A Theoretical Guide on Differentiation and a Practical Guide to JAX

(or, how never to compute a derivative by hand again)

The Basics

JAX is a lot like numpy

```
import numpy as np
  import jax.numpy as jnp
  x = np.array([1., 2., 3.])
  y = np.array([0., 1., 5.])
  z = np.array([2., 3., 4.])
  print(f"with numpy: \{x * y + z\}")
  x_{-} = jnp.array([1., 2., 3.])
  y_{-} = jnp.array([0., 1., 5.])
  z_{-} = jnp.array([2., 3., 4.])
  print(f"with jax: \{x_* + y_+ z_-\}")
✓ 0.5s
                                                                  Python
```

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   import jax.numpy as jnp
   x = np.array([1., 2., 3.])
   y = np.array([0., 1., 5.])
   z = np.array([2., 3., 4.])
   print(f"with numpy: \{x * y + z\}")
   x_{-} = jnp.array([1., 2., 3.])
   y_{-} = jnp.array([0., 1., 5.])
   z_{-} = jnp.array([2., 3., 4.])
   print(f"with jax: \{x_* + y_+ z_-\}")
 ✓ 0.5s
                                                                   Python
with numpy: [ 2. 5. 19.]
with jax: [ 2. 5. 19.]
```

Most np functions have a jnp counterpart

```
np_linspace = np.linspace(0, 1, 3)
jnp_linspace = jnp.linspace(0, 1, 3)

print(f"np_linspace: {np_linspace}")
print(f"jnp_linspace: {jnp_linspace}\n")

A = np.random.normal(size = (10, 10))
np_2norm = np.linalg.norm(A, ord = 2)
jnp_2norm = jnp.linalg.norm(A, ord = 2) # notice that we can feed np array into jnp function!

print(f"np_2norm: {np_2norm:.4f}")
print(f"jnp_2norm: {jnp_2norm:.4f}\n")

$\square$ 0.6s

Python
```

Most np functions have a jnp counterpart

```
np_linspace = np.linspace(0, 1, 3)
   jnp_linspace = jnp.linspace(0, 1, 3)
   print(f"np_linspace: {np_linspace}")
   print(f"jnp_linspace: {jnp_linspace}\n")
   A = np.random.normal(size = (10, 10))
   np_2norm = np.linalg.norm(A, ord = 2)
   jnp_2norm = jnp.linalg.norm(A, ord = 2) # notice that we can feed np array into jnp function!
   print(f"np_2norm: {np_2norm:.4f}")
   print(f"jnp_2norm: {jnp_2norm:.4f}\n")
 ✓ 0.6s
                                                                                            Python
np_linspace: [0. 0.5 1.]
jnp_linspace: [0. 0.5 1.]
np_2norm: 5.2232
jnp_2norm: 5.2232
```

matplotlib can accept jnp arrays

```
import matplotlib.pyplot as plt

x = jnp.linspace(0, 2 * jnp.pi)
y = jnp.sin(x)
plt.plot(x, y)

$\square$ 0.9s

Python
```

matplotlib can accept jnp arrays

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import matplotlib.pyplot as plt
   x = jnp.linspace(0, 2 * jnp.pi)
   y = jnp.sin(x)
   plt.plot(x, y)
✓ 0.9s
                                                                                                     Python
[<matplotlib.lines.Line2D at 0x7f5d24561dc0>]
 1.00
 0.75
 0.50
 0.25
 0.00
-0.25
-0.50
-0.75
-1.00
```

RNG is different

```
from jax import random

key = random.PRNGKey(0) # initialize key from your favorite integer

A = random.normal(key, shape = (2, 2))
print(f"A: {A}")
B = random.normal(key, shape = (2, 2)) # will get the same thing as A!
print(f"B: {B}")

key, subkey = random.split(key) # new key and subkey are different from original key
C = random.normal(key, shape = (2, 2))
print(f"C: {C}")
D = random.normal(subkey, shape = (2, 2))
print(f"D: {D}")

$\times 0.2s$

Python
```

