DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING



Machine Learning Preliminary

COMP4901Y

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Audit Policy



- You are always welcome to come to my class or view the online resource;
- If you want an audit credit in your HKUST transcript:
 - Get 60% on the final exam.
 - No mid-term or homework is required.





Linear Algebra

Some material in this section is modified from https://courses.d2l.ai/berkeley-stat-157





• Sample operations

$$c = a + b$$

$$c = a \cdot b$$

$$c = \sin a$$

• Length

$$|a| = \begin{cases} a & if \ a > 0 \\ -a & otherwise \end{cases}$$

$$|a+b| \le |a| + |b|$$

$$|a \cdot b| = |a| \cdot |b|$$



• Vector in n-dimensions
$$\mathbf{a} \in \mathbb{R}^n$$
, $\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$

• Sample operations:

$$c = a + b$$
 where $c_i = a_i + b_i$
 $c = \alpha \cdot b$ where $c_i = \alpha b_i$
 $c = \sin a$ where $c_i = \sin a_i$



- Some properties of vector addition:
 - Commutative:

$$a+b=b+a$$
, $a,b\in\mathbb{R}^n$

• Associative:

$$(a+b)+c=a+(b+c),$$
 $a,b,c\in\mathbb{R}^n$

• <u>Distibutive</u>:

$$\alpha(\boldsymbol{a}+\boldsymbol{b})=\alpha\boldsymbol{a}+\alpha\boldsymbol{b}, \qquad \boldsymbol{a},\boldsymbol{b}\in\mathbb{R}^n$$



• Euclidean Length

$$\|\mathbf{a}\|_{2} = \left[\sum_{i=1}^{m} a_{i}^{2}\right]^{\frac{1}{2}}$$

$$\|\mathbf{a}\| \ge 0 \ \forall \ \mathbf{a}$$

$$\|\mathbf{a} + \mathbf{b}\| \le \|\mathbf{a}\| + \|\mathbf{b}\|$$

$$\|\alpha \cdot \mathbf{b}\| \le |\alpha| \|\mathbf{b}\|$$

• p-norm

$$\|\boldsymbol{a}\|_p = \left[\sum_{i=1}^m a_i^p\right]^{\frac{1}{p}}$$



• The <u>span</u> of a set of vectors:

$$\operatorname{span}\{\boldsymbol{a_1},\boldsymbol{a_2},\ldots,\boldsymbol{a_k}\} = \left\{\alpha_1\boldsymbol{a_1} + \alpha_2\boldsymbol{a_2} + \cdots + \alpha_k\boldsymbol{a_k} \middle| \alpha_k \in \mathbb{R}, \; \boldsymbol{a_k} \in \mathbb{R}^n\right\}$$

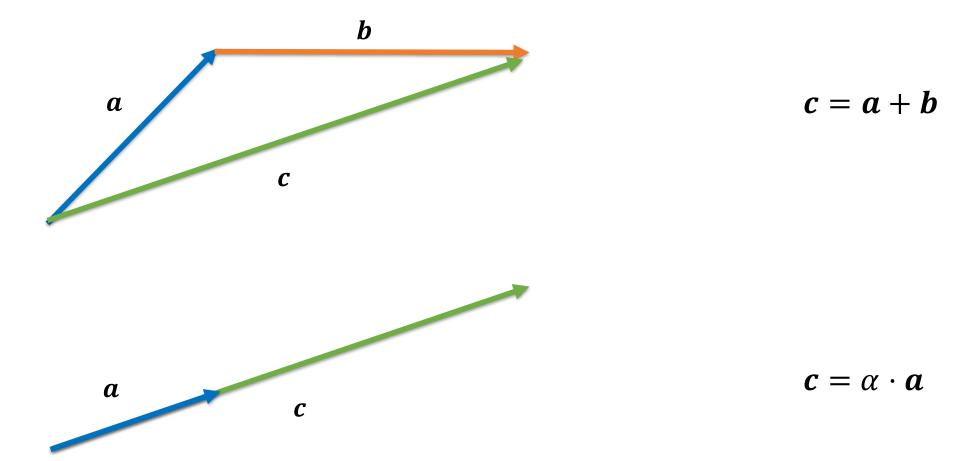
• <u>Linear independence</u>:

$$\alpha_1 \boldsymbol{a_1} + \alpha_2 \boldsymbol{a_2} + \dots + \alpha_k \boldsymbol{a_k} = \boldsymbol{0} \Rightarrow \alpha_i = 0, \forall i$$

