Cagri Ozcinar, PhD

LTTI.00.032 – Machine Learning in Synthetic Biology

Recap

- The essence of deep learning is to find best weights for the network that minimizes the error (loss)

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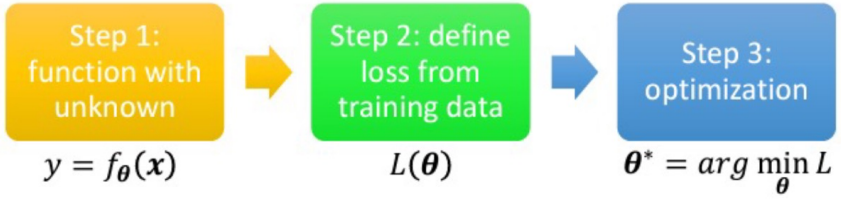
Recap



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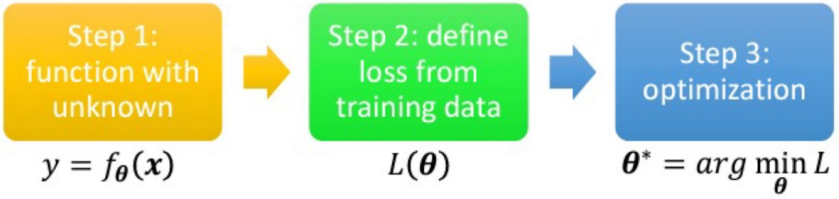
Recap



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- This is done via an iterative process where weights are updated in each iteration in a direction that minimizes the loss

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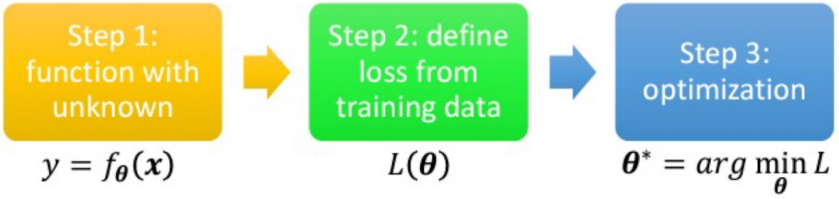
Recap



- The essence of deep learning is to find best weights for the network that minimizes the error (loss)
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- To find this direction we need the slope of the loss function for a given weight. This is achieved by computing the derivatives (gradient)

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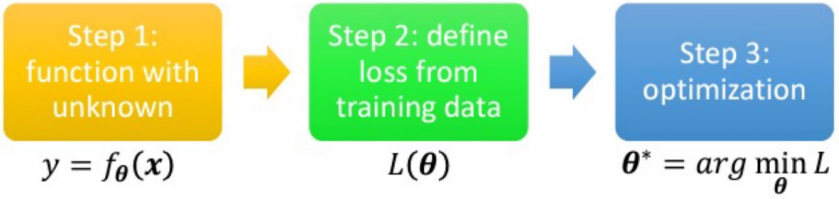
Recap



- The essence of deep learning is to find best weights for the network that minimizes the error (loss)
- This is done via an iterative process where weights are updated in each iteration in a direction that minimizes the loss
- To find this direction we need the slope of the loss function for a given weight. This is achieved by computing the derivatives (gradient)
- It is computationally expensive to compute derivatives for millions of weights

Recap

- Backpropagation makes this computation possible by using the chain rule in calculus

Rumelhart, D. E., Hinton, G. E., & Williams, R. J. (1986). Learning representations by back-propagating errors. nature, 323(6088), 533-536.

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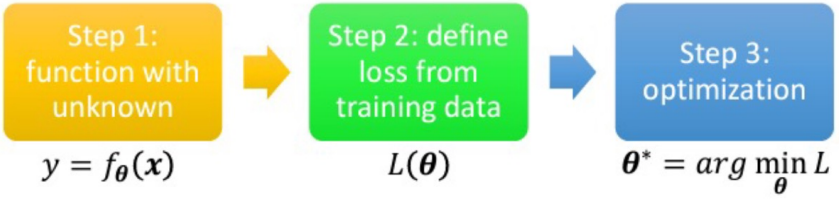
Recap



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Rumelhart, D. E., Hinton, G. E., & Williams, R. J. (1986). Learning representations by back-propagating errors. nature, 323(6088), 533-536.

- Gradient decent is a general term for calculating the gradient and updating the weights

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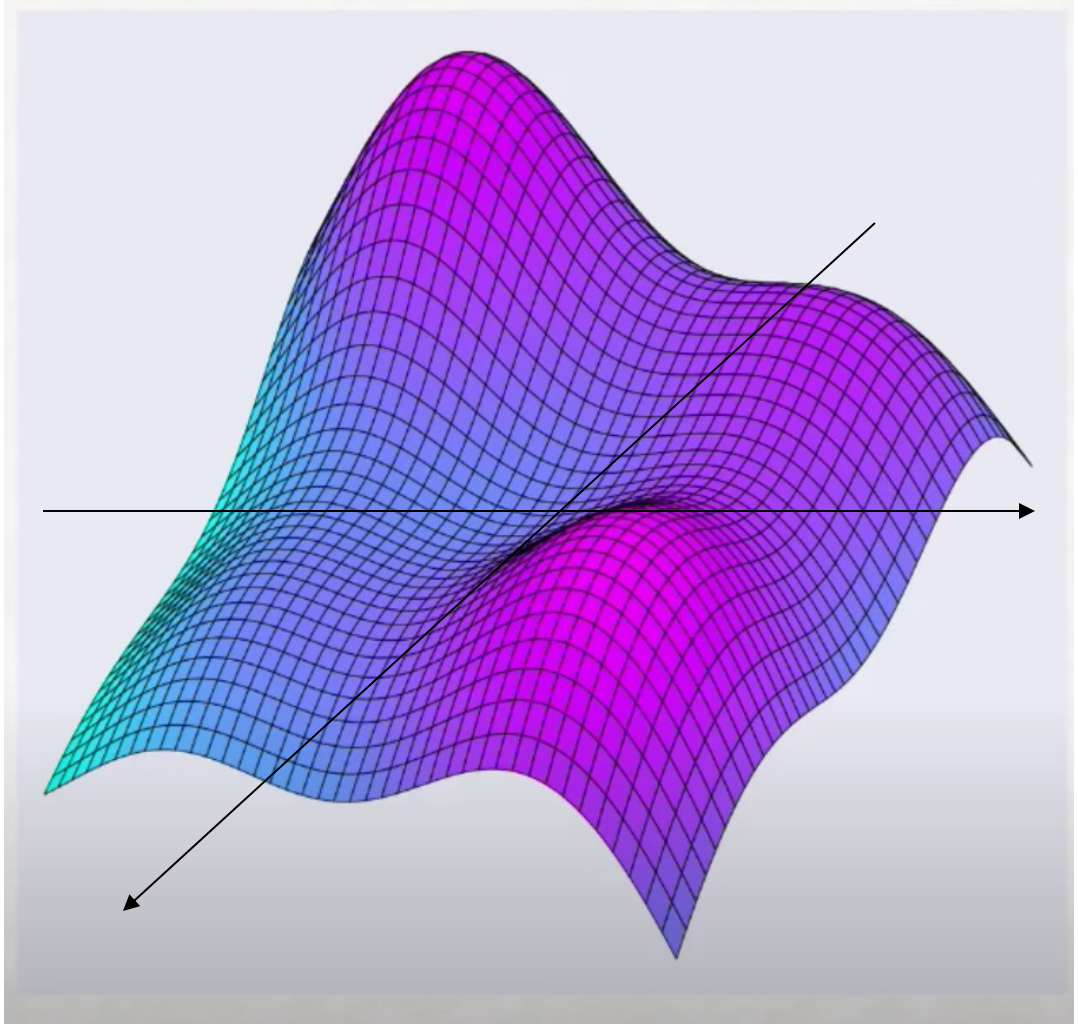
Gradient Decent



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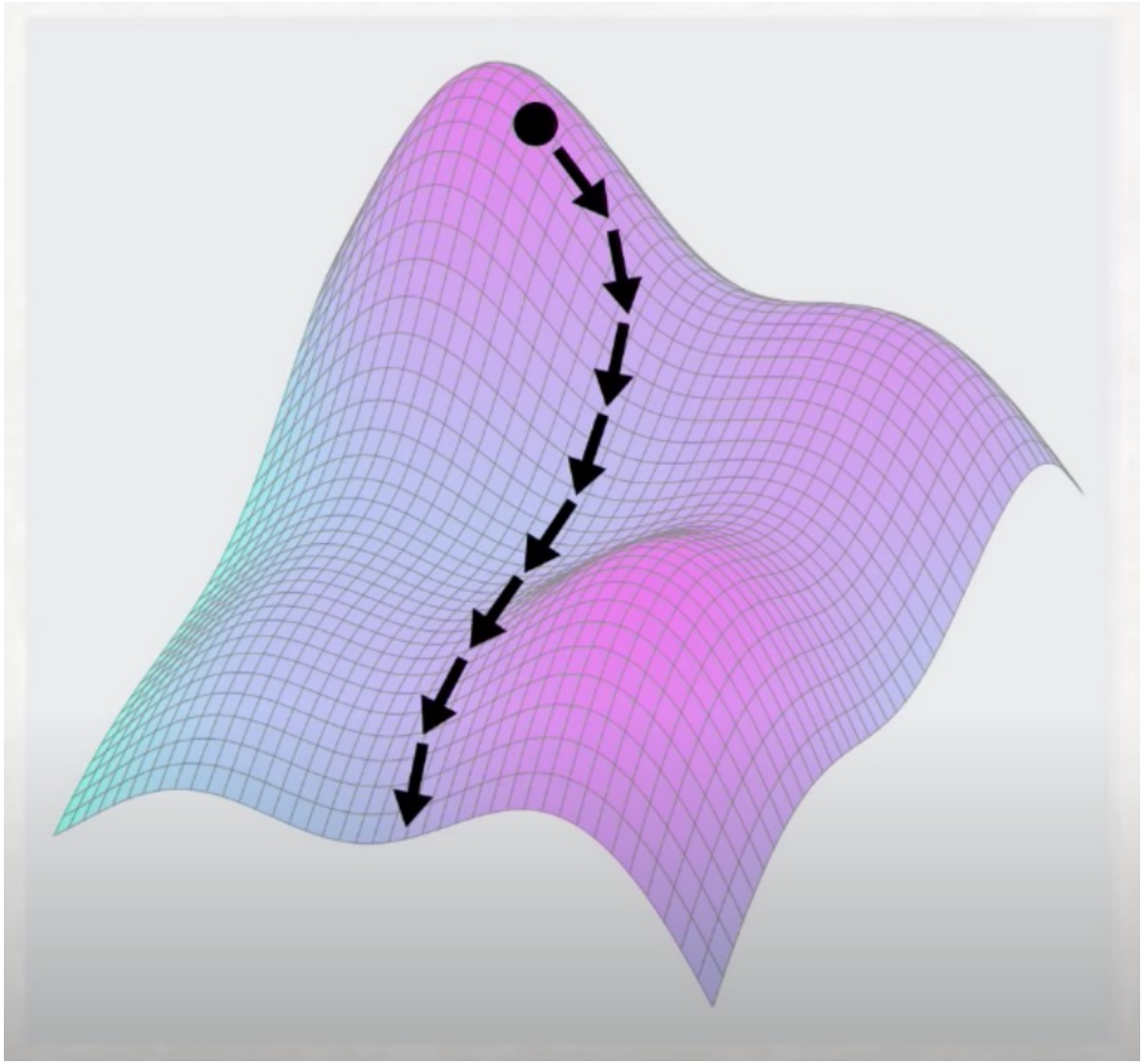
Gradient Decent



