PyTorch

Tutorial II

Course CS 419

Instructor Prof Abir De

Aditya Pande

[22m2108 @iitb.ac.in]

Ninad Gandhi

[22m2151 @iitb.ac.in]

</ 0. Recap />

Previously Discussed

1. MNIST Dataset
2. Neural Network Architecture
    a. Activations
    b. Mathematical Form
    c. Probability and Logits

Previously Discussed: Activations

$\underline{Sigmoid}$

$$\sigma(x) = \frac{1}{1 + e^{-(x)}}$$

$\underline{Tanh}$

$$\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$\underline{ReLU}$

$$\sigma(x) = max(x, 0)$$

$\underline{LeakyReLU}$

$$\sigma(x) = max(0.1x, x)$$

[Visualization]

Previously Discussed: Mathematical Form

$$y_i = f(x_i)$$

$$y_i = W_1^T \cdot x_i + b_1$$

$$h_1 = \sigma_1(W_1^T \cdot x_i + b_1)$$

$$h_2 = \sigma_2(W_2^T \cdot (h_1) + b_2)$$

$$\vdots$$

$$h_l = \sigma_l(W_l^T \cdot (h_{l-1}) + b_l)$$

$$logits = W_{out}^T \cdot (h_l) + b_{out}$$

Next in line…

1. Tensors
2. Datasets and Dataloaders
3. Batching
4. Model Architecture
5. Forward Pass
6. Optimizer
7. Loss Objective
8. Device: GPU v CPU
9. Train Trajectory
10. Early Stopping
11. Reproducibility

</ 1. Tensors />

Tensor: What is a tensor?

A torch tensor is a multi-dimensional array used for data and computations in PyTorch

```python
import torch

# Create a tensor
x = torch.tensor([1.0, 2.0, 3.0])

# Print the tensor
print("Tensor x:", x)

# Perform basic operations
y = x + 2.0          # Addition
z = x * 3.0          # Multiplication

# Print results
print("x + 2:", y)   # Output: tensor([3.0, 4.0, 5.0])
print("x * 3:", z)   # Output: tensor([3.0, 6.0, 9.0])
```

</ TENSOR : go in BATCHES />

Always use BATCHES !!!!!!!!!

- Groups of data samples processed together
- Batch processing speeds up training and improves efficiency by enabling parallel computation and reducing memory usage

```
any_data_tensor .shape == [batch_size, .,
.]
```

</ TENSOR : Attributes : .shape />

How to access attribute ?

An attribute in is a characteristic or of that tensor

An attribute can be accessed with .

```python
import torch

# Create a larger tensor
tensor = torch.randn(10, 20, 30)  # A tensor with shape (10, 20, 30)

# Print the shape of the tensor
print("Shape of the tensor:", tensor.shape)
```

</ Dataloader />

- handles batching, shuffling, and loading data efficiently for training and evaluation

- It works with a Dataset to streamline data handling during model training

```python
import torch
from torch.utils.data import DataLoader, TensorDataset

# Generate random data
num_samples = 1000
num_features = 20
# Random features
X = torch.randn(num_samples, num_features)
 # Random 10-ary labels
y = torch.randint(0, 10, (num_samples,))

# Create a TensorDataset from the random data
dataset = TensorDataset(X, y)

# Create DataLoader
batch_size = 64
data_loader = DataLoader(dataset, batch_size=batch_size,
                         shuffle=True, num_workers=2)
```

Tensor: Methods

- transpose(T)
- squeeze
- unsqueeze
- size
- log, log10, log2, …
- mean, median, mode, std
- nelement, element_size
- dtype: fp16, fp32, fp64
- relu, sigmoid, tanh, softmax
- Topk, sort, sum

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- relu, sigmoid, tanh, softmax
- Topk, sort, sum
- flatten, reshape
- view
- max, min
- logsumexp
- ndim
- norm
- Permute
- multinomial, random
- requires_grad

Tensor: Methods (more)