• How does k compare to n, the vector dimension?

$$k \leq n$$



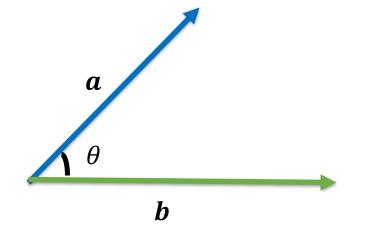


Mathematician's 'parallel for all do'



• Inner product

$$\boldsymbol{a}^T \boldsymbol{b} = \sum_i a_i b_i = \|\boldsymbol{a}\| \cdot \|\boldsymbol{b}\| \cdot \cos \theta$$



Orthogonality

$$\boldsymbol{a}^T\boldsymbol{b} = \sum_i a_i b_i = 0$$

• If we have two vectors that are orthogonal with a third, their linear combination is, too.



• Matrix in m, n-dimensions: $A \in \mathbb{R}^{m \times n}$:

$$\mathbf{A} = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mn} \end{bmatrix}$$

• <u>Transpose</u> of matrix:

$$\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} A_{11} & \cdots & A_{m1} \\ \vdots & \ddots & \vdots \\ A_{1n} & \cdots & A_{mn} \end{bmatrix} \in \mathbb{R}^{n \times m}$$

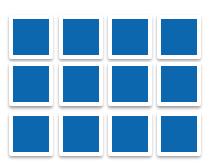
$$(\boldsymbol{A} + \boldsymbol{B})^T = \boldsymbol{A}^T + \boldsymbol{B}^T, \forall \boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{m \times n}$$



• Simple operations

$$C = A + B$$
 where $C_{ij} = A_{ij} + B_{ij}$
 $C = \alpha \cdot B$ where $C_{ij} = \alpha B_{ij}$

$$C = \sin A \text{ where } C_{ij} = \sin A_{ij}$$





- Some properties of matrix addition:
 - Commutative:

$$A + B = B + A$$
, $A, B \in \mathbb{R}^{m \times n}$

• Associative:

$$(A + B) + C = A + (B + C),$$
 $A, B, C \in \mathbb{R}^{m \times n}$

• <u>Distibutive</u>:

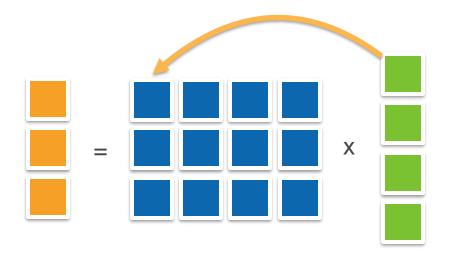
$$\alpha(\mathbf{A} + \mathbf{B}) = \alpha \mathbf{A} + \alpha \mathbf{B}, \qquad \mathbf{A}, \mathbf{B} \in \mathbb{R}^{m \times n}$$



