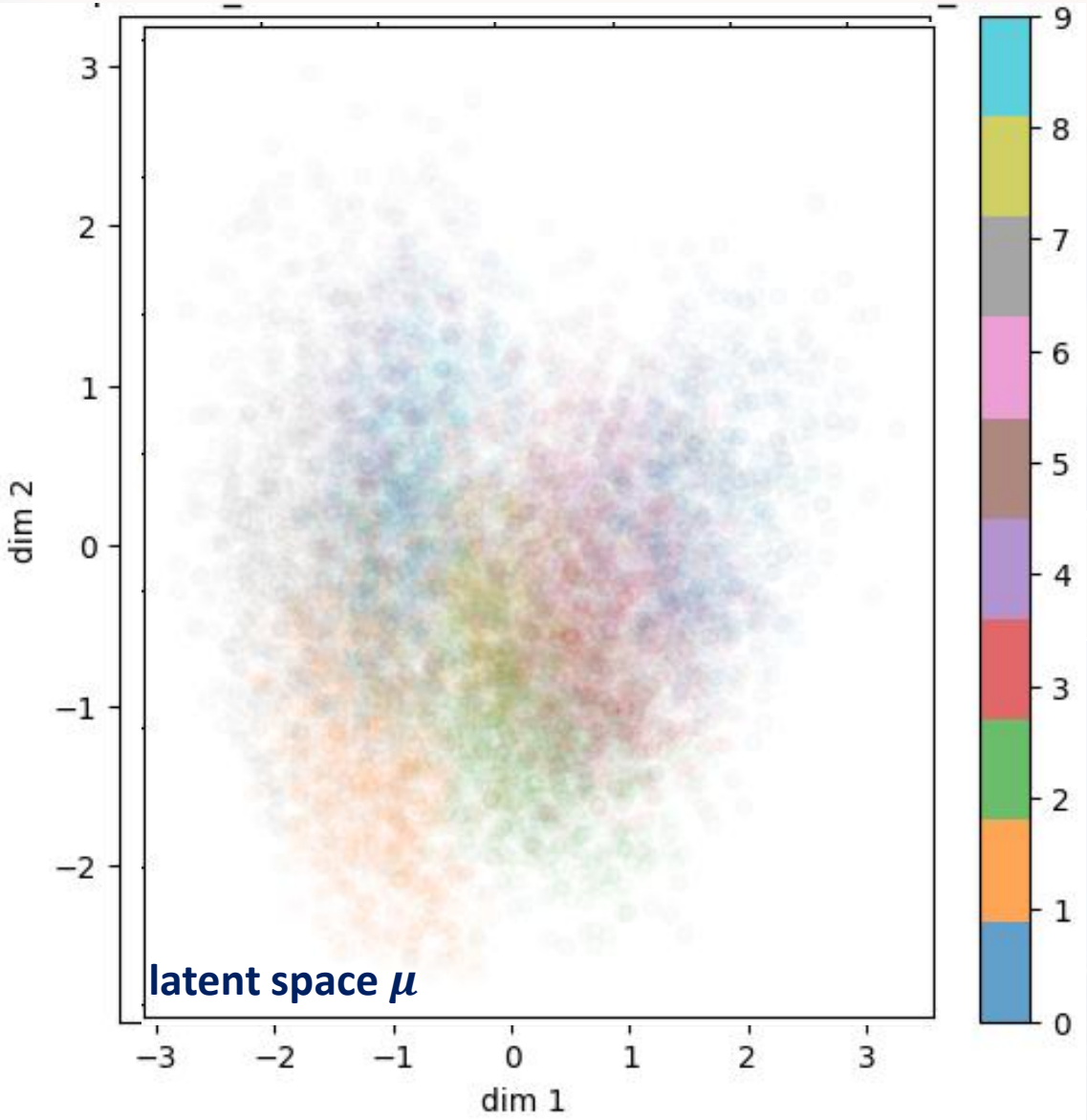
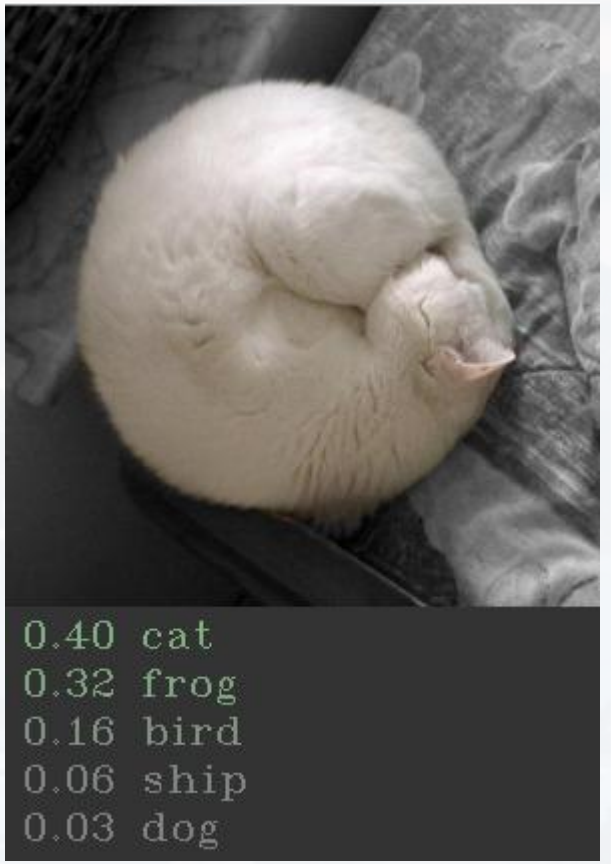
reconstruction



generated

Convolution, Image Classification & Segmentation

check out `VAR architecture.ipynb`



Thank you very much for your attention!