CSC 561: Neural Networks and Deep Learning

Preliminaries

Marco Alvarez

Department of Computer Science and Statistics
University of Rhode Island

Spring 2024

Linear Algebra

Subset of most relevant concepts to Deep Learning

Credit: Deep Learning by Ian Goodfellow, Yoshua Bengio, Aaron Courville

Scalars and vectors

- Scalars
  - integers, real numbers, rational numbers, etc.
  - usually denoted by lowercase letters
- Vectors
  - 1-D array of elements (scalars)

$$\mathbf{x} \in \mathbb{R}^n \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Norms

- Functions that measure the magnitude ("length") of a vector
  - strictly positive, except for the zero vector
  - think about the distance between zero and the point represented by the vector

$$f(\mathbf{x}) = 0 \Rightarrow \mathbf{x} = \mathbf{0}$$
$$f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y}) \text{ (triangle inequality)}$$
$$\forall \alpha \in \mathbb{R}, f(\alpha \mathbf{x}) = |\alpha| f(\mathbf{x})$$

Norms

ℓ_1-norm: $\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|$

ℓ_2-norm: $\|\mathbf{x}\|_2 = \left(\sum_{i=1}^{n} x_i^2 \right)^{\frac{1}{2}}$

max norm: $\|\mathbf{x}\|_\infty = \max_i |\mathbf{x}_i|$

Matrices and tensors

- Matrices
  - 2-D array of elements

$$\begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} \quad A \in \mathbb{R}^{m \times n}$$

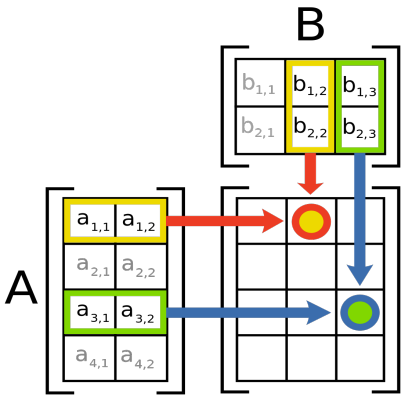
- Tensors
  - homogeneous arrays that may have zero (scalar) or more dimensions

Basics

- Matrix Multiplication

$C = AB$

$C_{i,j} = \sum_k A_{i,k} B_{k,j}$



Number of columns in A must be equal to the number of rows in B

https://en.wikipedia.org/wiki/Matrix_multiplication

Dot product

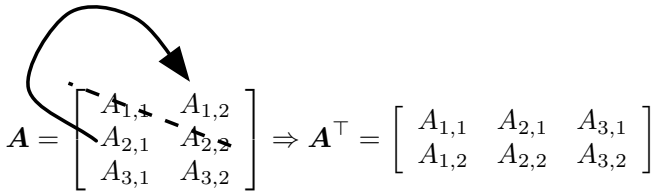
$$[x_1 \quad x_2 \quad \dots \quad x_n] \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$\mathbf{x}^T\mathbf{y} = \sum_{i=1}^{n} x_i y_i$

$\mathbf{x}^T\mathbf{y} = \|\mathbf{x}\| \|\mathbf{y}\| \cos\theta$

$\mathbf{x}^T\mathbf{y} \in \mathbb{R}$

Matrix transpose



$$\left(A^T\right)_{i,j} = A_{j,i} \qquad (AB)^T = B^T A^T$$

Identity matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\forall x \in \mathbb{R}^n, I_n x = x$$

$$A^{-1}A = I_n$$

Special matrices and vectors

- Unit vector

$$\|\mathbf{x}\|_2 = 1$$

- Symmetric matrix

$$A = A^T$$

- Orthogonal matrix

$$A^T A = AA^T = I$$
$$A^{-1} = A^T$$

Programming with Tensors

Non-negotiable (Python)

- Basic data types
  - booleans, integers, floating point values, strings
- Control flow
- Built-in data structures
  - lists, tuples, dictionaries, sets
  - iterators
- Functions
  - functions can be assigned, passed, returned, and stored
  - lambda functions (inline and anonymous)
- Classes

