ML.init(0): Dive into PyTorch

A Beginner's Guide to AI & ML Exploration!

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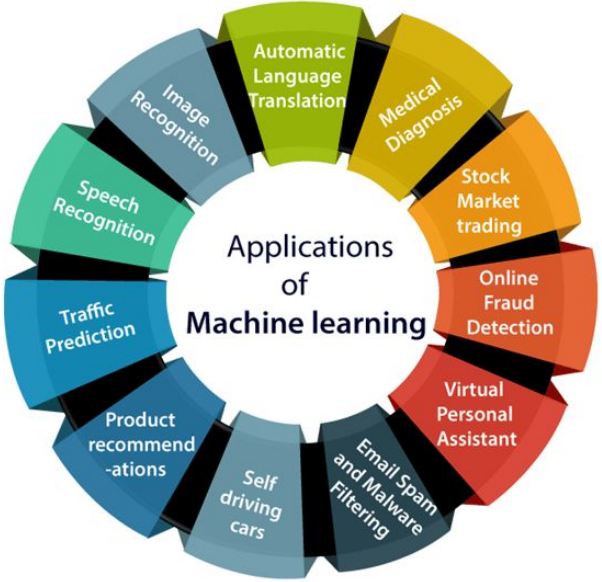
Objectives

- Set up a machine learning project in PyTorch
- Train and test a machine learning (ML) model
- Run inferences using the trained model

What is PyTorch?

- Open-source deep learning library for Python
- Mainly used by data scientists for R&D
- Tensor computation, great for GPU use
- **Important modules:** autograd, optim, nn



How does it compare with TensorFlow?

PyTorch	TensorFlow
• **Pythonic implementation**; APIs easier to write, understand and debug • **Flexible** for experimentation, prototyping and data visualisation • **Rapidly expanding** community	• **Mature, extensive** documentation with a large, established community • Optimised for **production deployment** • Compatible with **existing** frameworks and industry standards

AI research project workflow

1. Pre-process & partition **data**

2. Create or use an existing ML **model**

3. Select **loss function** to compute error

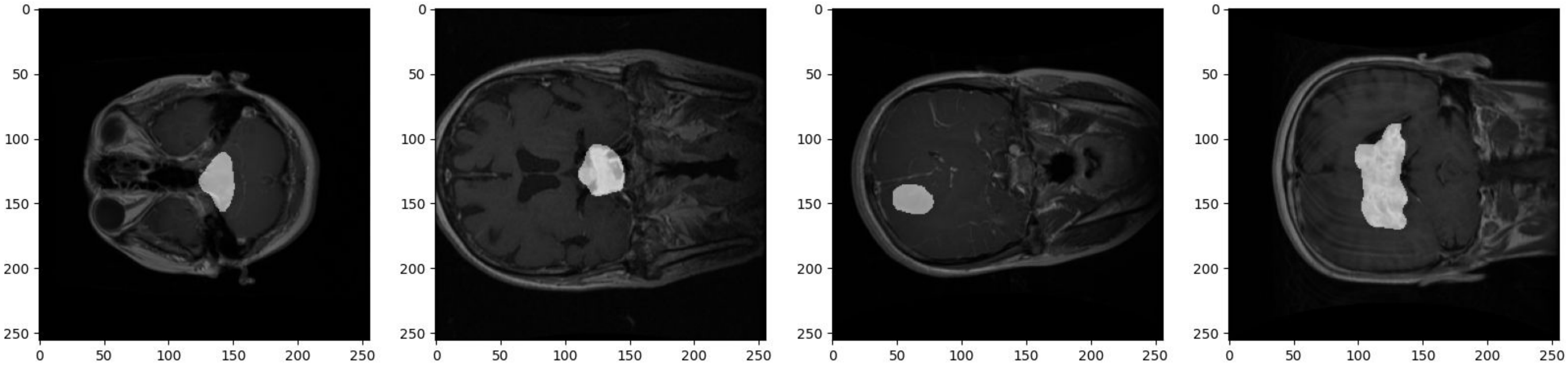
imizer to
el learning

5. **Train** ML model

6. Make model **inferences**

← *Scan here for code*

Example: Brain Tumor Segmentation



- 3064 T1 MRI slices from 233 patients
- Three brain tumor types:
  - Meningioma
  - Glioma
  - Pituitary tumor