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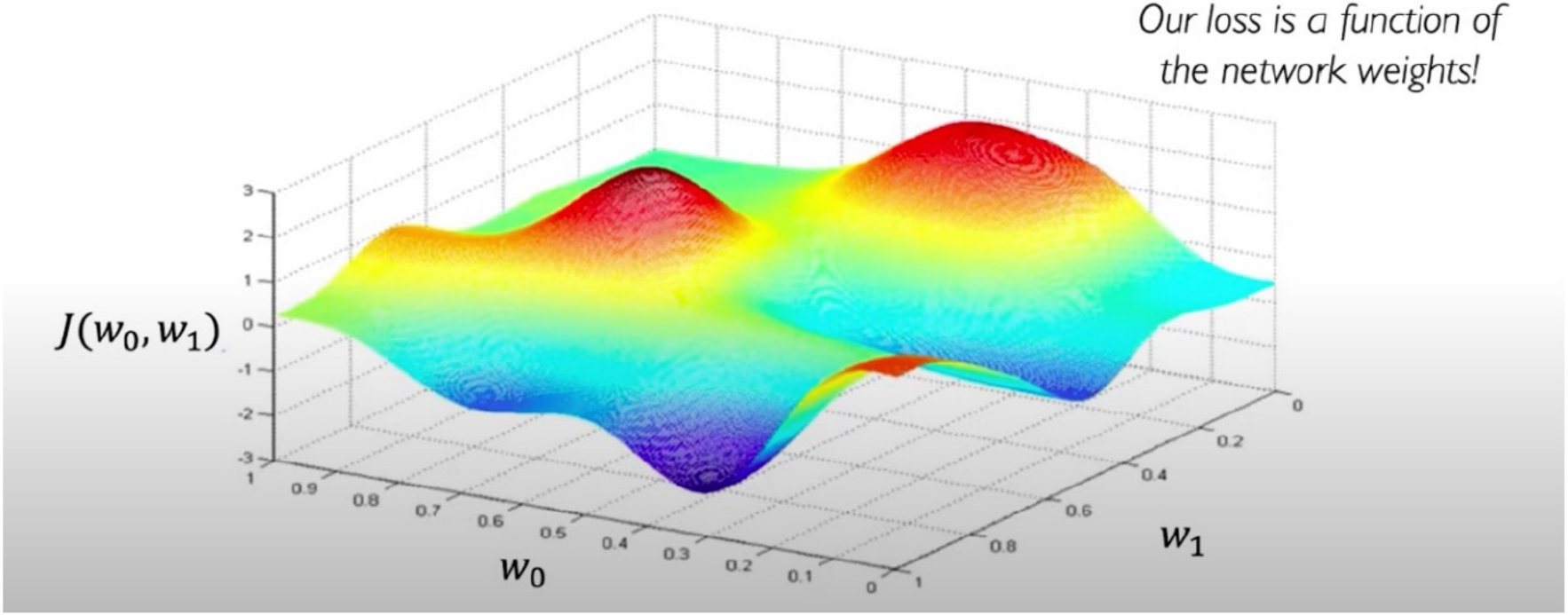
Loss optimization

$$W^* = \underset{W}{\operatorname{argmin}} J(W)$$

Remember:
Our loss is a function of the network weights!



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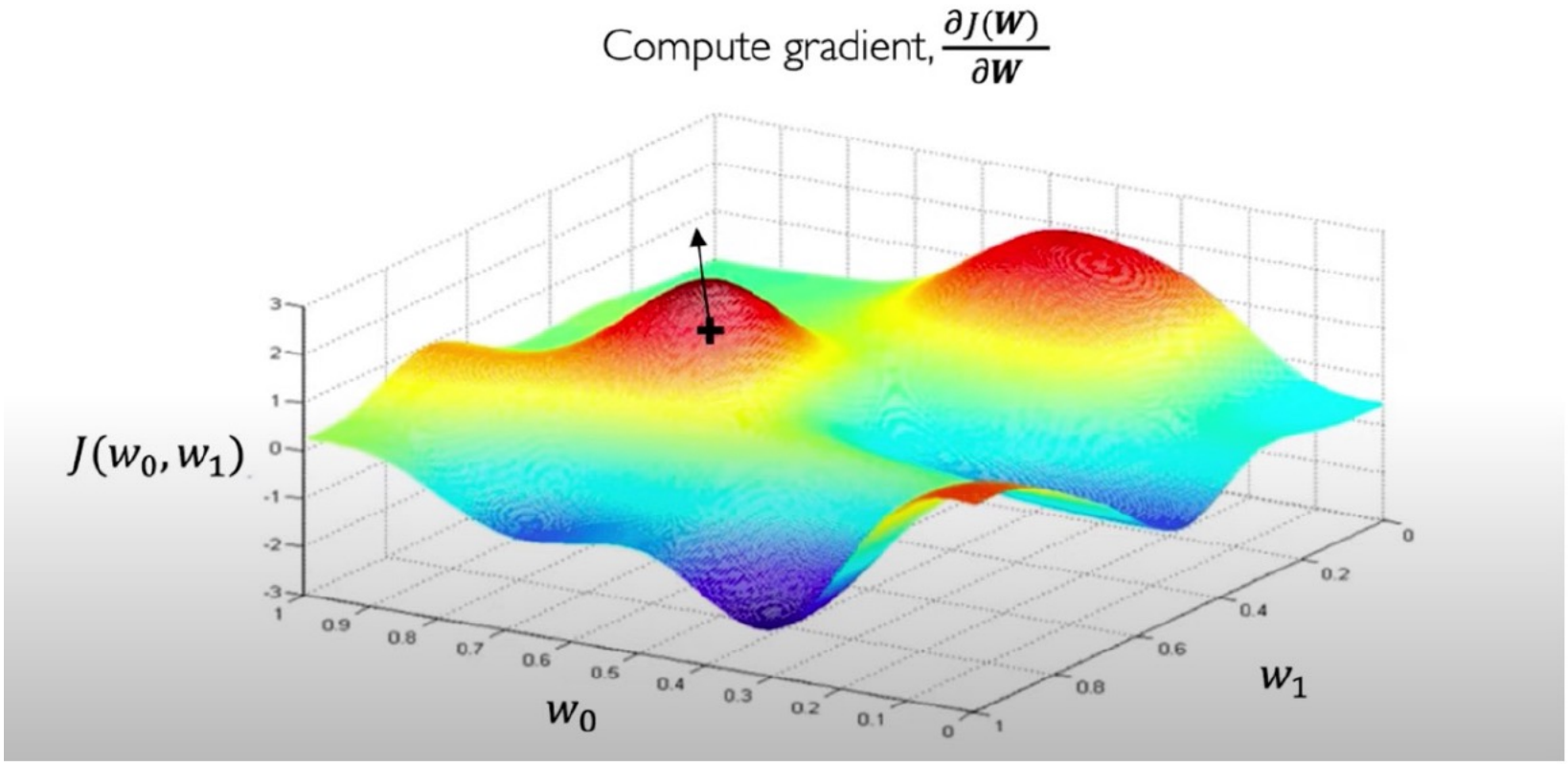
Loss optimization



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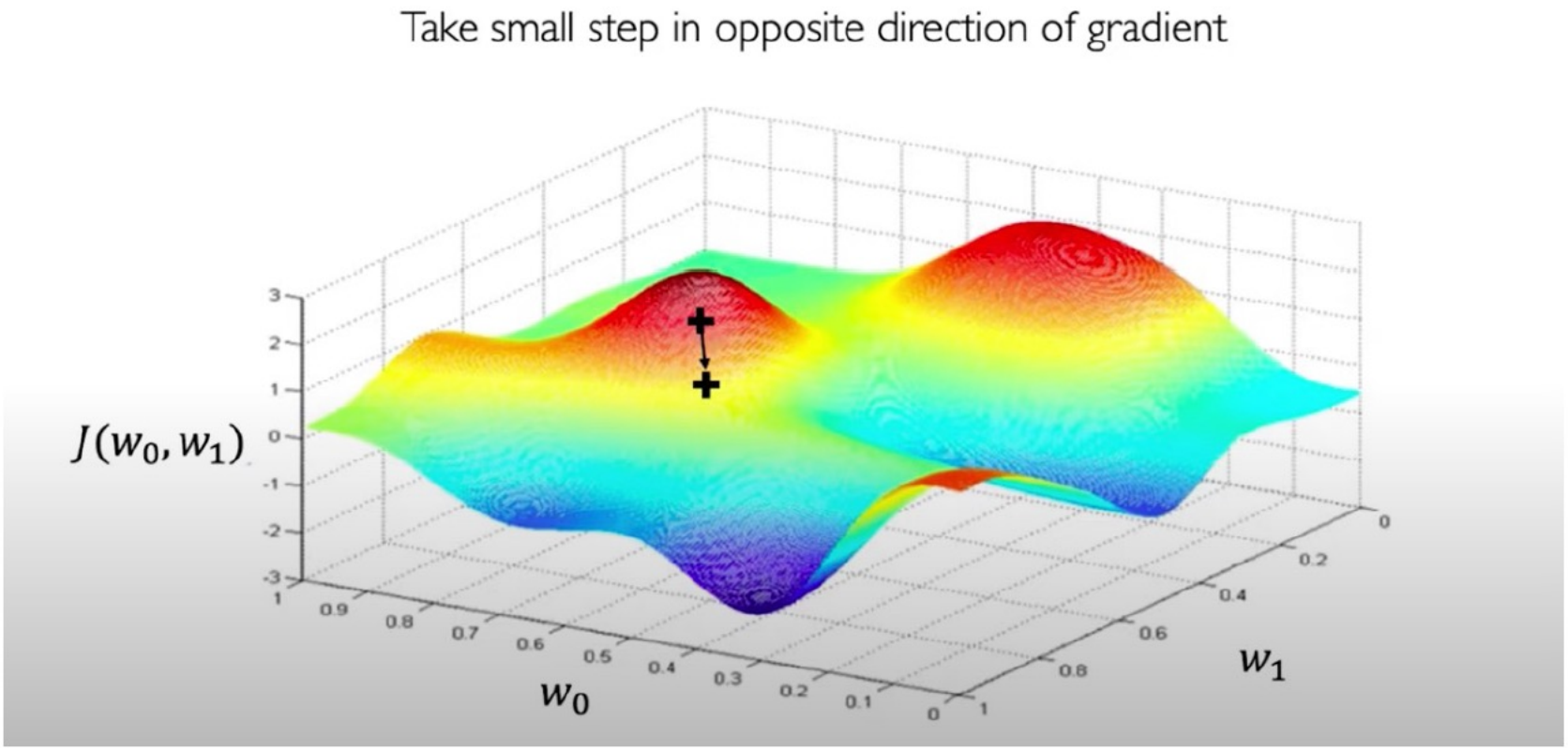
Loss optimization



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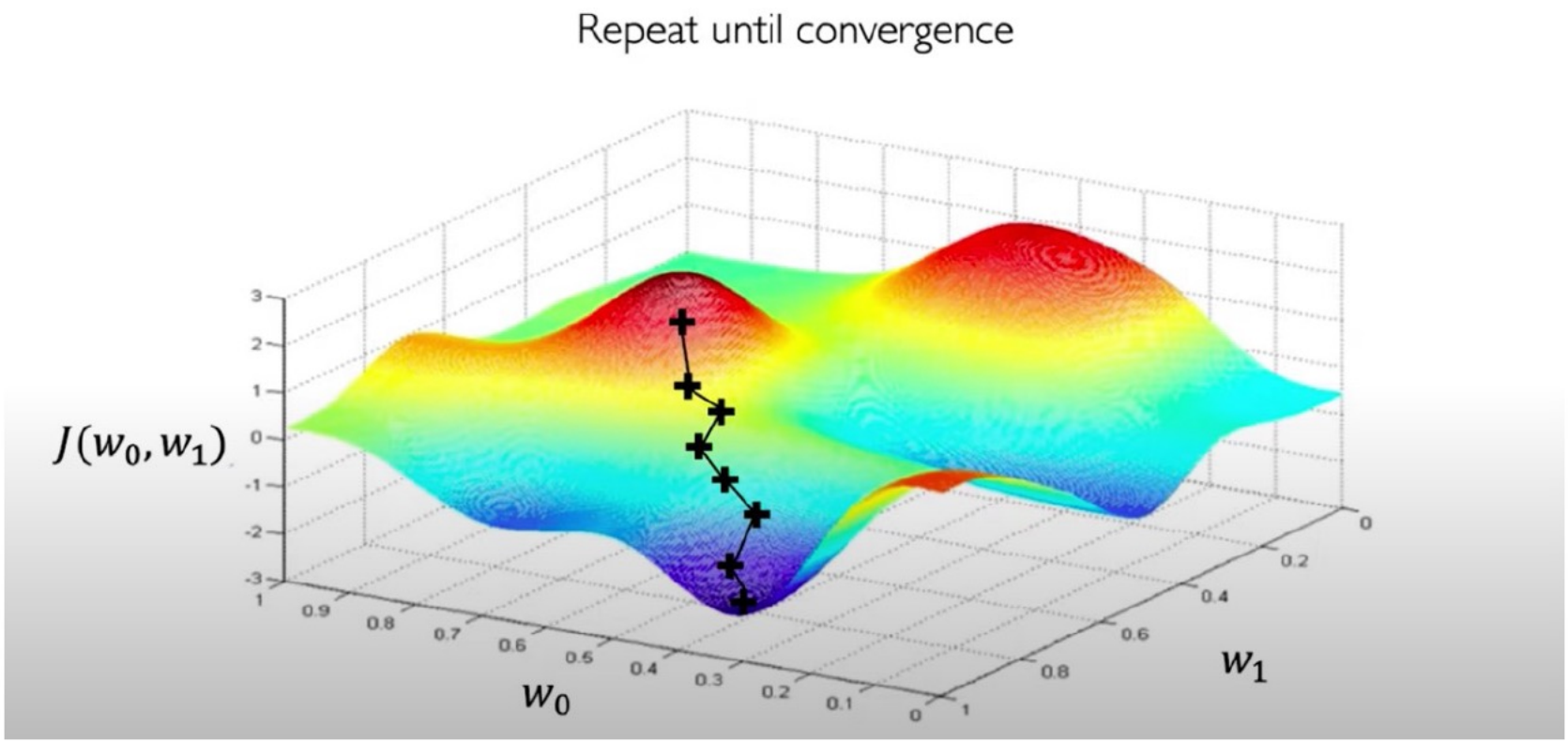
Gradient decent