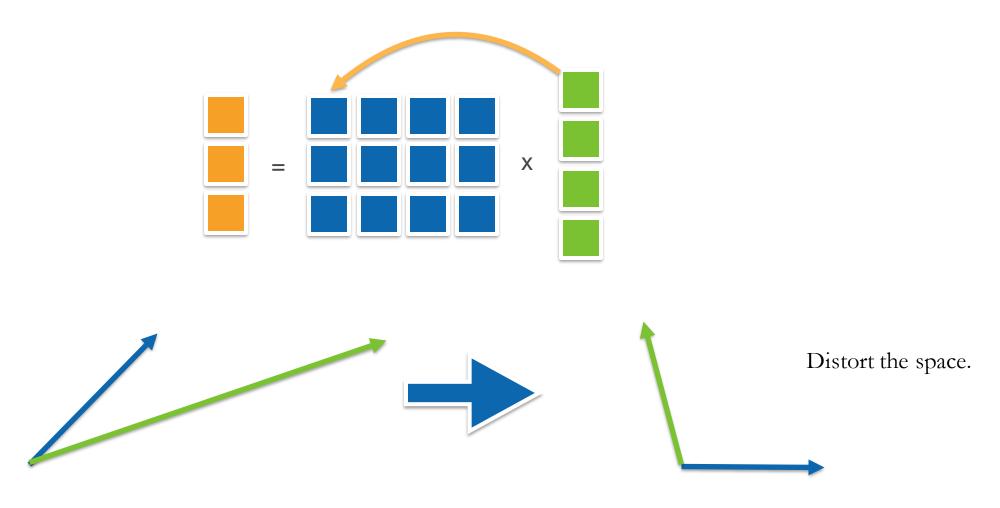


• Multiplications (matrix-vector), c = Ab, $c \in \mathbb{R}^m$, $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^n$

$$\begin{bmatrix} c_1 \\ \cdots \\ c_m \end{bmatrix} = \mathbf{c} = \mathbf{A}\mathbf{b} = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \cdots \\ b_n \end{bmatrix} \text{ where } c_i = \sum_{j=1}^n A_{ij}b_j$$



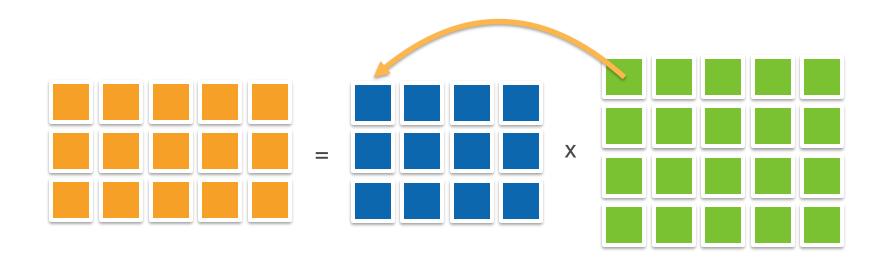






• Multiplications (matrix-matrix) C = AB, $C \in \mathbb{R}^{m \times p}$, $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$

$$\begin{bmatrix} C_{11} & \cdots & C_{1p} \\ \vdots & \ddots & \vdots \\ C_{m1} & \cdots & C_{mp} \end{bmatrix} = \mathbf{C} = \mathbf{A}\mathbf{B} = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} B_{11} & \cdots & A_{1p} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & A_{np} \end{bmatrix} \text{ where } C_{ik} = \sum_{j=1}^{n} A_{ij} B_{jk}$$





- Some properties of matrix multiplication:
 - Non-commutative!

$$AB \neq BA$$

• Associative:

$$(AB)C = A(BC), \qquad \forall A, B, C$$

 $\alpha(AB) = (\alpha A)B, \qquad \forall A, B$

• <u>Distibutive</u>:

$$A(B+C)=AB+AB, \forall A,B,C$$

• Transpose:

$$(AB)^T = B^T A^T$$

Matrix



• Norm

$$\|\mathbf{A}\| = \sup \left\{ \frac{\|\mathbf{A}\mathbf{x}\|_p}{\|\mathbf{x}\|_p}, \forall \mathbf{x} \neq 0 \right\}$$

- Interpretation: how much can the mapping induced by A can stretch vectors?
- Choices depend on how to measure the length of vectors:
- Popular norms
 - Frobenius norm (p=2):

$$||A||_{Frob} = \left[\sum_{ij} A_{ij}^2\right]^{\frac{1}{2}}$$

• Max norm ($p=\infty$):

$$||A||_{Max} = \max |a_{ij}|$$

Matrix



- Eigenvectors and egienvalue
 - Vectors that are not changed by the matrix (\boldsymbol{x} is the vector, $\boldsymbol{\lambda}$ is the eginvalue):

$$Ax = \lambda x$$



• For symmetric matrices, we can always find the eigenvalue and eigenvector.

