



COMP9444: Neural Networks and Deep Learning

Week 2c. PyTorch

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Comparison 1






<https://jamesmccaffrey.wordpress.com/2019/08/22/a-subjective-comparison-of-tensorflow-pytorch-keras-and-scikit-learn/>

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Comparison 2

	Keras 	TensorFlow 	PyTorch 
Level of API	high-level API ¹	Both high & low level APIs	Lower-level API ²
Speed	Slow	High	High
Architecture	Simple, more readable and concise	Not very easy to use	Complex ³
Debugging	No need to debug	Difficult to debugging	Good debugging capabilities
Dataset Compatibility	Slow & Small	Fast speed & large	Fast speed & large datasets
Popularity Rank	1	2	3
Uniqueness	Multiple back-end support	Object Detection Functionality	Flexibility & Short Training Duration
Created By	Not a library on its own	Created by Google	Created by Facebook ⁴
Ease of use	User-friendly	Incomprehensive API	Integrated with Python language
Computational graphs used	Static graphs	Static graphs	Dynamic computation graphs ⁵

<https://medium.com/analytics-vidhya/ml03-9de2f0dbd62d>



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Comparison 3

Aspect	Keras	TensorFlow	PyTorch
Best For	Beginners, rapid prototyping	Production environments, enterprise apps	Research, dynamic models, academic use
Ease of Use	High (Simple and intuitive)	Moderate (Can be complex)	High (Pythonic and intuitive)
Flexibility	Low (Limited control)	High (Full control over architecture)	High (Dynamic graph for flexibility)
Performance	Moderate (High-level abstraction)	High (Optimized for large-scale models)	High (Efficient, especially for research)
Ecosystem	Strong (Through TensorFlow integration)	Very Strong (Production-ready ecosystem)	Growing (Improving deployment features)
Deployment	Moderate (Through TensorFlow)	Excellent (Highly scalable, many options)	Improving (TorchServe, but less mature)
Popularity	High (Part of TensorFlow)	Very High (Widely used in the industry)	Very High (Popular in research)

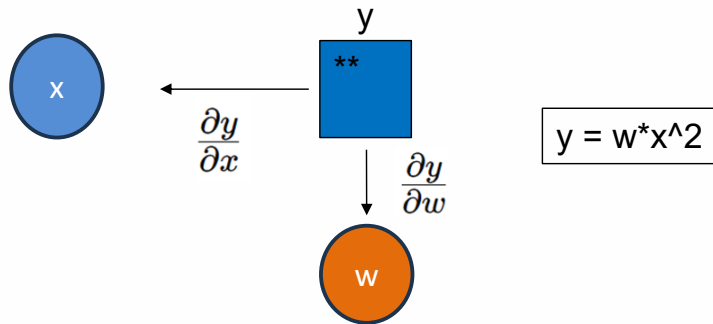
Keras vs. TensorFlow vs. PyTorch
Which ML Framework is Right for You?

https://medium.com/@avijitsur_8327/keras-vs-tensorflow-vs-pytorch-which-ml-framework-is-right-for-you-c44299e79a8b



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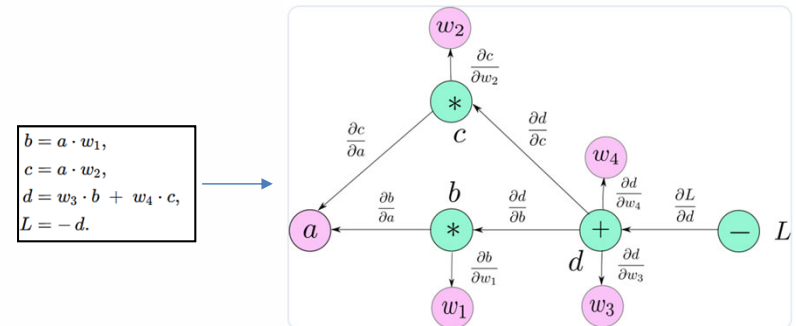
Computational graph and auto-differentiation (COMP9444_demo0_autoDiff)



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Computational graph and auto-differentiation example



<https://www.digitalocean.com/community/tutorials/pytorch-101-understanding-graphs-and-automatic-differentiation>

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Computational Graphs

- PyTorch automatically builds a computational graph, enabling it to backpropagate derivatives.
- Every parameter includes `.data` and `.grad` components, for example:
`A.data`
`A.grad`
- If we need to stop the gradients from being backpropagated through a certain variable (or expression) `A`, we can exclude it from the computational graph by using:

`A.detach()`

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Typical Structure of a PyTorch Program

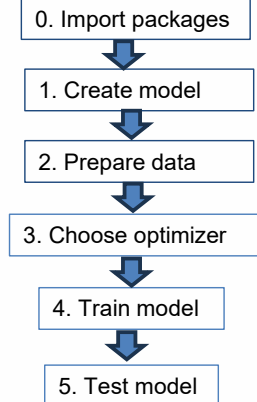
0. Import packages
1. Create model
2. Prepare data
3. Choose optimizer
4. Train model
5. Test model

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Example 1: COMP9444_demo1_simpleLinear

$$y=wx$$

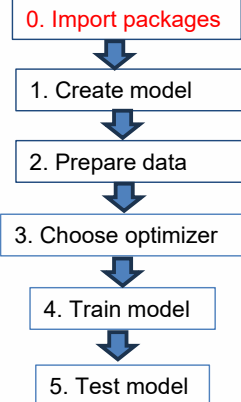


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Example 1: COMP9444_demo1_simpleLinear

$$y=wx$$



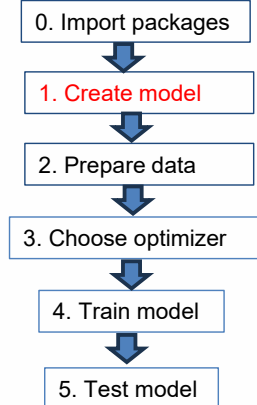
```
# 0. Import packages
import torch
```

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Example 1: COMP9444_demo1_simpleLinear

$$y=wx$$



```
# 1. Create model
class MyModel(torch.nn.Module):
    def __init__(self):
        super(MyModel, self).__init__()
        self.weight = torch.nn.Parameter(torch.zeros(1), requires_grad=True)
    def forward(self, input):
        output = self.weight * input
        return(output)
model = MyModel()
```

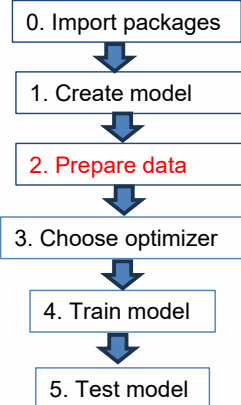
- a) Initializes MyModel when first created (constructor)
- b) Inherits functionality from PyTorch's base model class
- c) Define and initializes the parameter "weight"
- d) Forward pass – Define function on how the model processes input
- e) Output – define the actual processing
- f) Create an instance of MyModel

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Example 1: COMP9444_demo1_simpleLinear

$$y=wx$$



```
# 2. Prepare data
input_train = [[1]]
output_train = [[2.343434]]
# Convert to tensors
input_train_tensor = torch.tensor(input_train, dtype=torch.float32)
output_train_tensor = torch.tensor(output_train, dtype=torch.float32)
# Load training
batch_size=1
train_dataset = torch.utils.data.TensorDataset(input_train_tensor, output_train_tensor)
train_loader = torch.utils.data.DataLoader(train_dataset, batch_size=batch_size)
```

- a) Set input and output data (manually in this case)
- b) Convert to tensors, required as input in later functions
- c) Wraps input and output tensors to form a dataset – allows for easy iteration over (input, output) pairs during training
- d) Create DataLoader object which allows loading of data batches efficiently, iteration over dataset, and others

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Example 1: COMP9444_demo1_simpleLinear

$$y = WX$$

0. Import packages

1. Create model

2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

```
# 3. Choose optimizer
# Neural network parameters
learning_rate = 1.9 # Learning rate

# Optimizer
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)
```

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Choosing an Optimizer

Adadelta	Implements Adadelta algorithm.
Adafactor	Implements Adafactor algorithm.
Adagrad	Implements Adagrad algorithm.
Adam	Implements Adam algorithm.
AdamW	Implements AdamW algorithm.
SparseAdam	SparseAdam implements a masked version of the Adam algorithm suitable for sparse gradients.
Adamax	Implements Adamax algorithm (a variant of Adam based on infinity norm).
ASGD	Implements Averaged Stochastic Gradient Descent.
LBFGS	Implements L-BFGS algorithm.
NAdam	Implements NAdam algorithm.
RAdam	Implements RAdam algorithm.
RMSprop	Implements RMSprop algorithm.
Rprop	Implements the resilient backpropagation algorithm.
SGD	Implements stochastic gradient descent (optionally with momentum).