- abs
- abs_
- absolute
- absolute_
- acos
- acos_
- acosh
- acosh_
- add
- add_
- addbmm
- addbmm_
- addcdiv
- addcdiv_
- addcmul
- addcmul_
- addmm
- addmm_
- addmv
- addmv_
- addr
- addr_
- adjoint
- align_as
- align_to
- all
- allclose
- amax
- amin
- aminmax
- angle
- any
- apply_
- arccos
- arccos_
- arccosh
- arccosh_
- arcsin
- arcsin_
- arcsinh
- arcsinh_
- arctan
- arctan2
- arctan2_
- arctan_
- arctanh
- arctanh_
- argmax
- argmin
- argsort
- argwhere
- as_strided
- as_strided_
- as_strided_scatter
- as_subclass
- asin
- asin_
- asinh
- asinh_
- atan
- atan2
- atan2_
- atan_
- atanh
- atanh_
- backward
- baddbmm
- baddbmm_
- bernoulli
- bernoulli_
- bfloat16
- bincount
- bitwise_and
- bitwise_and_
- bitwise_left_shift
- bitwise_left_shift_
- bitwise_not
- bitwise_not_
- bitwise_or
- bitwise_or_
- bitwise_right_shift
- bitwise_right_shift_
- bitwise_xor
- bitwise_xor_
- bmm
- bool
- broadcast_to
- byte
- cauchy_
- ccol_indices
- double
- ceil
- ceil_
- cfloat
- chalf
- char
- cholesky
- cholesky_inverse
- cholesky_solve
- chunk
- clamp
- clamp_
- clamp_max
- lamp_max_
- clamp_min
- clamp_min_
- clip
- clip_
- clone
- coalesce
- col_indices
- conj
- conj_physical
- conj_physical_
- contiguous
- copy_
- copysign
- copysign_
- corrcoef
- cos
- cos_
- cosh
- cosh_
- count_nonzero
- cov
- cpu
- cross
- crow_indices
- cuda
- cummax
- cummin
- cumprod
- cumprod_
- cumsum
- cumsum_
- data
- data_ptr
- deg2rad
- deg2rad_
- dense_dim
- dequantize
- det
- detach
- detach_
- device
- diag
- diag_embed
- diagflat
- diagonal
- diagonal_scatter
- diff
- digamma
- digamma_
- dim
- dim_order
- dist
- div
- div_
- divide
- divide_
- dot
- double
- dsplit
- dtype
- eig
- element_size
- eq
- eq_
- equal
- erf
- erf_
- erfc
- erfc_
- erfinv
- erfinv_
- exp
- exp2
- exp2_
- exp_
- expand
- expand_as
- expm1
- expm1_
- exponential_
- fill_
- fill_diagonal_
- fix
- fix_
- flatten
- flip
- fliplr
- flipud
- float
- float_power
- float_power_
- floor
- floor_
- floor_divide
- floor_divide_
- fmax
- fmin
- fmod
- fmod_
- frac
- frac_
- frexp
- gather
- gcd
- gcd_
- ge
- ge_
- geometric_
- geqrf
- ger
- get_device
- grad
- grad_fn
- greater
- greater_
- greater_equal
- greater_equal_
- gt
- gt_
- half
- hardshrink
- has_names
- heaviside
- heaviside_
- histc
- histogram
- hsplit
- hypot
- hypot_
- i0
- i0_
- igamma
- igamma_
- igammac
- igammac_
- imag
- index_add
- index_add_
- index_copy
- index_copy_
- index_fill
- index_fill_
- index_put
- index_put_
- index_reduce
- index_reduce_
- index_select
- indices
- inner
- int
- int_repr
- inverse
- ipu
- is_coalesced
- is_complex
- s_conj
- is_contiguous
- is_cpu
- is_cuda
- is_distributed
- is_floating_point
- is_inference
- is_ipu
- is_leaf
- is_maia
- is_meta
- is_mkldnn
- is_mps
- is_mtia
- is_neg
- is_nested
- is_nonzero
- is_pinned
- is_quantized
- is_same_size
- is_set_to
- is_shared
- is_signed
- is_sparse
- is_sparse_csr
- is_vulkan
- is_xla
- is_xpu
- isclose…

</ 2. Dataset and Dataloaders />

Built-in Datasets

Torchvision: (https://pytorch.org/vision/stable/datasets.html)

- MNIST
- CIFAR-10
- CIFAR-100
- ImageNet

Torchaudio: (https://pytorch.org/audio/stable/datasets.html)

- VoxCeleb1Identification
- CMUARCTIC

</ MNIST : dataset example />

```python
# 1. Data Loading and Preprocessing
transform = transforms.Compose([
    transforms.ToTensor(),  # Convert image to tensor
    transforms.Normalize((0.5,), (0.5,))  # Normalize data
])

# Download and load training data
trainset = torchvision.datasets.MNIST(root='./data', train=True, download=True, transform=transform)
trainloader = torch.utils.data.DataLoader(trainset, batch_size=64, shuffle=True, num_workers=2)

# Download and load test data
testset = torchvision.datasets.MNIST(root='./data', train=False, download=True, transform=transform)
testloader = torch.utils.data.DataLoader(testset, batch_size=64, shuffle=False, num_workers=2)
```

Custom Dataset

Object type: torch.utils.data.Dataset

Implement 3 methods:

1. __init__()
2. __len__()
3. __getitem__()

```python
class CustomDataset(torch.utils.data.Dataset):
    def __init__(self, data, labels):
        self.data = data
        self.labels = labels

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

    def __getitem__(self, idx):
        return self.data[idx], self.labels[idx]
```

Dataloaders

- The DataLoader class in PyTorch handles *batching*, *shuffling*, and *parallel* data loading using multiple workers.

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- The DataLoader class in PyTorch handles *batching*, *shuffling*, and *parallel* data loading using multiple workers.
- Dataloader wraps around the Dataset object.
- You must split the dataset into train test and val before using the dataloader.