Numpy

- Library for scientific computing
  - provides a high-performance multidimensional array object and routines for fast operations on these arrays
- The `ndarray` object encapsulates n-dimensional arrays of homogeneous data types
  - many operations performed in compiled code for higher performance
  - have a fixed size at creation
    - changing the size of an ndarray will create a new array and delete the original


```
n = 100000000
array1 = np.random.rand(n)
array2 = np.random.rand(n)
```

```
def dot_python(x, y):
    sum = 0
    for i in range(len(x)):
        sum += x[i] * y[i]
    return sum

def dot_numpy(x, y):
    return np.dot(x, y)
```

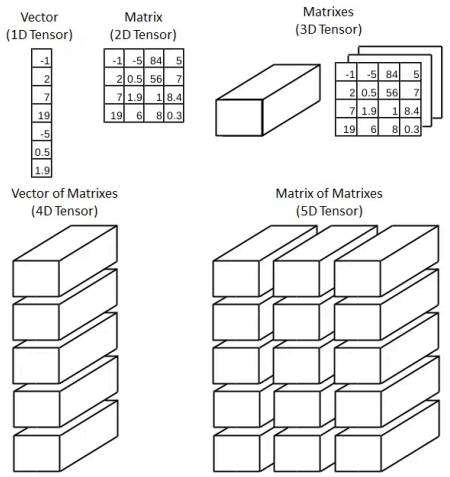
```
time_taken = timeit.timeit(lambda: dot_numpy(array1, array2), number=1)
print(f'Numpy Time: {time_taken} seconds')
```

```
Numpy Time: 0.05994947799996453 seconds
```

```
array1 = array1.tolist()
array2 = array2.tolist()
time_taken = timeit.timeit(lambda: dot_python(array1, array2), number=1)
print(f'Python Time: {time_taken} seconds')
```

```
Python Time: 8.325287125999978 seconds
```


Tensors



https://towardsdatascience.com/deep-learning-introduction-to-tensors-tensorflow-36ce3663528f

The following figures are from:

"*NumPy Illustrated: The Visual Guide to NumPy*" by Lev Maximov

https://betterprogramming.pub/numpy-illustrated-the-visual-guide-to-numpy-3b1d4976de1d

Elegant code

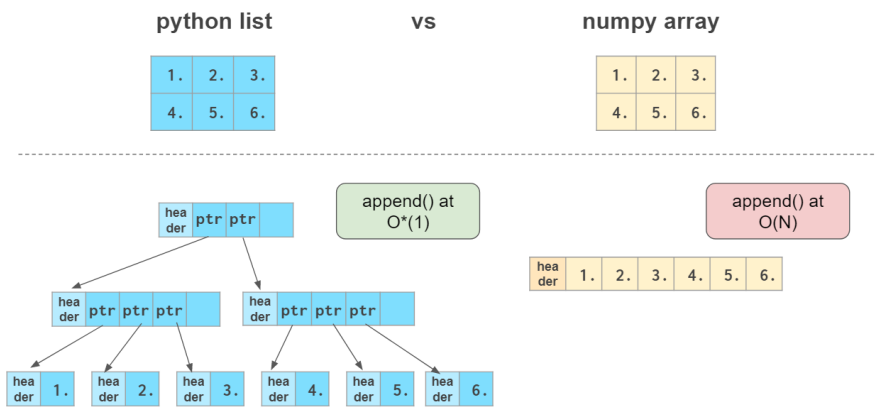
```
In [3]: a = [1, 2, 3]
        [q*2 for q in a]
Out[3]: [2, 4, 6]
```

```
In [4]: a = np.array([1, 2, 3])
        a * 2
Out[4]: array([2, 4, 6])
```

