Software Intelligence

The Center for Research and Development

Full Documentation Link: 👨‍🎓 Day 02: PyTorch Tensors Basics

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Welcome to Day 2 of your Deep Learning journey! Today, we delve into the foundational building blocks of PyTorch: **Tensors**. Understanding tensors is crucial as they are the primary data structure used in PyTorch for representing and manipulating data. This day is meticulously designed to equip you with a comprehensive understanding of tensors, their attributes, and the myriad ways to create and manipulate them effectively.

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1. Understanding Tensors

1.1. What is a Tensor?

At its core, a **tensor** is a multi-dimensional array that generalizes scalars, vectors, and matrices to higher dimensions. Tensors are the fundamental data structure in PyTorch and are pivotal for representing inputs, outputs, weights, and activations in neural networks.

- **Scalar (0D Tensor):** A single number (e.g., `torch.tensor(5)`).
- **Vector (1D Tensor):** A one-dimensional array (e.g., `torch.tensor([1, 2, 3])`).
- **Matrix (2D Tensor):** A two-dimensional array (e.g., `torch.tensor([[1, 2], [3, 4]])`).
- **3D and Higher Tensors:** Used to represent more complex data structures, such as batches of images or sequences.

1.2. Tensors vs. NumPy Arrays

While tensors and NumPy arrays share similarities, there are key differences that make tensors particularly suited for deep learning:

Feature	NumPy Arrays	PyTorch Tensors
Backend	CPU-based computations	CPU and GPU-based computations
Automatic Gradients	Not supported	Supported via Autograd
Interoperability	Integrates seamlessly with Python and various scientific libraries	Integrates seamlessly with deep learning workflows and supports GPU acceleration
Memory Sharing	Limited support for GPU	Efficient memory sharing between CPU and GPU
Performance	Optimized for CPU	Optimized for both CPU and GPU

1.3. Tensors in Deep Learning

In the realm of deep learning, tensors serve as the conduit for data flow within neural networks. They facilitate:

- **Data Representation:** Inputs (e.g., images, text), targets (labels), and model parameters (weights and biases) are all represented as tensors.
- **Parallel Computation:** Leveraging GPUs, tensors enable parallel processing, significantly accelerating training and inference.
- **Gradient Computation:** Tensors support automatic differentiation, allowing for efficient backpropagation during training.

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2. Tensor Creation and Manipulation

2.1. Creating Tensors

PyTorch provides a variety of methods to create tensors, each suited for different scenarios:

1. **From Data:**

```
import torch

# Creating a tensor from a Python list
data = [[1, 2], [3, 4]]
x_data = torch.tensor(data)
```

2. **Using Factory Methods:**

   - `torch.zeros`: Creates a tensor filled with zeros.

     ```
     x_zeros = torch.zeros(2, 3)  # 2x3 tensor of zeros
     ```

   - `torch.ones`: Creates a tensor filled with ones.

     ```
     x_ones = torch.ones(2, 3)  # 2x3 tensor of ones
     ```

   - `torch.rand`: Creates a tensor with random values uniformly distributed between 0 and 1.

     ```
     x_rand = torch.rand(2, 3)
     ```

   - `torch.randn`: Creates a tensor with random values from a standard normal distribution.

     ```
     x_randn = torch.randn(2, 3)
     ```

   - `torch.arange`: Creates a 1D tensor with values from a specified range.

     ```
     x_arange = torch.arange(0, 10, step=2)  # tensor([0, 2, 4, 6, 8])
     ```

- `torch.linspace`: Creates a 1D tensor with a specified number of points linearly spaced between two values.

```
x_linspace = torch.linspace(0, 1, steps=5)  # tensor([0.0000, 0.2500, 0.5000, 0.7500,
```

3. **From NumPy Arrays:**

```
import numpy as np

np_array = np.array([[1, 2], [3, 4]])
x_np = torch.from_numpy(np_array)
```

4. **From Existing Tensors:**

- `torch.empty_like`: Creates an uninitialized tensor with the same shape as another tensor.

```
x_empty = torch.empty_like(x_data)
```

- `torch.clone`: Creates a copy of a tensor.

```
x_clone = x_data.clone()
```

2.2. Tensor Attributes

Understanding tensor attributes is essential for effective manipulation and debugging.