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<https://pytorch.org/docs/stable/optim.html>



SGD optimizer

```
class torch.optim.SGD(optimizer.Optimizer):
    """Implements stochastic gradient descent (optionally with momentum)."""
    def __init__(self, params, lr=0.01, momentum=0, dampening=0, weight_decay=0,
                 nesterov=False, maximize=False, foreach=None, differentiable=False, fused=None):
        super().__init__(params)
        self.lr = lr
        self.momentum = momentum
        self.dampening = dampening
        self.weight_decay = weight_decay
        self.nesterov = nesterov
        self.maximize = maximize
        self.foreach = foreach
        self.differentiable = differentiable
        self.fused = fused

    def step(self):
        for group in self.param_groups:
            for p in group['params']:
                if p.grad is None:
                    continue
                grad = p.grad.data
                if grad.is_sparse:
                    raise RuntimeError('SGD does not support sparse gradients')
                # Compute weight decay
                if self.weight_decay > 0:
                    grad.add_._(self.weight_decay, p.data)
                # Compute momentum
                if self.momentum == 0:
                    p.data.add_._(-self.lr, grad)
                else:
                    # Compute momentum buffer for "Nesterov" momentum
                    prev_grad = torch.zeros_like(grad)
                    self.set_grad_prev(prev_grad)
                    # Compute the momentum buffer for the first step
                    grad.add_._(self.momentum, grad)
                    # Update the momentum buffer
                    self.set_grad_prev(grad)
                    # Update the parameter
                    p.data.add_._(-self.lr, grad)
```

SGD stands for "Stochastic Gradient Descent"

```
optimizer = torch.optim.SGD(
    net.parameters(), lr=0.01,
    momentum=0.9, weight_decay=0.0001)
```

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Adam optimizer

```
class torch.optim.Adam(optimizer.Optimizer):
    """Implements Adam algorithm."""
    def __init__(self, params, lr=0.001, betas=(0.9, 0.999), eps=1e-08, weight_decay=0,
                 amsgrad=False, foreach=None, maximize=False, differentiable=False, fused=None):
        super().__init__(params)
        self.lr = lr
        self.betas = betas
        self.eps = eps
        self.weight_decay = weight_decay
        self.amsgrad = amsgrad
        self.foreach = foreach
        self.maximize = maximize
        self.differentiable = differentiable
        self.fused = fused

    def step(self):
        for group in self.param_groups:
            for p in group['params']:
                if p.grad is None:
                    continue
                grad = p.grad.data
                if grad.is_sparse:
                    raise RuntimeError('Adam does not support sparse gradients')
                # Compute the Adam step
                state = self.get_state(p)
                if state is None:
                    state = {}
                # Initialize state
                if 'm' not in state:
                    state['m'] = torch.zeros_like(p.data)
                if 'v' not in state:
                    state['v'] = torch.zeros_like(p.data)
                if 'm_sq' not in state:
                    state['m_sq'] = torch.zeros_like(p.data)
                if 'v_sq' not in state:
                    state['v_sq'] = torch.zeros_like(p.data)
                # Compute the Adam step
                m = state['m']
                v = state['v']
                m_sq = state['m_sq']
                v_sq = state['v_sq']
                # Compute the Adam step
                m.add_._(1 - self.betas[0], grad)
                v.add_._(1 - self.betas[1], grad * grad)
                m_sq.add_._(1 - self.betas[0], m * m)
                v_sq.add_._(1 - self.betas[1], v * v)
                # Compute the Adam step
                m_hat = m / (1 - self.betas[0])
                v_hat = v / (1 - self.betas[1])
                # Compute the Adam step
                m_hat_sq = m_hat * m_hat
                v_hat_sq = v_hat * v_hat
                # Compute the Adam step
                m_hat_sq.add_._(self.weight_decay, m_hat_sq)
                # Compute the Adam step
                v_hat_sq.add_._(self.weight_decay, v_hat_sq)
                # Compute the Adam step
                m_hat_sq_sqrt = m_hat_sq.sqrt()
                v_hat_sq_sqrt = v_hat_sq_sqrt.add_._(self.eps, v_hat_sq_sqrt)
                # Compute the Adam step
                step = m_hat / v_hat_sq_sqrt
                # Update the parameter
                p.data.add_._(-self.lr, step * grad)
```

Adam = Adaptive Moment Estimation
(good for deep networks)

```
optimizer = torch.optim.Adam(net.parameters(), eps=
0.000001, lr=0.01,
betas=(0.5, 0.999),
weight_decay=0.0001)
```