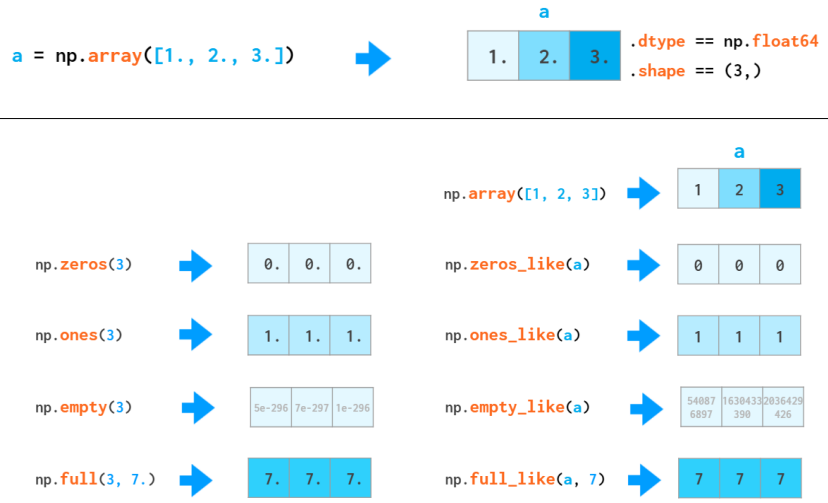
```
In [1]: a = [1, 2, 3]
        b = [4, 5, 6]
        [q+r for q, r in zip(a, b)]
Out[1]: [5, 7, 9]
```

```
In [2]: a = np.array([1, 2, 3])
        b = np.array([4, 5, 6])
        a + b
Out[2]: array([5, 7, 9])
```