- **Shape (`size` or `shape`):** The dimensions of the tensor.

```
print(x_data.shape)  # torch.Size([2, 2])
```

- **Data Type (`dtype`):** The type of elements stored in the tensor (e.g., `torch.float32`, `torch.int64`).

```
print(x_data.dtype)  # torch.int64
```

- **Device (`device`):** Indicates whether the tensor is stored on the CPU or GPU.

```
print(x_data.device)  # cpu
```

- **Requires Grad (`requires_grad`):** Specifies whether gradients should be computed for the tensor during backpropagation.

```
x = torch.ones(2, 2, requires_grad=True)
print(x.requires_grad)  # True
```

2.3. Tensor Operations

PyTorch supports a wide range of tensor operations, enabling efficient data manipulation and computation.

1. **Arithmetic Operations:**

```
x = torch.tensor([1, 2, 3])
y = torch.tensor([4, 5, 6])

# Addition
print(x + y)  # tensor([5, 7, 9])

# Subtraction
print(x - y)  # tensor([-3, -3, -3])

# Multiplication
print(x * y)  # tensor([ 4, 10, 18])

# Division
print(x / y)  # tensor([0.2500, 0.4000, 0.5000])
```

2. **Matrix Multiplication:**

```
A = torch.rand(2, 3)
B = torch.rand(3, 2)

# Matrix multiplication
C = torch.mm(A, B)
print(C.shape)  # torch.Size([2, 2])
```

3. **Element-wise Operations:**

```
# Element-wise square
print(x.pow(2))  # tensor([1, 4, 9])

# Exponential
print(x.exp())  # tensor([ 2.7183,  7.3891, 20.0855])
```

4. **In-place Operations:**

```
x.add_(y)  # Adds y to x in-place
print(x)    # tensor([5, 7, 9])
```

5. **Indexing, Slicing, and Joining:**

```
# Indexing
print(x[0])  # tensor(5)

# Slicing
print(x[1:3])  # tensor([7, 9])

# Concatenation
z = torch.cat((x, y), dim=0)
print(z)  # tensor([5, 7, 9, 4, 5, 6])
```

2.4. Advanced Tensor Manipulations

1. **Reshaping and Transposing:**

```
x = torch.arange(1, 13)
x = x.view(3, 4)  # Reshape to 3x4
print(x)
# tensor([[ 1,  2,  3,  4],
#         [ 5,  6,  7,  8],
#         [ 9, 10, 11, 12]])

# Transpose
x_t = x.t()
print(x_t)
# tensor([[ 1,  5,  9],
#         [ 2,  6, 10],
#         [ 3,  7, 11],
#         [ 4,  8, 12]])
```

2. **Broadcasting:** PyTorch automatically expands tensors with smaller dimensions to match larger ones during operations, following broadcasting rules.

```
x = torch.ones(3, 1)
y = torch.ones(1, 4)
z = x + y  # Broadcasted to 3x4
print(z)
# tensor([[2., 2., 2., 2.],
#         [2., 2., 2., 2.],
#         [2., 2., 2., 2.]])
```

3. **Cloning and Detaching:**

- **Cloning:** Creates a copy of the tensor.

```
x_clone = x.clone()
```

- **Detaching:** Creates a new tensor detached from the computational graph.

```
x_detached = x.detach()
```

4. **Type Conversion:**

```
x = torch.tensor([1, 2, 3], dtype=torch.int32)
x_float = x.float()
print(x_float.dtype)  # torch.float32
```

5. **Moving Tensors Between Devices:**

```
# Assuming a GPU is available
if torch.cuda.is_available():
    device = torch.device('cuda')
    x = x.to(device)
    print(x.device)  # cuda:0
```

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3. Practical Activities

Engaging in hands-on activities solidifies theoretical knowledge. Below are structured exercises to enhance your understanding of tensors.

3.1. Exploring Tensor Attributes

Objective: Familiarize yourself with various tensor attributes and understand how to access and modify them.

