Awkward Array's JAX backend and complex-step autodiff as an alternative

Jim Pivarski

Princeton University – IRIS-HEP

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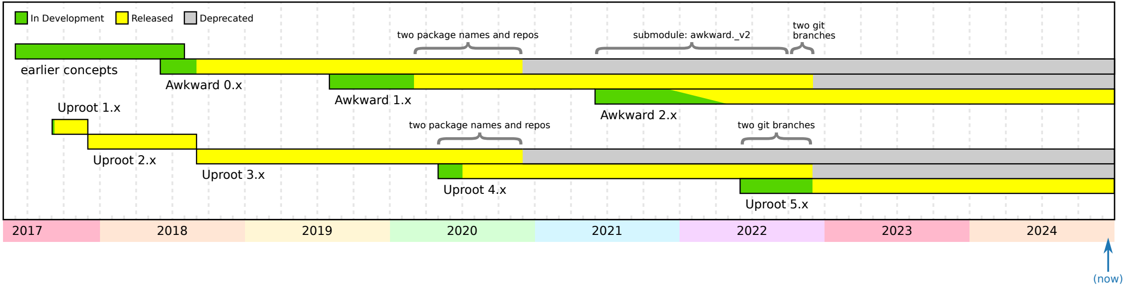
When a backend is untested, it gets out of date. `"jax"` has 44 tests. (`"cuda"` has 459 tests and `"cpu"` + `"typetracer"` has 2214 tests and are used daily.)

JAX backend development



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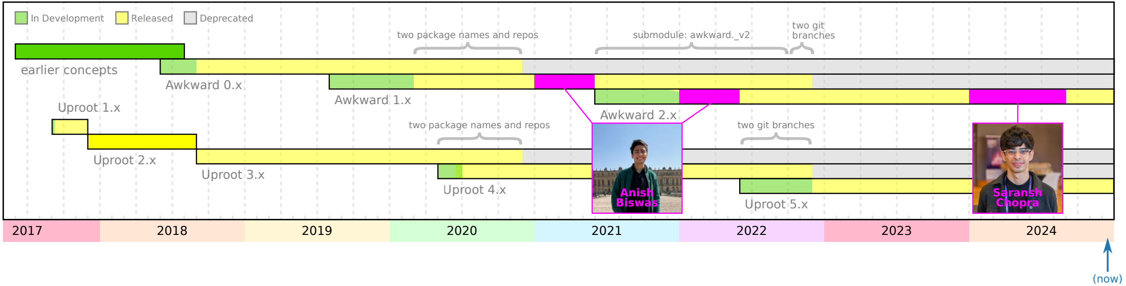

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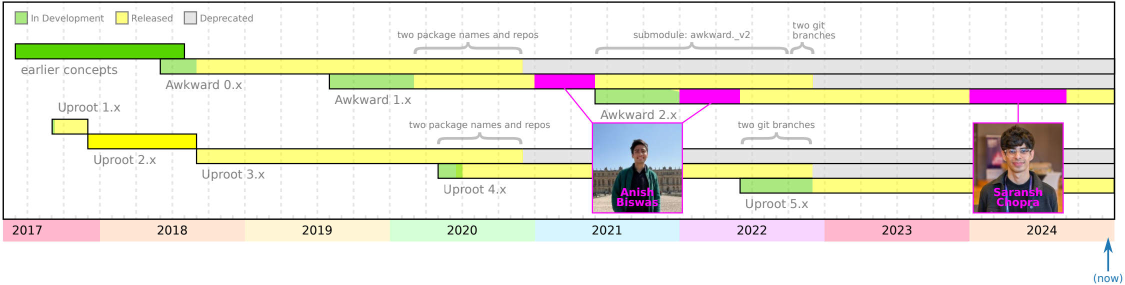