</ MNIST : dataloader example />

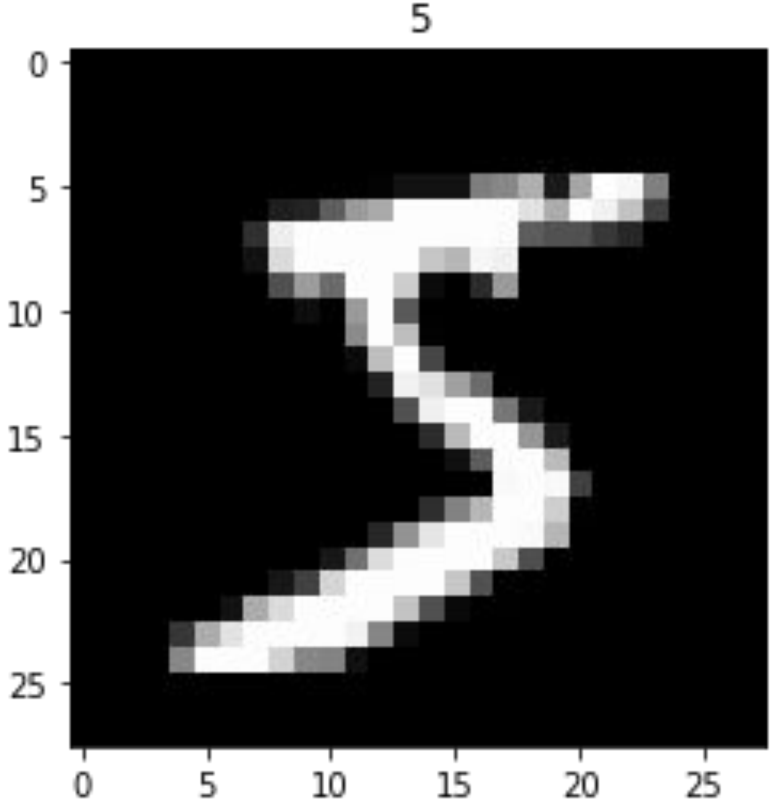
- handles batching, shuffling, and loading data efficiently for training and evaluation

- It works with a Dataset to streamline data handling during model training

```python
import torch
from torch.utils.data import DataLoader, TensorDataset

# Generate random data
num_samples = 1000
num_features = 20
# Random features
X = torch.randn(num_samples, num_features)
 # Random 10-ary labels
y = torch.randint(0, 10, (num_samples,))

# Create a TensorDataset from the random data
dataset = TensorDataset(X, y)

# Create DataLoader
batch_size = 64
data_loader = DataLoader(dataset, batch_size=batch_size,
                         shuffle=True, num_workers=2)
```