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Example 1: COMP9444_demo1_simpleLinear

$$y=wx$$

0. Import packages

1. Create model

2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

```
# 4. Train model
epochs = 100
for epoch in range(1, epochs):
    for batch_id, (data, target) in enumerate(train_loader):
        optimizer.zero_grad() # zero the gradients (a)
        output = model(data) # apply network (some of model.forward(data)) (b)
        loss = 0.5 * torch.mean((output - target) ** 2) # calculate loss (c)
        print('Epoch{:3d}: zero_grad(): weight.data={:7.4f} loss={:7.4f} target={:7.4f} \
              % (epoch, model.weight.data, loss, output, target)) (d)

        loss.backward() # compute gradients (e)
        optimizer.step() # update weights (f)
        print('step(): w.grad={:7.4f} w.data={:7.4f} \
              % (model.weight.grad, model.weight.data))
```

- a) Iterate over epochs. Iterate over each training sample
- b) Zero the gradients because PyTorch accumulates gradients
- c) Forward pass
- d) Calculate loss
- e) Calculate the gradients
- f) Update the weights

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Example 1: COMP9444_demo1_simpleLinear

$$y=wx$$

0. Import packages

1. Create model

2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

```
Epoch 1: zero_grad(): weight.data= 0.0000 loss= 2.7458 output= 0.0000 target= 2.3434
step(): w.grad= -1.3434 w.data= 4.4525
Epoch 2: zero_grad(): weight.data= 4.4525 loss= 2.2241 output= 4.4525 target= 2.3434
step(): w.grad= 2.1891 w.data= 0.4453
Epoch 3: zero_grad(): weight.data= 0.4453 loss= 1.8815 output= 0.4453 target= 2.3434
step(): w.grad= -1.8982 w.data= 4.8518
Epoch 4: zero_grad(): weight.data= 4.8518 loss= 1.5375 output= 4.8518 target= 2.3434
step(): w.grad= 1.5375 w.data= 3.7272
Epoch 5: zero_grad(): weight.data= 0.8859 loss= 1.1820 output= 0.8859 target= 2.3434
step(): w.grad= -1.5375 w.data= 3.7272
Epoch 6: zero_grad(): weight.data= 3.7272 loss= 0.9574 output= 3.7272 target= 2.3434
step(): w.grad= 1.3838 w.data= 1.8980
Epoch 7: zero_grad(): weight.data= 1.8980 loss= 0.7755 output= 1.8980 target= 2.3434
step(): w.grad= -1.2454 w.data= 3.4643
```

```
Epoch 92: zero_grad(): weight.data= 2.3436 loss= 0.0000 output= 2.3436 target= 2.3434
step(): w.grad= 0.0002 w.data= 2.3433
Epoch 93: zero_grad(): weight.data= 2.3433 loss= 0.0000 output= 2.3433 target= 2.3434
step(): w.grad= -0.0001 w.data= 2.3436
Epoch 94: zero_grad(): weight.data= 2.3436 loss= 0.0000 output= 2.3436 target= 2.3434
step(): w.grad= 0.0001 w.data= 2.3433
Epoch 95: zero_grad(): weight.data= 2.3433 loss= 0.0000 output= 2.3433 target= 2.3434
step(): w.grad= -0.0001 w.data= 2.3435
Epoch 96: zero_grad(): weight.data= 2.3435 loss= 0.0000 output= 2.3435 target= 2.3434
step(): w.grad= 0.0001 w.data= 2.3433
Epoch 97: zero_grad(): weight.data= 2.3433 loss= 0.0000 output= 2.3433 target= 2.3434
step(): w.grad= -0.0001 w.data= 2.3435
Epoch 98: zero_grad(): weight.data= 2.3435 loss= 0.0000 output= 2.3435 target= 2.3434
step(): w.grad= 0.0001 w.data= 2.3434
Epoch 99: zero_grad(): weight.data= 2.3434 loss= 0.0000 output= 2.3434 target= 2.3434
step(): w.grad= -0.0001 w.data= 2.3435
```

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Example 2: COMP9444_demo2_LinearMultipleTraining

$$y=wx+b$$

0. Import packages

1. Create model

2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

Add bias term ??