RNG is different

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from jax import random
   key = random.PRNGKey(0) # initialize key from your favorite integer
   A = random.normal(key, shape = (2, 2))
   print(f"A: {A}")
   B = random.normal(key, shape = (2, 2)) # will get the same thing as A!
   print(f"B: {B}")
   key, subkey = random.split(key) # new key and subkey are different from original key
   C = random.normal(key, shape = (2, 2))
   print(f"C: {C}")
   D = random.normal(subkey, shape = (2, 2))
   print(f"D: {D}")
 ✓ 0.2s
                                                                                                Python
A: [[ 1.8160863 -0.75488514]
 [ 0.33988908 -0.53483534]]
B: [[ 1.8160863 -0.75488514]
 [ 0.33988908 -0.53483534]]
C: [[ 0.13893168  1.370668 ]
 [-0.53116107 0.02033782]]
D: [[ 1.1378784 -0.14331433]
 [-0.59153634 0.79466224]]
```

```
# in numpy, we can do in-place array updates:
A = np.array([1, 2, 3])
print(f"this is A: {A}")

A[0] = 0
print(f"this is the new A in numpy: {A}")

$\square$ 0.3s

Python
```

```
# in jax, this doesn't work:
A = jnp.array([1, 2, 3])
print(f"this is A: {A}")

A[0] = 0 # this will throw an error

Street

Python
```

```
# instead, we have to do this:

A = A.at[0].set(0)
print(f"this is the new A: {A}")

$\square$ 0.1s

Python
```

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✓ 0.3s

Python

this is A: [1 2 3]
this is the new A in numpy: [0 2 3]

# in jax, this doesn't work:

A = jnp.array([1, 2, 3])
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② 1.2s
```

```
# instead, we have to do this:

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$\square$ 0.1s
Python
```

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 ✓ 0.3s
                                                                                                                                        Python
this is A: [1 2 3]
this is the new A in numpy: [0 2 3]
   # in jax, this doesn't work:
   A = jnp.array([1, 2, 3])
   print(f"this is A: {A}")
   A[0] = 0 \# this will throw an error
 Python
this is A: [1 2 3]
                                          Traceback (most recent call last)
 /data/philliplo125/jax-tutorial/tutorial.ipynb Cell 15' in <cell line: 5>()
       2 A = jnp.array([1, 2, 3])
        print(f"this is A: {A}")
 ---> 5 A[0] = 0
 File ~/anaconda3/envs/jax-tutorial/lib/python3.9/site-packages/jax/_src/numpy/lax_numpy.py:4512, in _unimplemented_setitem(self, i, x)
    4507 def _unimplemented_setitem(self, i, x):
         msg = ("'{}' object does not support item assignment. JAX arrays are "
                 "immutable. Instead of ``x[idx] = y``, use ``x = x.at[idx].set(y)`` "
   4510
                  "or another .at[] method: "
                  "https://jax.readthedocs.io/en/latest/_autosummary/jax.numpy.ndarray.at.html")
         raise TypeError(msg.format(type(self)))
TypeError: '<class 'jaxlib.xla_extension.DeviceArray'>' object does not support item assignment. JAX arrays are immutable. Instead of ``x[id
 x] = y``, use ``x = x.at[idx].set(y)`` or another .at[] method: https://jax.readthedocs.io/en/latest/_autosummary/jax.numpy.ndarray.at.html
   # instead, we have to do this:
   A = A.at[0].set(0)
   print(f"this is the new A: {A}")
                                                                                                                                       Python
 ✓ 0.1s
```

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# in numpy, we can do in-place array updates:
   A = np.array([1, 2, 3])
   print(f"this is A: {A}")
   A[0] = 0
   print(f"this is the new A in numpy: {A}")
 ✓ 0.3s
                                                                                                                                        Python
this is A: [1 2 3]
this is the new A in numpy: [0 2 3]
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 Python
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   # instead, we have to do this:
   A = A.at[0].set(0)
   print(f"this is the new A: {A}")
 ✓ 0.1s
                                                                                                                                        Python
this is the new A: [0 2 3]
```

Computing Gradients

JAX is highly functional

Use grad() to map a scalar-valued function to its derivative

```
from jax import grad

sin_grad = grad(jnp.sin)
print(f"sin'(1): {sin_grad(1.0):.4f}")
print(f"cos(1): {jnp.cos(1.0):.4f}")

$\square$ 0.4s

Python
```