Special Matrices $A \in \mathbb{R}^{n \times n}$



• Symmetric matrix: $A^T = A$

$$A_{ij} = A_{ji}$$

• Antisymmetric matrix: $A^T = -A$

$$A_{ij} = -A_{ji}$$

• Positive definite:

$$x^T A x \ge 0, \quad \forall x$$





- Orthogonal Matrices:
 - All rows of the matrix are orthogonal to each other;
 - All rows of the matrix have unit length.

$$\sum_{j} U_{ij} U_{kj} = \delta_{ik}$$

• Rewrite in matrix form:

$$UU^T = I$$

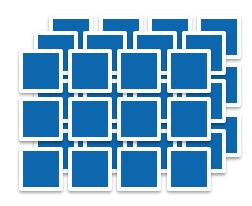
- Permutation Matrices:
 - There is only one 1 in each row or column:

$$P_{ij} = \begin{cases} 1 & if \ and \ only & if \ j = \pi(i) \\ 0. & otherwise \end{cases}$$

Tensor



- A tensor is a collection of numbers labelled by indices.
- The rank of a tensor is the number of indices required to specify an entry in the tensor:
 - A vector is a rank–1 tensor;
 - A matrix is a rank–2 tensor.



Tensor



- Einstein summation convention:
 - Each index can appear at most twice in any term.
 - Repeated indices are implicitly summed over.
 - Each term must contain identical non-repeated indices.

$$M_{ij}v_j \equiv \sum_i M_{ij}v_j$$



Matrix multiplication between matrix M and vector v

$$M_{ij}u_jv_j$$



The index j appears three times in the first term.

$$T_{ijk}u_k + M_{ip}$$



The first term contains the non-repeated index j whereas the second term contains p.



Tensors in PyTorch





• Tensors are the central data abstraction in PyTorch.

Code	Output				
<pre>import torch import math</pre>	<pre><class 'torch.tensor'=""> tensor([[-1.9609e-04, 4.5654e-41, 4.4115e-04, 0.0000e+00], [8.0387e+26, 4.5654e-41, 8.9824e-06, 0.0000e+00], [1.3431e-14, 0.0000e+00, 0.0000e+00, 0.0000e+00]])</class></pre>				
<pre>x = torch.empty(3, 4) print(type(x)) print(x)</pre>	[1.54516-14, 0.00006+00, 0.00006+00]])				





Code	Output				
<pre>import torch import math x = torch.empty(3, 4) print(type(x)) print(x)</pre>	<pre><class 'torch.tensor'=""> tensor([[-1.9609e-04, 4.5654e-41, 4.4115e-04, 0.0000e+00], [8.0387e+26, 4.5654e-41, 8.9824e-06, 0.0000e+00], [1.3431e-14, 0.0000e+00, 0.0000e+00, 0.0000e+00]])</class></pre>				

- Create a tensor using one of the numerous factory methods attached to the torch module.
- The tensor itself is 2-dimensional, having 3 rows and 4 columns.
- The type of the object returned is torch. Tensor, which is an alias for torch. Float Tensor; by default, PyTorch tensors are populated with 32-bit floating point numbers.
- You will probably see some random-looking values when printing your tensor.
- The torch.empty() call allocates memory for the tensor, but does not initialize it with any values.
- What you're seeing is whatever was in memory at the time of allocation.





• Initialize your tensor with some value.

Code	Output
<pre>zeros = torch.zeros(2, 3) print(zeros)</pre>	tensor([[0., 0., 0.],
<pre>ones = torch.ones(2, 3) print(ones)</pre>	[1., 1., 1.]]) tensor([[0.3126, 0.3791, 0.3087],
<pre>torch.manual_seed(1729) random = torch.rand(2, 3) print(random)</pre>	





• Manually setting your random number generator's seed assures reproducibility.

Code	Output
torch.manual_seed(1729)	tensor([[0.3126, 0.3791, 0.3087],
<pre>random1 = torch.rand(2, 3)</pre>	[0.0736, 0.4216, 0.0691]])
<pre>print(random1)</pre>	tensor([[0.2332, 0.4047, 0.2162],
	[0.9927, 0.4128, 0.5938]])
<pre>random2 = torch.rand(2, 3)</pre>	tensor([[0.3126, 0.3791, 0.3087],
<pre>print(random2)</pre>	[0.0736, 0.4216, 0.0691]])
	tensor([[0.2332, 0.4047, 0.2162],
torch.manual_seed(1729)	[0.9927, 0.4128, 0.5938]])
<pre>random3 = torch.rand(2, 3)</pre>	
<pre>print(random3)</pre>	
<pre>random4 = torch.rand(2, 3) print(random4)</pre>	





- A pseudorandom number generator is a *deterministic* random bit generator:
 - An algorithm for generating a sequence of numbers whose properties approximate the properties of sequences of random numbers.
 - The generated sequence is not truly random, it is completely determined by an initial value.