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Gradient decent

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
4. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Return weights

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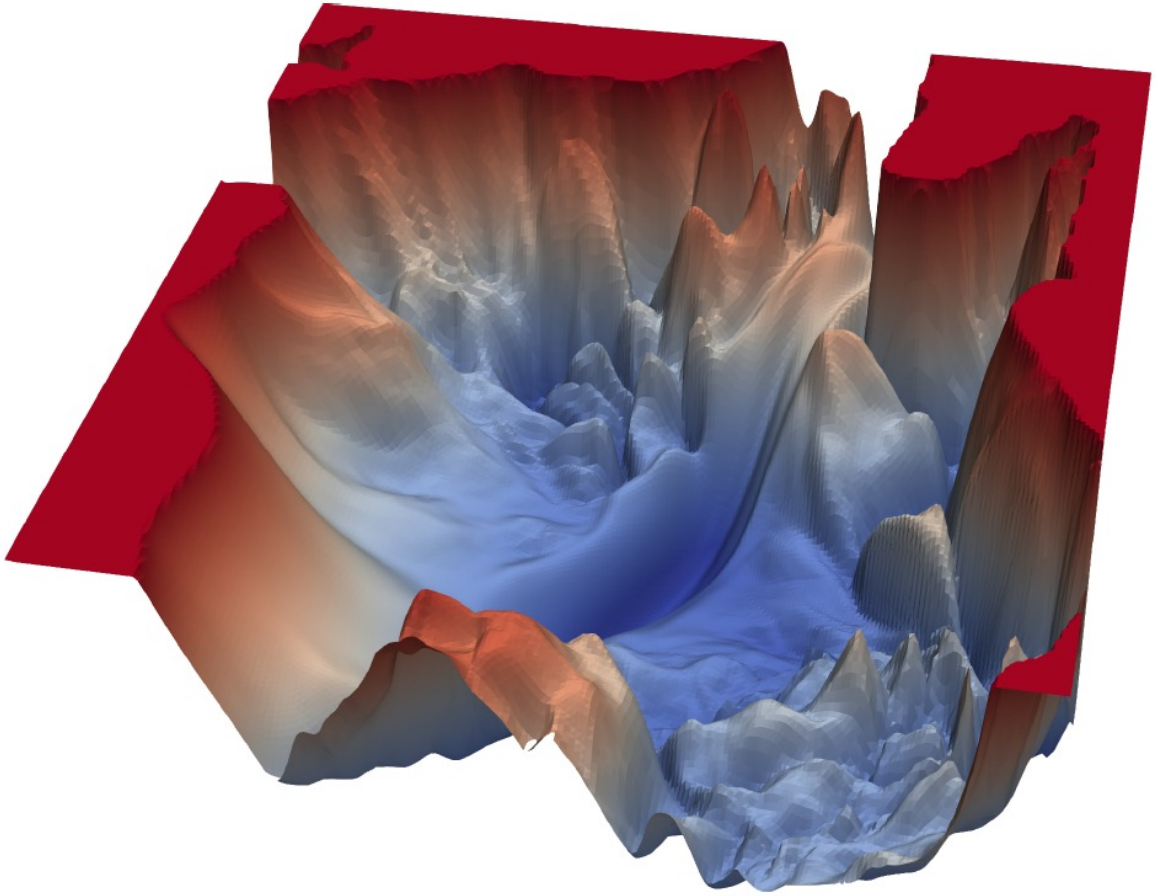
Gradient decent



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Loss function optimization

Remember:

Optimization through gradient descent

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$

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Loss function optimization

Remember:

Optimization through gradient descent

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$

How can we set the learning rate?

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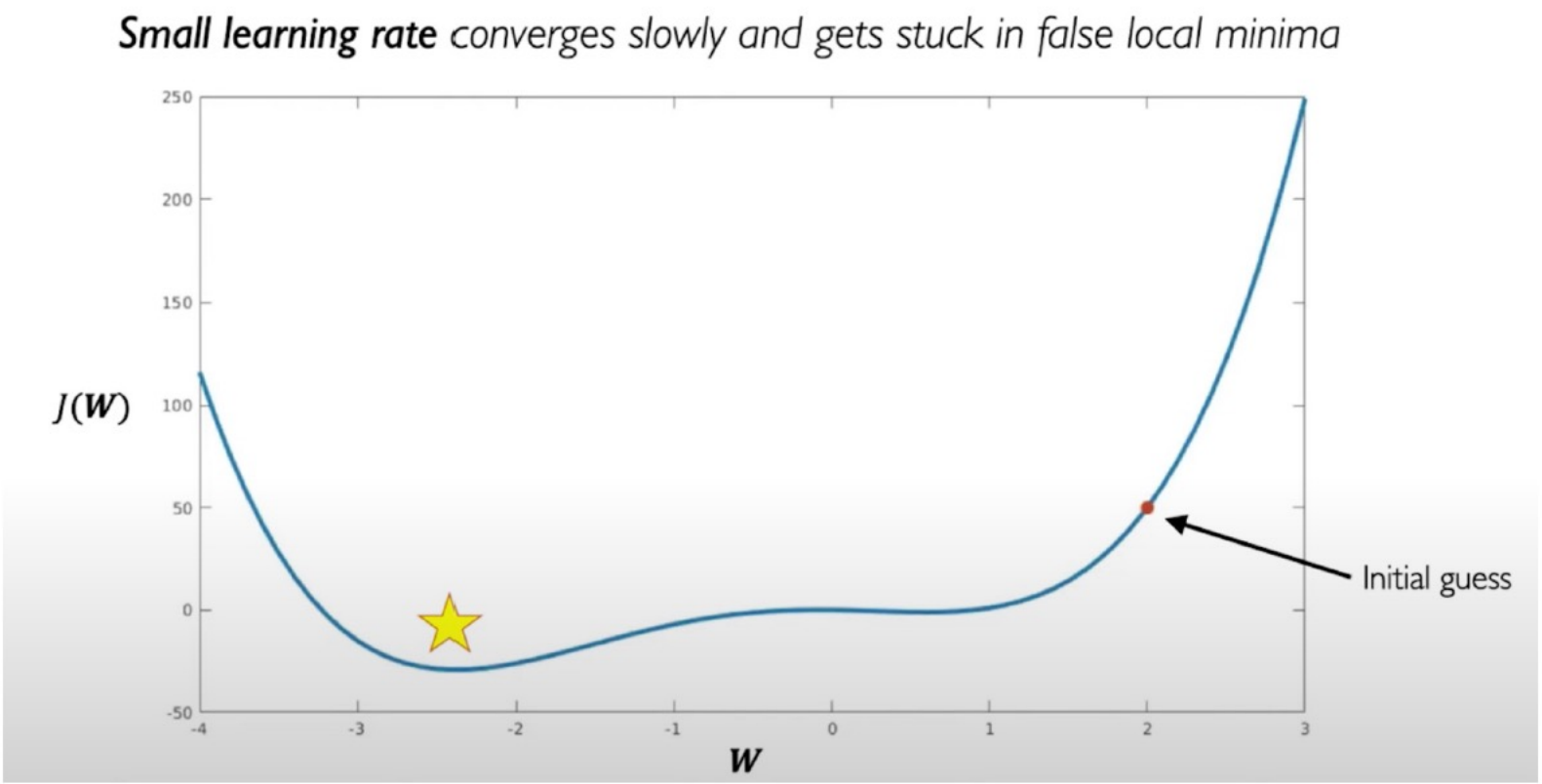
Setting the learning rate



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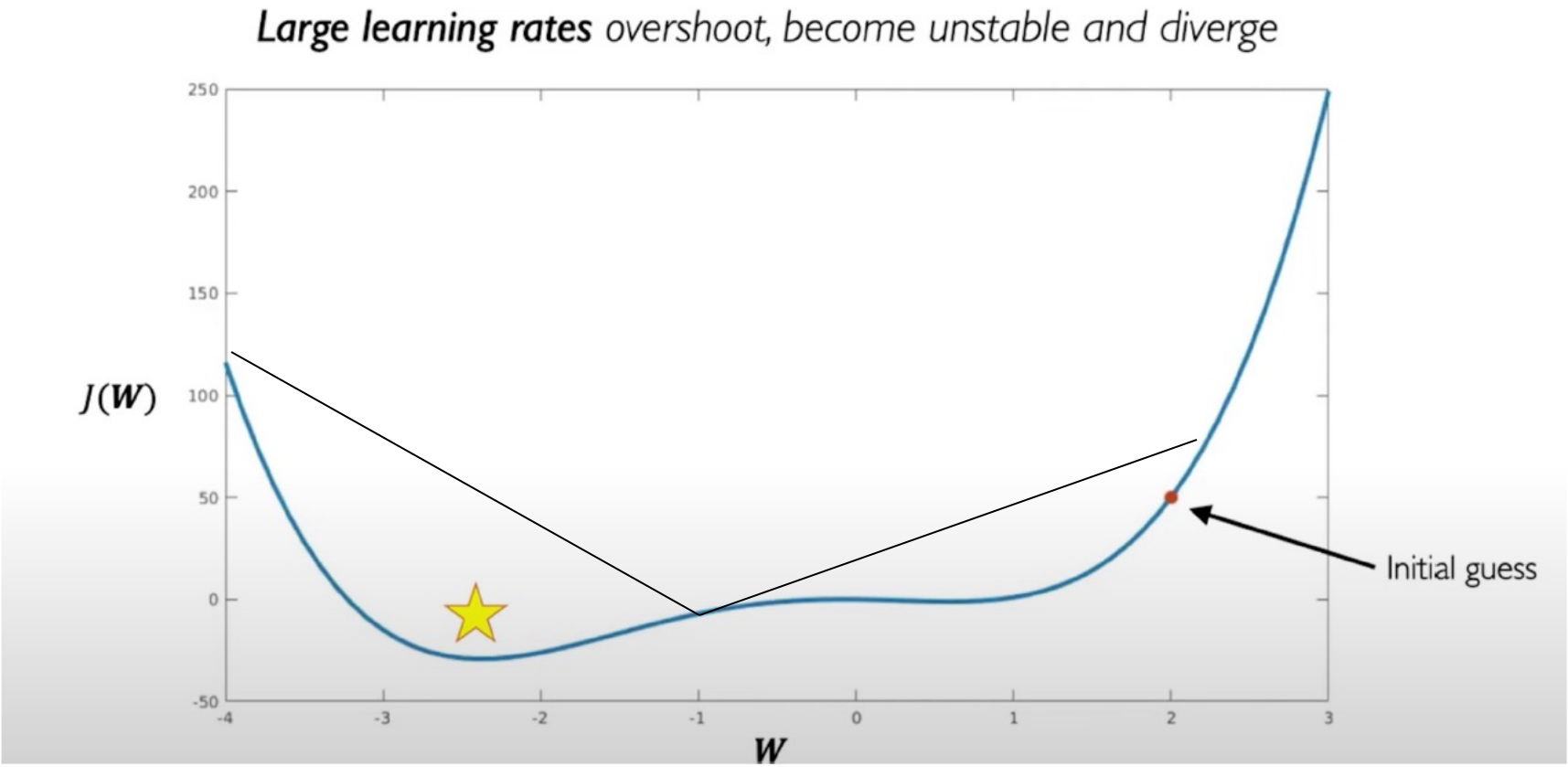
Setting the learning rate



