A basic introduction to NumPy's einsum

The `einsum` function is one of NumPy's jewels. It can often outperform familiar array functions in terms of speed and memory efficiency, thanks to its expressive power and smart loops. On the downside, it can take a little while understand the notation and sometimes a few attempts to apply it correctly to a tricky problem.

There are quite a few questions on sites like Stack Overflow which about what `einsum` does and how it works, so this post hopes to serve as a basic introduction to the function and what you need to know to begin using it.

What `einsum` does

Using the `einsum` function, we can specify operations on NumPy arrays using the **Ein**stein **sum**mation convention.

Suppose we have two arrays, `A` and `B`. Now suppose that we want to:

- **multiply** `A` with `B` in a particular way to create new array of products, *and then maybe*
- **sum** this new array along particular axes, *and/or*
- **transpose** the axes of the array in a particular order.

Then there's a good chance `einsum` will help us do this much faster and more memory-efficiently that combinations of the NumPy functions `multiply`, `sum` and `transpose` would allow.

As a small example of the function's power, here are two arrays that we want to multiply element-wise and then sum along axis 1 (the rows of the array):

```
A = np.array([0, 1, 2])

B = np.array([[ 0,  1,  2,  3],
              [ 4,  5,  6,  7],
              [ 8,  9, 10, 11]])
```

(3,) (3,4) → Outer most bracket is first shape!

How do we normally do this in NumPy? The first thing to notice is that we need to reshape `A` so that we can broadcast it with `B` (specifically `A` needs to be column vector). Then we can multiply `0` with the first row of `B`, multiply `1` with the second row, and `2` with the third row. This will give us a new array and the three rows can then be summed.

Putting this together, we have:

3,1 3,4 / 3,4 → Diff from dot prod!

```
>>> (A[:, np.newaxis] * B).sum(axis=1)
array([ 0, 22, 76])
```

3,

This works fine, but using `einsum` we can do better:

```
>>> np.einsum('i,ij->i', A, B)
array([ 0, 22, 76])
```

Why better? In short because we didn't need to reshape `A` at all and, most importantly, the multiplication didn't create a temporary array like `A[:, np.newaxis] * B` did. Instead, `einsum` simply summed the products along the rows as it went. Even for this tiny example, I timed `einsum` to be about three times faster.

How to use `einsum`

The key is to choose the correct labelling for the axes of the inputs arrays and the array that we want to get out.

The function lets us do that in one of two ways: using a string of letters, or using lists of integers. For simplicity, we'll stick to the strings (this appears to be the more commonly used of the two options).

A good example to look at is matrix multiplication, which involves multiplying rows with columns and then summing the products. For two 2D arrays `A` and `B`, matrix multiplication can be done with `np.einsum('ij,jk->ik', A, B)`.

What does this string mean? Think of `'ij,jk->ik'` as split in two at the arrow `->`. The left-hand part labels the axes of the *input* arrays: `'ij'` labels `A` and `'jk'` labels `B`. The right-hand part of the string labels the axes of the single *output* array with the letters `'ik'`. In other words, we're putting two 2D arrays in and we want a new 2D array out.

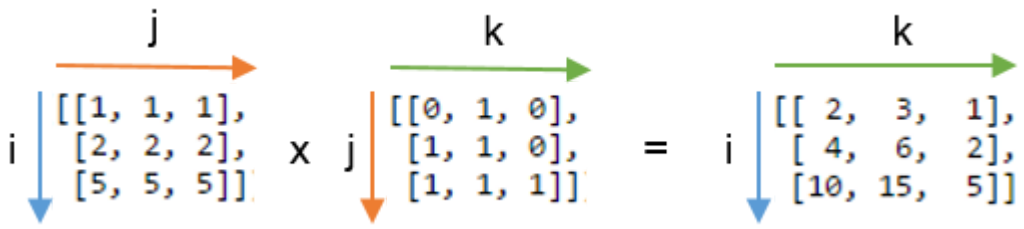
The two arrays we'll multiply are:

```
A = np.array([[1, 1, 1],
              [2, 2, 2],
              [5, 5, 5]])

B = np.array([[0, 1, 0],
```

```
[1, 1, 0],
[1, 1, 1]])
```