TORCH.MANUAL_SEED

torch.manual_seed(seed) [SOURCE]

Sets the seed for generating random numbers. Returns a torch.Generator object.

Parameters

seed (*int*) – The desired seed. Value must be within the inclusive range [-ox8000_0000_0000_0000, oxffff_ffff_ffff_fffff]. Otherwise, a RuntimeError is raised. Negative inputs are remapped to positive values with the formula oxffff_ffff_fffff_fffff+seed.

Return type

Generator



Creating Tensors

• torch.shape contains a list of the extent of each dimension of a tensor.

Code	Output
<pre>x = torch.empty(2, 2, 3) print(x.shape)</pre>	torch.Size([2, 2, 3])
empty_like_x =	torch.Size([2, 2, 3])
<pre>torch.empty_like(x) print(empty_like_x.shape)</pre>	torch.Size([2, 2, 3])
<pre>zeros_like_x = torch.zeros_like(x)</pre>	torch.Size([2, 2, 3])
<pre>print(zeros_like_x.shape)</pre>	torch.Size([2, 2, 3])
<pre>ones_like_x = torch.ones_like(x)</pre>	
<pre>print(ones_like_x.shape)</pre>	
<pre>rand_like_x = torch.rand_like(x)</pre>	
<pre>print(rand_like_x.shape)</pre>	





• Create a tensor by specifying its data directly from a Python collection.

Code	Output
<pre>some_constants = torch.tensor([[3.1415926, 2.71828], [1.61803, 0.0072897]]) print(some_constants) some_integers = torch.tensor((2, 3, 5, 7, 11, 13, 17, 19)) print(some_integers) more_integers = torch.tensor(((2, 4, 6), [3, 6, 9])) print(more_integers)</pre>	tensor([[3.1416, 2.7183],





• Setting the datatype of a tensor.

Code	Output
<pre>a = torch.ones((2, 3), dtype=torch.int16) print(a)</pre>	<pre>tensor([[1, 1, 1],</pre>
<pre>b = torch.rand((2, 3), dtype=torch.float64) * 20. print(b)</pre>	tensor([[0, 1, 5], [11, 11, 11]], dtype=torch.int32)
<pre>c = b.to(torch.int32) print(c)</pre>	





- Available data types include:
 - torch.bool
 - torch.int8
 - torch.uint8
 - torch.int16
 - torch.int32
 - torch.int64
 - torch.half
 - torch.float
 - torch.double
 - torch.bfloat

32-bit floating point	torch.float32 or torch.float	torch.FloatTensor	torch.cuda.FloatTensor
64-bit floating point	torch.float64 or torch.double	torch.DoubleTensor	torch.cuda.DoubleTensor
16-bit floating point 1	torch.float16 or torch.half	torch.HalfTensor	torch.cuda.HalfTensor
16-bit floating point 2	torch.bfloat16	torch.BFloat16Tensor	torch.cuda.BFloat16Tenso

8-bit integer (unsigned)	torch.uint8	torch.ByteTensor	torch.cuda.ByteTensor
8-bit integer (signed)	torch.int8	torch.CharTensor	torch.cuda.CharTensor
16-bit integer (signed)	torch.int16 or torch.short	torch.ShortTensor	torch.cuda.ShortTensor
32-bit integer (signed)	torch.int32 or torch.int	torch.IntTensor	torch.cuda.IntTensor
64-bit integer (signed)	torch.int64 or torch.long	torch.LongTensor	torch.cuda.LongTensor





• Basic arithmetic: how tensors interact with simple scalars.

