Demystifying Pytorch's Strides Format

Intro

Even though I have been using Numpy and Pytorch for a long time, I never really knew how they implemented the underlying tensors and why they are **so efficient**. Recently, while studying the course Deep Learning Systems, I finally got the opportunity to try implementing tensors on my own. After going through the process, my understanding of tensors is much better 🧐

As a Pytorch user, is it necessary to understand the underlying tensor storage mechanism? I believe **it is essential**. In most cases, understanding the underlying principles helps you grasp higher-level concepts better. For example, understanding the tensor storage mechanism can help you answer the following questions:

- Does broadcasting involve copying arrays?
- What does `contiguous` do in Pytorch, and why is this function needed?

Row-major and column-major

Let's start with a simple 2D array, **A 2D array occupies a contiguous location in memory**, but how it is stored, whether using row-major or column-major, may vary.

Let's say we have a 2D array `A` *whose size is* 2×3 2×3

```
[[0.2949, 0.9608, 0.0965],
 [0.5463, 0.4176, 0.8146]]
```

If we use row-major, then the memory layout(denoted as `A_in_row`) would be:

```
[0.2949, 0.9608, 0.0965, 0.5463, 0.4176, 0.8146]
```

To access `(i, j)` when using row-major, the equations says:

```
A[i][j] = A_in_row[i * A.shape[1] + j]
```

If we use column-major, then the memory layout(denoted as `A_in_col`) would be:

```
[0.2949, 0.5463, 0.9608, 0.4176, 0.0965, 0.8146]
```

To access `(i, j)` when using column-major, the equations says:

```
A[i][j] = A_in_col[j * A.shape[0] + i]
```

Strides format

Note: I will use continuous/contiguous/compact interchangeably.

At the low level, tensors can be stored either by rows or columns. Both Numpy and PyTorch adopt the approach of storing tensors by rows. Regardless of the tensor's dimension, **the underlying storage always occupies continuous memory space**. Now, the question arises: How do we access the data at the desired positions?

The answer is **strides format**. We may regard the strides format as a generalization version of the two previous indexing formats. Let's consider a tensor of *N*N dimensions(0-based), and its underlying storage is represented as `A_internal`. If we want to access `A[i0][i1][i2]...`, the indexing is done as follows:

```
A[i0][i1][i2]... = A_internal[
    stride_offset
    + i0 * A.strides[0]
    + i1 * A.strides[1]
    + i2 * A.strides[2]
    + ...
    + in-1 * A.strides[n-1]
]
```

The strides format has two components:

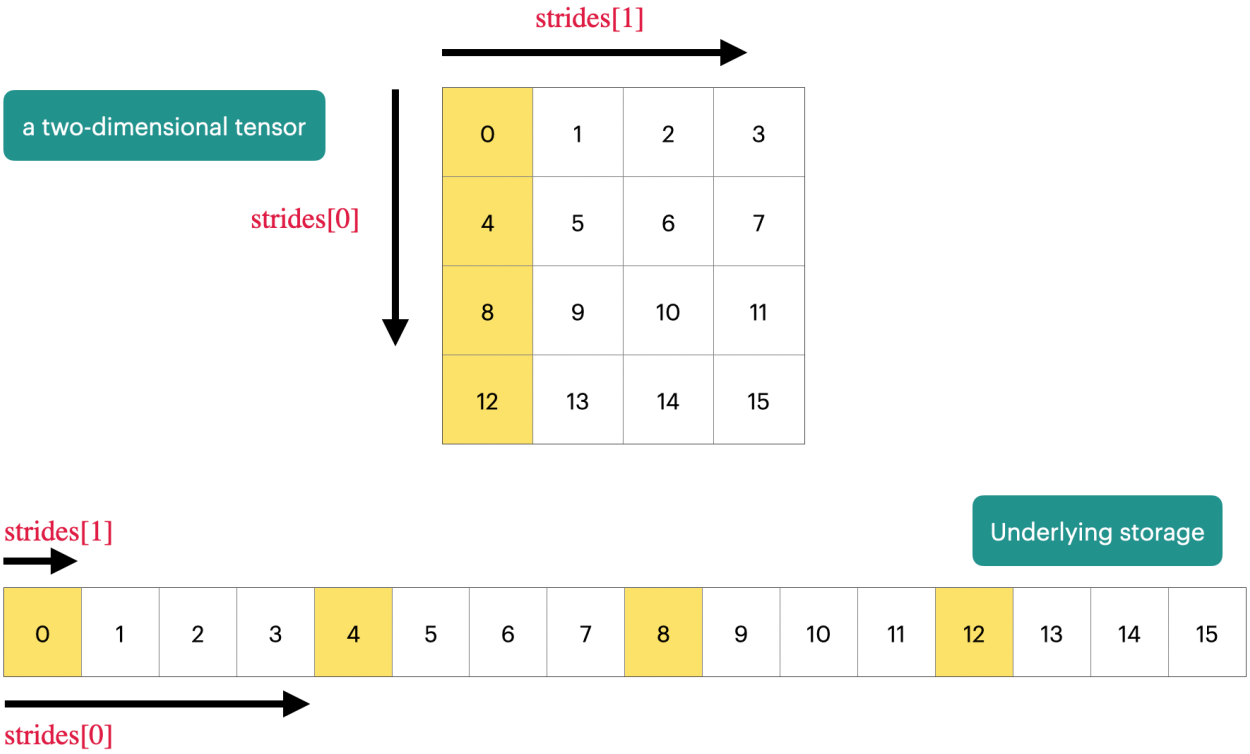
- `offset` - the offset of the tensor relative to the underlying storage
- `strides` array, whose length is equal to the number of dimensions of the tensor. `strides[i]` indicates how many "elements" need to be skipped in memory to move "one unit" in the *i*i-th dimension of the tensor