Cheng (2017). Brain tumor dataset. figshare. Dataset.
https://doi.org/10.6084/m9.figshare.1512427.v5

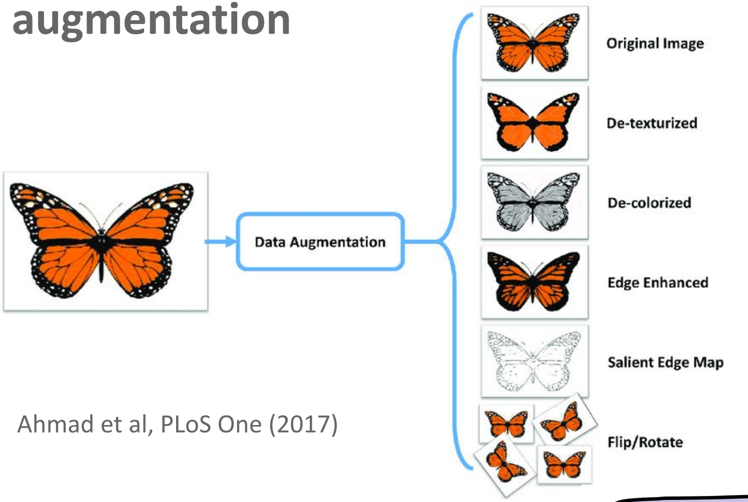
Important necessary libraries
Data -> Get Dataset
Data -> Data visualization

1. Data

Pre-process data using the **Transform** class

- Numpy arrays ⟶ Tensor (*torch.from_numpy*)
  - Tensor designed to work with GPU acceleration and backpropagation
- Resize image

Can also enlarge dataset by **data augmentation**



Ahmad et al, PLoS One (2017)

Data -> Dataset class
Data -> Transform class

1. Data

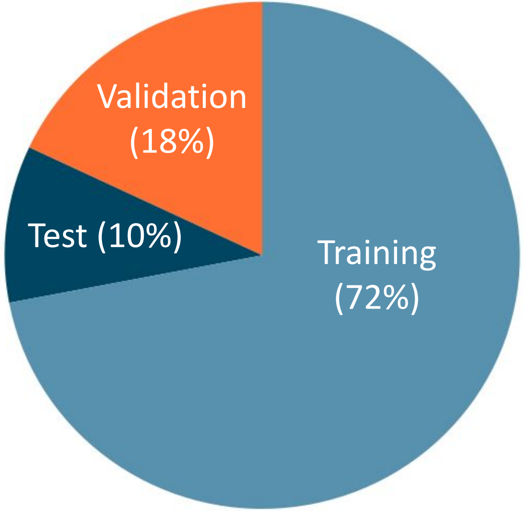
```python
class Resize(object):
    """Resize the image and mask.

    Args:
        output_size (tuple or int): Desired output size. If tuple, output is
            matched to output_size. If int, smaller of image edges is matched
            to output_size keeping aspect ratio the same.
    """

    def __init__(self, output_size):
        assert isinstance(output_size, (int, tuple))
        self.output_size = output_size

    def __call__(self, sample):
        image = sample['image']
        mask = sample['mask']

        h, w = image.shape[:2]
        if isinstance(self.output_size, int):
            if h > w:
                new_h, new_w = self.output_size * h / w, self.output_size
            else:
                new_h, new_w = self.output_size, self.output_size * w / h
        else:
            new_h, new_w = self.output_size

        new_h, new_w = int(new_h), int(new_w)

        image = transform.resize(image, (new_h, new_w)) * 255.0
        image = np.stack((image,) * 3, axis=-1)
        mask = transform.resize(mask, (new_h, new_w)) * 255.0
        mask = np.expand_dims(mask,axis=-1)

        sample['image'] = image
        sample['mask'] = mask

        return sample
```

```python
aset):
"""

ot_dir, transform=None):

ing): Directory with all the images.
llable, optional): Optional transform to be applied
le.

oot_dir
listdir(self.root_dir)
transform

mages)

 idx):
r(idx):
ist()

h.join(self.root_dir,self.imag
filename,'r').get('cjdata')
'image')[()]
tumorMask')[()]

: image, 'mask': mask}

:
.transform(sample)
```

```python
class ToTensor(object):
    """Convert ndarrays to Tensors."""

    def __call__(self, sample):
        # swap color axis because
        # numpy image: H x W x C
        # torch image: C x H x W
        image = sample['image'].transpose((2, 0, 1))
        mask = sample['mask'].transpose((2, 0, 1))
        sample['image'] = torch.from_numpy(image)
        sample['mask'] = torch.from_numpy(mask)

        return sample
```