Code	Output		
ones = $torch.zeros(2, 2) + 1$	tensor([[1., 1.],		
twos = torch.ones $(2, 2) * 2$	[1., 1.]])		
threes = $(torch.ones(2, 2) * 7$	tensor([[2., 2.],		
- 1) / 2	[2., 2.]])		
fours = twos ** 2	tensor([[3., 3.],		
sqrt2s = twos ** 0.5	[3., 3.]])		
	tensor([[4., 4.],		
<pre>print(ones)</pre>	[4., 4.]])		
<pre>print(twos)</pre>	tensor([[1.4142, 1.4142],		
<pre>print(threes)</pre>	[1.4142, 1.4142]])		
<pre>print(fours)</pre>			
<pre>print(sqrt2s)</pre>			





• Basic arithmetic operations between two tensors.

Code	Output
<pre>powers2 = twos ** torch.tensor([[1, 2], [3, 4]]) print(powers2)</pre>	tensor([[2., 4.],
<pre>fives = ones + fours print(fives)</pre>	tensor([[12., 12.], [12., 12.]])
<pre>dozens = threes * fours print(dozens)</pre>	





- Tensor broadcasting:
 - Perform an operation between tensors that have similarities in their shapes;
 - E.g., a common example:
 - Multiply a tensor of learning weights by a batch of input tensors;
 - Apply the operation to each instance in the batch separately;
 - Return a tensor of identical shape.
- Four rule for broadcasting:
 - Each tensor must have at least one dimension (no empty tensors).
 - Comparing the dimension sizes of the two tensors, going from last to first.
 - Each dimension must be equal, or
 - One of the dimensions must be of size 1, or
 - The dimension does not exist in one of the tensors.





• Examples allow broadcasting.

Code	Output		
a = torch.ones(4, 3, 2)	tensor([[[0.6493, 0.2633], [0.4762, 0.0548], [0.2024, 0.5731]],	tensor([[[0.7191, 0.7191], [0.4067, 0.4067], [0.7301, 0.7301]],	tensor([[[0.6276, 0.7357], [0.6276, 0.7357], [0.6276, 0.7357]],
<pre># 3rd & 2nd dims identical to a, dim 1 absent b = a * torch.rand(3, 2)</pre>	[[0.6493, 0.2633], [0.4762, 0.0548], [0.2024, 0.5731]],	[[0.7191, 0.7191], [0.4067, 0.4067], [0.7301, 0.7301]],	[[0.6276, 0.7357], [0.6276, 0.7357], [0.6276, 0.7357]],
<pre>print(b)</pre>	[[0.6493, 0.2633], [0.4762, 0.0548], [0.2024, 0.5731]],	[[0.7191, 0.7191], [0.4067, 0.4067], [0.7301, 0.7301]],	[[0.6276, 0.7357], [0.6276, 0.7357], [0.6276, 0.7357]],
<pre># 3rd dim = 1, 2nd dim identical to a c = a * torch.rand(3, 1)</pre>	[[0.6493, 0.2633], [0.4762, 0.0548], [0.2024, 0.5731]]])	[[0.7191, 0.7191], [0.4067, 0.4067], [0.7301, 0.7301]]])	[[0.6276, 0.7357], [0.6276, 0.7357], [0.6276, 0.7357]]])
print(c) # 2nd dim identical to a 2nd			
<pre># 3rd dim identical to a, 2nd dim = 1 d = a * torch.rand(1, 2)</pre>			
print(d)			





• Examples attempt at broadcasting that will fail.

```
Code
a = torch.ones(4, 3, 2)
b = a * torch.rand(4, 3) # dimensions must match last-to-first
c = a * torch.rand( 2, 3) # both 3rd & 2nd dims different
d = a * torch.rand((0, )) # can't broadcast with an empty tensor
```





- Most binary operations on tensors will return a third, new tensor that takes a region of memory distinct from the other tensors.
- Most of the math functions have a version with an appended underscore (_) that will alter a tensor in place.

```
Code
a = torch.tensor([0, math.pi / 4, math.pi / 2, 3 * math.pi / 4])
print('a:')
print(a)
print(torch.sin(a))
                     # this operation creates a new tensor in memory
print(a)
                     # a has not changed
b = torch.tensor([0, math.pi / 4, math.pi / 2, 3 * math.pi / 4])
print('\nb:')
print(b)
print(torch.sin (b)) # note the underscore
print(b)
                     # b has changed
```





• Set up an out argument to specify a tensor to receive the output. If the out tensor is the correct shape and dtype, this can happen without a new memory allocation.