Drawing on the labels, our matrix multiplication with `np.einsum('ij,jk->ik', A, B)` looks like this:



matrix mul
= matmul
dot product

To understand how the output array is calculated, remember these three rules:

- **Repeating letters between input arrays means that values along those axes will be multiplied together. The products make up the values for the output array.**

In this case, we used the letter `j` twice: once for `A` and once for `B`. This means that we're multiplying each row of `A` with each column of `B`. This will only work if the axis labelled by `j` is the same length in both arrays (or the length is 1 in either array).

↳ Broadcasting

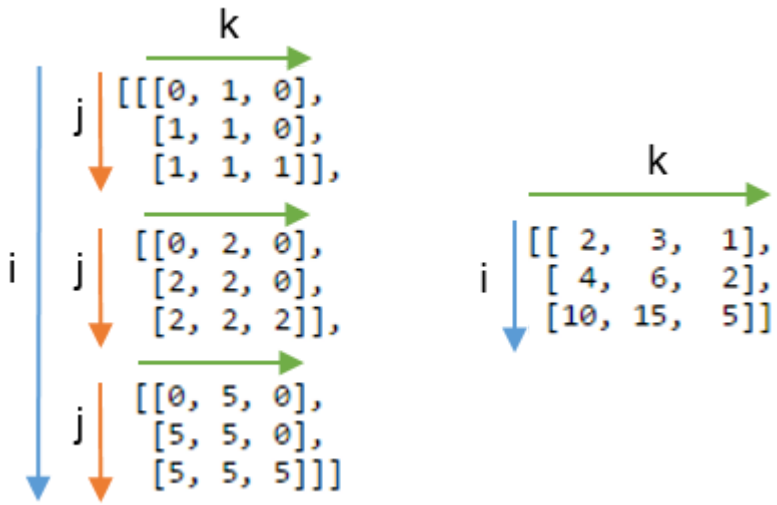
- **Omitting a letter from the output means that values along that axis will be summed.**

Here, `j` is not included among the labels for the output array. Leaving it out sums along the axis and explicitly reduces the number of dimensions in the final array by 1. Had the output signature been `'ijk'` we would have ended up with a 3x3x3 array of products. (And if we gave *no* output labels but just write the arrow, we'd simply sum the whole array.)

- **We can return the unsummed axes in any order we like.**

If we leave out the arrow `'->'`, NumPy will take the labels that appeared once and arrange them in alphabetical order (so in fact `'ij,jk->ik'` is equivalent to just `'ij,jk'`). If we want to control what our output looked like we can choose the order of the output labels ourself. For example, `'ij,jk->ki'` delivers the transpose of the matrix multiplication (notice that `k` and `i` were switched in the output labelling).

It should now be easier to see how the matrix multiplication worked. This image shows what we'd get if we *didn't* sum the `j` axis and instead included it in the output by writing `np.einsum('ij,jk->ijk', A, B)`). To the right, axis `j` has been summed:



Note that with `np.einsum('ij,jk->ik', A, B)`, the function doesn't construct a 3D array and then sum, it just accumulates the sums into a 2D array.

A handful of simple operations

That's all we need to know to start using `einsum`. Knowing how to multiply different axes together and then how to sum the products, we can express a lot of different operations succinctly. This allows us to generalise problems to higher-dimensions relatively easily.

For example, we don't have to insert new axes or transpose arrays to get them to line up correctly.

Below are two tables showing how `einsum` can stand in for various NumPy operations. It's useful to play about with these to get the hang of the notation.