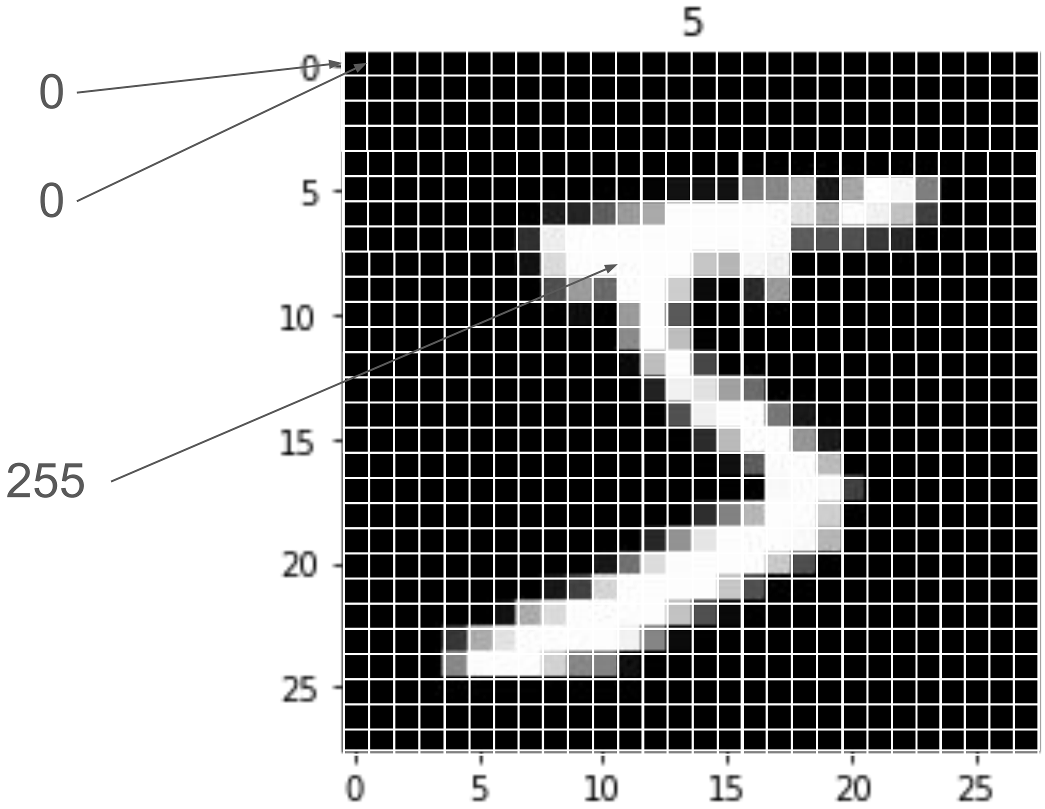
</ 3. Batching />

Batching: One Example

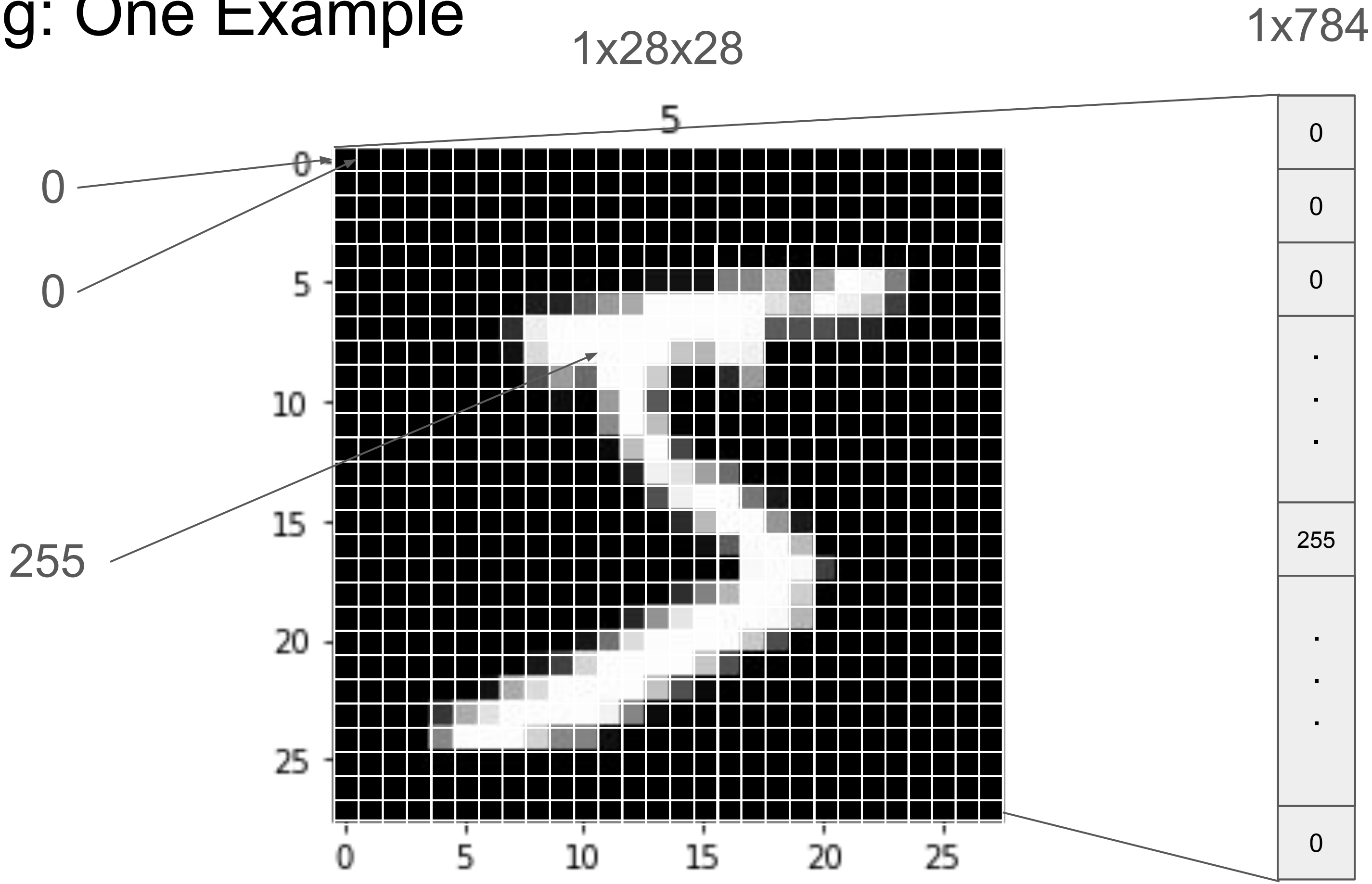


Batching: One Example

1x28x28



Batching: One Example



Batching: Sending multiple examples

0	0	0	0	117	0		0	0
0	0	0	0	140	0		0	0
0	120	0	50	20	0		0	0
. . .	. . .	. . .	. . .	. . .	. . .		. . .	. . .
255	255	200	0	255	255	• • •	255	255
. . .	. . .	. . .	. . .	. . .	. . .		. . .	. . .
0	0	0	0	0	0		0	0

Bx784

</ 4. Model Architecture />

Architecture: Mathematical Form

$$h_1 = \sigma_1(W_1^T \cdot x_i + b_1)$$

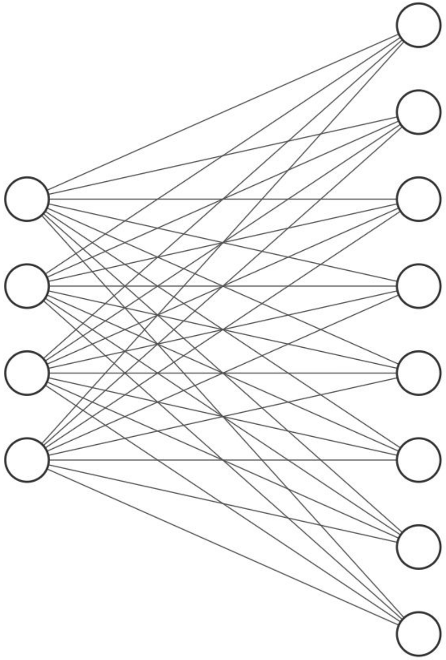
$$h_2 = \sigma_2(W_2^T \cdot (h_1) + b_2)$$

