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Top 10 Matrix Operations in Numpy with Examples

Perform Linear Algebra with Python



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About 30–40% of the mathematical knowledge required for Data Science and

Machine Learning comes from linear algebra. Matrix operations play a significant role in linear algebra. Today, we discuss 10 of such matrix operations with the help of the powerful numpy library. Numpy is generally used to perform numerical calculations in Python. It also has special classes and sub-packages for matrix operations. The use of vectorization allows numpy to perform matrix operations more efficiently by avoiding many for loops.

I will include the meaning, background description and code examples for each matrix operation discussing in this article. The “Key Takeaways” section at the end of this article will provide you with some more specific facts and a brief summary of matrix operations. So, make sure to read that section as well.

I will discuss each matrix operation in the following order. Here is the list of the top 10 matrix operations I have chosen for you carefully.

1. Inner product
2. Dot product
3. Transpose
4. Trace
5. Rank
6. Determinant
7. True inverse
8. Pseudo inverse
9. Flatten
10. Eigenvalues and eigenvectors

Prerequisites

To get the full advantage of this article, you should know the numpy basics and array creation methods. If you don't have that knowledge, read the following article written by me.

- [NumPy for Data Science: Part 1 \(NumPy Basics and Array Creation\)](#)

Let's get started with the first one, the *inner product*.

Inner product

The *inner product* takes two vectors of equal size and returns a single number (scalar). This is calculated by multiplying the corresponding elements in each vector and adding up all of those products. In numpy, vectors are defined as one-dimensional numpy arrays.

To get the inner product, we can use either `np.inner()` or `np.dot()`. Both give the same results. The inputs for these functions are two vectors and they should be the same size.

```
1 import numpy as np
2
3 # Vectors as 1D numpy arrays
4 a = np.array([1, 2, 3])
5 b = np.array([4, 5, 6])
6
7 print("a= ", a)
8 print("b= ", b)
9 print("\ninner:", np.inner(a, b))
10 print("dot:", np.dot(a, b))
```

[matrix_operations_in_numpy_1.py](#) hosted with ❤ by [GitHub](#)

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Wait till loading the Python code!

```
a= [1 2 3]
b= [4 5 6]

inner: 32
dot: 32
```

The inner product of two vectors (Image by author)

Dot product

The *dot product* is defined for matrices. It is the sum of the products of the corresponding elements in the two matrices. To get the dot product, the number of columns in the first matrix should be equal to the number of rows in the second matrix.

There are two ways to create matrices in numpy. The most common one is to use the numpy *ndarray class*. Here we create two-dimensional numpy arrays (ndarray

objects). The other one is to use the numpy *matrix class*. Here we create matrix objects.

The dot product of both ndarray and matrix objects can be obtained using `np.dot()`.

```
1 import numpy as np
2
3 # Matrices as ndarray objects
4 a = np.array([[1, 2], [3, 4]])
5 b = np.array([[5, 6, 7], [8, 9, 10]])
6 print("a", type(a))
7 print(a)
8 print("\nb", type(b))
9 print(b)
10
11 # Matrices as matrix objects
12 c = np.matrix([[1, 2], [3, 4]])
13 d = np.matrix([[5, 6, 7], [8, 9, 10]])
14 print("\nc", type(c))
15 print(c)
16 print("\nd", type(d))
17 print(d)
18 print("\ndot product of two ndarray objects")
19 print(np.dot(a, b))
20 print("\ndot product of two matrix objects")
21 print(np.dot(c, d))
```

Wait till loading the Python code!

```
a <class 'numpy.ndarray'>
[[1 2]
 [3 4]]

b <class 'numpy.ndarray'>
[[ 5  6  7]
 [ 8  9 10]]

c <class 'numpy.matrix'>
[[1 2]
 [3 4]]

d <class 'numpy.matrix'>
[[ 5  6  7]
 [ 8  9 10]]

dot product of two ndarray objects
[[21 24 27]
 [47 54 61]]

dot product of two matrix objects
[[21 24 27]
 [47 54 61]]
```

The dot product of two matrices (Image by author)