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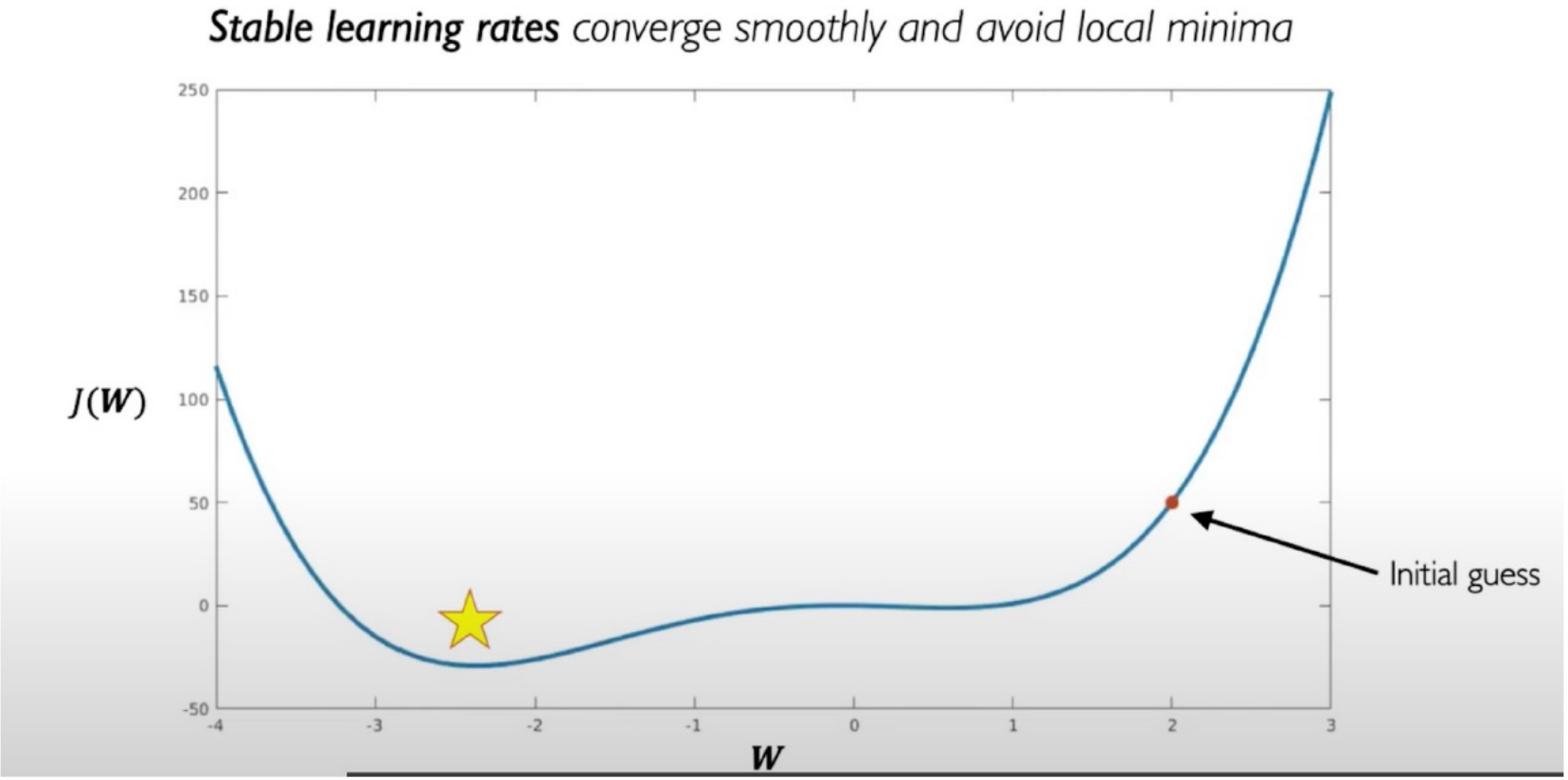
Setting the learning rate



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How to deal with this

Idea 1.

Try lots of different learning rates and see what works “just right”

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How to deal with this

Idea 1.

Try lots of different learning rates and see what works “just right”

Idea 2.

Design an adaptive learning rate that adapts to the landscape

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Gradient decent algorithms

SGD

Adam

Adadelta

Adagrad

RMSProp

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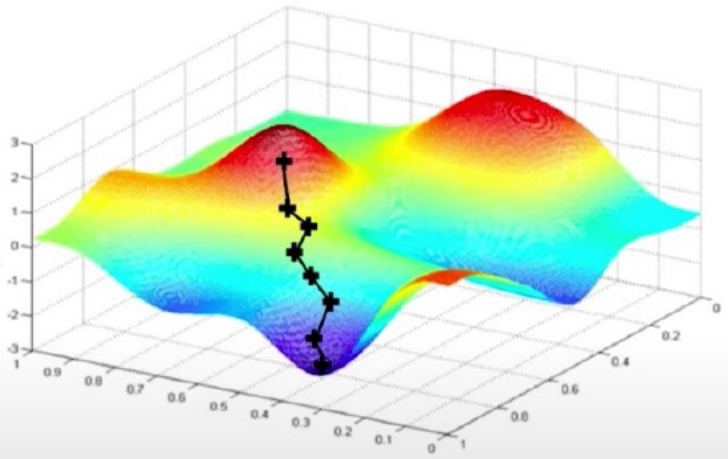
Gradient decent

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
4. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Return weights



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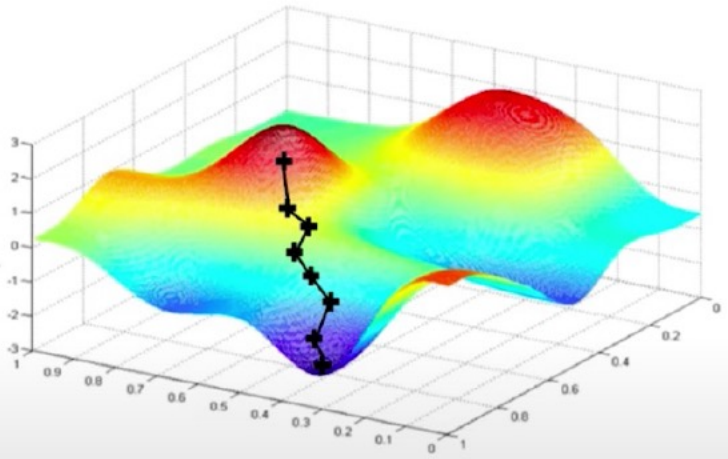

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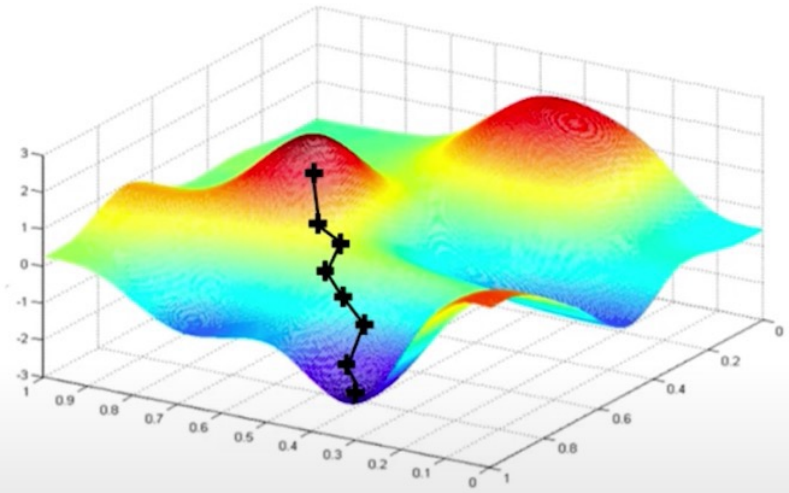
Stochastic Gradient Decent

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Pick single data point i
4. Compute gradient, $\frac{\partial J_i(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
6. Return weights



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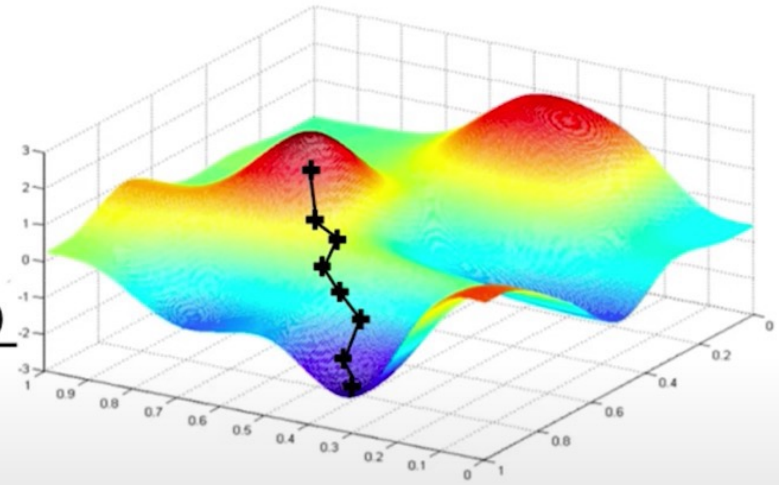
Stochastic Gradient Decent

Algorithm

1. Initialize weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence:
3. Pick batch of B data points
4. Compute gradient, $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}} = \frac{1}{B} \sum_{k=1}^{B} \frac{\partial J_k(\boldsymbol{W})}{\partial \boldsymbol{W}}$
5. Update weights, $\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
6. Return weights



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Mini-batches while training

- More accurate estimation of gradient
- Smoother convergence
- Allows for larger learning rates
- Leads to fast training

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Practical

What is PyTorch?

- An **machine learning framework** in Python
- Two main features:
  - N-dimensional **Tensor** computation on **GPUs**
  - Automatic differentiation for training deep neural networks

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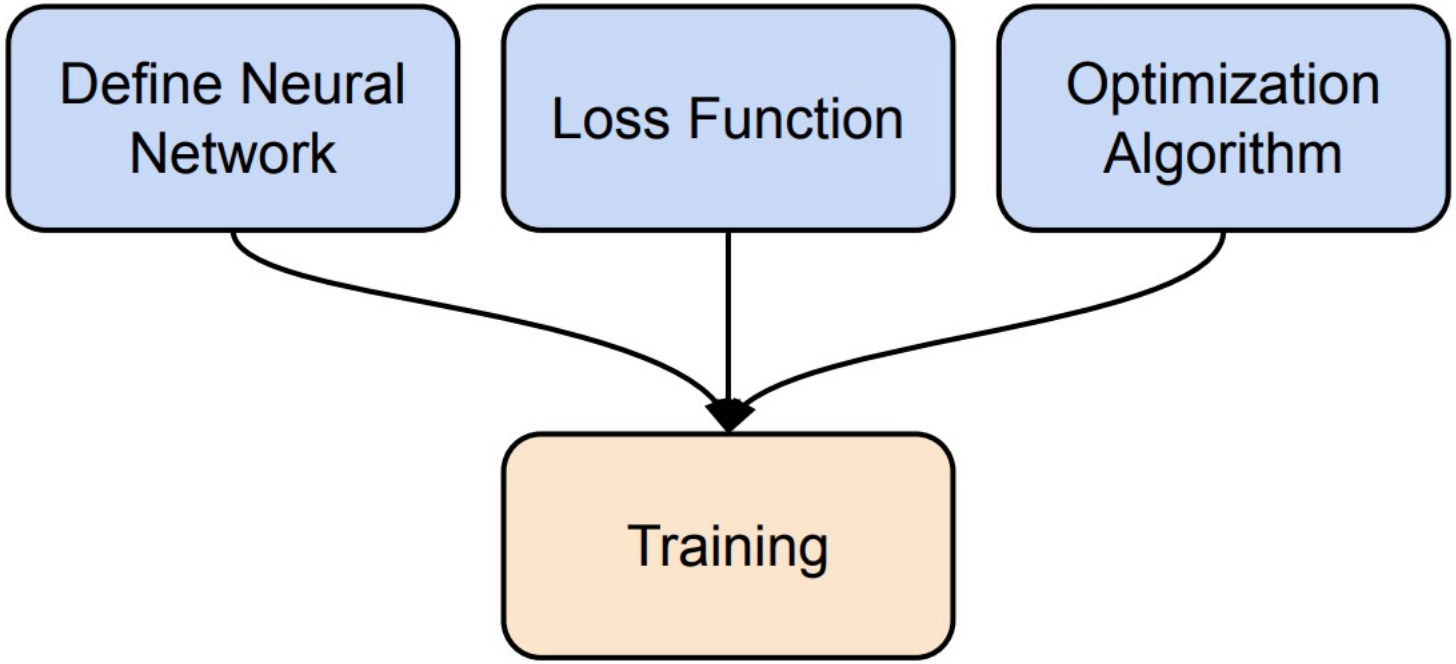
Training Neural Networks