Multiple training samples

Learning rate

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Example 2: COMP9444_demo2_LinearMultipleTraining

Learning rate=1.9

0. Import packages

1. Create model

2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

```
Epoch 1: zero_grad(): weight.data= 0.4528 loss= 0.3615 output= 0.8407 target= 1.7000
step(): w.grad= -2.8059 w.data= 1.7841
Epoch 1: zero_grad(): weight.data= 1.7841 loss= 0.7979 output= -26.4238 target= 2.7600
step(): w.grad= 184.1882 w.data= 352.8214
Epoch 1: zero_grad(): weight.data= 352.8214 loss= 104.0214 output= -1380.1828 target= 2.0000
step(): w.grad= -4802.4001 w.data= 1325.8026
Epoch 1: zero_grad(): weight.data= 1325.8026 loss= 104.0214 output= -78846.9219 target= 3.1000
step(): w.grad= 12367.4488 w.data= 91363.4071
Epoch 1: zero_grad(): weight.data= 91363.4071 loss= 104.0214 output= -692953.0000 target= 1.0000
step(): w.grad= -4023372.0000 w.data= 90077506.0000
Epoch 1: zero_grad(): weight.data= 90077506.0000 loss= 104.0214 output= -39118844.0000 target= 1.5700
step(): w.grad= 1430181814.0000 w.data= 1000187448.0000
Epoch 1: zero_grad(): weight.data= 1000187448.0000 loss= 104.0214 output= -3913410556.0000 target= 3.3600
step(): w.grad= -28451545128.0000 w.data= 15082702848.0000
Epoch 1: zero_grad(): weight.data= 15082702848.0000 loss= 104.0214 output= -354000787512.0000 target= 2.5900
step(): w.grad= 2161818181440.0000 w.data= 405405405440.0000
Epoch 1: zero_grad(): weight.data= 405405405440.0000 loss= 104.0214 output= -354291002006784.0000 target= 2.5000
step(): w.grad= -405405405440.0000 w.data= 405405405440.0000
```

```
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 3.3600
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 2.5900
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 2.5000
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 1.2210
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 2.8270
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 3.4650
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 1.6500
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 2.9000
step(): w.grad= nan w.data= nan
Epoch 99: zero_grad(): weight.data= nan loss= nan output= nan target= 1.3000
step(): w.grad= nan w.data= nan
```

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Example 2: COMP9444_demo2_LinearMultipleTraining

0. Import packages

1. Create model

2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

Learning rate=0.001

```
Epoch 1: zero_grad(): weight.data= 2.4533 loss=68.2164 output=-0.2760 target= 1.7000
step(): w.grad=-16.2288 w.data= 2.4391
Epoch 1: zero_grad(): weight.data= 2.4391 loss=180.8914 output=-11.8065 target= 2.7000
step(): w.grad=-66.8928 w.data= 2.3500
Epoch 1: zero_grad(): weight.data= 2.3500 loss=131.8648 output=-14.3064 target= 2.8000
step(): w.grad=-69.0873 w.data= 2.2500
Epoch 1: zero_grad(): weight.data= 2.2500 loss=109.6374 output=-16.3363 target= 3.1000
step(): w.grad=-121.8212 w.data= 2.1500
Epoch 1: zero_grad(): weight.data= 2.1500 loss=154.9822 output=-15.9873 target= 1.6544
step(): w.grad=-121.9798 w.data= 2.0520
Epoch 1: zero_grad(): weight.data= 2.0520 loss=61.1353 output=-9.4840 target= 1.6544
step(): w.grad=-66.0885 w.data= 1.9600
Epoch 1: zero_grad(): weight.data= 1.9600 loss=288.4530 output=-28.3175 target= 1.3660
step(): w.grad=-225.0080 w.data= 1.7553
Epoch 1: zero_grad(): weight.data= 1.7553 loss=181.4391 output=-11.7873 target= 2.5960
step(): w.grad=-66.9175 w.data= 1.6463
Epoch 1: zero_grad(): weight.data= 1.6463 loss=129.1424 output=-13.5412 target= 2.5300
step(): w.grad=-125.1987 w.data= 1.5244

|

Epoch 99: zero_grad(): weight.data= 0.4349 loss= 0.0763 output= 2.2853 target= 2.5960
step(): w.grad= 2.4354 w.data= 0.4373
Epoch 99: zero_grad(): weight.data= 0.4373 loss= 0.0469 output= 2.8363 target= 2.5300
step(): w.grad= 2.3249 w.data= 0.4358
Epoch 99: zero_grad(): weight.data= 0.4358 loss= 0.2899 output= 0.4596 target= 1.2210
step(): w.grad= 1.6581 w.data= 0.4366
Epoch 99: zero_grad(): weight.data= 0.4366 loss= 0.8275 output= 2.5924 target= 2.8270
step(): w.grad= 1.6522 w.data= 0.4383
Epoch 99: zero_grad(): weight.data= 0.4383 loss= 0.3868 output= 4.2473 target= 3.4650
step(): w.grad= 0.4620 w.data= 0.4298
Epoch 99: zero_grad(): weight.data= 0.4298 loss= 0.8214 output= 1.8880 target= 1.6500
step(): w.grad= 0.8815 w.data= 0.4298
Epoch 99: zero_grad(): weight.data= 0.4298 loss= 0.0018 output= 2.9479 target= 2.9040
step(): w.grad= 0.3514 w.data= 0.4287
Epoch 99: zero_grad(): weight.data= 0.4287 loss= 0.1831 output= 0.8459 target= 1.3800
step(): w.grad= 1.4878 w.data= 0.4393
```