When multiplying two ndarray objects using the * operator, the result is the *element-by-element multiplication*. On the other hand, when multiplying two matrix objects using the * operator, the result is the *dot (matrix) product* which is equivalent to the *np.dot()* as previous.

```
1 import numpy as np
2
3 # Matrices as ndarray objects
4 a = np.array([[1, 2], [3, 4]])
5 b = np.array([[5, 6], [8, 9]])
6 print("a", type(a))
7 print(a)
8 print("\nb", type(b))
9 print(b)
10
11 # Matrices as matrix objects
12 c = np.matrix([[1, 2], [3, 4]])
13 d = np.matrix([[5, 6], [8, 9]])
14 print("\nc", type(c))
15 print(c)
16 print("\nd", type(d))
17 print(d)
18 print("\n* operation on two ndarray objects (Elementwise)")
19 print(a * b)
20 print("\n* operation on two matrix objects (same as np.dot())")
21 print(c * d)
```

Wait till loading the Python code!

```
a <class 'numpy.ndarray'>
[[1 2]
 [3 4]]

b <class 'numpy.ndarray'>
[[5 6]
 [8 9]]

c <class 'numpy.matrix'>
[[1 2]
 [3 4]]

d <class 'numpy.matrix'>
[[5 6]
 [8 9]]

* operation on two ndarray objects (Elementwise)
[[ 5 12]
 [24 36]]

* operation on two matrix objects (same as np.dot())
[[21 24]
 [47 54]]
```

Different behaviour of * operator on matrix and ndarray objects (Image by author)

Transpose

The *transpose* of a matrix is found by switching its rows with its columns. We can use `np.transpose()` function or NumPy `ndarray.transpose()` method or `ndarray.T` (a special method which does not require parentheses) to get the transpose. All give the same output.

```
1 import numpy as np
2
3 a = np.array([[1, 2], [3, 4], [5, 6]])
4 print("a = ")
5 print(a)
6
7 print("\nWith np.transpose(a) function")
8 print(np.transpose(a))
9
10 print("\nWith ndarray.transpose() method")
11 print(a.transpose())
12
13 print("\nWith ndarray.T short form")
14 print(a.T)
```

matrix operations in numpy 4.py hosted with ❤ by [GitHub](#)

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Wait till loading the Python code!

```
a =
[[1 2]
 [3 4]
 [5 6]]

With np.transpose(a) function
[[1 3 5]
 [2 4 6]]

With ndarray.transpose() method
[[1 3 5]
 [2 4 6]]

With ndarray.T short form
[[1 3 5]
 [2 4 6]]
```

Getting transpose of a matrix (Image by author)

The transpose can also be applied to a vector. However, technically, a one-dimensional numpy array cannot be transposed.

```
import numpy as np

a = np.array([1, 2, 3])
print("a = ")
print(a)
print("\na.T = ")
print(a.T)
```

```
a =
[1 2 3]

a.T =
[1 2 3]
```

Image by author

If you really want to transpose a vector, it should be defined as a two-dimensional numpy array with double square brackets.

```
import numpy as np

a = np.array([[1, 2, 3]])
print("a = ")
print(a)
print("\na.T = ")
print(a.T)
```

```
a =
[[1 2 3]]

a.T =
[[1]
 [2]
 [3]]
```

Image by author

Trace

The *trace* is the sum of diagonal elements in a square matrix. There are two methods to calculate the trace. We can simply use the `trace()` method of an ndarray object or get the diagonal elements first and then get the sum.

```
import numpy as np

a = np.array([[2, 2, 1],
              [1, 3, 1],
              [1, 2, 2]])
print("a = ")
print(a)
print("\nTrace:", a.trace())
print("Trace:", sum(a.diagonal()))
```

```
a =
[[2 2 1]
 [1 3 1]
 [1 2 2]]
```

```
Trace: 7
Trace: 7
```

Image by author

Rank

The *rank* of a matrix is the dimensions of the vector space spanned (generated) by its columns or rows. In other words, it can be defined as the maximum number of linearly independent column vectors or row vectors.