$$\vdots$$

$$h_l = \sigma_l(W_l^T \cdot (h_{l-1}) + b_l)$$

$$logits = W_{out}^T \cdot (h_l) + b_{out}$$

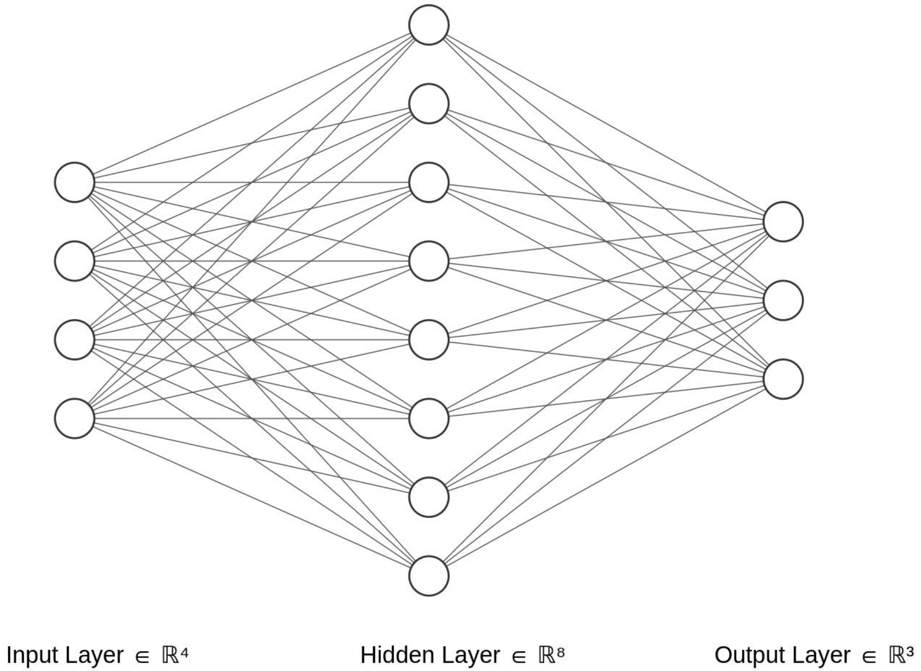
</ Building Block : nn.Linear(in_dim, out_dim) />



Input Layer $\in \mathbb{R}^4$ Output Layer $\in \mathbb{R}^8$

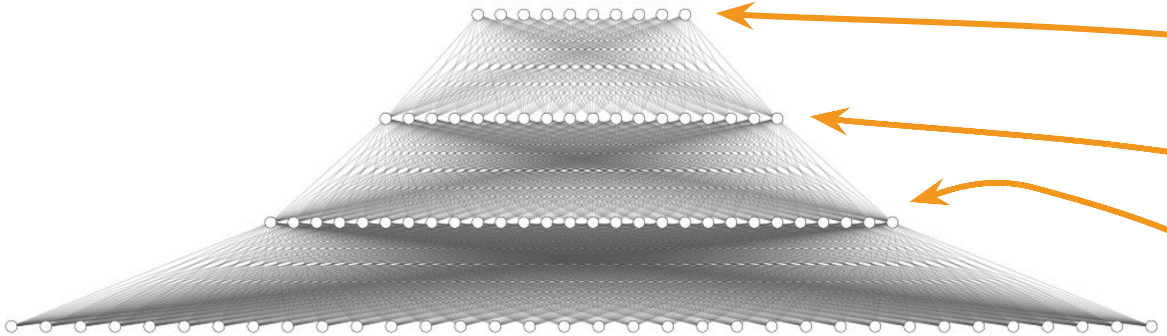
```python
layer = nn.Linear(4, 8)
out = layer(x)
```

</ Building Block : Linear & Activations />




```
layer1 = nn.Linear(4, 8)
layer2 = nn.Linear(8, 3)
out = layer(x)
out = torch.relu(out)
out = torch.relu(out)
```

</ Building Block : OUR MODEL />



```
self.fc1 = nn.Linear(28*28, 128)
self.fc2 = nn.Linear(128, 64)
self.fc3 = nn.Linear(64,  10)
```

</ 5. Forward Method />

</ .forward() />

```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.fc1 = nn.Linear(28*28, 128)
        self.fc2 = nn.Linear(128, 64)
        self.fc3 = nn.Linear(64,  10)

    def forward(self, x):
        x = x.view(-1, 28*28)

        h1 = torch.relu(self.fc1(x))
        h2 = torch.relu(self.fc2(h1))
        # ...
        h3 = self.fc3(h2)

        return x
```

$$h_1 = \sigma_1(W_1^T \cdot x_i + b_1)$$

$$h_2 = \sigma_2(W_2^T \cdot (h_1) + b_2)$$

$$\vdots$$

$$h_l = \sigma_l(W_l^T \cdot (h_{l-1}) + b_l)$$

$$logits = W_{out}^T \cdot (h_l) + b_{out}$$

</ 6. Loss Objective />

</ Loss : Cross Entropy />

For K-class classification using the softmax function, the cross-entropy loss $J(\theta)$ is given by:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} y_k^{(i)} \log \left(h_\theta(x^{(i)})_k \right)$$

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

Where:

- m is the number of training examples.
- K is the number of classes.
- $y_k^{(i)}$ is a binary indicator (0 or 1) that represents whether the class label k is the correct classification for the i-th example.
- $h_\theta(x^{(i)})_k$ is the predicted probability of the i-th example belonging to class k, given by the softmax function:

$$h_\theta(x^{(i)})_k = \frac{\exp(\theta_k^T x^{(i)})}{\sum_{j=1}^{K} \exp(\theta_j^T x^{(i)})}$$

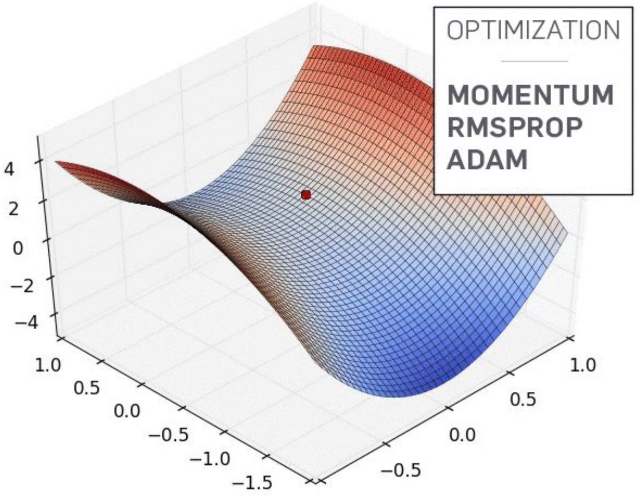
</ Loss : Gradient Descent />

$$\theta^{(t+1)} = \theta^{(t)} - \alpha \nabla_\theta J(\theta)$$

```
loss.backward()
```

</ 7. Optimizer />

Various Optimizers




```python
optimizer = optim.Adam(model.parameters(), lr=3e-4)
```