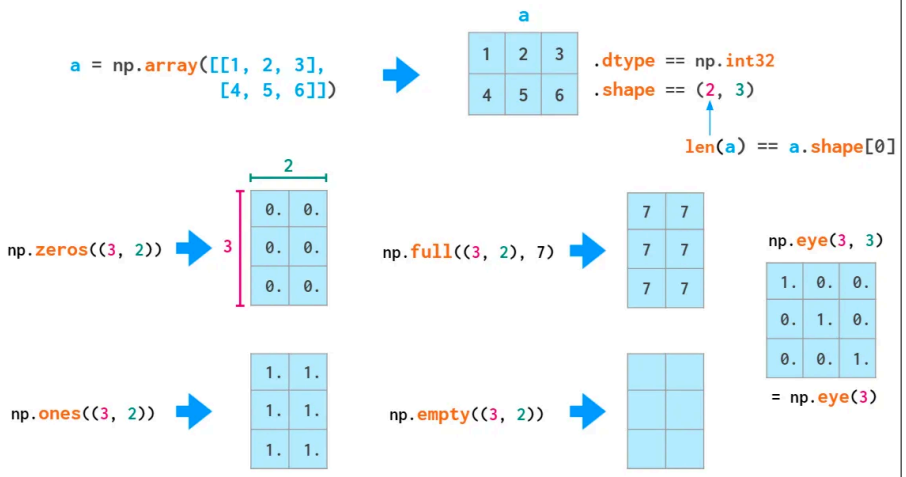

Homogeneous and fixed-length



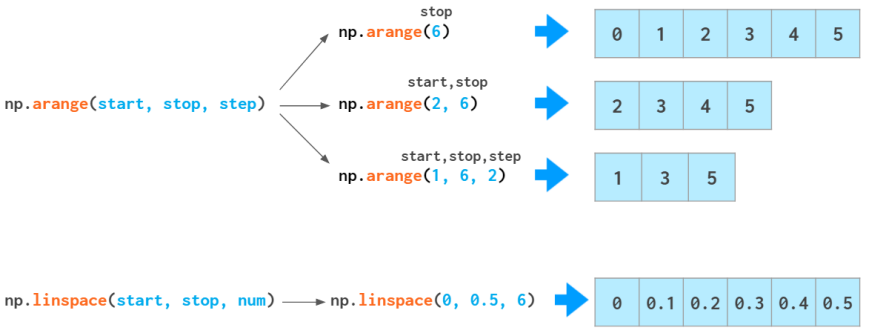
Creating numpy arrays



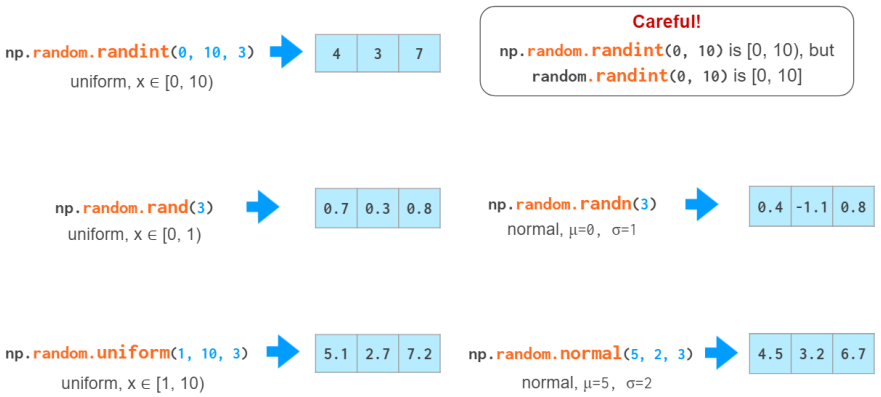
Creating numpy arrays



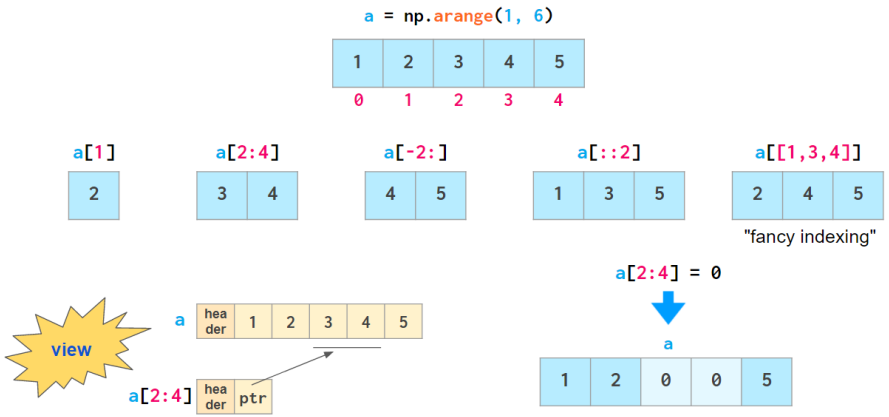
Creating numpy arrays



Creating numpy arrays



Indexing

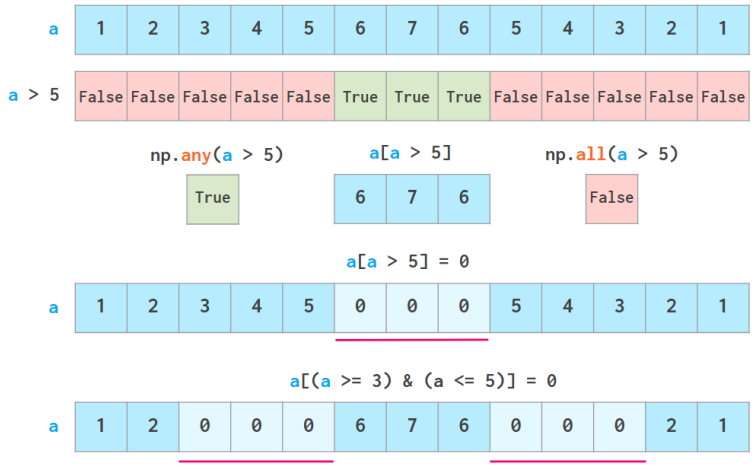


Careful when making copies

python list vs numpy array

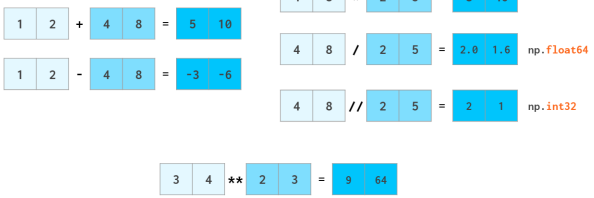
```
a = [1, 2, 3]                a = np.array([1, 2, 3])
b = a          # no copy     b = a          # no copy
c = a[:]       # copy        c = a[:]       # no copy!!!
d = a.copy() # copy          d = a.copy() # copy
```