1. Data

Split dataset and **save** to respective folders



Load data with DataLoader

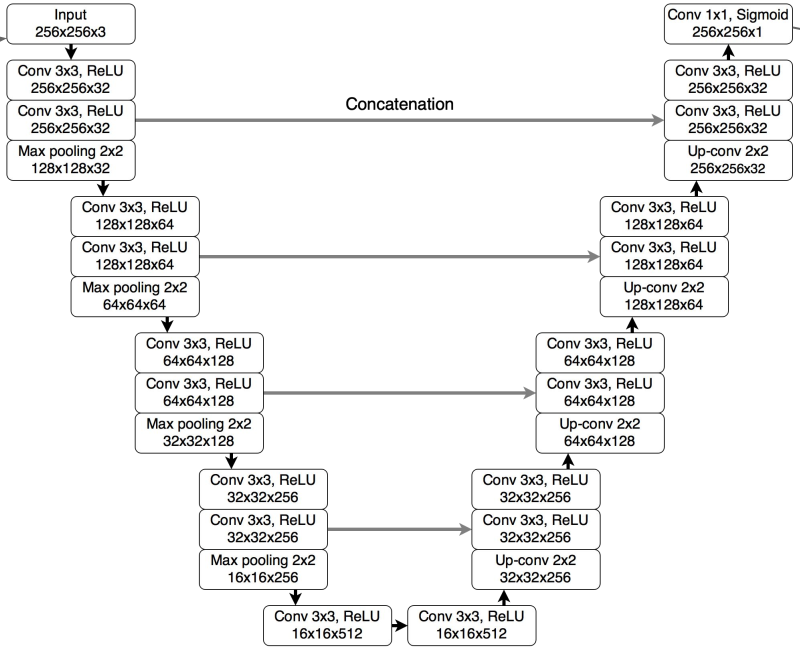
- *Batching:* Optimises memory usage
- *Shuffling:* Avoid learning patterns
- *Parallel loading:* Speeds up training

```
# Training data
train_dataloader = DataLoader(
    train_dataset,batch_size= 4, num_workers=2, shuffle=True)

# Test data
test_dataloader = DataLoader(
    test_dataset,batch_size= 4, num_workers=2, shuffle=False)

# Validation data
val_dataloader = DataLoader(
    val_dataset,batch_size= 4, num_workers=2, shuffle=False)
```