JAX is highly functional

Use grad() to map a scalar-valued function to its derivative

Get fancy with function composition

Let $f(x) = \sin(x^2) + 3x^2$, then $f'(x) = 2x\cos(x^2) + 6x$

```
def f(x):
    return jnp.sin(x**2) + 3 * x**2
  def grad_f_manual(x):
    return 2 * x * jnp.cos(x**2) + 6 * x
  grad_f_auto = grad(f)
  x = 2.0
  print(f"manual f'(1): {grad_f_manual(x):.4f}")
  print(f"auto f'(1): {grad_f_auto(x):.4f}")
✓ 0.1s
                                                  Python
```

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   def grad_f_manual(x):
     return 2 * x * jnp.cos(x**2) + 6 * x
   grad_f_auto = grad(f)
   x = 2.0
   print(f"manual f'(1): {grad_f_manual(x):.4f}")
   print(f"auto f'(1): {grad_f_auto(x):.4f}")
 ✓ 0.1s
                                                   Python
manual f'(1): 9.3854
auto f'(1): 9.3854
```

Multivariate Functions

$$f(x, y, z) = x^{2} + 3\sin(y) + \cos(z)$$
$$\nabla f(x, y, z) = (2x, 3\cos(y), -\sin(z))$$

```
\# denote X = (x, y, z)
  def f(X):
    return X[0]**2 + 3 * jnp.sin(X[1]) + jnp.cos(X[2])
  def grad_f_manual(X):
    return jnp.array([2 * X[0], 3 * jnp.cos(X[1]), -jnp.sin(X[2])])
  grad_f_auto = grad(f)
 X = jnp.array([2.0, 3.0, 1.0])
  print(f"manual f'(1): {grad_f_manual(X)}")
  print(f"auto f'(1): {grad_f_auto(X)}")
✓ 0.5s
                                                                   Python
```

Multivariate Functions

$$f(x, y, z) = x^{2} + 3\sin(y) + \cos(z)$$
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   grad_f_auto = grad(f)
   X = jnp.array([2.0, 3.0, 1.0])
   print(f"manual f'(1): {grad_f_manual(X)}")
   print(f"auto f'(1): {grad_f_auto(X)}")
 ✓ 0.5s
                                                                   Python
                       -2.9699774 -0.84147096]
manual f'(1): [ 4.
auto f'(1): [ 4. -2.9699774 -0.84147096]
```

Differentiate with respect to dictionaries

$$f(x, y, z) = x^{2} + 3\sin(y) + \cos(z)$$
$$\nabla f(x, y, z) = (2x, 3\cos(y), -\sin(z))$$

```
def f(X):
    return X['x']**2 + 3 * jnp.sin(X['y']) + jnp.cos(X['z'])

def grad_f_manual(X):
    return jnp.array([2 * X['x'], 3 * jnp.cos(X['y']), -jnp.sin(X['z'])])

grad_f_auto = grad(f)

X = {'x' : 2.0, 'y' : 3.0, 'z' : 1.0}
    print(f"manual f'(1): {grad_f_manual(X)}")

print(f"auto f'(1): {grad_f_auto(X)}")

$\square$ 0.5s

Python
```

Differentiate with respect to dictionaries

$$f(x, y, z) = x^{2} + 3\sin(y) + \cos(z)$$
$$\nabla f(x, y, z) = (2x, 3\cos(y), -\sin(z))$$

```
def f(X):
     return X['x']**2 + 3 * jnp.sin(X['y']) + jnp.cos(X['z'])
   def grad_f_manual(X):
     return jnp.array([2 * X['x'], 3 * jnp.cos(X['y']), -jnp.sin(X['z'])])
   grad_f_auto = grad(f)
   X = \{'x' : 2.0, 'y' : 3.0, 'z' : 1.0\}
   print(f"manual f'(1): {grad_f_manual(X)}")
   print(f"auto f'(1): {grad_f_auto(X)}")
 ✓ 0.5s
                                                                    Python
manual f'(1): [ 4. -2.9699774 -0.84147096]
auto f'(1): {'x': DeviceArray(4., dtype=float32, weak_type=True), 'y':
DeviceArray(-2.9699774, dtype=float32, weak_type=True), 'z':
DeviceArray(-0.84147096, dtype=float32, weak_type=True)}
```