For example, considering the earlier example of a 2D array, if we interpret it using the strides format

```
A[i][j] = A_in_row[
    0
    + i * A.shape[1]
    + j * 1
]
```

For a 2D array of size `(A.shape[0], A.shape[1])`, its offset is `0`, and the `strides` array is `[A.shape[1], 1]` (row-major). 🤔 *This means that moving "one unit" in the first dimension requires skipping `A.shape[1]` elements in the underlying memory, where `A.shape[1]` is the length of each row*

I made this image to give you better intuition :)



🧐 How to obtain the strides array for an NN dimensional tensor? Let's say we want to calculate `strides[k]` for the kk-th dimension. We know the semantic of `strides[k]` is *the elements to skip in the underlying memory to moving "one unit" in the kk-th dimension*, **If the memory layout of the tensor is continuous**, then the answer would be the product of $k+1, k+2, \ldots, N-1$k+1,k+2,…,N−1. If $k = N-1$k=N−1, then `strides[N - 1] = 1`

The mathematical formula is as follows:

$$strides[k] = \prod_{i=k+1}^{N-1} shape[i]$$

strides[k]=i=k+1∏N−1shape[i]

> 💡 *It is important to reiterate that the above formula holds only when the tensor's underlying memory layout is contiguous.*

Why strides?

After understanding the strides format. The next question would be: **Why do we need the strides format and what benefits it brings**? The most significant advantage is that many tensor operations can be performed in a **zero-copy** manner. By using the strides format, the concepts of "underlying storage" and "views" are separated. Now let's talk about some common tensor operations

print_internal function

Before we start to investigate the tensor operations, we need to write a helper function such that we can get the underlying storage.

Pytorch provides us with the `data_ptr` API, which will return the address of the first element of a tensor.

Then, by using the storage().nbytes() method provided by PyTorch, we can determine the amount of memory space the tensor's underlying storage occupies(in bytes)[1]. Additionally, the `dtype` attribute of the tensor informs us about the size of each element. *For example, `torch.float32` occupies 4 bytes*

Finally, we can use the `ctypes.string_at(address, size=-1)` function to read the tensor as a C-style string (buffer), and `torch.frombuffer` can be used to create a tensor from this buffer.

Putting it all together, we can write this helper function called `print_internal`:

```
def print_internal(t: torch.Tensor):
    print(
        torch.frombuffer(
            ctypes.string_at(t.data_ptr(), t.storage().nbytes()), dtype=t.dtype
        )
    )
```

Now we create a tensor `t` with dimension `(1, 2, 3, 4)` and observe its underlying representation. **The subsequent operations and explanations will be based on this tensor `t`**

```
torch.arange(0, 24).reshape(1, 2, 3, 4)
print(t)
# tensor([[[[ 0,  1,  2,  3],
#           [ 4,  5,  6,  7],
#           [ 8,  9, 10, 11]],

#          [[12, 13, 14, 15],
#           [16, 17, 18, 19],
#           [20, 21, 22, 23]]]])

print(t.stride())
# (24, 12, 4, 1)

print_internal(t)
# tensor([0,  1,  2,  3,
#         4,  5,  6,  7,
#         8,  9, 10, 11,
#         12, 13, 14, 15,
#         16, 17, 18, 19,
#         20, 21, 22, 23])
```