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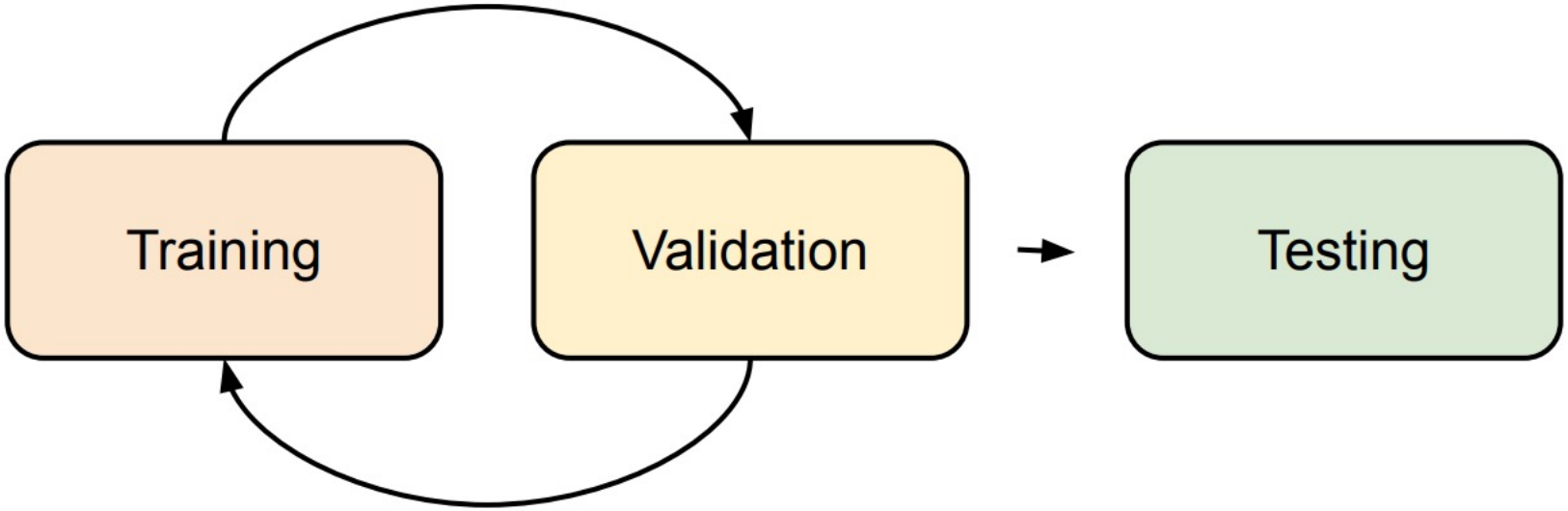
Training & Testing Neural Networks



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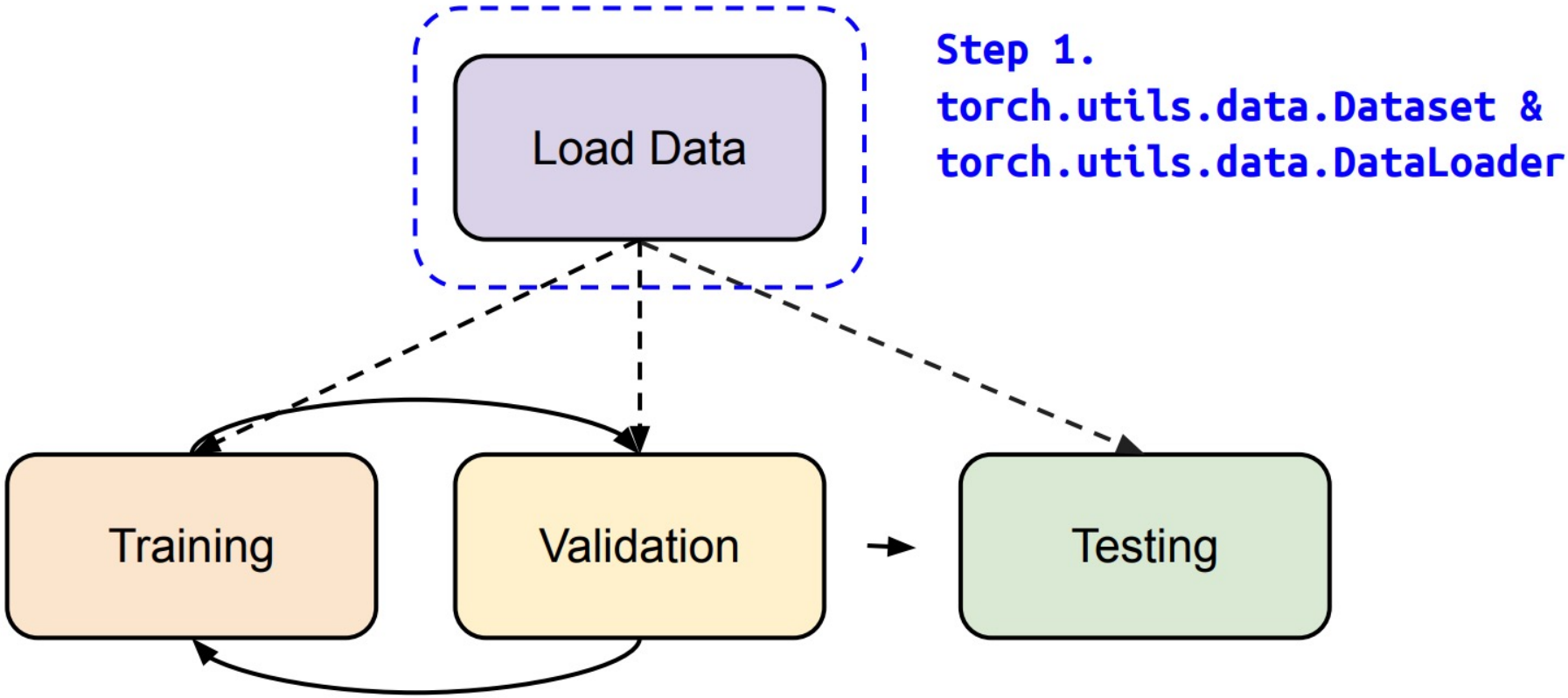
Training & Testing Neural Networks in PyTorch



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Dataset & Dataloader

- `Dataset:` stores data samples and expected values
- `Dataloader:` groups data in batches, enables multiprocessing

- `dataset = MyDataset(file)`
- `dataloader = DataLoader(dataset, batch_size, shuffle=True)`

Training: True
Testing: False

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Dataset & Dataloader

```
from torch.utils.data import Dataset, DataLoader

class MyDataset(Dataset):
    def __init__(self, file):
        self.data = ...

    def __getitem__(self, index):
        return self.data[index]

    def __len__(self):
        return len(self.data)
```

Read data & preprocess

Returns one sample at a time

Returns the size of the dataset

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Dataset & Dataloader

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```

Read data & preprocess

Returns one sample at a time

Returns the size of the dataset

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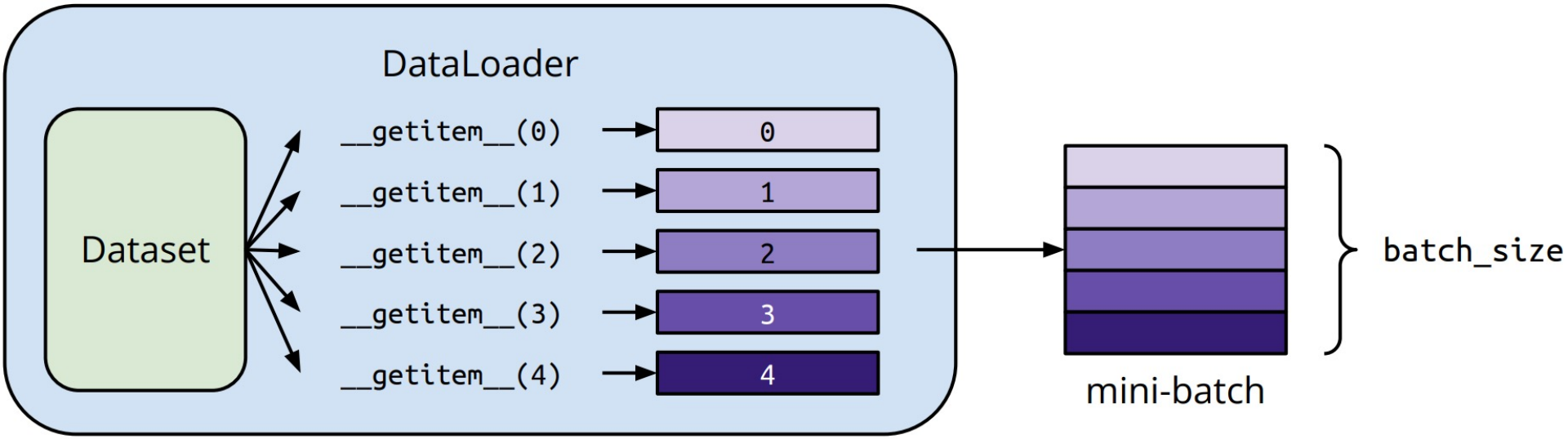
Dataset & Dataloader

```
dataset = MyDataset(file)

dataloader = DataLoader(dataset, batch_size=5, shuffle=False)
```



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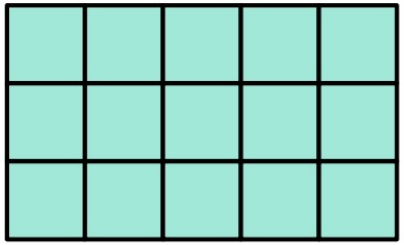
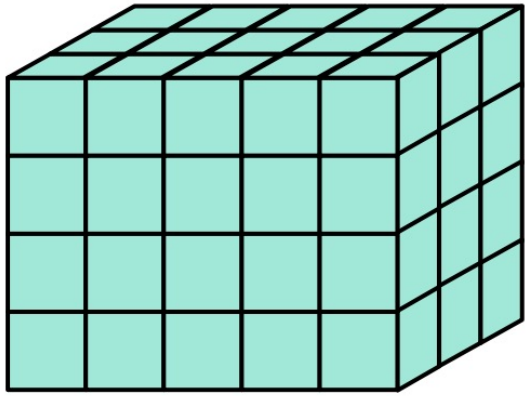
Tensors

- High-dimensional matrices (arrays)