Multiple multivariate arguments

$$f(x,y) = ||x||^2 + ||y|| + \langle x, y \rangle$$

$$D_x f(x,y) = 2x + y$$

$$D_y f(x,y) = \frac{y}{||y||} + x$$

$$x, y \in \mathbb{R}^3$$

```
def f(x, y):
    return jnp.linalg.norm(x)**2 + jnp.linalg.norm(y) + jnp.inner(x, y)

Dxf = grad(f, 0) # take the derivative wrt the zeroth argument
Dyf = grad(f, 1) # take the derivative wrt the first argument

x = jnp.array([1., 2., 3.])
y = jnp.array([0, -1., 1.])

print(f"derivative wrt x: {Dxf(x, y)}")
print(f"manually computed: {2 * x + y}\n")
print(f"derivative wrt y: {Dyf(x, y)}")
print(f"manually computed: {y / jnp.linalg.norm(y) + x}")

$\leftarrow$ 0.8s

Python
```

Multiple multivariate arguments

$$f(x,y) = ||x||^2 + ||y|| + \langle x, y \rangle$$

$$D_x f(x,y) = 2x + y$$

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```
def f(x, y):
     return jnp.linalg.norm(x)**2 + jnp.linalg.norm(y) + jnp.inner(x, y)
   Dxf = grad(f, 0) # take the derivative wrt the zeroth argument
   Dyf = grad(f, 1) # take the derivative wrt the first argument
   x = jnp.array([1., 2., 3.])
   y = jnp.array([0, -1., 1.])
   print(f"derivative wrt x: {Dxf(x, y)}")
   print(f"manually computed: \{2 * x + y\} \setminus n")
   print(f"derivative wrt y: {Dyf(x, y)}")
   print(f"manually computed: {y / jnp.linalg.norm(y) + x}")
 ✓ 0.8s
                                                                      Python
derivative wrt x: [2. 3. 7.]
manually computed: [2. 3. 7.]
derivative wrt y: [1.
                             1.2928932 3.7071068]
manually computed: [1.
                              1.2928932 3.7071068]
```

value_and_grad()

Useful for first-order optimization methods

```
from jax import value_and_grad

def f(x):
    return x ** 2

value, grad = value_and_grad(f)(3.0)
    print(f"value: {value}")
    print(f"grad: {grad}")