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Example 2: COMP9444_demo2_LinearMultipleTraining

0. Import packages

1. Create model

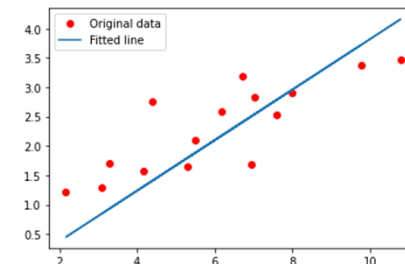
2. Prepare data

3. Choose optimizer

4. Train model

5. Test model

Learning rate=0.001



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Example 3: COMP9444_demo3_LinearExtension

0. Import packages

1. Create model

Run on GPU if available

2. Prepare data

Change batch size (batch)

3. Choose optimizer

Change optimizer to ADAM

4. Train model

Modify output to sum (because batch)

5. Test model

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Example 4: COMP9444_demo4_LinearExtensionTorch

0. Import packages

1. Create model

Use PyTorch predefined linear model

2. Prepare data

3. Choose optimizer

Use PyTorch predefined loss function

4. Train model

5. Test model

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Loss Functions

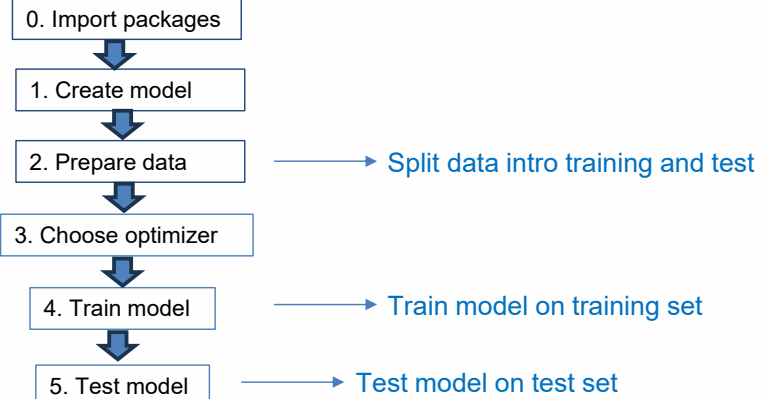
nn.L1Loss	Creates a criterion that measures the mean absolute error (MAE) between each element in the input xx and target yy.
nn.MSELoss	Creates a criterion that measures the mean squared error (squared L2 norm) between each element in the input xx and target yy.
nn.CrossEntropyLoss	This criterion computes the cross entropy loss between input logits and target.
nn.CTCLoss	The Connectionist Temporal Classification loss.
nn.NLLLoss	The negative log likelihood loss.
nn.PoissonNLLLoss	Negative log likelihood loss with Poisson distribution of target.
nn.GaussianNLLLoss	Gaussian negative log likelihood loss.
nn.KLDivLoss	The Kullback-Leibler divergence loss.
nn.BCELoss	Creates a criterion that measures the Binary Cross Entropy between the target and the input probabilities.
nn.BCEWithLogitsLoss	This loss combines a Sigmoid layer and the BCELoss in one single class.
nn.MarginRankingLoss	Creates a criterion that measures the loss given inputs x1x1, x2x2, two 1D mini-batch or 0D Tensors, and a label 1D mini-batch or 0D Tensor yy (containing 1 or -1).
nn.HingeEmbeddingLoss	Measures the loss given an input tensor xx and a labels tensor yy (containing 1 or -1).
nn.MultiLabelMarginLoss	Creates a criterion that optimizes a multi-class multi-label classification hinge loss (margin-based loss) between input xx (a 2D mini-batch Tensor) and output yy (which is a 2D Tensor of target class indices).
nn.HuberLoss	Creates a criterion that uses a squared term if the absolute element-wise error falls below delta and a delta-scaled L1 term otherwise.
nn.SmoothL1Loss	Creates a criterion that uses a squared term if the absolute element-wise error falls below beta and an L1 term otherwise.
nn.SoftMarginLoss	Creates a criterion that optimizes a two-class classification logistic loss between input tensor xx and target tensor yy (containing 1 or -1).
nn.MultiLabelSoftMarginLoss	Creates a criterion that optimizes a multi-label one-versus-all loss based on max-entropy, between input xx and target yy of size (N,C)(N,C).
nn.CosineEmbeddingLoss	Creates a criterion that measures the loss given input tensors x1x1, x2x2 and a Tensor label yy with values 1 or -1.
nn.MultiMarginLoss	Creates a criterion that optimizes a multi-class classification hinge loss (margin-based loss) between input xx (a 2D mini-batch Tensor) and output yy (which is a 1D tensor of target class indices, 0 ≤ y ≤ C-1).
nn.TripleMarginLoss	Creates a criterion that measures the triplet loss given input tensors x1x1, x2x2, x3x3 and a margin with a value greater than 0.0.
nn.TripleMarginWithDistanceLoss	Creates a criterion that measures the triplet loss given input tensors aa, pp, and nn (representing anchor, positive, and negative examples, respectively), and a nonnegative, real-valued function ("distance function") used to compute the relationship between the anchor and positive example ("distance") and between the anchor and negative example ("negative distance").