Boolean indexing

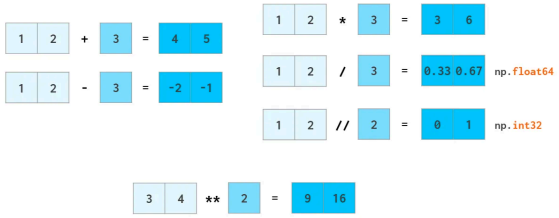


Vector operations

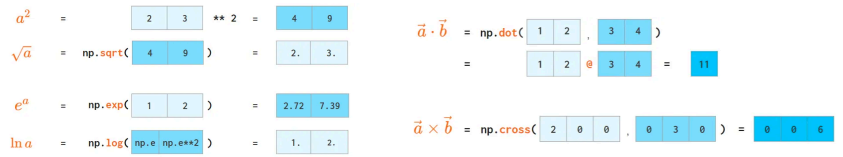
Element-wise operations

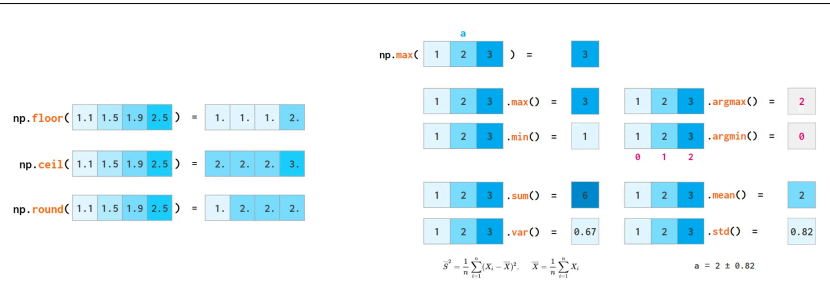


Broadcasting scalars

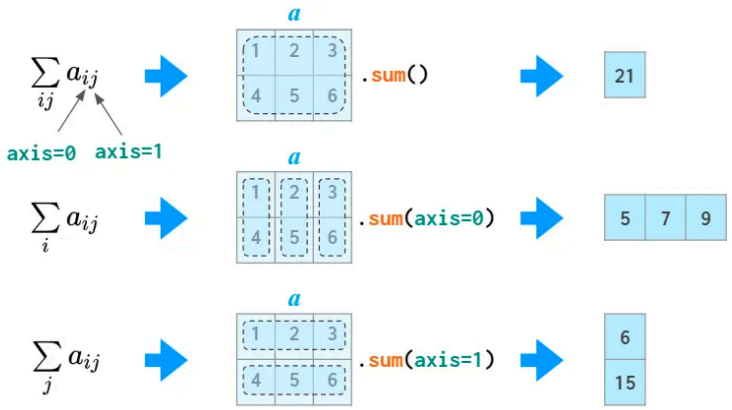


Math functions



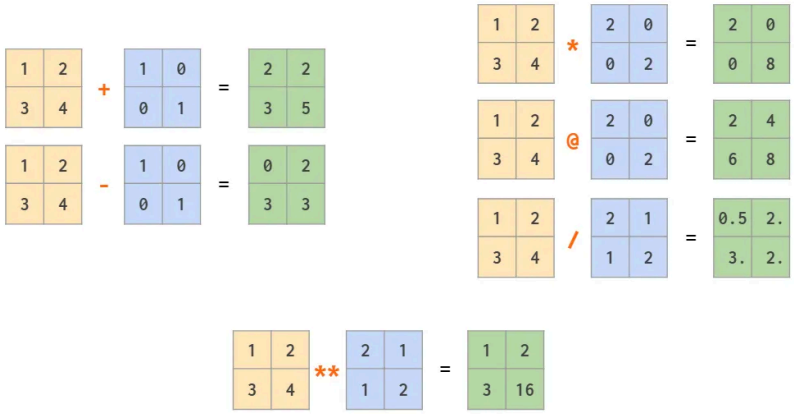


The axis



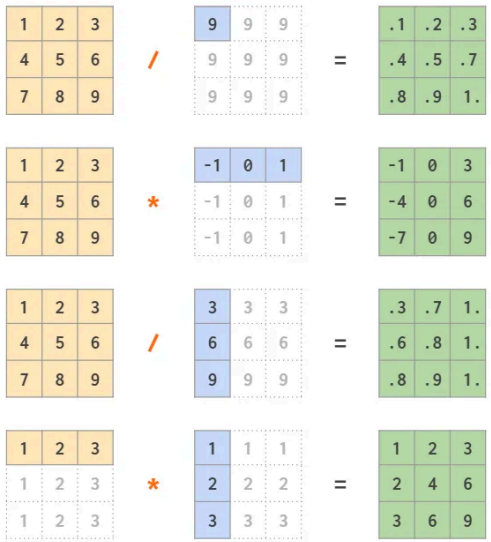
By specifying the **axis** parameter you can apply an operation along the specified axis of an array