Let `A` and `B` be two 1D arrays of compatible shapes (meaning the lengths of the axes we pair together either equal, or one of them has length 1):

Call signature	NumPy equivalent	Description
`('i', A)`	`A`	returns a view of A
`('i->', A)`	`sum(A)`	sums the values of A
`('i,i->i', A, B)`	`A * B`	element-wise multiplication of A and B
`('i,i', A, B)`	`inner(A, B)`	inner product of A and B
`('i,j->ij', A, B)`	`outer(A, B)`	outer product of A and B

Now let `A` and `B` be two 2D arrays with compatible shapes:

Call signature	NumPy equivalent	Description
`('ij', A)`	`A`	returns a view of A
`('ji', A)`	`A.T`	view transpose of A
`('ii->i', A)`	`diag(A)`	view main diagonal of A
`('ii', A)`	`trace(A)`	sums main diagonal of A
`('ij->', A)`	`sum(A)`	sums the values of A

`('ij->j', A)`	`sum(A, axis=0)`	sum down the columns of A (across rows)
`('ij->i', A)`	`sum(A, axis=1)`	sum horizontally along the rows of A
`('ij,ij->ij', A, B)`	`A * B`	element-wise multiplication of A and B
`('ij,ji->ij', A, B)`	`A * B.T`	element-wise multiplication of A and B.T
`('ij,jk', A, B)`	`dot(A, B)`	matrix multiplication of A and B
`('ij,kj->ik', A, B)`	`inner(A, B)`	inner product of A and B
`('ij,kj->ikj', A, B)`	`A[:, None] * B`	each row of A multiplied by B
`('ij,kl->ijkl', A, B)`	`A[:, :, None, None] * B`	each value of A multiplied by B

When working with larger numbers of dimensions, keep in mind that `einsum` allows the ellipses syntax `'...'`. This provides a convenient way to label the axes we're not particularly interested in, e.g. `np.einsum('...ij,ji->...', a, b)` would multiply just the last two axes of `a` with the 2D array `b`. There are more examples in the documentation.

A few quirks to watch out for

Here a few things to be mindful/wary of when using the function.

`einsum` does not promote data types when summing. If you're using a more limited datatype, you might get unexpected results:

```
>>> a = np.ones(300, dtype=np.int8)
>>> np.sum(a) # correct result
```

```
300
>>> np.einsum('i->', a) # produces incorrect result
44
```

Also `einsum` might not permute axes in the order inteded. The documentation highlights `np.einsum('ji', M)` as a way to transpose a 2D array. You'd be forgiven for thinking that for a 3D array, `np.einsum('kij', M)` moves the last axis to the first position and shifts the first two axes along. Actually, `einsum` creates its own output labelling by rearranging labels in alphabetical order. Therefore `'kij'` becomes `'kij->ijk'` and we have a sort of inverse permutation instead.

Finally, `einsum` is not always the fastest option in NumPy. Functions such as `dot` and `inner` often link to lightening-quick BLAS routines which can outperform `einsum` and certainly shouldn't be forgotten about. The `tensordot` function is also worth comparing for speed. If you search around, you'll find examples of posts highlighting cases where `einsum` appears to be slow, especially when operating on several input arrays (such as this GitHub issue).

Historical notes and links

The `einsum` function was written by Mark Wiebe. Here is a thread from the NumPy mailing list announcing its existence, followed by discussion about the motivation for introducing it into the library. In 2011, the function was included as part of NumPy 1.6.0.

Three further links that may be of interest:

- Official `einsum` documentation
- Source for `einsum` on GitHub
- `einsum` on Stack Overflow

Written on May 2, 2015

Anna-Chiara Bellini • 3 years ago

Super clear explanation, thank you! Just as a note, version 1.14 of Numpy makes einsum use BLAS like Tensordot does, fresh new!

14 • Reply • Share ›

Alex Mod → Anna-Chiara Bellini • 3 years ago

Thank you for the kind words! And thanks for the note about BLAS - it looks like there's been quite a bit of optimisation done around around einsum since I wrote this post.

• Reply • Share ›

TEJAS SHETTY • a year ago

Very nice article Alex. Far more helpful than numpy official reference.