Data -> Split Data and create Data sets
Data -> Data Loders

2. Model

Three-channel MRI slice



Single-channel probability map of abnormal regions

U-Net model

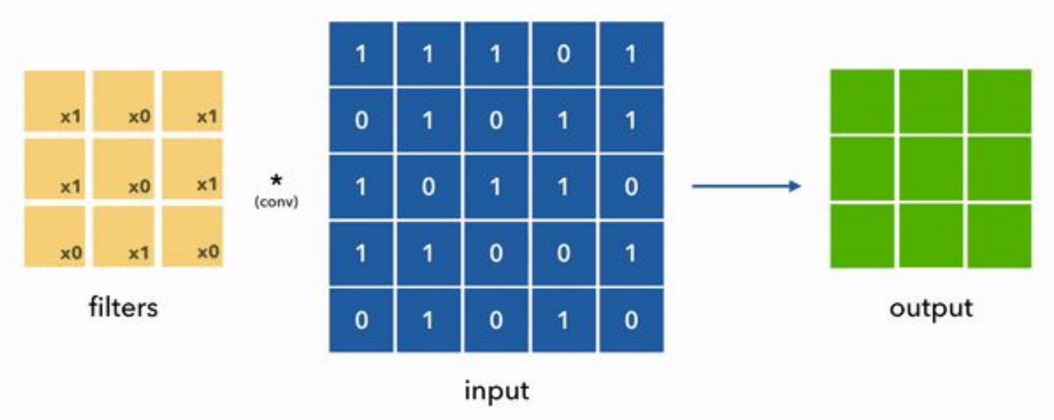
(developed specifically for segmenting abnormalities from brain MRI)

Buda et al, Computers in Biology and Medicine (2019)

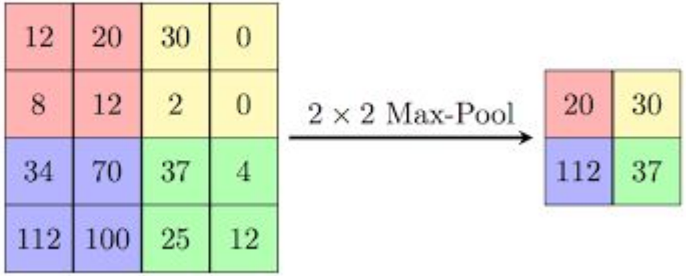
```python
model = torch.hub.load('mateuszbuda/brain-segmentation-pytorch', 'unet',
    in_channels=3, out_channels=1, init_features=32, pretrained=True)
```

Building blocks

Convolution



Max Pooling



3. Loss

- Quantify how well our model predictions **perform** v.s. ground truth
- Model **learns by reducing** the loss function
- Improve model's predictive ability by **minimising** the loss function
- **Choice** of loss function is important

3. Loss

DICE score
Accurate boundary localisation

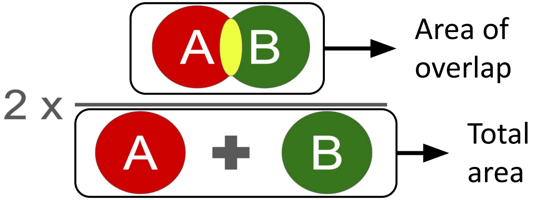
+

Binary Cross-Entropy (BCE)
Measures pixel-wise similarity between predicted & target mask

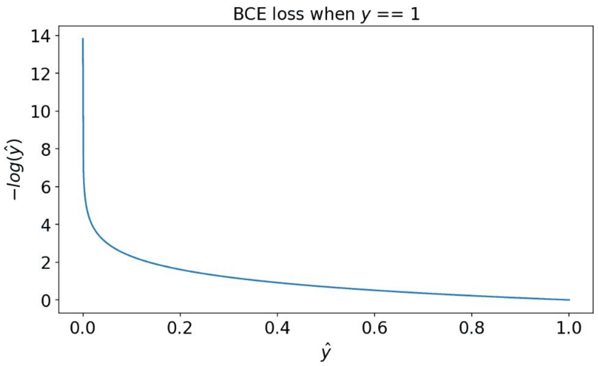
=

BCE Dice Loss
Accurate object localisation & overall segmentation accuracy

A = Prediction   B = Ground truth (target)