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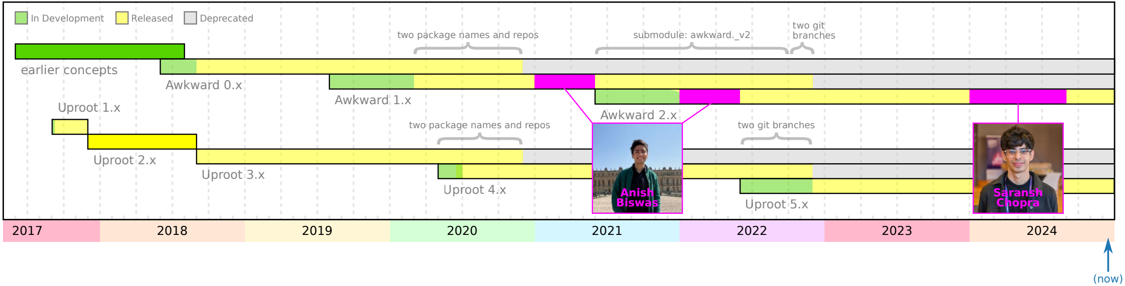

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- Jan 2024–Sep 2024: Saransh Chopra as IRIS-HEP Gap Year Fellow
  - "on call" for feedback from autograd users; received very little

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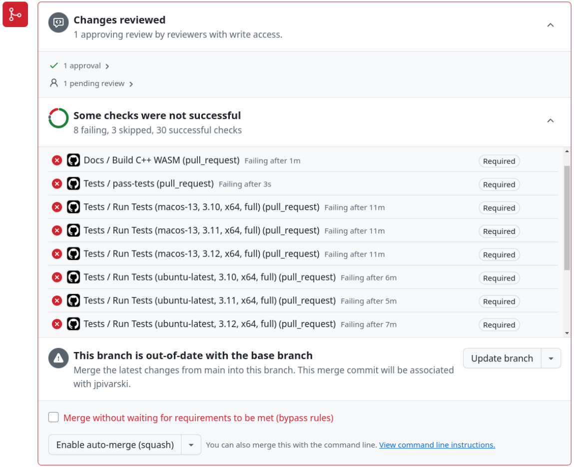
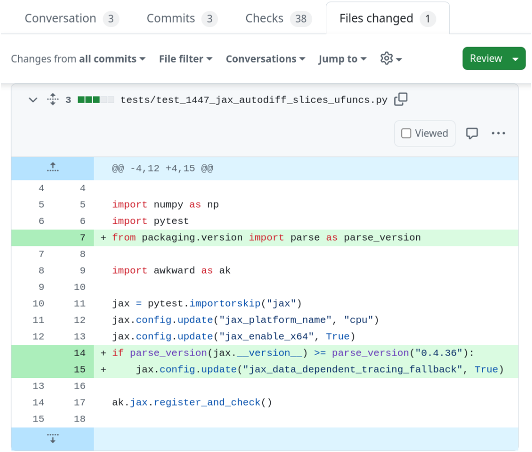
- We were lucky enough that JAX's LAX library has segmented reductions.
- I'm not completely sure all of the above works: Anish was fighting corner cases to the end and we don't have much user feedback.

Occasionally, the JAX tests fail and have to be patched





Can we get autodiff without JAX?

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- If backpropagation is necessary, we could at least get dask-awkward's coverage by using our own typetracer or Dask DAGs.
- How hard is it to implement autodiff, anyway?

Theory of autodiff: complex numbers

https://www.hedonisticlearning.com/posts/complex-step-differentiation.html

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Calculating a derivative of $f : \mathbb{R} \to \mathbb{R}$ to $\mathcal{O}(h^2)$ by finite differences:

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but too-small h has large cancellations and too-large h steps over bumps in f.

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No more additive cancellations and the step is perpendicular to bumps in f.

Theory of autodiff: dual numbers

The derivative of f from its complex extension F,

$$f'(x) \approx \mathrm{Im}\Big(F(x + i\varepsilon) \Big) / \varepsilon$$

is exact if $\varepsilon > 0$ and $\varepsilon^2 = 0$. The complex numbers don't have this property, but imagine an abstract algebra in which this is true.