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Amit Chaudhary • 2 years ago

Super useful.

• Reply • Share ›

Sergey Kojoian • 3 years ago • edited

Excellent article!

I am having trouble understanding one of the examples. Specifically,
I don't think A[:, None] * B is the same as ('ij,jk->ijk', A, B).

E.g.
A = [[1, 2],
[3, 4]]
B = [[0, 1],
[1, 0]]
np.einsum('ij,jk->'ijk', A, B) equals [[[0, 1],
[2, 0]],
[[0, 3],
[4, 0]]

where as A[:, None] * B equals [[[0, 2],
[1, 0]],
[[0, 4],
[3, 0]]]

If in stead, you transpose the inner 2 by 2 sub-matrix of A[:, None], and then multiply by B, the results match.

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Alex Mod → Sergey Kojoian • 3 years ago

Apologies for my very late reply. Thank you for your compliment, and thank you very much for identifying an error! The signature for einsum in this case should be 'ij,kj->ikj' (unless I am mistaken again). I have updated the table in the post.

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Gurpreet Singh Kakar • 3 years ago

np.inner(A,B) should be np.einsum('ij,kj->ik',A,B). Otherwise good article.

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Alex Mod → Gurpreet Singh Kakar • 3 years ago

You're absolutely right - thanks for the correction!

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Sam Kirkiles • 3 years ago

Big thanks for this explanation

^ | v • Reply • Share ›

Alex Mod ➚ Sam Kirkiles • 3 years ago

Thanks Sam - glad it was helpful.

^ | v • Reply • Share ›

dacheatbot • 5 years ago

Doesn't sum(A, axis=0) sum the rows of A and sum(A, axis=1) the columns?

^ | v • Reply • Share ›

Alex Mod ➚ dacheatbot • 5 years ago

For 2D arrays in NumPy, sum(A, axis=0) sums the columns (i.e. down each column), while sum(A, axis=0) sums the values across each row.

^ | v • Reply • Share ›

dacheatbot ➚ Alex • 5 years ago

I think you made a typo, as you have "axis=0" in both.

I understand what you're saying. The confusion arises in saying "sums each column" as if one thinks of the matrix as composed as a collection of columns, i.e. A = (a_i), then sum(A, axis=1) would indeed be the sum of those columns, i.e. sum(A, axis=1) = ∑a_i. Exclusively describing the sum axis as being the axis *along* which a sum takes place is clearer, and is the vocabulary used in the documentation.

I hope this doesn't come off as disparaging. This article is great and I thank you for writing it; np.einsum is super useful.

^ | v • Reply • Share ›

Alex Mod ➚ dacheatbot • 5 years ago

Oops, you're quite right: the second sum in my comment should have read sum(A, axis=1). Regarding the wording, I'll edit the article to make the description of these operations clearer. Sticking to the same terminology as

the documentation is preferable, as you suggest. Thank you for raising this point, it's very helpful (your comments didn't come off as disparaging at all).

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Egor Panfilov • 5 years ago

Thanks for the interesting and informative article!
I've got confused by "('ij,ji->ij', A, B) | A * B.T | element mult. of A and B.T". Input 'i' and 'j' have to be equal, but it is not obvious from the notation. Other examples look useful!

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Alex Mod → Egor Panfilov • 5 years ago

Thank you for the feedback! You're right that the axes labelled by i and j must be equal in length for that example; I'll see if I can make it clearer in the post.

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Francesc Alted • 5 years ago

Really cool. Its introduction 5 years ago in NumPy by Mark Wiebe could be an interesting historical note: http://numpy-discussion.109...

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Alex Mod → Francesc Alted • 5 years ago

Thank you for the interesting link, I'd not seen that discussion before. I've included it in a new section at the foot of the article for additional visibility, along with a few other links.

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Mertin • 5 years ago

Just implemented Einsum in a research code for the first time today. Great article, thanks!!

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Alex Mod → Mertin • 5 years ago

Thank you, Mertin! Glad it helped.

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