DICE score



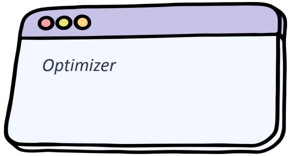

```python
def bce_dice_loss(inputs, target):
    dicescore = dice_loss(inputs, target)
    bcescore = nn.BCELoss()
    bceloss = bcescore(inputs, target)

    return bceloss + dicescore
```

Balanced approach for image segmentation

4. Optimizer

- Optimizer **updates the value of weights** using the gradient from loss.backward to **minimize loss**
  - Gradient = change in loss function w.r.t. weight of model
  - Gradient ⟶ 0: minimise loss, achieve **optimal model configuration**
- Lr scheduler to update learning rate depending on the training behaviour

```
optimizer = AdamW(model.parameters(), 0.1)
scheduler = lr_scheduler.StepLR(optimizer, step_size=5, gamma=0.5)
```

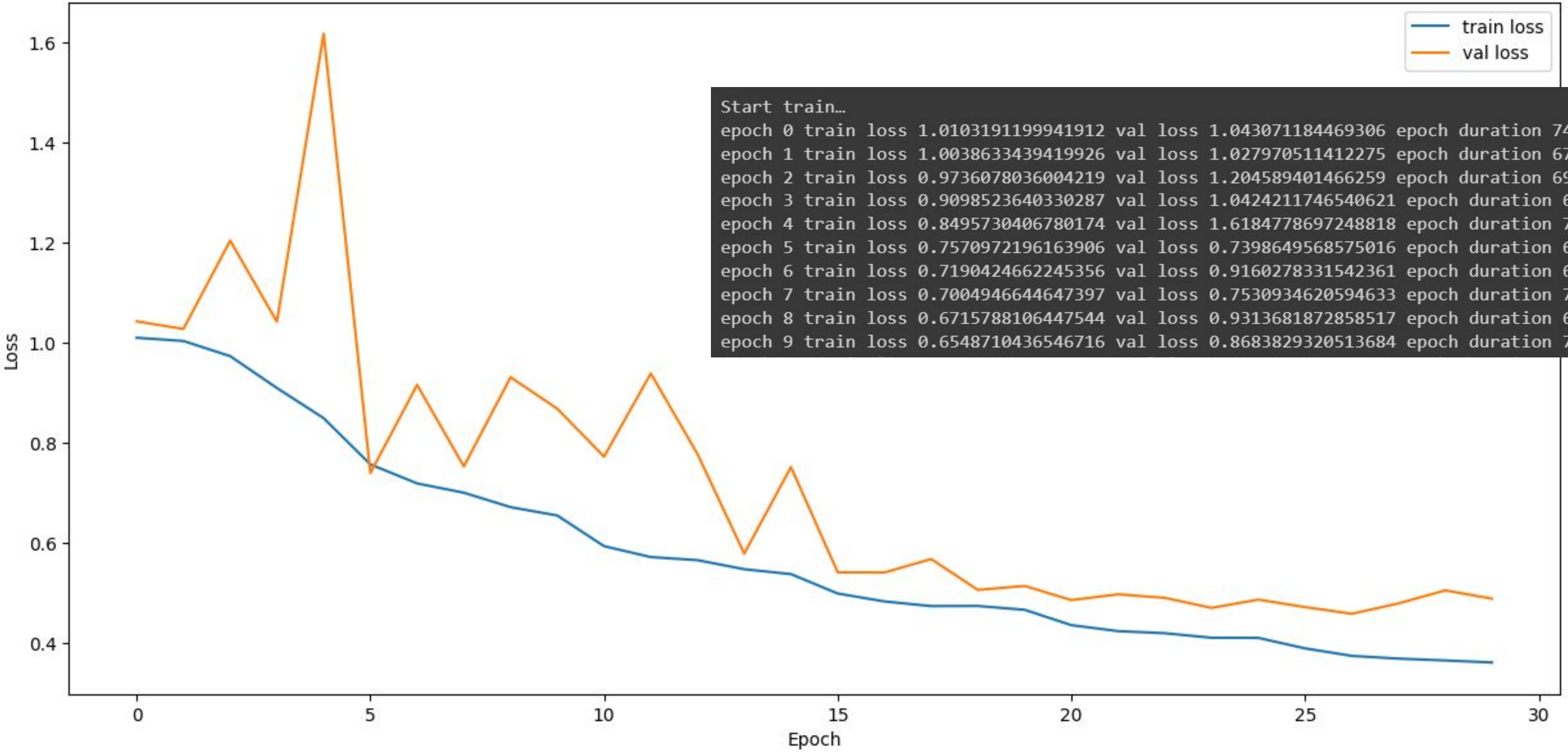


5. Training

Training loop:

- Train
  - Predict
  - Compute loss
  - Optimize
- Validate
  - Predict
  - Compute loss
- Save best model
- Adjust learning rate
- Repeat

5. Training




```
Start train…
epoch 0 train loss 1.0103191199941912 val loss 1.043071184469306 epoch duration 74.04199075698853
epoch 1 train loss 1.0038633439419926 val loss 1.027970511412275 epoch duration 67.39683508872986