The rank of a matrix can be found using the **matrix_rank()** function which comes from the numpy *linalg* package.

```
import numpy as np

a = np.arange(1, 10)
a.shape = (3, 3)
print("a = ")
print(a)
rank = np.linalg.matrix_rank(a)
print("\nRank:", rank)
```

```
a =
[[1 2 3]
 [4 5 6]
 [7 8 9]]
```

```
Rank: 2
```

Image by author

Determinant

The *determinant* of a square matrix can be calculated **det()** function which also comes from the numpy *linalg* package. If the determinant is 0, that matrix is not invertible. It is known as a singular matrix in algebra terms.

```
import numpy as np

a = np.array([[2, 2, 1],
              [1, 3, 1],
              [1, 2, 2]])
print("a = ")
print(a)
det = np.linalg.det(a)
print("\nDeterminant:", np.round(det))
```

```
a =
[[2 2 1]
 [1 3 1]
 [1 2 2]]

Determinant: 5.0
```

Image by author

True inverse

The *true inverse* of a square matrix can be found using the **inv()** function of the numpy *linalg* package. If the determinant of a square matrix is not 0, it has a true inverse.

```
import numpy as np

a = np.array([[2, 2, 1],
              [1, 3, 1],
              [1, 2, 2]])
print("a = ")
print(a)
det = np.linalg.det(a)
print("\nDeterminant:", np.round(det))
inv = np.linalg.inv(a)
print("\nInverse of a = ")
print(inv)
```

```
a =  
[[2 2 1]  
 [1 3 1]  
 [1 2 2]]  
  
Determinant: 5.0  
  
Inverse of a =  
[[ 0.8 -0.4 -0.2]  
 [-0.2  0.6 -0.2]  
 [-0.2 -0.4  0.8]]
```

Image by author

If you try to compute the true inverse of a singular matrix (a square matrix whose determinant is 0), you will get an error.

```
import numpy as np  
  
a = np.array([[2, 8],  
             [1, 4]])  
print("a = ")  
print(a)  
det = np.linalg.det(a)  
print("\nDeterminant:", np.round(det))  
inv = np.linalg.inv(a)  
print("\nInverse of a = ")  
print(inv)
```

```
a =  
[[2 8]  
 [1 4]]  
  
Determinant: 0.0  
  
-----  
LinAlgError                                 Traceback (most recent call last)  
<ipython-input-110-df20cbc6f696> in <module>
```

Image by author

Pseudo inverse

The *pseudo (not genuine) inverse* can be calculated even for a singular matrix (a square matrix whose determinant is 0) using the `pinv()` function of the numpy `linalg` package.

```
import numpy as np

a = np.array([[2, 8],
              [1, 4]])
print("a = ")
print(a)
det = np.linalg.det(a)
print("\nDeterminant:", np.round(det))
pinv = np.linalg.pinv(a)
print("\nPseudo Inverse of a = ")
print(pinv)
```

```
a =
[[2 8]
 [1 4]]

Determinant: 0.0

Pseudo Inverse of a =
[[0.02352941 0.01176471]
 [0.09411765 0.04705882]]
```

Image by author

There is no difference between true inverse and pseudo-inverse if a square matrix is non-singular (determinant is *not* 0).

Flatten

Flatten is a simple method to transform a matrix into a one-dimensional numpy array. For this, we can use the **flatten()** method of an ndarray object.

```
import numpy as np

a = np.arange(1, 10)
a.shape = (3, 3)
print("a = ")
print(a)
print("\nAfter flattening")
print("-----")
print(a.flatten())
```

```
a =  
[[1 2 3]  
 [4 5 6]  
 [7 8 9]]  
  
After flattening  
-----  
[1 2 3 4 5 6 7 8 9]
```

Image by author

Eigenvalues and eigenvectors

Let A be an $n \times n$ matrix. A scalar λ is called an *eigenvalue* of A if there is a non-zero vector x satisfying the following equation.

$$Ax = \lambda x$$

Image by author

The vector x is called the *eigenvector* of A corresponding to λ .

In numpy, both eigenvalues and eigenvectors can be calculated simultaneously using the `eig()` function.

```
import numpy as np  
  
a = np.array([[2, 2, 1],  
              [1, 3, 1],  
              [1, 2, 2]])  
print("a = ")  
print(a)  
w, v = np.linalg.eig(a)  
print("\nEigenvalues:")  
print(w)  
print("\nEigenvectors:")  
print(v)
```

```
a =  
[[2 2 1]  
 [1 3 1]  
 [1 2 2]]  
  
Eigenvalues:  
[1. 5. 1.]  
  
Eigenvectors:  
[[-0.90453403  0.57735027  0.04093652]  
 [ 0.30151134  0.57735027 -0.46313831]  
 [ 0.20000000  0.00000000  1.00000000]]
```

Numpy Matrix Linear Algebra Python Arrays

Image by author

The sum of eigenvalues ($1+5+1=7$) is equal to the trace ($2+3+2=7$) of the same matrix! The product of the eigenvalues ($1 \times 5 \times 1 = 5$) is equal to the determinant (5) of the same matrix!