Steps:

1. **Create Tensors of Different Dimensions:**

```
import torch

scalar = torch.tensor(7)
vector = torch.tensor([1, 2, 3])
matrix = torch.tensor([[1, 2], [3, 4]])
tensor3d = torch.tensor([[[1], [2]], [[3], [4]]])
```

2. **Inspect Attributes:**

```
print("Scalar:", scalar)
print("Shape:", scalar.shape)        # torch.Size([])
print("Data Type:", scalar.dtype)    # torch.int64
print("Device:", scalar.device)      # cpu

print("\nVector:", vector)
print("Shape:", vector.shape)        # torch.Size([3])

print("\nMatrix:", matrix)
print("Shape:", matrix.shape)        # torch.Size([2, 2])

print("\n3D Tensor:", tensor3d)
print("Shape:", tensor3d.shape)      # torch.Size([2, 2, 1])
```

3. **Modify Attributes:**

   - **Change Data Type:**

     ```
     tensor_float = matrix.float()
     print(tensor_float.dtype)  # torch.float32
     ```

   - **Move to GPU (if available):**

     ```
     if torch.cuda.is_available():
         tensor_gpu = tensor_float.to('cuda')
         print(tensor_gpu.device)  # cuda:0
     ```

3.2. Creating and Manipulating Tensors

Objective: Gain proficiency in creating various types of tensors and performing basic manipulations.

Steps:

1. **Create Tensors Using Different Factory Methods:**

```
zeros = torch.zeros(3, 3)
ones = torch.ones(2, 4)
rand = torch.rand(5)
randn = torch.randn(2, 2)
arange = torch.arange(0, 10, step=2)
linspace = torch.linspace(0, 1, steps=5)
```

2. **Manipulate Tensors:**

   - **Reshape Tensors:**

```
reshaped = rand.view(1, 5)
print(reshaped.shape)  # torch.Size([1, 5])
```

- **Transpose Tensors:**

```
matrix = torch.tensor([[1, 2, 3], [4, 5, 6]])
transposed = matrix.t()
print(transposed)
# tensor([[1, 4],
#         [2, 5],
#         [3, 6]])
```

- **Squeeze and Unsqueeze:**

```
tensor = torch.zeros(2, 1, 2, 1, 2)
print(tensor.shape)  # torch.Size([2, 1, 2, 1, 2])

squeezed = tensor.squeeze()
print(squeezed.shape)  # torch.Size([2, 2, 2])

unsqueezed = squeezed.unsqueeze(0)
print(unsqueezed.shape)  # torch.Size([1, 2, 2, 2])
```

3. **Combine Tensors:**

```
a = torch.tensor([1, 2, 3])
b = torch.tensor([4, 5, 6])
combined = torch.stack((a, b), dim=0)
print(combined)
# tensor([[1, 2, 3],
#         [4, 5, 6]])
```

3.3. Implementing Tensor Operations

Objective: Apply tensor operations to perform computations, essential for neural network training and data processing.

Steps:

1. **Arithmetic Operations:**

```
x = torch.tensor([1.0, 2.0, 3.0])
y = torch.tensor([4.0, 5.0, 6.0])

# Addition
z_add = x + y
print(z_add)  # tensor([5., 7., 9.])
```

```
# Multiplication
z_mul = x * y
print(z_mul)  # tensor([ 4., 10., 18.])
```

2. **Matrix Multiplication:**

```
A = torch.tensor([[1, 2], [3, 4]])
B = torch.tensor([[5, 6], [7, 8]])

C = torch.mm(A, B)
print(C)
# tensor([[19, 22],
#         [43, 50]])
```

3. **Element-wise Operations:**

```
x = torch.tensor([1.0, 2.0, 3.0], requires_grad=True)
y = x.pow(2) + 3 * x + 1
print(y)  # tensor([ 5., 11., 19.], grad_fn=<AddBackward0>)
```

4. **In-place Operations:**

```
x = torch.ones(2, 2)
print(x)
# tensor([[1., 1.],
#         [1., 1.]])

x.add_(2)
print(x)
# tensor([[3., 3.],
#         [3., 3.]])
```

5. **Broadcasting Example:**

```
x = torch.tensor([[1, 2, 3], [4, 5, 6]])
y = torch.tensor([1, 2, 3])
z = x + y  # y is broadcasted to match x's shape
print(z)
# tensor([[2, 4, 6],
#         [5, 7, 9]])
```