	Code	Output
<pre>a = torch.rand(2, 2) b = torch.rand(2, 2) c = torch.zeros(2, 2) old_id = id(c) print(c) d = torch.matmul(a, b, print(c)</pre>	out=c) # contents of c have changed	tensor([[0., 0.],
	<pre># test c & d are same object, not just containing equal values # make sure that our new c is the same object as the old one</pre>	
<pre>print(c)</pre>	<pre># works for creation too! # c has changed again # still the same object!</pre>	





- As with any object in Python, assigning a tensor to a variable makes the variable a label of the tensor, and does not copy it.
- If you want a separate copy of the data to work on? The clone() method is there for you.

	Code	Output
<pre>a = torch.ones(2, 2) b = a.clone()</pre>		<pre>tensor([[True, True],</pre>
	<pre># different objects in memory #but still with the same contents!</pre>	[1., 1.]])
a[0][1] = 561 print(b)	<pre># a changes #but b is still all ones</pre>	





- Define string or torch device handle to move the tensor to GPU.
- To do computation involving two or more tensors, all of the tensors must be on the *same* device.

Code	Output
<pre>if torch.cuda.is_available(): my_device = torch.device('cuda') x = torch.rand(2, 2, device='cuda') print(gpu rand)</pre>	tensor([[0.3344, 0.2640],
else: my_device = torch.device('cpu') print('Device: {}'.format(my_device))	tensor([[0.0024, 0.6778],
<pre>y = torch.rand(2, 2, device=my_device) print(y)</pre>	





 $\texttt{torch.squeeze(}\textit{input,dim=None)} \rightarrow \texttt{Tensor}$

Returns a tensor with all specified dimensions of input of size 1 removed.

For example, if input is of shape: $(A \times 1 \times B \times C \times 1 \times D)$ then the input.squeeze() will be of shape: $(A \times B \times C \times D)$.

When dim is given, a squeeze operation is done only in the given dimension(s). If input is of shape: $(A \times 1 \times B)$, squeeze(input, 0) leaves the tensor unchanged, but squeeze(input, 1) will squeeze the tensor to the shape $(A \times B)$.

• NOTE

The returned tensor shares the storage with the input tensor, so changing the contents of one will change the contents of the other.

• WARNING

If the tensor has a batch dimension of size 1, then *squeeze(input)* will also remove the batch dimension, which can lead to unexpected errors. Consider specifying only the dims you wish to be squeezed.

The squeeze() method has the in-place versions squeeze_().

Manipulating Tensor Shapes - Unsqueeze



```
torch.unsqueeze(\textit{input}, \textit{dim}) \rightarrow \mathsf{Tensor}
```

Returns a new tensor with a dimension of size one inserted at the specified position.

The returned tensor shares the same underlying data with this tensor.

A dim value within the range [-input.dim() - 1, input.dim() + 1) can be used. Negative dim will correspond to unsqueeze() applied at dim = dim + input.dim() + 1.

Parameters

- **input** (*Tensor*) the input tensor.
- **dim** (*int*) the index at which to insert the singleton dimension

The unsqueeze() method has the in-place versions unsqueeze_().

Manipulating Tensor Shapes - Reshape



torch.reshape(input, shape) → Tensor

Returns a tensor with the same data and number of elements as input, but with the specified shape. When possible, the returned tensor will be a view of input. Otherwise, it will be a copy. Contiguous inputs and inputs with compatible strides can be reshaped without copying, but you should not depend on the copying vs. viewing behavior.

See torch.Tensor.view() on when it is possible to return a view.

A single dimension may be -1, in which case it's inferred from the remaining dimensions and the number of elements in input.

Parameters

- **input** (*Tensor*) the tensor to be reshaped
- shape (tuple of int) the new shape

reshape() will return a *view* on the tensor to be changed: a separate tensor object looking at the same underlying region of memory. That means any change made to the source tensor will be reflected in the view on that tensor, unless you clone() it.

References



- https://d2l.ai/
- https://www.dr-qubit.org/teaching/summation_delta.pdf
- https://pytorch.org/tutorials/beginner/introyt/tensors_deeper_tutorial.html