Matrix operations



Not every operator or operation in NumPy is element-wise

Broadcasting



General broadcasting rules

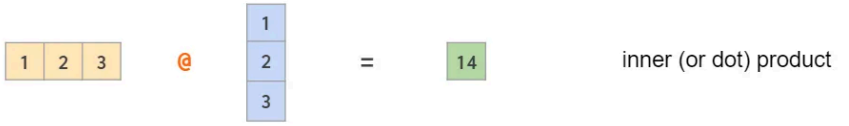
- Numpy follows a set of rules to determine how the smaller array is **broadcasted** to match the shape of the larger array
  - start with the rightmost dimension and work backwards
  - two dimensions are compatible if they are equal, or one of them is 1
    - otherwise throw a ValueError exception: "operands could not be broadcast together"
  - if the arrays have a different number of dimensions, pad the smaller array's shape with ones on its left
- Resulting array will have the same number of dimensions as the input array with the greatest number of dimensions
  - the size of each dimension is the largest size of the corresponding dimension among the input arrays

Practice

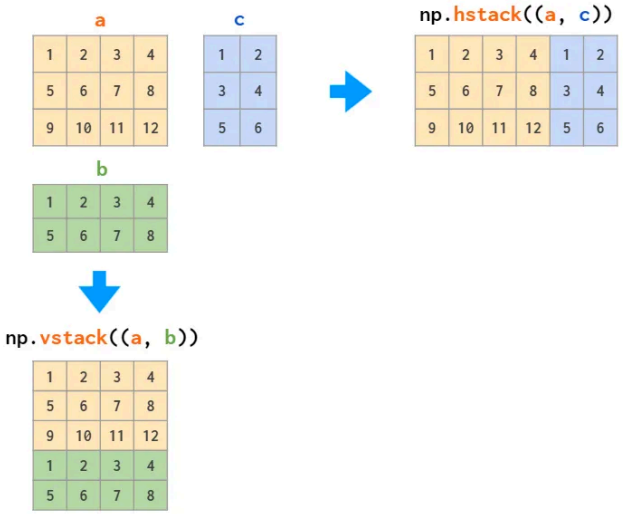
Arrays	Result
8 x 1 x 6 x 1 7 x 1 x 5	8 x 7 x 6 x 5
5 x 4 1	5 x 4
5 x 4 4	5 x 4
15 x 3 x 5 15 x 1 x 5	15 x 3 x 5
15 x 3 x 5 3 x 5	15 x 3 x 5
15 x 3 x 5 3 x 1	15 x 3 x 5
3 4	mistmatch
2 x 1 8 x 4 x 3	mismatch

Arrays	Result
4 x 3 3	
5 x 4 x 3 1 x 3	
8 x 1 x 6 7 x 1	
5 x 2 5	
3 x 1 3 x 5	
2 x 4 x 1 8	
6 x 3 3 x 1	
3 x 5 x 2 3	

Must know your shapes …



Concatenation



Practice

- Task
  - **MSE loss** for a batch of predictions and corresponding ground truth labels

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- Input
  - predictions (batch_size, num_outputs)
  - ground_truth (batch_size, num_outputs)
- Output
  - scalar value representing the average MSE across the batch
- Hint
  - element-wise subtraction followed by squaring and averaging

Practice

- Task
  - **softmax** for a batch of input vectors
- Input
  - input_vectors (batch_size, num_inputs)
- Output
  - output_vectors(batch_size, num_inputs)
- Hint
  - consider numerical instability (behavior of the exponential with very small and very large numbers)
    - subtract the max of each input vector
  - make it efficient by using broadcasting
    - may need `keepdims=True`

$$\frac{e^{x_i}}{\sum_{j=1}^{d} e^{x_j}}$$

$$\begin{bmatrix}1\\2\\3\\4\\5\end{bmatrix} \Rightarrow \begin{bmatrix}0.0117\\0.0317\\0.0861\\0.2341\\0.6364\end{bmatrix}$$

Practice

- Task
  - given N data points, find the nearest neighbor to a query data point
- Input:
  - input vector (vector_dim)
  - data (num_vectors, vector_dim)
- Output:
  - nearest_neighbor_idx (scalar)
- Hint:
  - calculate the euclidean distance
  - use vectorized and broadcasting operations

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}$$