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<https://pytorch.org/docs/stable/nn.html#loss-functions>



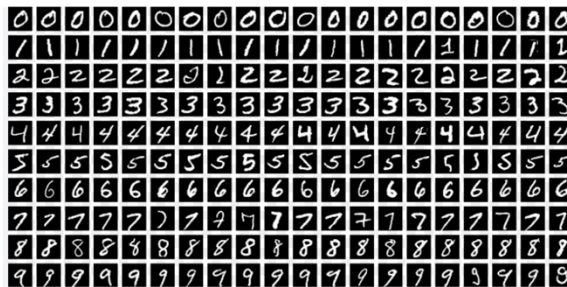
Example 5: COMP9444_demo5_LinearExtensionTest



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Example 6: COMP9444_demo6_NeuralNetwork (Dataset)

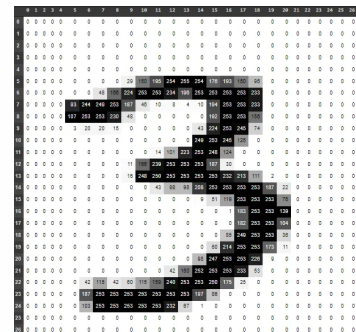


10 classes

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Example 6: COMP9444_demo6_NeuralNetwork (Dataset)

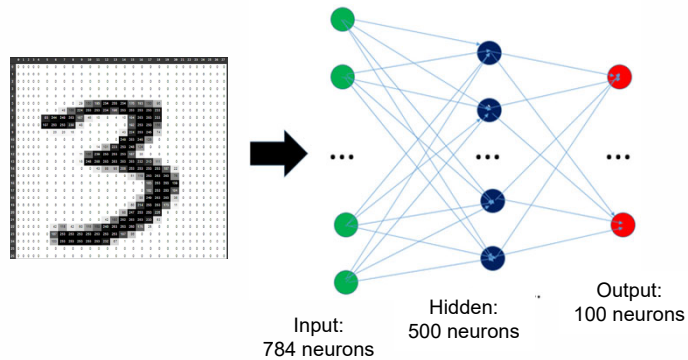


- 28 x 28 = 784 inputs
- Number indicate darkness

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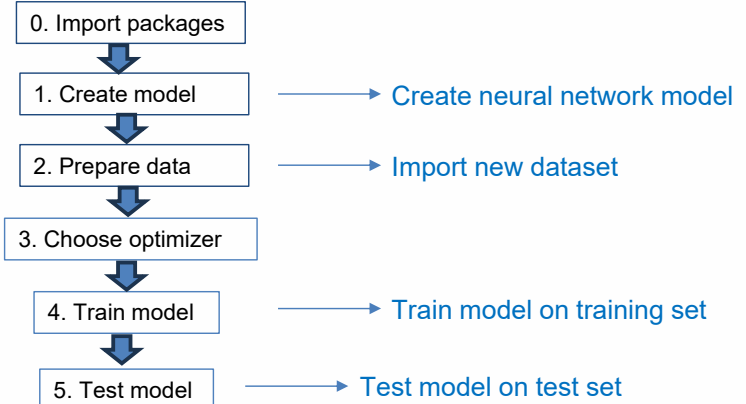
Example 6: COMP9444_demo6_NeuralNetwork (Model)