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4. Resources

Enhance your learning by exploring the following resources:

1. **Official Documentation and Guides:**
   - PyTorch Tensors Documentation: Detailed explanation of tensors, their properties, and operations.
   - PyTorch Tutorial: Tensors: Beginner-friendly tutorial on tensor basics.
   - PyTorch API Reference: Comprehensive API documentation.
2. **Books and Reading Materials:**
   - "*Deep Learning with PyTorch*" by Eli Stevens, Luca Antiga, and Thomas Viehmann: Practical insights and projects to build real-world deep learning applications using PyTorch.
   - "*Programming PyTorch for Deep Learning*" by Ian Pointer: A guide to leveraging PyTorch for deep learning tasks.
   - "*Neural Networks and Deep Learning*" by Michael Nielsen: Available online.
3. **Online Courses and Lectures:**
   - Fast.ai's Practical Deep Learning for Coders: Hands-on approach with PyTorch.
   - Deep Learning Specialization by Andrew Ng on Coursera: Comprehensive courses covering various aspects of deep learning.
   - Udacity's Intro to Deep Learning with PyTorch: Focused on PyTorch implementations.
4. **Community and Support:**
   - PyTorch Forums: Engage with the community for questions and discussions.
   - Stack Overflow PyTorch Tag: Find solutions to common problems.
   - Reddit's r/PyTorch: Stay updated with the latest news, tutorials, and discussions related to PyTorch.
5. **Tools and Extensions:**
   - **Visualization:**
     - TensorBoard with PyTorch: Visualizing training metrics.
     - Visdom: Real-time visualization tool.
   - **Performance Optimization:**
     - PyTorch Lightning: Simplifies training loops and scalability.
     - TorchScript: Transition models from research to production.
   - **Debugging and Profiling:**
     - PyTorch Profiler: Analyze and optimize the performance of PyTorch models.
     - Visual Studio Code with PyTorch Extensions: Enhance your development environment with debugging and IntelliSense for PyTorch.

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5. Learning Objectives

By the end of Day 2, you should be able to:

1. **Comprehend Tensor Fundamentals:**
    - Grasp the concept of tensors and their role in deep learning.
    - Differentiate between tensors and other data structures like NumPy arrays.
2. **Master Tensor Creation:**
    - Utilize various PyTorch methods to create tensors tailored to different needs.
    - Understand factory methods and their applications.
3. **Manipulate Tensor Attributes:**
    - Access and modify tensor attributes such as shape, dtype, and device.
    - Perform type conversions and move tensors between devices.
4. **Execute Tensor Operations:**
    - Perform arithmetic and matrix operations with tensors.
    - Implement advanced manipulations like reshaping, transposing, and broadcasting.
5. **Optimize Tensor Usage:**
    - Employ in-place operations to enhance computational efficiency.
    - Understand and apply broadcasting rules to simplify operations.

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6. Expected Outcomes

By the end of Day 2, you will have:

- **Proficient Tensor Manipulation Skills:** Ability to create, modify, and perform operations on tensors with ease.
- **Deep Understanding of Tensor Attributes:** Comprehensive knowledge of tensor properties and how to leverage them in various scenarios.
- **Practical Experience:** Hands-on practice through exercises, solidifying your grasp on tensor operations and manipulations.
- **Foundation for Advanced Topics:** Preparedness to tackle more complex deep learning concepts that build upon tensor operations, such as neural network layers and data processing pipelines.

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7. Tips for Success

1. **Hands-On Practice:** Actively code along with examples to reinforce your understanding of tensor operations.
2. **Experiment:** Modify code snippets to observe different outcomes and deepen your comprehension.
3. **Visualize:** Use visualization tools like TensorBoard to gain insights into tensor operations and their effects.
4. **Document Learning:** Keep notes of key concepts, commands, and observations to reference in future projects.
5. **Seek Clarification:** Don't hesitate to ask questions in forums or consult resources when encountering challenges.