1-D tensor
e.g. audio



2-D tensor
e.g. black&white images



3-D tensor
e.g. RGB images

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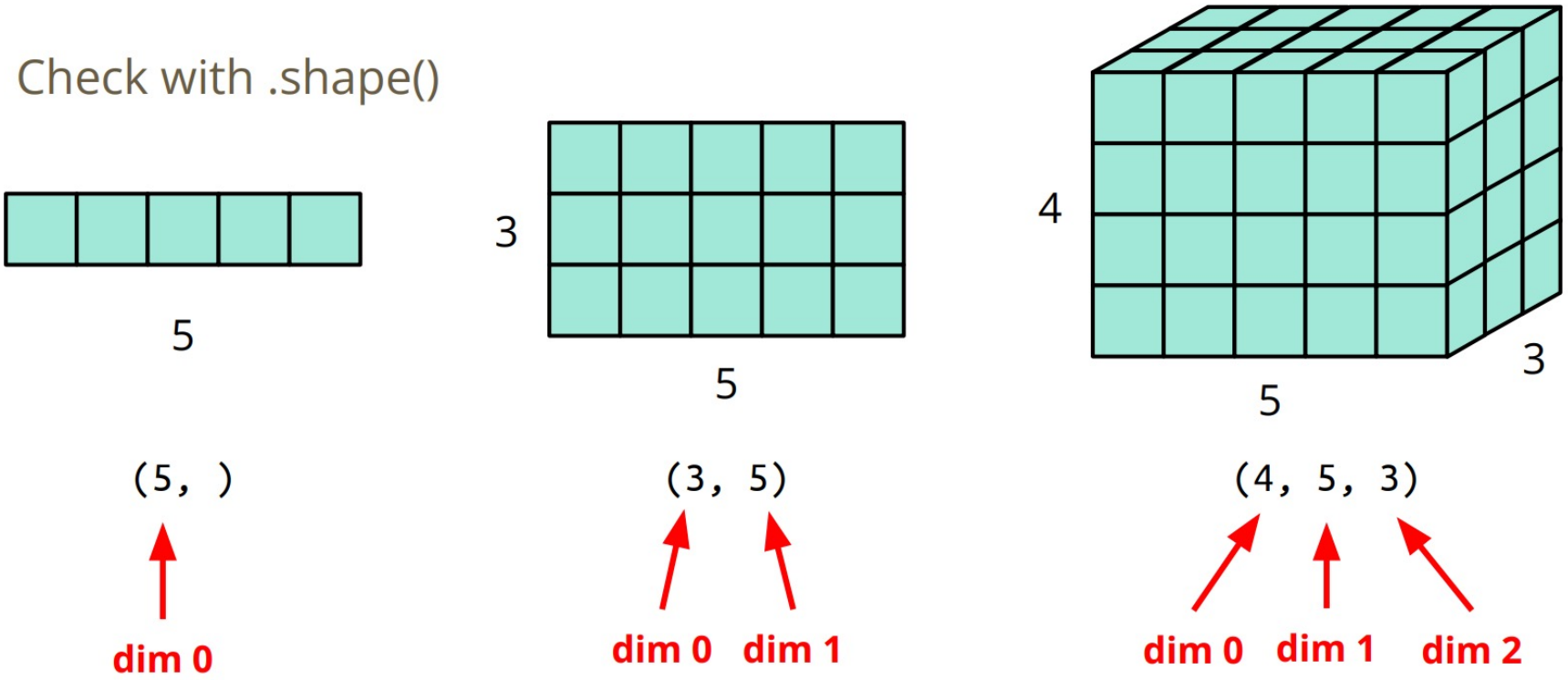
Tensors – Shape of Tensors

- Check with .shape()



Note: `dim` in PyTorch == `axis` in NumPy

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Tensors – Creating Tensors

- Directly from data (list or numpy.ndarray)

```
x = torch.tensor([[1, -1], [-1, 1]])
```

```
tensor([[1., -1.],
        [-1., 1.]])
```

```
x = torch.from_numpy(np.array([[1, -1], [-1, 1]]))
```

- Tensor of constant zeros & ones

```
x = torch.zeros([2, 2])
```

```
tensor([[0., 0.],
        [0., 0.]])
```

```
x = torch.ones([1, 2, 5])
```

shape

```
tensor([[[1., 1., 1., 1., 1.],
         [1., 1., 1., 1., 1.]]])
```

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Tensors – Common Operations

Common arithmetic functions are supported, such as:

- Addition

```
z = x + y
```

- Subtraction

```
z = x - y
```

- Power

```
y = x.pow(2)
```

- Summation

```
y = x.sum()
```

- Mean

```
y = x.mean()
```

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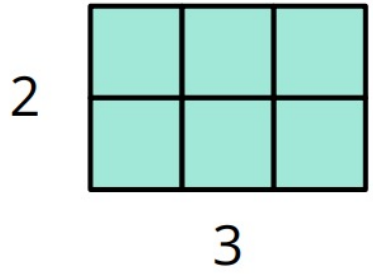
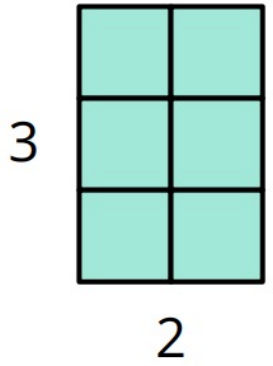
Tensors – Common Operations

- **Transpose**: transpose two specified dimensions

```
>>> x = torch.zeros([2, 3])
>>> x.shape
torch.Size([2, 3])
>>> x = x.transpose(0, 1)
>>> x.shape
torch.Size([3, 2])
```





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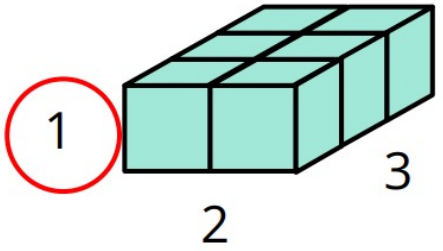
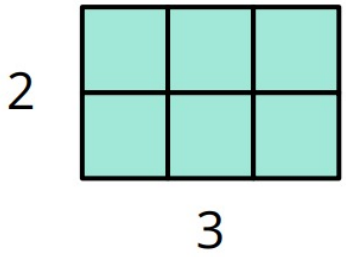
Tensors – Common Operations

- **Squeeze**: remove the specified dimension with length = 1

```
>>> x = torch.zeros([1, 2, 3])
>>> x.shape
torch.Size([1, 2, 3])
>>> x = x.squeeze(0)
>>> x.shape
torch.Size([2, 3])
```

(dim = 0)





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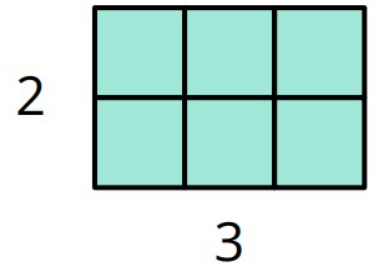
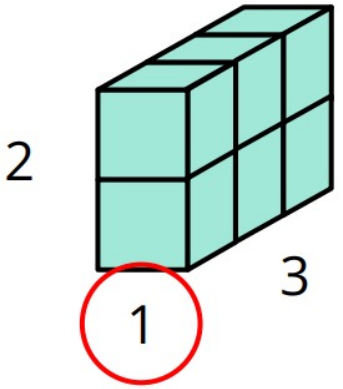
Tensors – Common Operations

- **Unsqueeze**: expand a new dimension

```
>>> x = torch.zeros([2, 3])
>>> x.shape
torch.Size([2, 3])
>>> x = x.unsqueeze(1)
>>> x.shape
torch.Size([2, 1, 3])
```

(dim = 1)





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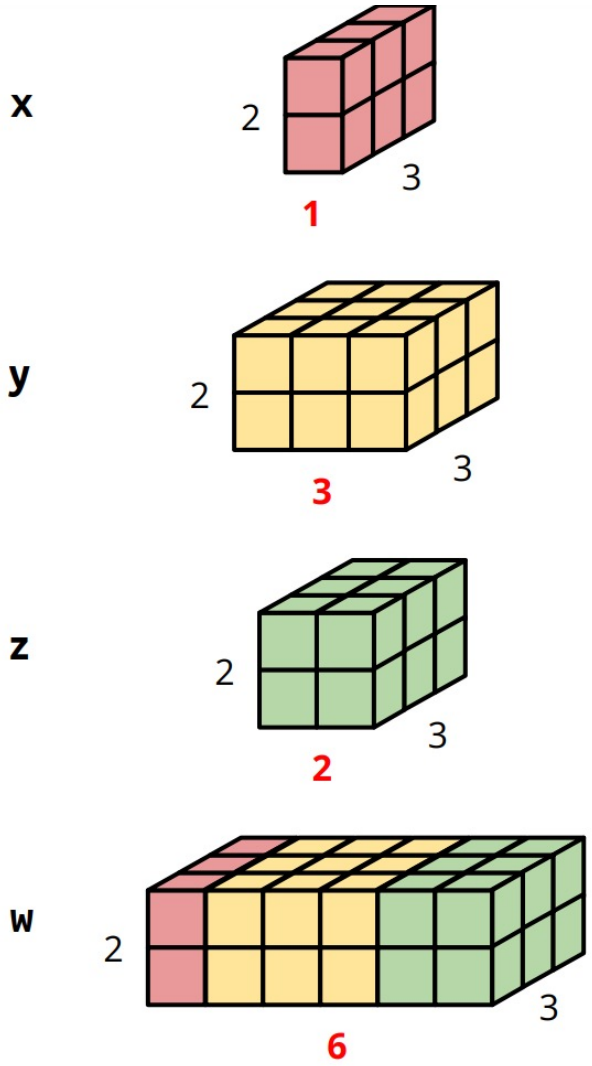
Tensors – Common Operations

- **Cat**: concatenate multiple tensors

```
>>> x = torch.zeros([2, 1, 3])
>>> y = torch.zeros([2, 3, 3])
>>> z = torch.zeros([2, 2, 3])
>>> w = torch.cat([x, y, z], dim=1)
>>> w.shape
torch.Size([2, 6, 3])
```



more operators: https://pytorch.org/docs/stable/tensors.html

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Tensors – Data Type

- Using different data types for model and data will cause errors.

Data type	dtype	tensor
32-bit floating point	`torch.float`	`torch.FloatTensor`
64-bit integer (signed)	`torch.long`	`torch.LongTensor`

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Tensors – PyTorch vs Numpy

- Similar attributes

PyTorch	NumPy
`x.shape`	`x.shape`
`x.dtype`	`x.dtype`

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Tensors – PyTorch vs Numpy

- Many functions have the same names as well

PyTorch	NumPy
`x.reshape / x.view`	`x.reshape`
`x.squeeze()`	`x.squeeze()`
`x.unsqueeze(1)`	`np.expand_dims(x, 1)`

Tensors – Device

- Tensors & modules will be computed with **CPU** by default

  Use **.to()** to move tensors to appropriate devices.

- CPU

```
x = x.to('cpu')
```

- GPU

```
x = x.to('cuda')
```

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Tensors – Device (GPU)

- Check if your computer has NVIDIA GPU

```
torch.cuda.is_available()
```

- Multiple GPUs: specify `'cuda:0'`, `'cuda:1'`, `'cuda:2'`, ...

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Tensors – Gradient Calculation

1
```
>>> x = torch.tensor([[1., 0.], [-1., 1.]], requires_grad=True)
```
2
```
>>> z = x.pow(2).sum()
```
3
```
>>> z.backward()
```
4
```
>>> x.grad
tensor([[ 2.,  0.],
        [-2.,  2.]])
```

1
$$x = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}$$

2
$$z = \sum_i \sum_j x_{i,j}^2$$

3
$$\frac{\partial z}{\partial x_{i,j}} = 2x_{i,j}$$

4
$$\frac{\partial z}{\partial x} = \begin{bmatrix} 2 & 0 \\ -2 & 2 \end{bmatrix}$$

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Tensors – Gradient Calculation

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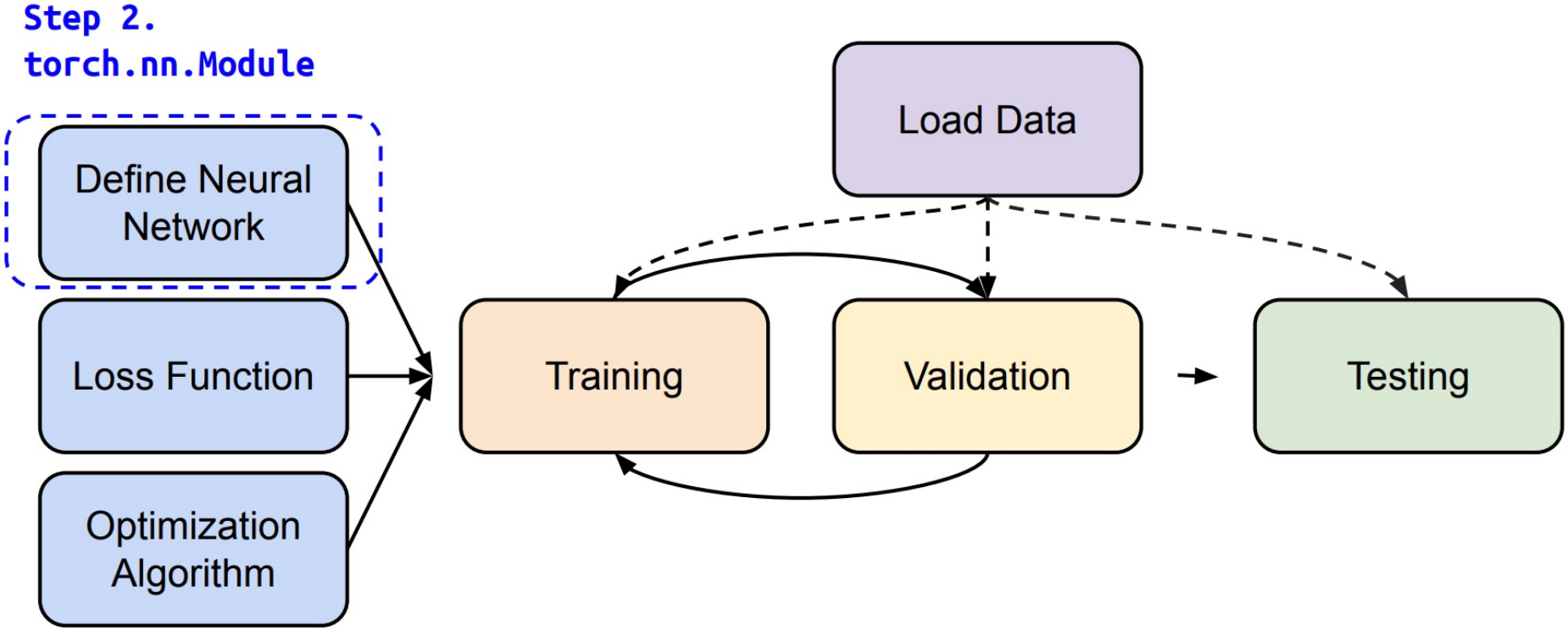
Training & Testing NN in PyTorch