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But if we already have a complex implementation of all of our functions, we can set $\varepsilon = 10^{-8}$ to get 10^{-16} errors (typical errors in double-precision floating-point).

A complete autodiff library on one slide (NumPy & CuPy)

```python
import numpy as np
from numpy.lib.mixins import NDArrayOperatorsMixin

class diffarray(NDArrayOperatorsMixin):
    @classmethod
    def _build(cls, complex_array):
        self = cls.__new__(cls); self._array = complex_array
        return self

    def __init__(self, primal, tangent=None):
        if issubclass(primal.dtype.type, np.float32):
            self._array = primal.astype(np.complex64)
        elif issubclass(primal.dtype.type, np.float64):
            self._array = primal.astype(np.complex128)
        else:
            raise TypeError("array must be float32 or float64")
        if tangent is None:
            self._array += 1j * self._step_scale
        else:
            self._array += tangent * 1j * self._step_scale
    @property
    def _step_scale(self):
        return 1e-4 if issubclass(
            self._array.dtype.type, np.complex128) else 1e-8

    @property
    def primal(self):
        return np.real(self._array)
    @property
    def tangent(self):
        return np.imag(self._array) / self._step_scale
```

```python
def __array_ufunc__(self, ufunc, method, *args, **kwargs):
    return self.__array_function__(ufunc, None, args, kwargs)

def __array_function__(self, func, types, args, kwargs):
    # functions that would be misinterpreted on complex
    if func.__name__ == "abs":
        out = args[0].copy()
        out[out.real < 0] *= -1
        return type(self)._build(out)
    if func.__name__ == "real":
        return type(self)._build(args[0]._array)
    if func.__name__ == "imag":
        return type(self)._build(args[0]._array * 0)
    if func.__name__ in ("less", "less_equal", "equal",
                         "not_equal", "greater", "greater_equal"):
        args = [getattr(x, "_array", x).real for x in args]
        return func(*args, **kwargs)

    # all other functions
    args = [getattr(x, "_array", x) for x in args]
    kwargs = {
        k: getattr(v, "_array", v) for k, v in kwargs.items()
    }
    out = func(*args, **kwargs)
    return type(self)._build(out) if issubclass(
        out.dtype.type, np.complexfloating) else out

def __getitem__(self, where):
    out = self._array[where]
    return type(self)._build(np.asarray(out)) if isinstance(
        out, np.complexfloating) else out
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A complete autodiff library on one slide (NumPy & CuPy)

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt

>>> x = np.linspace(-20, 20, 10000)
>>> da_x = diffarray(x)
>>> da_y = np.sin(da_x) / da_x
>>> abs(da_y.tangent - ((x*np.cos(x) - np.sin(x)) / x**2)).max()
3.9683650809863025e-10

>>> plt.plot(x, da_y.tangent)
>>> plt.plot(x, (x*np.cos(x) - np.sin(x)) / x**2, ls="--")
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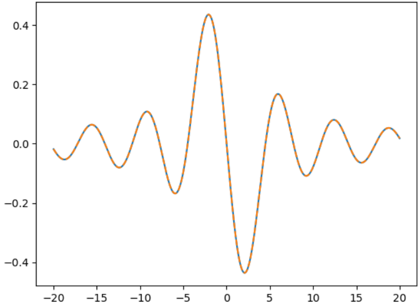

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What else? Can anyone find a reason why this is not sufficient?

What are our options?

1. Keep the JAX backend in Awkward Array, tweaking as necessary.
2. Drop the JAX backend and...
    2.1 give up on autodiff.
    2.2 make a new autodiff mini-library that is Awkward-friendly that...
        2.2.1 just uses the complex-valued implementations we already have.
        2.2.2 implements a conventional autodiff.
    2.3 hide an autodiff implementation inside Awkward that...
        2.3.1 just uses the complex-valued implementations we already have.
        2.3.2 implements a conventional autodiff.