By using the formula we previously talked about, we know the strides of `t` should be `(2 * 3 * 4, 3 * 4, 4, 1)`, that is, `(24, 12, 4, 1)`. The `t.stride()` will give us the strides array maintained by Pytorch. Indeed, it gives us the answer which is exactly what we expected.

permute operations

Suppose we rearrange the dimensions with `permute`, how does `strides` change?

```
print(t.stride())
# (24, 12, 4, 1)

print(t.permute((1, 2, 3, 0)).is_contiguous())
# True

print(t.permute((1, 2, 3, 0)).stride())
# (12, 4, 1, 24)

print_internal(t.permute((1, 2, 3, 0)))
# tensor([0,  1,  2,  3,
#         4,  5,  6,  7,
#         8,  9, 10, 11,
#         12, 13, 14, 15,
#         16, 17, 18, 19,
#         20, 21, 22, 23])
```

The `permute` operation will not change `offset`. And **the underlying storage is still compact**(indicated by `is_contiguous`). So we can use the `new_shape` after permuting to re-calculate the `strides` array. However, we can **just permute the original `strides` array**. The output of `print_internal` indicates that the underlying storage doesn't change.

broadcast_to operation

Broadcast_to operation is an interesting operation. Before knowing the internals, you *might* think that broadcasting involves copying along the corresponding dimensions. However, there is **no** copying under the hood. Pytorch just change the `strides` array. More specifically, Pytorch will set `stride[k] = 0` if its size is one before broadcasting[2].

Let's try to do broadcasting along the first dimension of tensor `t` and observe how the shape and strides will change

```
print(t.broadcast_to((2, 2, 3, 4)).is_contiguous())
# False

print(t.broadcast_to((2, 2, 3, 4)).shape)
# torch.Size([2, 2, 3, 4])

print(t.stride())
# (24, 12, 4, 1)

print(t.broadcast_to((2, 2, 3, 4)).stride())
# (0, 12, 4, 1)

print_internal(t.broadcast_to((2, 2, 3, 4)))
# tensor([0,  1,  2,  3,
#         4,  5,  6,  7,
#         8,  9, 10, 11,
```

```
#         12, 13, 14, 15,
#         16, 17, 18, 19,
#         20, 21, 22, 23])
```

Surprisingly, Pytorch does not allocate memory, and copy elements in the dimension got broadcasted. The only thing that changed is the `strides` array. Pause for a second and try to figure out what's the meaning of setting stride as 0. It means we don't need to skip any elements along this dimension, which indicates we are referring to the same data(same memory location).

reshape operation and contiguous operation

The indexing operation may modify the `offset` because the resulting tensor after indexing may not start from the first element of the original underlying storage. Moreover, the indexing operation **may access the non-contiguous parts** of the underlying storage. So the indexing operation will help us to understand the `reshape` and `contiguous` operations better.

Let's say we want to get the following tensor from `t`

```
[[[2,
   6,
   10],
  [14,
   18,
   22]]]
```

The corresponding indexing operation is

```
print(t[:, :, :, 2])
# tensor([[[ 2,  6, 10],
#          [14, 18, 22]]])
```

Note that this operation aligns with what I mentioned earlier:

- the `offset` will change because the resulting tensor starts from `2` rather than `0`
- The elements accessed by indexing are not contiguous in the original memory

The following code proves our speculation

```
print(t.storage_offset())
# 0

print(t[:, :, :, 2].storage_offset())
# 2

print(t[:, :, :, 2].is_contiguous())
# False
```

Now let's observe the underlying storage

```
print_internal(t[:, :, :, 2])
# tensor([        2,  3,
#         4,  5,  6,  7,
#         8,  9, 10, 11,
#         12, 13, 14, 15,
#         16, 17, 18, 19,
#         20, 21, 22, 23
#         1152921504606846976, -8070441752123218147]])
# ignore the last row because t.data_ptr() has changed but t.storage().nbytes()
# kept the same.
# As a result, we read 2 invalid elements and get 2 meaningless values
```

Pytorch's tensor has a method called `storage_offset()` which shows the offset in the underlying storage. As we can see, now it starts from the second position in the underlying storage, which corresponds to the first element `2` of `t[:, :, :, 2]`. And the underlying storage is still the same