https://blog.paperspace.com/intro-to-optimization-momentum-rmsprop-adam/

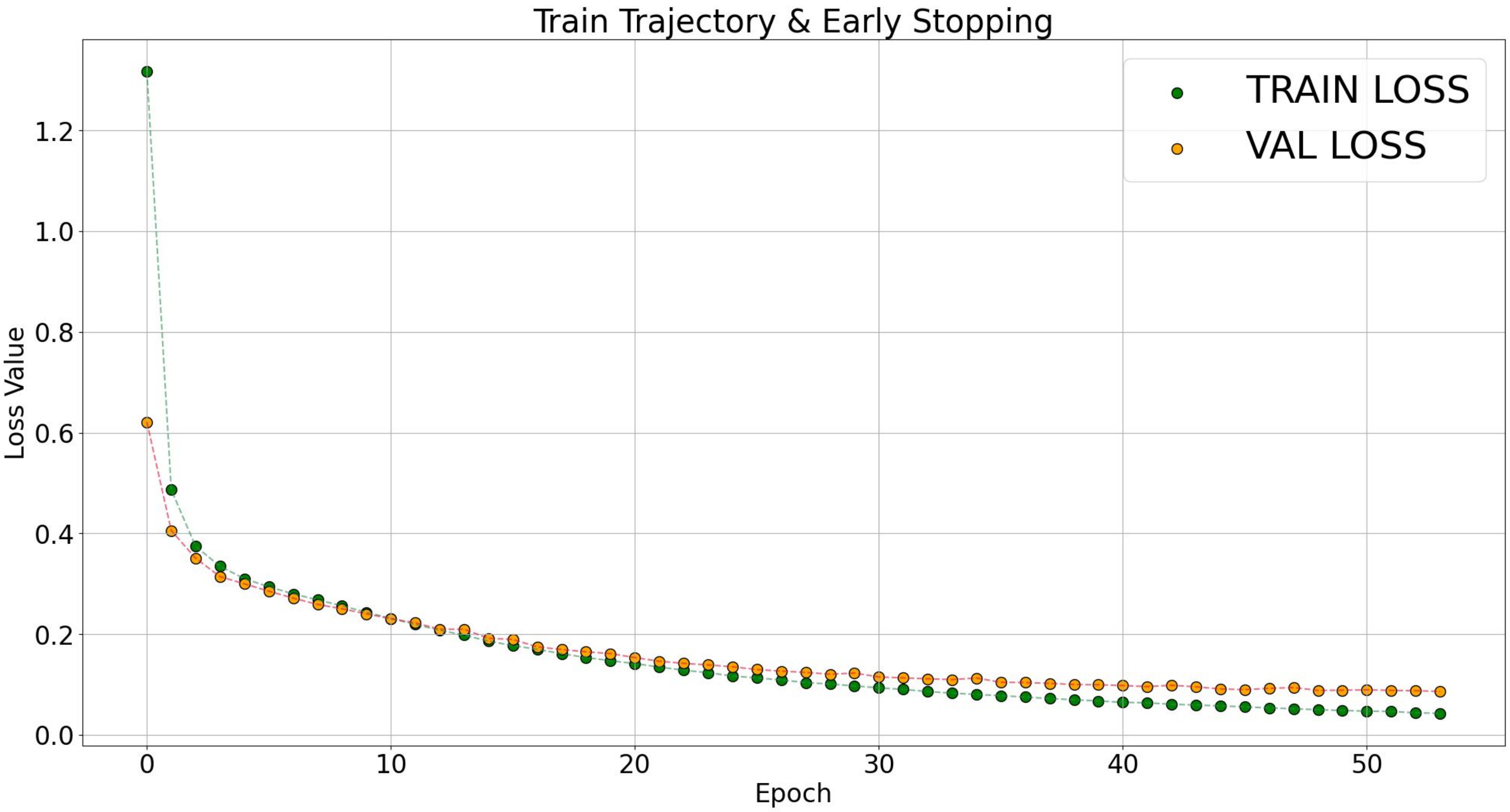
</ Loss : Gradient Descent />

$$\theta^{(t+1)} = \theta^{(t)} - \alpha \nabla_\theta J(\theta)$$

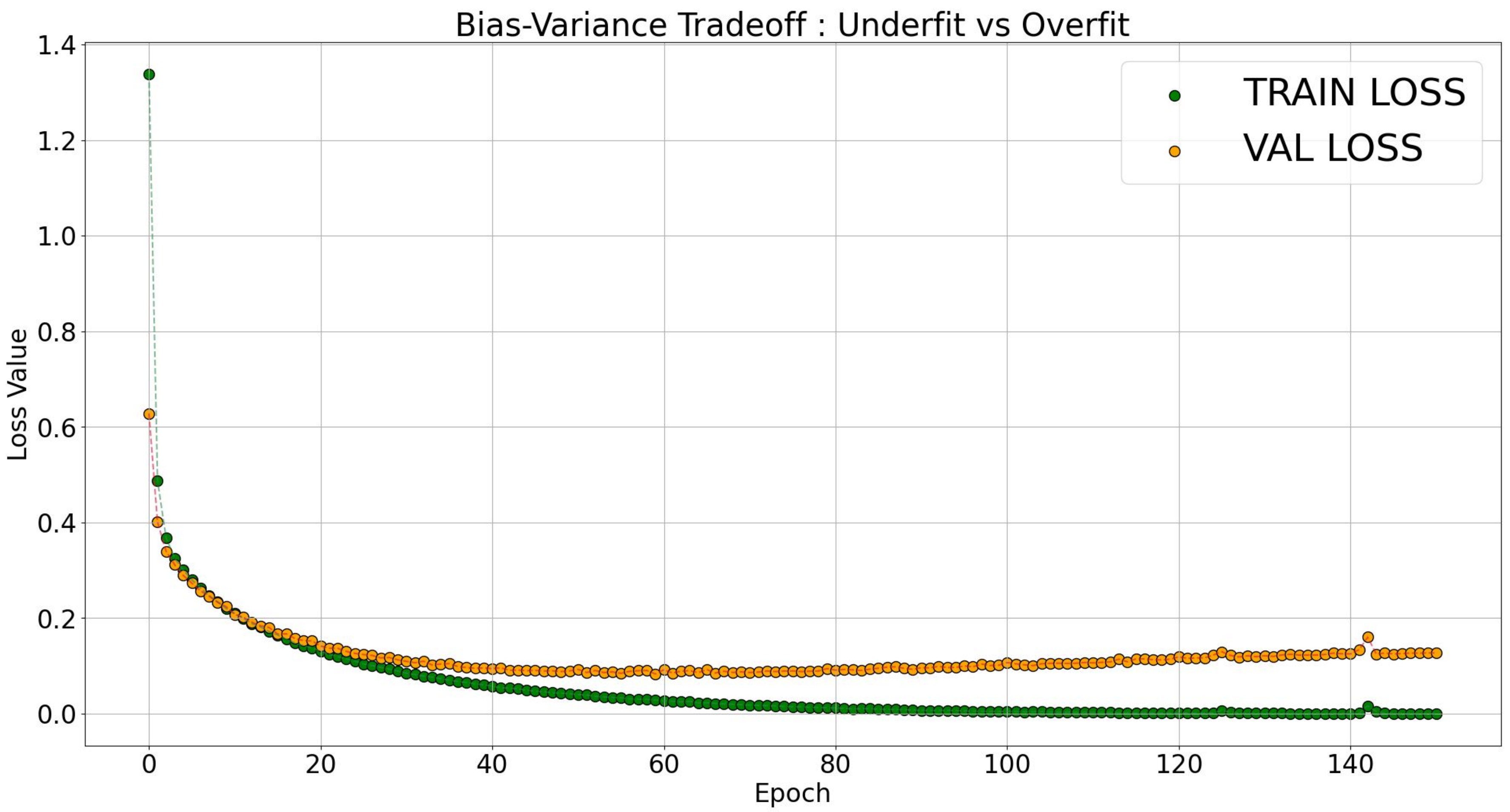
```
loss.backward()

optimizer.step()
```

</ 8. Device: GPU v CPU />

</ 9. Train Trajectory />



Train Trajectory & Early Stopping
TRAIN LOSS
VAL LOSS
Loss Value
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50
Epoch



Bias-Variance Tradeoff : Underfit vs Overfit
TRAIN LOSS
VAL LOSS
Loss Value
Epoch
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
20
40
60
80
100
120
140

</ 10. Reproducibility />

Random Number Generators

- **torch**, **numpy**, and **random** libraries have their own random number generators.

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- **Dropout** uses a RNG.