epoch 2 train loss 0.9736078036004219 val loss 1.204589401466259 epoch duration 69.68581986427307
epoch 3 train loss 0.9098523640330287 val loss 1.0424211746540621 epoch duration 67.49174499511719
epoch 4 train loss 0.8495730406780174 val loss 1.6184778697248818 epoch duration 70.41903424263
epoch 5 train loss 0.7570972196163906 val loss 0.7398649568575016 epoch duration 67.40357279777527
epoch 6 train loss 0.7190424662245356 val loss 0.9160278331542361 epoch duration 68.81970643997192
epoch 7 train loss 0.7004946644647397 val loss 0.7530934620594633 epoch duration 70.83153796195984
epoch 8 train loss 0.6715788106447544 val loss 0.9313681872858517 epoch duration 69.40048336982727
epoch 9 train loss 0.6548710436546716 val loss 0.8683829320513684 epoch duration 73.2097098827362
```

6. Inference

- **Save & load** models
- Use **best model weights** to segment tumours (test set)

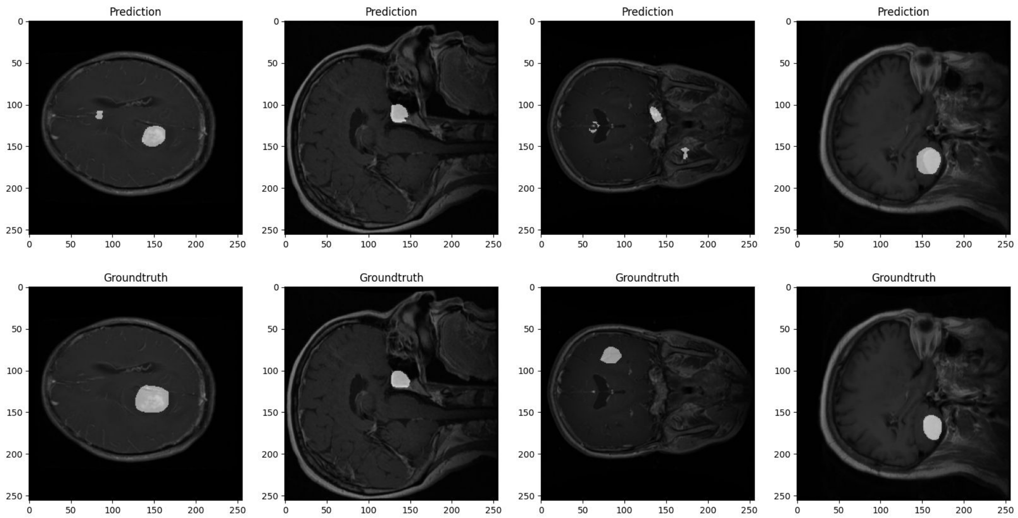
```
if curr_loss_val < best_loss_val:
    best_loss_val = curr_loss_val
    torch.save(model.state_dict(), r'/content/best_model.pth')
```

```
checkpoint = torch.load(
    '/content/best_model.pth', map_location=torch.device('cpu'))
model.load_state_dict(checkpoint)
```