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8. Advanced Tips and Best Practices

1. **Leverage GPU Acceleration:**
   - **Move Tensors to GPU:**

     ```
     if torch.cuda.is_available():
         device = torch.device('cuda')
         x_gpu = x.to(device)
         print(x_gpu.device)  # cuda:0
     ```

   - **Ensure All Tensors Are on the Same Device:** Prevent runtime errors by maintaining consistency in tensor devices.
2. **Efficient Memory Management:**
   - **Use In-Place Operations Sparingly:** While they save memory, they can complicate the computational graph.
   - **Detach Tensors When Necessary:**

     ```
     y = x.detach()
     ```

3. **Avoid Common Pitfalls:**
   - **Understanding Broadcasting Rules:** Ensure tensor dimensions are compatible to avoid unexpected results.
   - **Gradient Tracking:** Be mindful of `requires_grad` to manage which tensors should track gradients.
4. **Optimizing Performance:**

- **Batch Operations:** Perform operations on batches of data to leverage parallel computation.
- **Minimize Data Transfers:** Reduce the number of times tensors are moved between CPU and GPU.

5. **Code Readability and Maintenance:**
   - **Use Descriptive Variable Names:** Enhance code clarity by naming tensors meaningfully.
   - **Modularize Code:** Break down complex operations into smaller, reusable functions.
6. **Integrate with Other Libraries:**
   - **Seamless Conversion Between PyTorch and NumPy:**

     ```
     # From Tensor to NumPy
     np_array = x.numpy()

     # From NumPy to Tensor
     tensor_from_np = torch.from_numpy(np_array)
     ```

   - **Interoperability with Pandas:**

     ```
     import pandas as pd

     df = pd.DataFrame(np_array)
     tensor_from_df = torch.tensor(df.values)
     ```

7. **Utilize Built-in Functions:**
   - **Aggregation Functions:** `torch.sum`, `torch.mean`, `torch.max`, etc.
   - **Statistical Operations:** `torch.std`, `torch.var`, etc.
8. **Implement Custom Operations:**
   - **Extend PyTorch Functionality:** Create custom functions for specialized tensor manipulations.

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9. Comprehensive Summary

Today, we've embarked on an in-depth exploration of **PyTorch Tensors**, the cornerstone of data representation in deep learning. Key takeaways include:

- **Tensor Fundamentals:** A solid understanding of what tensors are, their various dimensions, and how they differ from NumPy arrays.
- **Creation Techniques:** Mastery of multiple methods to create tensors, from basic factory functions to converting from existing data structures.

- **Attribute Mastery:** Ability to access and manipulate tensor attributes, ensuring flexibility in handling diverse data scenarios.
- **Operational Proficiency:** Competence in performing a wide range of tensor operations, from simple arithmetic to complex matrix multiplications and broadcasting.
- **Advanced Manipulations:** Insights into reshaping, transposing, and other advanced tensor manipulations that are essential for building and training neural networks.

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10. Moving Forward

With a robust understanding of tensors, you are now prepared to delve into more intricate aspects of PyTorch and deep learning. Here's a glimpse of upcoming topics:

- **Day 3:** PyTorch Autograd and Automatic Differentiation
- **Day 4:** Building Neural Networks with `torch.nn`
- **Day 5:** Data Loading and Preprocessing with `torch.utils.data`
- **Day 6:** Training Loops and Optimization Strategies
- **Day 7:** Model Evaluation and Deployment

Each subsequent day will build upon the foundation established today, gradually guiding you towards mastering deep learning with PyTorch.

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11. Final Encouragement

Embarking on the journey to master PyTorch tensors is a significant stride towards becoming proficient in deep learning. Remember, the key to mastery lies in consistent practice, curiosity, and a willingness to explore beyond the basics. Embrace challenges as opportunities to learn, and don't hesitate to leverage the wealth of resources and community support available. Here's to your continued success in harnessing the power of PyTorch!

Appendix

Example Code Snippets

To reinforce your learning, here are some example code snippets that encapsulate the concepts discussed today.