Vo.4s
```

value_and_grad()

Useful for first-order optimization methods

What is Automatic Differentiation?



• Finite differences: $\frac{d}{dx}f(x) \approx \frac{f(x+h) - f(x)}{h}$

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$$\frac{d}{dx}f(x) \approx \frac{f(x+h) - f(x)}{h}$$

Numerically unstable

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- Numerically unstable
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Chain rule

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$$h(x) = f(g(x))$$

$$\frac{dh}{dx} = \frac{df}{dg} \frac{dg}{dx}$$

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$$h(x) = f(g(x))$$

$$\frac{dh}{dx} = \frac{df}{dg} \frac{dg}{dx}$$

$$\frac{d}{dx}f(g_1(x),...,g_K(x)) = \sum_{k=1}^K \left(\frac{d}{dx}g_k(x)\right) D_k f(g_1(x),...,g_K(x))$$

Chain rule

$$h(x) = f(g(x))$$

$$\frac{dh}{dx} = \frac{df}{dg} \frac{dg}{dx}$$

$$\frac{d}{dx}f(g_1(x),...,g_K(x)) = \sum_{k=1}^K \left(\frac{d}{dx}g_k(x)\right) D_k f(g_1(x),...,g_K(x))$$

Idea: the chain rule is <u>modular</u>; as long as we know the derivatives of elementary functions, we can compute the derivatives of arbitrary compositions of these functions