Random Number Generators

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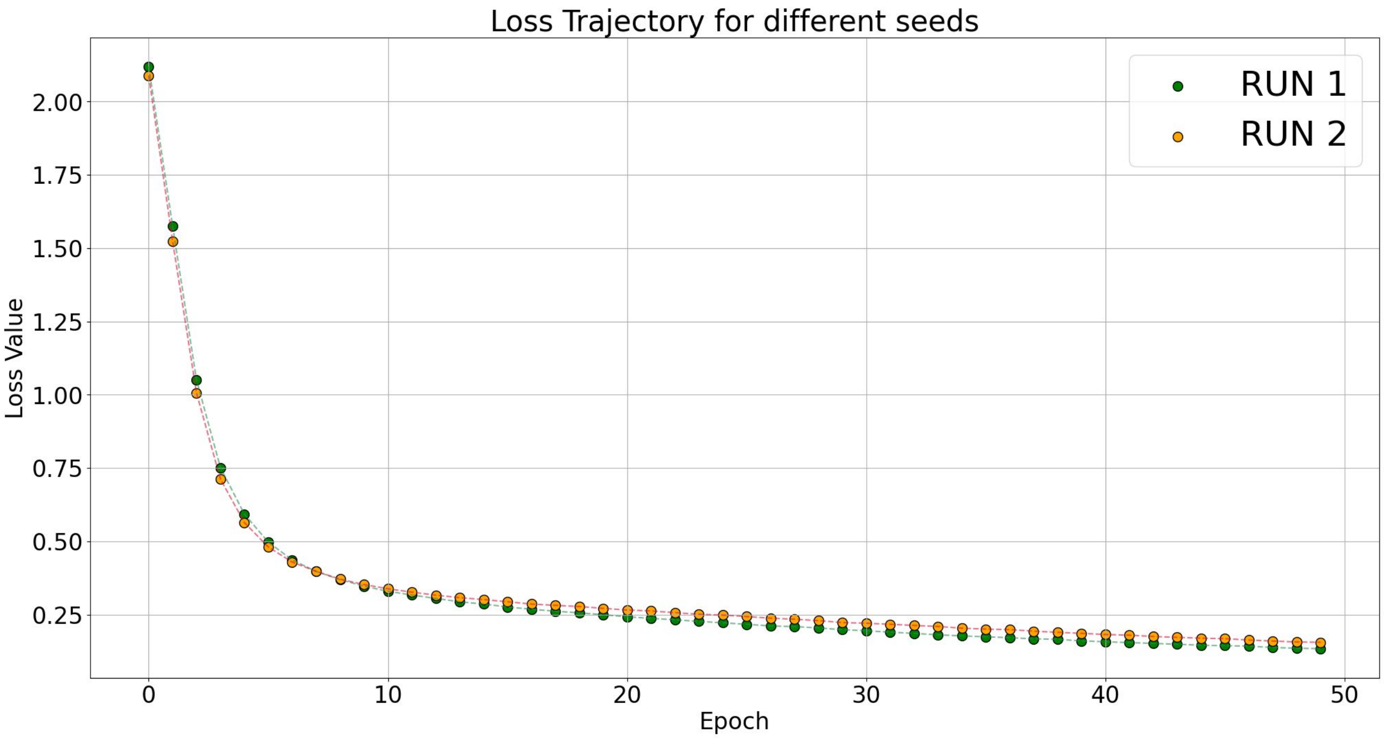
- **Initializing models** generates parameter vectors with random weights.
- **Shuffling** of data also uses an RNG.
- **Dropout** uses a RNG.

- These RNGs are used in the backend implicitly.
- What are the consequences?

Multiple train runs through the epochs



How to reproduce runs?

Initialize the random seeds for each RNG

- One can write a function as shown.
- Seeding everything is a good practice in machine learning.
- Reproducibility is a big aspect of machine learning research so that people can verify your work.

```
def seed_everything(seed):
    random.seed(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
```

Non Determinism (Pro stuff)

- It is possible that the training runs are not reproducible even after seeding.
- Non-Deterministic code is because of the hardware and non-deterministic algorithms used by torch in the background.

```
void nll_loss2d_forward_out_cuda_template(
    Tensor& output,
    Tensor& total_weight,
    const Tensor& input,
    const Tensor& target,
    const c10::optional<Tensor>& weight_opt,
    int64_t reduction,
    int64_t ignore_index) {
  // See Note [Writing Nondeterministic Operations]
  // Nondeterministic because of atomicAdd usage in 'sum' or 'mean' reductions.
  if (reduction != at::Reduction::None) {
    at::globalContext().alertNotDeterministic("nll_loss2d_forward_out_cuda_template");
  }
```

https://github.com/pytorch/pytorch/blob/8f1c3c68d3aba5c8898bfb3144988aab6776d549/aten/src/ATen/native/cuda/NLLLoss2d.cu#L236-L240

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- It is possible that the training runs are not reproducible even after seeding.
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- Sometimes asking pytorch to use deterministic algorithms can solve problems. For example, NLLLoss becomes deterministic.

```
torch.use_deterministic_algorithms(True)
```

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- But you may still have other dependencies that introduce non-determinism. :(

</ 11. Important Points/>

These are the things you should do in practice

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These are the things you should do in practice

Always:

1. Use git.
2. Write modular code.
3. Document your code.
4. Seed everything before training.
5. Reuse the available implementations. (Don’t reinvent the wheel)
6. Use chatGPT to code.

…

</ Thank You />