Creating and Inspecting Tensors

```
import torch

# Creating tensors
scalar = torch.tensor(5)
vector = torch.tensor([1, 2, 3])
matrix = torch.tensor([[1, 2], [3, 4]])
tensor3d = torch.tensor([[[1], [2]], [[3], [4]]])

# Inspecting attributes
print("Scalar:", scalar)
print("Shape:", scalar.shape)
print("Data Type:", scalar.dtype)
print("Device:", scalar.device)

print("\nVector:", vector)
print("Shape:", vector.shape)

print("\nMatrix:", matrix)
print("Shape:", matrix.shape)

print("\n3D Tensor:", tensor3d)
print("Shape:", tensor3d.shape)
```

Performing Tensor Operations

```
import torch

# Arithmetic operations
x = torch.tensor([1.0, 2.0, 3.0])
y = torch.tensor([4.0, 5.0, 6.0])

print("Addition:", x + y)
print("Subtraction:", x - y)
print("Multiplication:", x * y)
print("Division:", x / y)

# Matrix multiplication
A = torch.rand(2, 3)
B = torch.rand(3, 2)
C = torch.mm(A, B)
print("Matrix Multiplication:\n", C)

# Element-wise operations
print("Element-wise Square:", x.pow(2))
print("Exponential:", x.exp())

# Reshaping and Transposing
x = torch.arange(1, 13)
x = x.view(3, 4)
print("Reshaped Tensor:\n", x)
```

```
x_t = x.t()
print("Transposed Tensor:\n", x_t)

# Broadcasting
a = torch.ones(3, 1)
b = torch.ones(1, 4)
c = a + b
print("Broadcasted Tensor:\n", c)
```

Moving Tensors to GPU

```
import torch

# Check if CUDA is available
if torch.cuda.is_available():
    device = torch.device('cuda')
    print("CUDA is available. Using GPU.")
else:
    device = torch.device('cpu')
    print("CUDA is not available. Using CPU.")

# Create a tensor and move it to the selected device
x = torch.tensor([1, 2, 3], dtype=torch.float32)
x = x.to(device)
print("Tensor Device:", x.device)
```

Frequently Asked Questions (FAQ)

Q1: What is the difference between `torch.tensor` and `torch.Tensor`?

A1: `torch.tensor` is a function used to create a tensor from data (e.g., lists, NumPy arrays), whereas `torch.Tensor` is a constructor that creates an uninitialized tensor. It's recommended to use factory methods like `torch.tensor`, `torch.zeros`, etc., for creating tensors to ensure clarity and avoid confusion.

Q2: How do I ensure tensors are on the same device before performing operations?

A2: Before performing operations, explicitly move tensors to the same device using the `.to(device)` method. For example:

```
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
x = torch.tensor([1, 2, 3]).to(device)
```

```
y = torch.tensor([4, 5, 6]).to(device)
z = x + y
```

Q3: What are the implications of using in-place operations on tensors that require gradients?

A3: In-place operations can potentially overwrite values needed to compute gradients, leading to errors during backpropagation. Use them cautiously and ensure they do not interfere with the computational graph. When in doubt, prefer out-of-place operations.

Q4: Can I create tensors with custom data types?

A4: Yes, PyTorch supports various data types. You can specify the `dtype` parameter during tensor creation:

```
x = torch.tensor([1, 2, 3], dtype=torch.float64)
```

Refer to the PyTorch Dtypes Documentation for a comprehensive list of supported data types.

Q5: How do I convert a tensor to a NumPy array and vice versa?

A5: Use the `.numpy()` method to convert a tensor to a NumPy array and `torch.from_numpy()` to convert a NumPy array to a tensor:

```
import torch
import numpy as np

# Tensor to NumPy
tensor = torch.tensor([1, 2, 3])
np_array = tensor.numpy()

# NumPy to Tensor
new_tensor = torch.from_numpy(np_array)
```

Note: The tensor and NumPy array share the same memory. Modifying one will affect the other.

Conclusion

Mastering PyTorch tensors is a pivotal step in your deep learning journey. Today, you've acquired the skills to create, inspect, and manipulate tensors, laying a robust foundation for more complex tasks

like building neural networks and processing data pipelines. Continue practicing these concepts, explore the provided resources, and engage with the community to solidify your understanding. Tomorrow, we will build upon this knowledge by exploring PyTorch's automatic differentiation capabilities with Autograd.

Stay curious, stay persistent, and enjoy the process of learning!