$$z = mx + b$$

$$\hat{y} = \sigma(z)$$

$$L^{m,b}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$$

$$R(m) = \frac{1}{2}m^2$$

$$L_R^{m,b} = L^{m,b}(\hat{y}, y) + \lambda R(m)$$

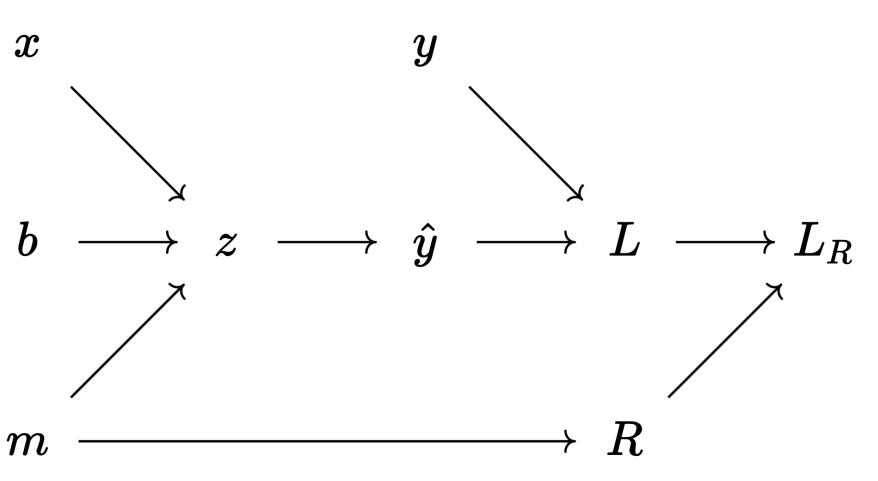
$$z = mx + b$$

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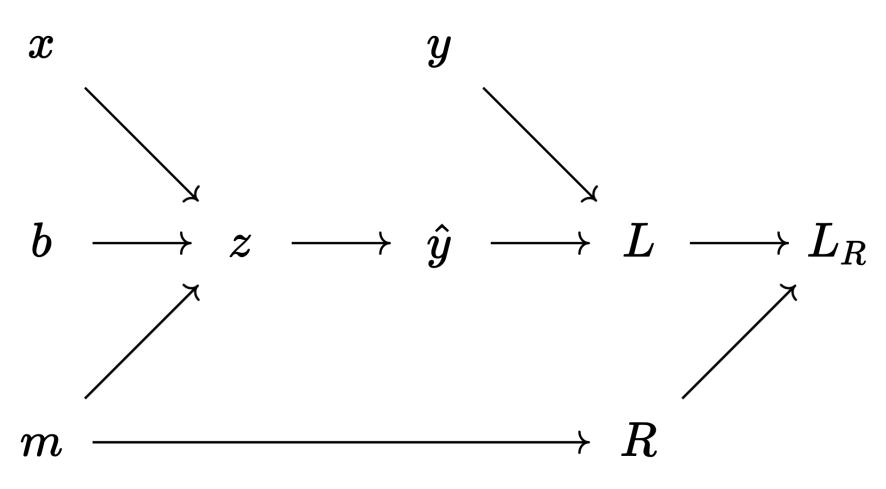
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parent → child, <u>derivative w.r.t.</u>

<u>parent requires derivatives w.r.t</u>

<u>children</u>

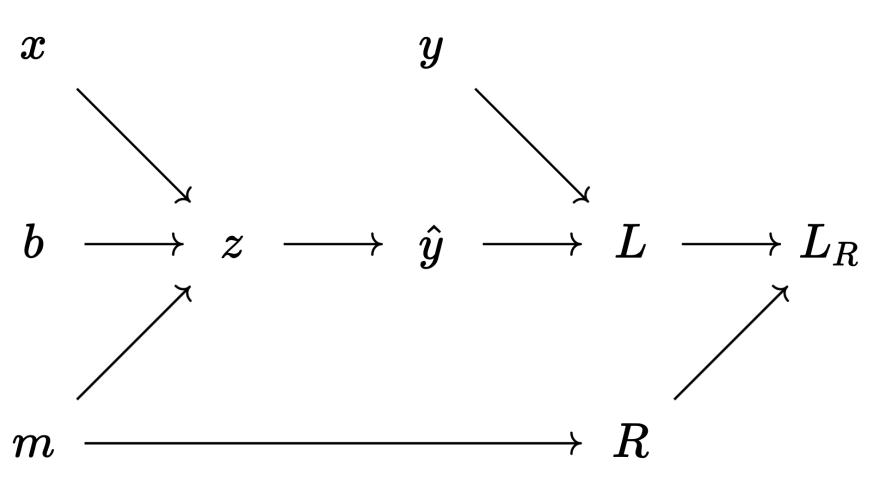
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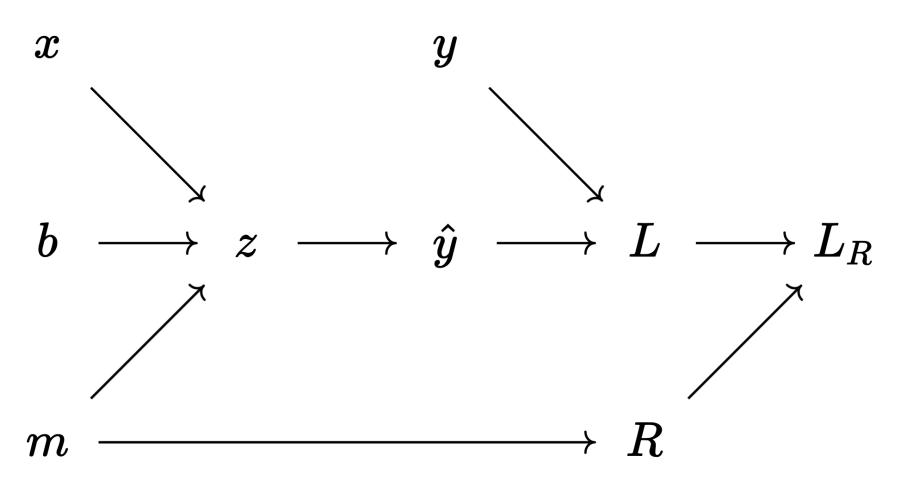
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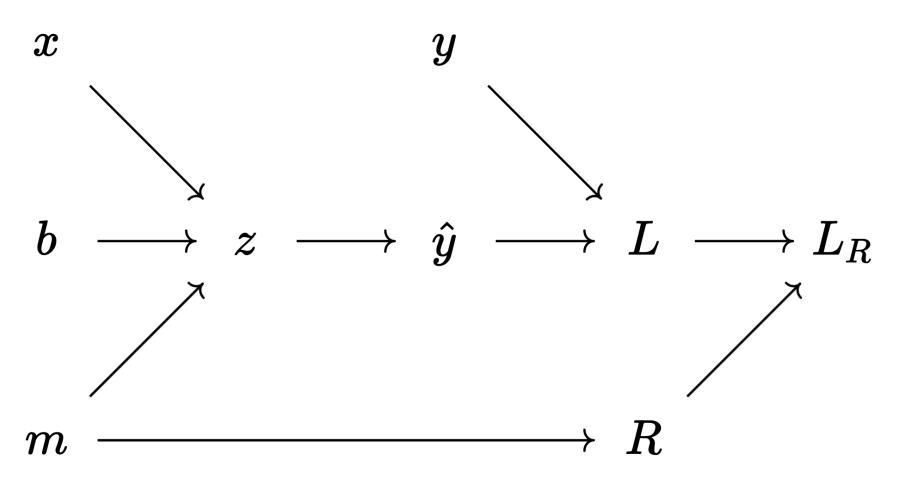
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$$\hat{y} = \sigma(z)$$

$$L^{m,b}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$$

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$$L_R^{m,b} = L^{m,b}(\hat{y}, y) + \lambda R(m)$$



parent → child, <u>derivative w.r.t.</u>

<u>parent requires derivatives w.r.t</u>

<u>children</u>

$$D_{L_R}=1$$

$$D_L = D_{L_R} \frac{dL_R}{dL} = D_{L_R}$$

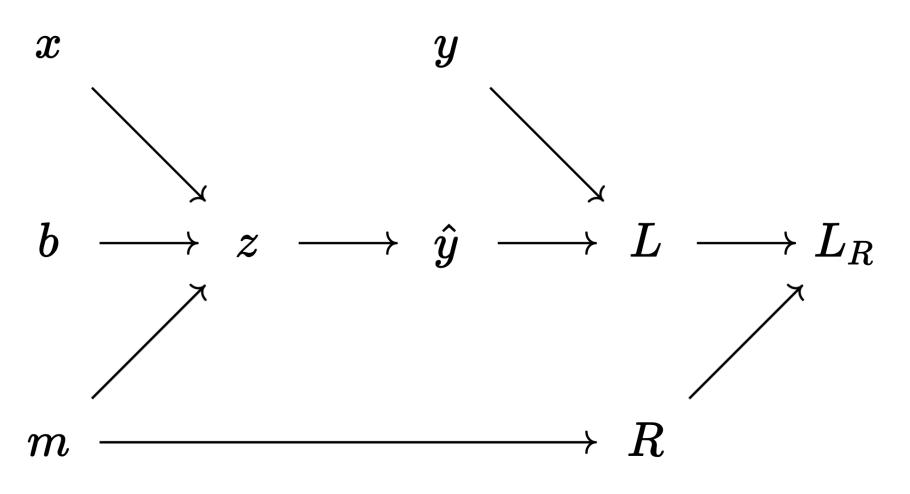