Eigenvalues and eigenvectors are extremely useful in the Principal Component Analysis (PCA). In PCA, the eigenvectors of the correlation or covariance matrix represent the principal components (the directions of maximum variance) and corresponding eigenvalues represent the amount of variation explained by each principal component. If you want to learn more about the following articles written by me.

Written by Rukshan Pramoditha

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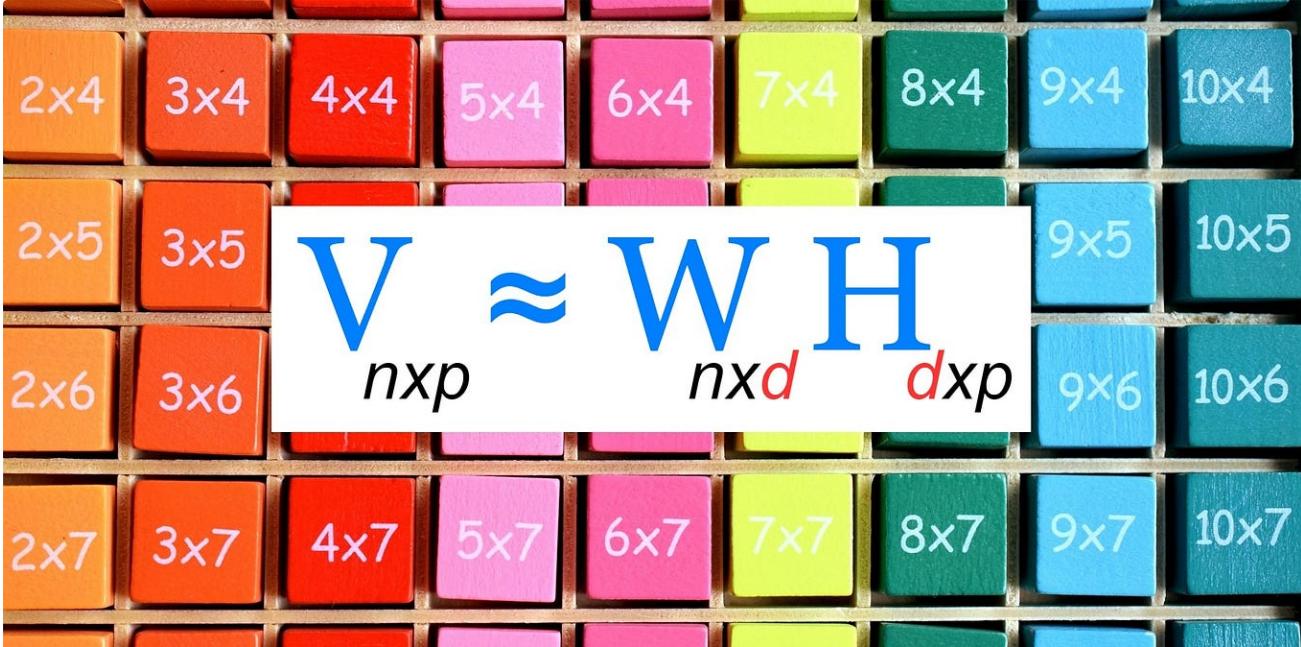
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Key Takeaways

Thanks to the numpy library, you can perform matrix operations easily with just a few lines of code. Today we learned 10 matrix operations in numpy. Numpy has common functions as well as special functions dedicated to linear algebra, for example, the *linalg* package has some special functions dedicated to linear algebra.

In numpy, matrices and ndarrays are two different things. The best way to get familiar with them is by experimenting with the codes by yourself. It is always better to check the dimensions of matrices and ndarrays.

In Scikit-learn machine learning libraries, most of the matrix operations



This tutorial was designed and created by [Rukshan Pramoditha](#), the Author of [Data Science 365 Blog](#).