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Example 6: COMP9444_demo6_NeuralNetwork (Model)



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Sequential Components

Network layers:

- `nn.Linear()`
- `nn.Conv2d()` (Week 4)

Intermediate Operators:

- `nn.Dropout()`
- `nn.BatchNorm()` (Week 4)

Activation Functions:

- `nn.Sigmoid()`
- `nn.Tanh()`
- `nn.ReLU()` (Week 3)

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More on the computational graph

- `optimizer.zero_grad()` sets all `.grad` components to zero.
- `loss.backward()` updates the `.grad` component of all Parameters by backpropagating gradients through the computational graph.
- `optimizer.step()` updates the `.data` components.
- By default, `loss.backward()` discards the computational graph after computing the gradients.
- If needed, we can force it to keep the computational graph by calling it this way:

```
loss.backward(retain_graph=True)
```

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In summary...

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Typical Structure of a PyTorch Program

```
# create neural network
net = MyNetwork().to(device) # CPU or GPU

# prepare to load the training and test data
train_loader = torch.utils.data.DataLoader(...)
test_loader = torch.utils.data.DataLoader(...)

# choose between SGD, Adam or other optimizer
optimizer = torch.optim.SGD(net.parameters,...)

for epoch in range(1, epochs): # training loop
    train(args, net, device, train_loader, optimizer)
    # periodically evaluate network on test data
    if epoch % 10 == 0:
        test( args, net, device, test_loader)
```

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Defining a Network Structure

```
class MyNetwork(torch.nn.Module):

    def __init__(self):
        super(MyNetwork, self).__init__()
        # define structure of the network here

    def forward(self, input):
        # apply network and return output
```

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Declaring Data Explicitly

```
import torch.utils.data

# input and target values for the XOR task
input = torch.Tensor([[0,0],[0,1],[1,0],[1,1]])
target = torch.Tensor([[0],[1],[1],[0]])

xdata = torch.utils.data.TensorDataset(input,target)
train_loader = torch.utils.data.DataLoader(xdata,batch_size=4)
```

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Loading Data from a .CSV File

```
import pandas as pd

df = pd.read_csv("sonar.all-data.csv")
df = df.replace('R',0)
df = df.replace('M',1)
data = torch.tensor(df.values, dtype=torch.float32)
num_input = data.shape[1] - 1
input = data[:,0:num_input]
target = data[:,num_input:num_input+1]
dataset = torch.utils.data.TensorDataset(input, target)
```

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Custom Datasets

```
from data import ImageFolder

# load images from a specified directory
dataset = ImageFolder(folder, transform)

import torchvision.datasets as dsets
# download popular image datasets remotely
mnistset = dsets.MNIST(...)
cifarset = dsets.CIFAR10(...)
celebset = dsets.CelebA(...)
```

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Choosing an Optimizer

```
# SGD stands for "Stochastic Gradient Descent"
optimizer = torch.optim.SGD( net.parameters(),
    lr=0.01, momentum=0.9,
    weight_decay=0.0001)

# Adam = Adaptive Moment Estimation (good for deep networks)
optimizer = torch.optim.Adam(net.parameters(), eps=0.000001,
    lr=0.01, betas=(0.5, 0.999),
    weight_decay=0.0001)
```

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Training

```
def train(args, net, device, train_loader, optimizer):

    for batch_idx, (data, target) in enumerate(train_loader):

        optimizer.zero_grad() # zero the gradients
        output = net(data)     # apply network
        loss = ...             # compute loss function
        loss.backward()        # compute gradients
        optimizer.step()       # update weights
```

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Loss Functions

```
loss = torch.sum((output-target)*(output-target))
loss = F.nll_loss(output,target)           # (Week 3)
loss = F.binary_cross_entropy(output,target) # (Week 3)
loss = F.softmax(output,dim=1)             # (Week 3)
loss = F.log_softmax(output,dim=1)         # (Week 3)
```

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Testing

```
def test(args, net, device, test_loader):

    with torch.no_grad(): # suppress updating of gradients
        net.eval() # toggle batch norm, dropout
        for data, target in test_loader:
            output = model(data)
            test_loss = ...
            print(test_loss)
        net.train() # toggle batch norm, dropout back again
```

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