Inference -> Load best model weights
Inference -> Visualization
Inference -> Accuracy

6. Inference

- Save & load models
- Use best model weights to segment tumours (test set)
- **Visualize** predicted and ground truth images
- Compute **model accuracy** using test cases




```
[27] # Test set
     acc_test = compute_acc(test_dataloader, model)
     print(f'Acccuracy on the train set is {acc_test}')

     Acccuracy on the train set is 0.6898969995913493
```

Inference -> Load best model weights
Inference -> Visualization
Inference -> Accuracy

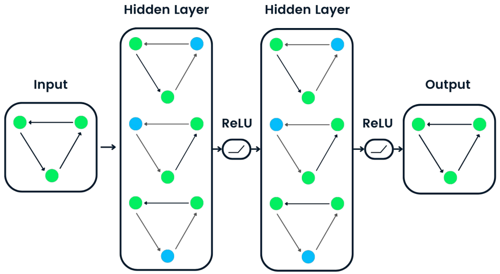
Summary

- **Learnt** how to **set up** a machine learning project in PyTorch
- **Trained** and **tested** a machine learning model to perform brain tumour **segmentation**
- Performed **inferences** with the trained model

Now, let's head over to the code!

What’s next?

Graph Convolution Network



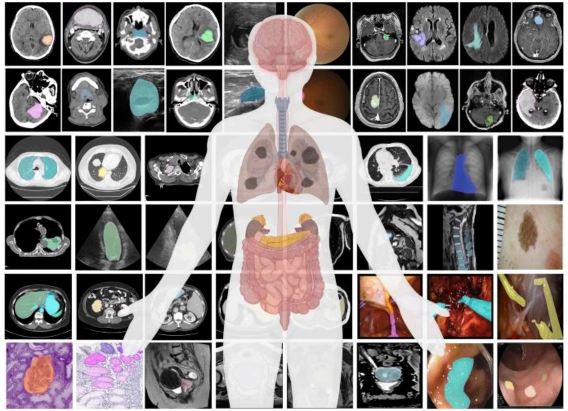
Diffusion Models

Article | Open access | Published: 22 January 2024

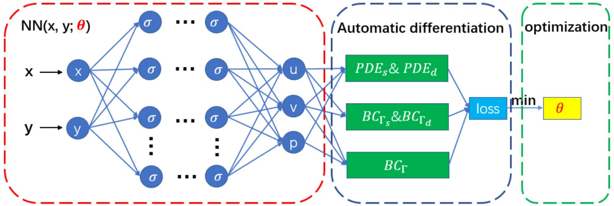
Segment anything in medical images

Jun Ma, Yuting He, Feifei Li, Lin Han, Chenyu You & Bo Wang

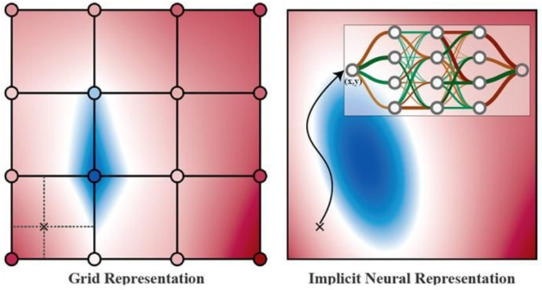
Nature Communications 15, Article number: 654 (2024) | Cite this article



Physics-Informed Neural Networks (PINNs)



Neural Implicit Representation (NIR)



ML.init() team

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If you’re interested to use ML in your work, or are just curious:

feel free to reach out for a chat!