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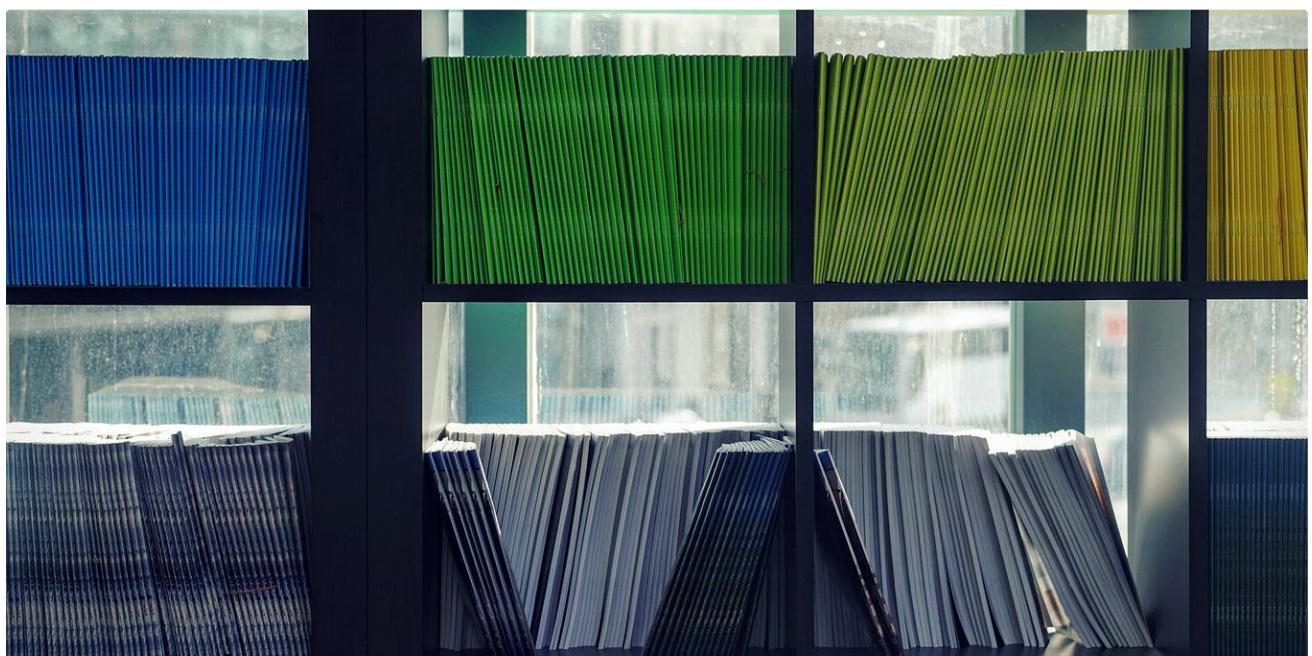
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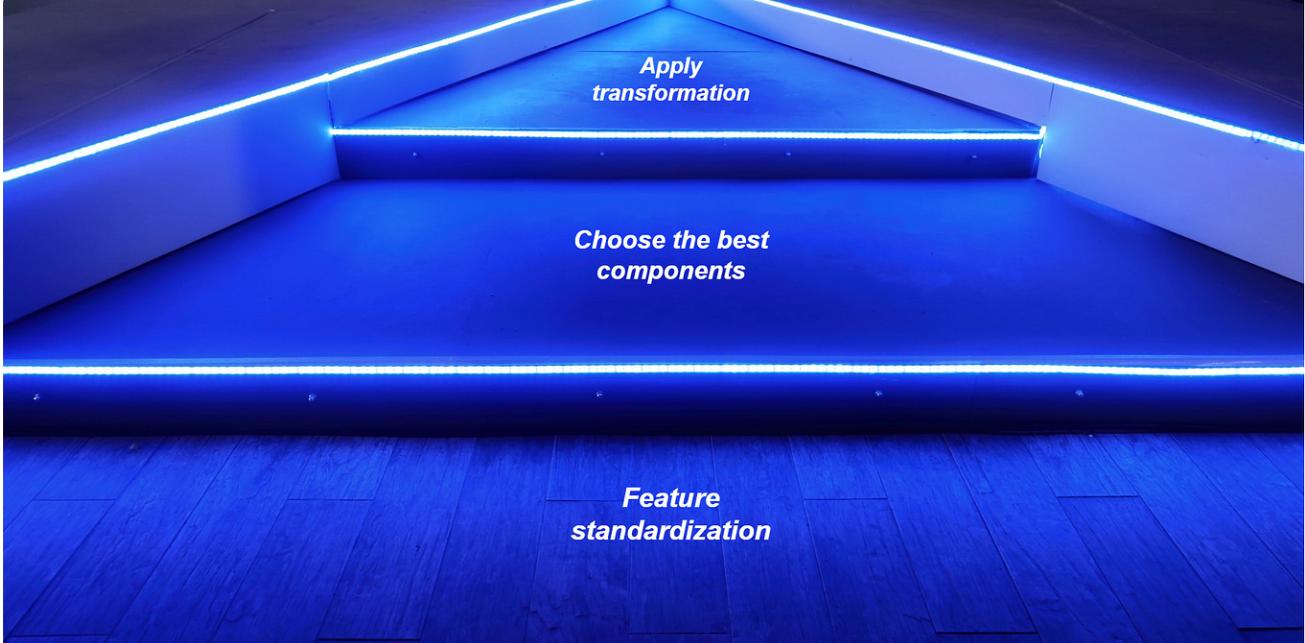