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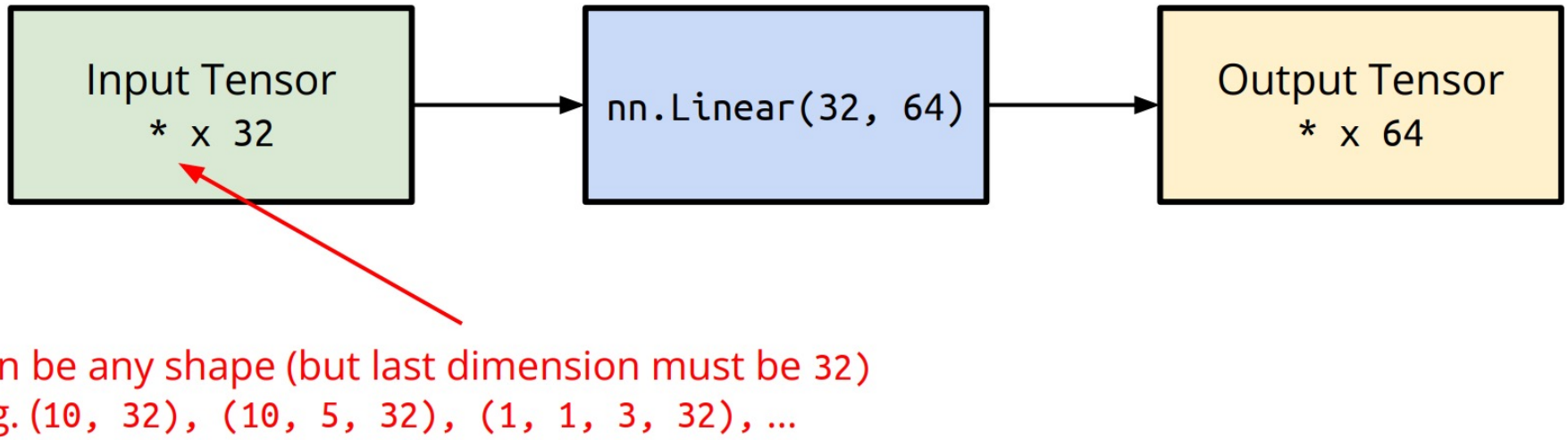
Network Layers

- Linear Layer (**Fully-connected** Layer)

```
nn.Linear(in_features, out_features)
```



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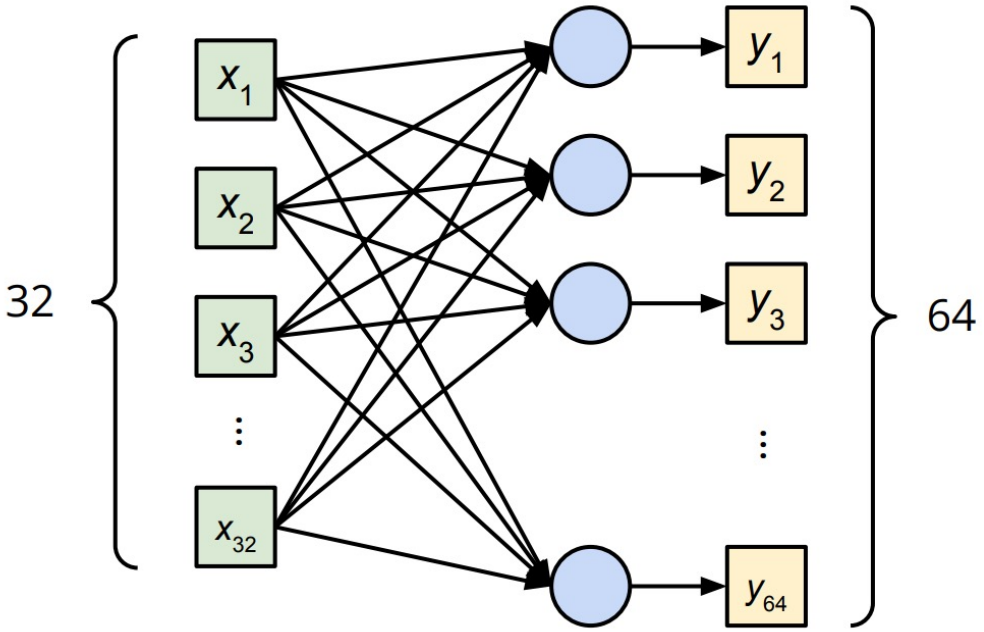
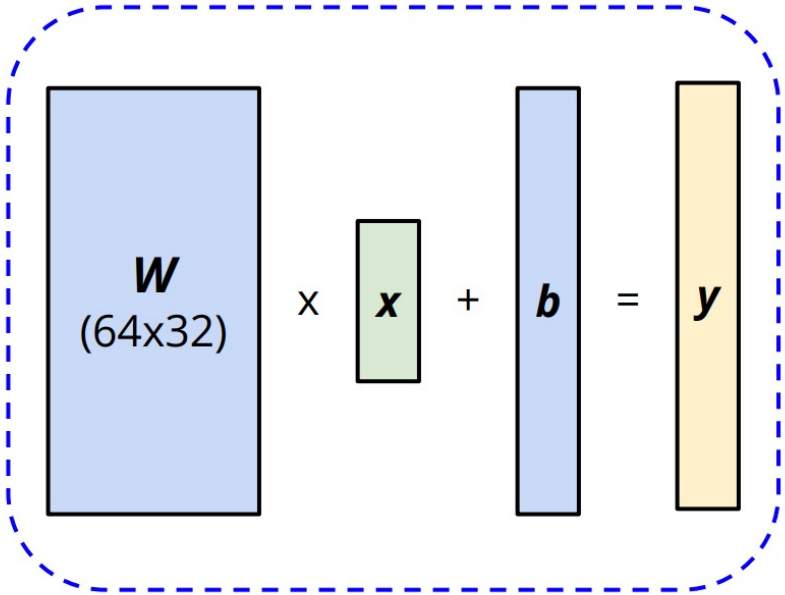
Network Layers

- Linear Layer (**Fully-connected** Layer)





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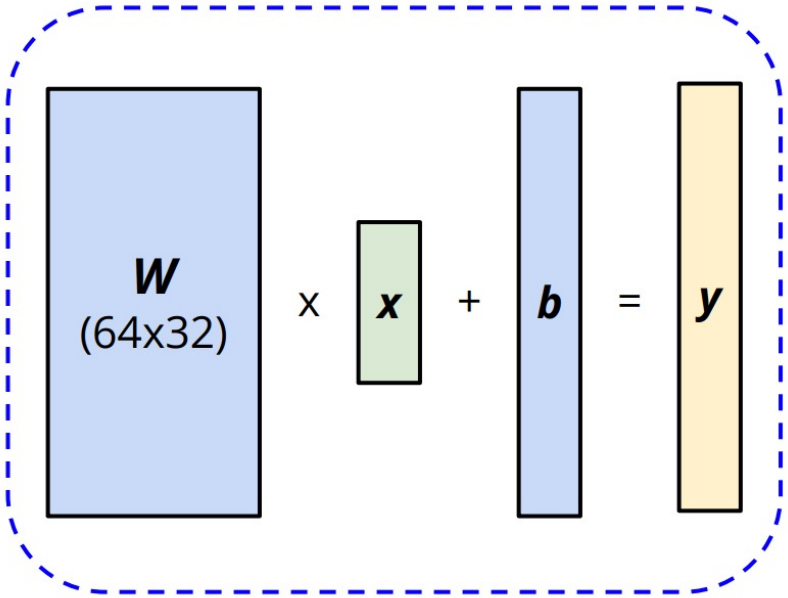
Network Layers

- Linear Layer (**Fully-connected** Layer)

```
>>> layer = torch.nn.Linear(32, 64)
>>> layer.weight.shape
torch.Size([64, 32])
>>> layer.bias.shape
torch.Size([64])
```



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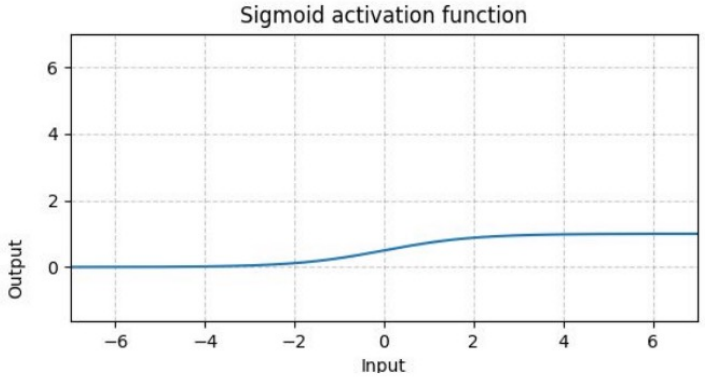
Non-Linear Activation Functions

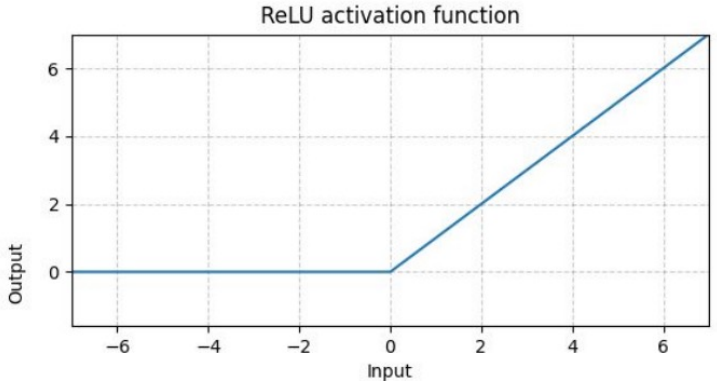
- Sigmoid Activation

```
nn.Sigmoid()
```



- ReLU Activation

```
nn.ReLU()
```



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Build your own NN

```
import torch.nn as nn

class MyModel(nn.Module):
    def __init__(self):
        super(MyModel, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(10, 32),
            nn.Sigmoid(),
            nn.Linear(32, 1)
        )

    def forward(self, x):
        return self.net(x)
```