> *Note: Because the underlying storage remains unchanged, `t.storage().nbytes()` remains the same. The `data_ptr()` will give us the address of the second element. As a result, the printed underlying array will have two additional meaningless positions (as seen in the last row), resulting in two extra irrelevant numbers.*

🧐 *Let's try to use `reshape(3, 2)` after indexing and observe the underlying storage*

```
print_internal(t[:, :, :, 2].reshape(3, 2))
# tensor([        2,  3,
#         4,  5,  6,  7,
#         8,  9, 10, 11,
#         12, 13, 14, 15,
#         16, 17, 18, 19,
#         20, 21, 22, 23
#         1152921504606846976, -8070441752123218147]])
```

We find that **the `reshape` operation does not change the underlying storage**. This aligns with what the documentation states: *When possible*, the returned tensor will be a view of input[3]

What if we want the tensor after `reshape` to have compact storage? We can use the `contiguous` method

```
print_internal(t[:, :, :, 2].reshape(3, 2).contiguous())
# tensor([ 2,  6, 10, 14, 18, 22])
```

😼 By chaining `reshape` and `contiguous` operations, we make the underlying storage compact. And the `strides` array should align with the aforementioned formula:

```
# before contiguous
print(t[:, :, :, 2].reshape(3, 2).stride())
# (8, 4)

# after contiguous
```

```
print(t[:, :, :, 2].reshape(3, 2).contiguous().shape)
# (3, 2)
print(t[:, :, :, 2].reshape(3, 2).contiguous().stride())
# (2, 1)
```

🧐 One **challenging** question for you, how indexing operation will change the `strides` array?

Let's use the previous indexing operation as an example. First, after indexing, the new dimensions should be `(1, 2, 3)`. The indexing pattern `[:, :, :, 2]` results in a non-compact underlying storage. So we can not just compute the `strides` array by the rule. Therefore, we have to reason the `strides` array based on the definitions. Let's assume the `strides` array of `t[:, :, :, 2]` is `[x, y, z]`

We can observe which elements are included in `t[:, :, :, 2]`

```
print(t[:, :, :, 2])
# tensor([[[ 2,  6, 10],
#          [14, 18, 22]]])
```

Because the tensor `t` starts from `0` and increments by one, we can just compute the strides based on the values(a little trick)

- for `z`, we find `2 -> 6 -> 10`, that is, we skip 4 elements each time. So `z = 4`
- for `y`, we find `2 -> 14`, `6 -> 18`, `10 -> 22`, we skip 12 elements each time. So `y = 12`
- for `x`, **since the underlying storage has not changed**, the original tensor `t` has `strides[0] = 24`. **Imagining that the first dimension is not 1 but a bigger value, we would need to skip `strides[0]` elements each time**. So `x = 24`

We claim that the `strides` of `t[:, :, :, 2]` should be `(24, 12, 4)`

Let's call the API to check if our claim is correct

```
print(t.stride())
# (24, 12, 4, 1)

print(t[:, :, :, 2].stride())
# (24, 12, 4)

# what if the first dimension is not 1 but 2?
another_t = torch.arange(0, 48).reshape(2, 2, 3, 4)
print(another_t[:, :, :, 2])
# tensor([[[ 2,  6, 10],
#          [14, 18, 22]],

#         [[26, 30, 34],
#          [38, 42, 46]]])

# you can see that 2 -> 26, 6 -> 30, 10 -> 35
# , so the stride[0] = 24 is true
```

The output meets our expectations

However, the indexing operations can be much more complex than our naive `[:, :, :, 2]` like `[2, 1:3, 1:6:3]`, and in such cases, how do `strides` and `offset` change? I won't elaborate on this, but here's a **hint**: convert each format into Python's Slice object and then reason through the definition of `strides[i]`

Wrap up

As you can see, many operations on Pytorch tensors are achieved by modifying the `offset` or(and) `strides` array. **This approach allows many operations to maintain zero-copy overhead, leading to high efficiency**. Moreover, this enables the *lazy* operations. Understanding the strides format **helps in constructing a mental model of tensors and facilitates a better understanding of tensor operation code**. I would also recommend watching the awesome video which talks about the cool tricks that manipulating strides to perform convolution efficiently

Now we can answer the questions raised earlier:

- Does broadcasting involve copying arrays?
    - No, broadcasting will only change the `strides` array
- What does `contiguous` do in Pytorch, and why is this function needed?
    - By using `contiguous`, we can make the underlying storage compact. Although this may involve copying, it is beneficial for later calculation because of the memory locality.