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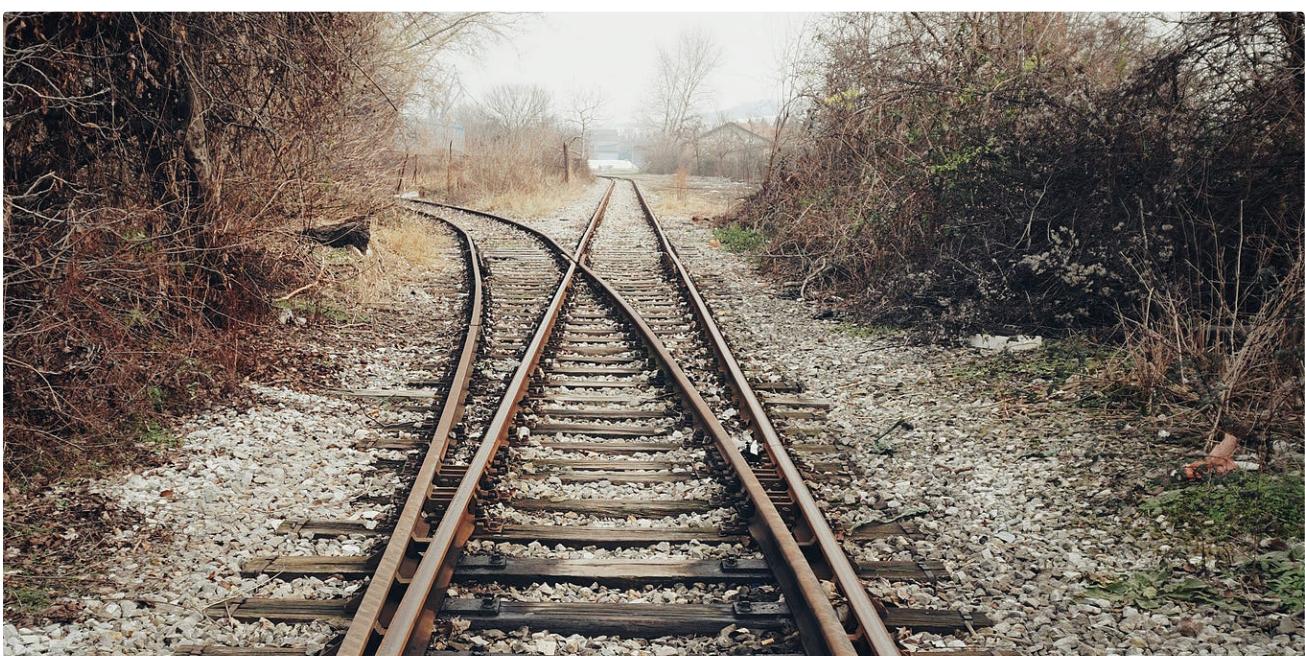
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