Initialize your model & define layers

Compute output of your NN

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Build your own NN

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            nn.Sigmoid(),
            nn.Linear(32, 1)
        )

    def forward(self, x):
        return self.net(x)
```

=

```
import torch.nn as nn

class MyModel(nn.Module):
    def __init__(self):
        super(MyModel, self).__init__()
        self.layer1 = nn.Linear(10, 32)
        self.layer2 = nn.Sigmoid(),
        self.layer3 = nn.Linear(32,1)

    def forward(self, x):
        out = self.layer1(x)
        out = self.layer2(out)
        out = self.layer3(out)
        return out
```

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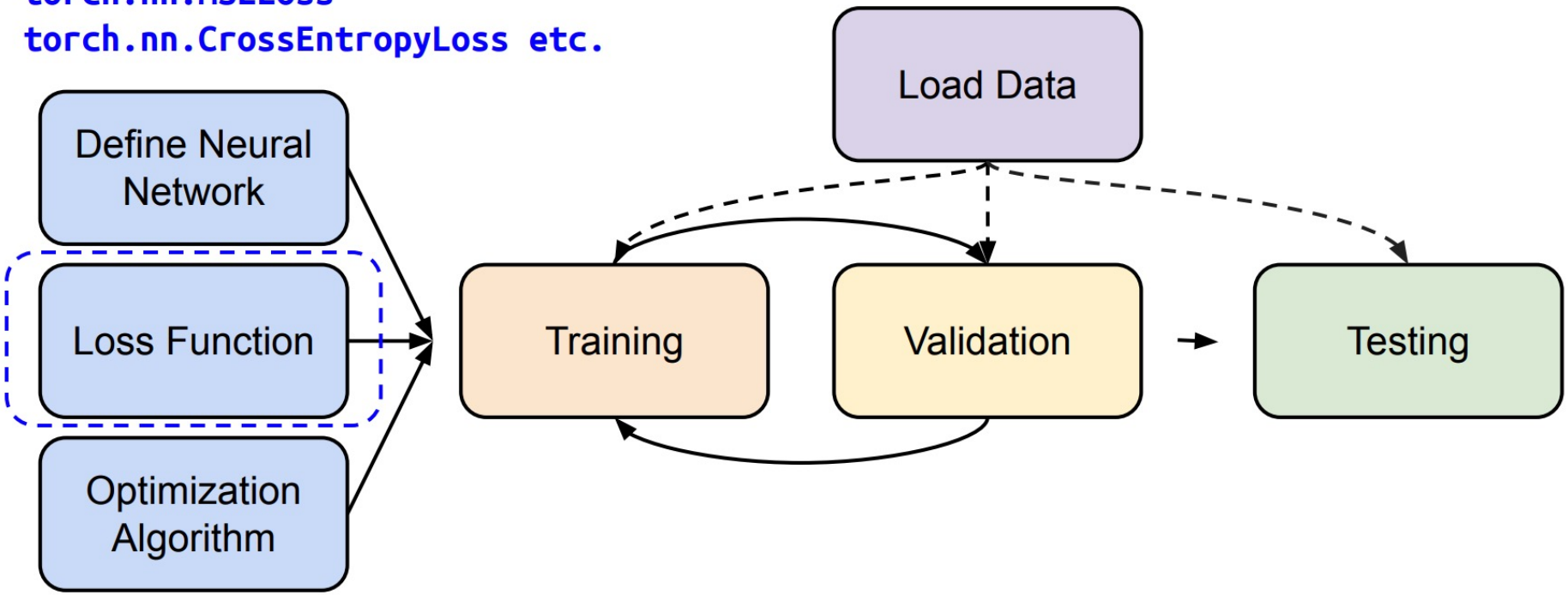
Training & Testing NN in PyTorch

```
Step 3.
torch.nn.MSELoss
torch.nn.CrossEntropyLoss etc.
```



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Loss Functions

- Mean Squared Error (for regression tasks)

```
criterion = nn.MSELoss()
```

- Cross Entropy (for classification tasks)

```
criterion = nn.CrossEntropyLoss()
```

- `loss = criterion(model_output, expected_value)`

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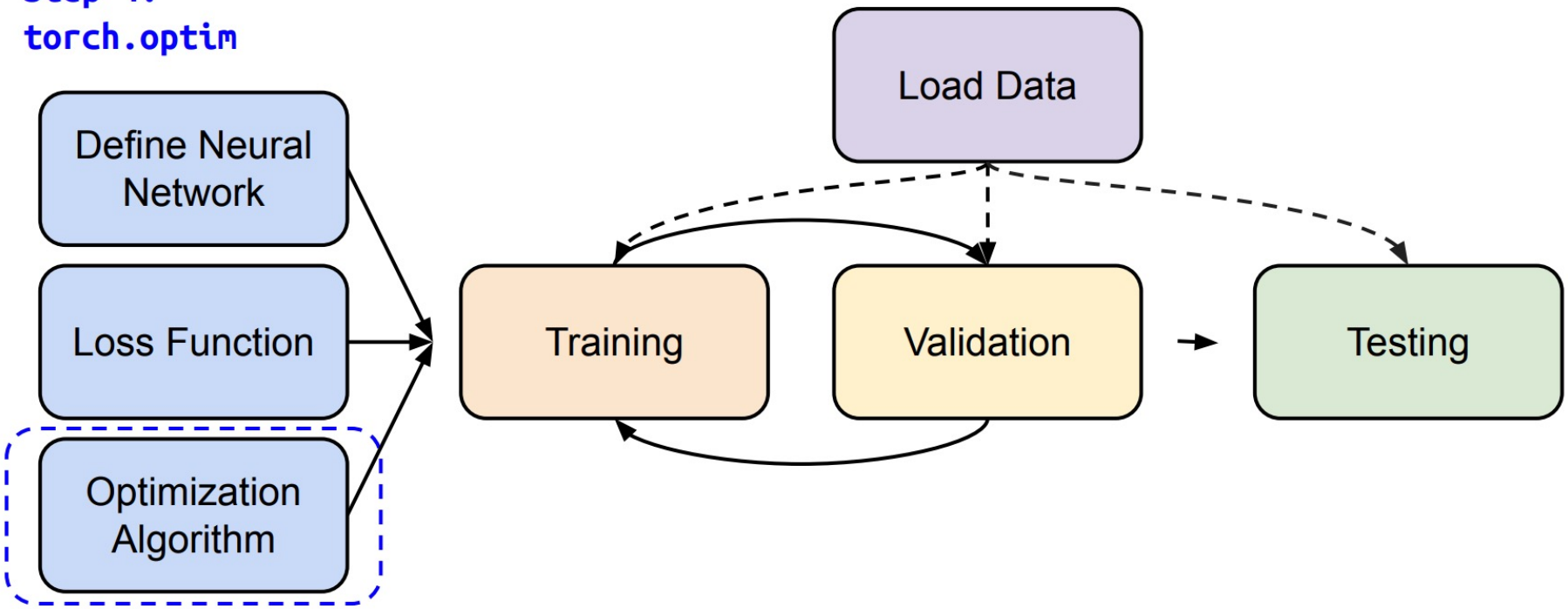
Training & Testing NN in PyTorch

Step 4.
torch.optim



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Optimization

- Gradient-based **optimization algorithms** that adjust network parameters to reduce error.

- E.g. Stochastic Gradient Descent (SGD)

```
torch.optim.SGD(model.parameters(), lr, momentum = 0)
```

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Optimization

```
optimizer = torch.optim.SGD(model.parameters(), lr, momentum = 0)
```

- For every batch of data:
  1. Call `optimizer.zero_grad()` to reset gradients of model parameters.
  2. Call `loss.backward()` to backpropagate gradients of prediction loss.
  3. Call `optimizer.step()` to adjust model parameters.

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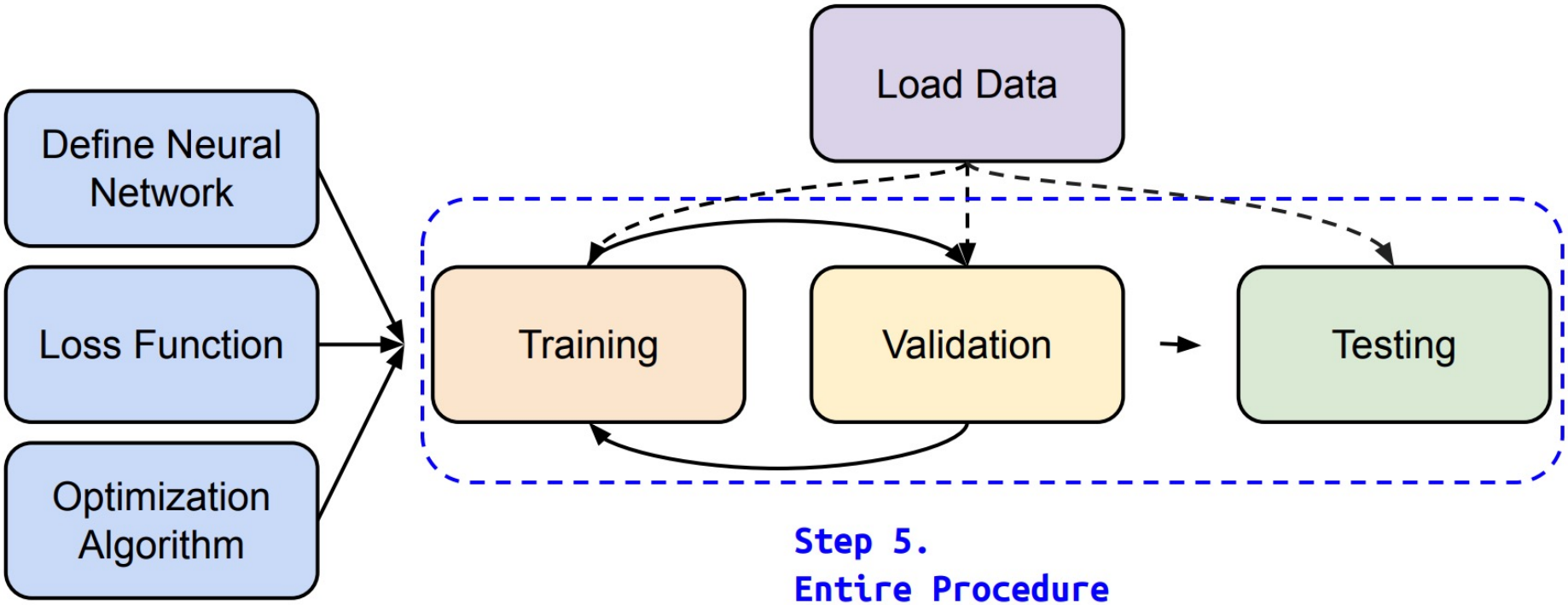
Training & Testing NN in PyTorch



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NN Training Setup

```
dataset = MyDataset(file)                                read data via MyDataset

tr_set = DataLoader(dataset, 16, shuffle=True)           put dataset into Dataloader

model = MyModel().to(device)                             construct model and move to device (cpu/cuda)

criterion = nn.MSELoss()                                 set loss function

optimizer = torch.optim.SGD(model.parameters(), 0.1)     set optimizer
```

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NN Training Loop

```
for epoch in range(n_epochs):                    iterate n_epochs
    model.train()                                set model to train mode
    for x, y in tr_set:                          iterate through the dataloader
        optimizer.zero_grad()                    set gradient to zero
        x, y = x.to(device), y.to(device)        move data to device (cpu/cuda)
        pred = model(x)                          forward pass (compute output)
        loss = criterion(pred, y)                compute loss
        loss.backward()                          compute gradient (backpropagation)
        optimizer.step()                         update model with optimizer
```

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NN Validation Loop

```
model.eval()                                        set model to evaluation mode

total_loss = 0

for x, y in dv_set:                                 iterate through the dataloader

    x, y = x.to(device), y.to(device)               move data to device (cpu/cuda)

    with torch.no_grad():                           disable gradient calculation

        pred = model(x)                             forward pass (compute output)

        loss = criterion(pred, y)                   compute loss

    total_loss += loss.cpu().item() * len(x)        accumulate loss

    avg_loss = total_loss / len(dv_set.dataset)     compute averaged loss
```

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NN Testing Loop

```
model.eval()                                    set model to evaluation mode

preds = []

for x in tt_set:                                iterate through the dataloader

    x = x.to(device)                            move data to device (cpu/cuda)

    with torch.no_grad():                       disable gradient calculation

        pred = model(x)                         forward pass (compute output)

        preds.append(pred.cpu())                collect prediction
```

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- `model.eval()`

  Changes behaviour of some model layers, such as dropout and batch normalization.

- `with torch.no_grad()`

  Prevents calculations from being added into gradient computation graph. Usually used to prevent accidental training on validation/testing data.

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Save/Load Trained Models

- Save

```
torch.save(model.state_dict(), path)
```

- Load

```
ckpt = torch.load(path)
model.load_state_dict(ckpt)
```

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More About PyTorch

- torchaudio
  - speech/audio processing
- torchtext
  - natural language processing
- torchvision
  - computer vision
- skorch
  - scikit-learn + pyTorch

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