$$z = mx + b$$

$$\hat{y} = \sigma(z)$$

$$L^{m,b}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$$

$$R(m) = \frac{1}{2}m^2$$

$$L_R^{m,b} = L^{m,b}(\hat{y}, y) + \lambda R(m)$$



$$D_{L_R}=1$$

$$D_L = D_{L_R} \frac{dL_R}{dL} = D_{L_R}$$

$$D_R = D_{L_R} \frac{dL_R}{dR} = \lambda D_{L_R}$$

$$z = mx + b \qquad x \qquad y$$

$$\hat{y} = \sigma(z)$$

$$L^{m,b}(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2 \qquad b \longrightarrow z \longrightarrow \hat{y} \longrightarrow L \longrightarrow$$

$$R(m) = \frac{1}{2}m^2 \qquad m \longrightarrow R$$

$$D_{L_R} = 1$$

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$$D_L = D_{L_R} \frac{dL_R}{dL} = D_{L_R}$$

$$D_R = D_{L_R} \frac{dL_R}{dR} = \lambda D_{L_R}$$

$$D_{\hat{y}} = D_L \frac{dL}{dy} = (\hat{y} - y)D_L$$

parent → child, <u>derivative w.r.t.</u> parent requires derivatives w.r.t children

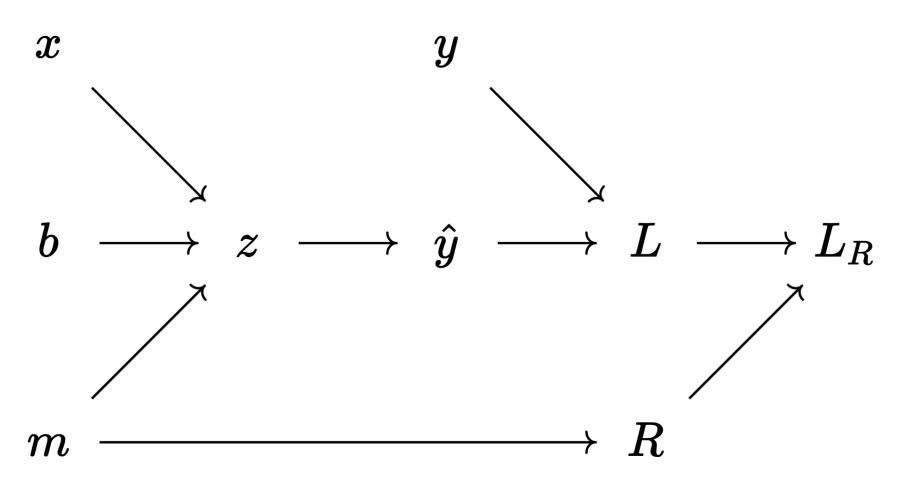
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Automatic differentiation algorithm: work backwards through the computation tree, computing derivatives of parents w.r.t children

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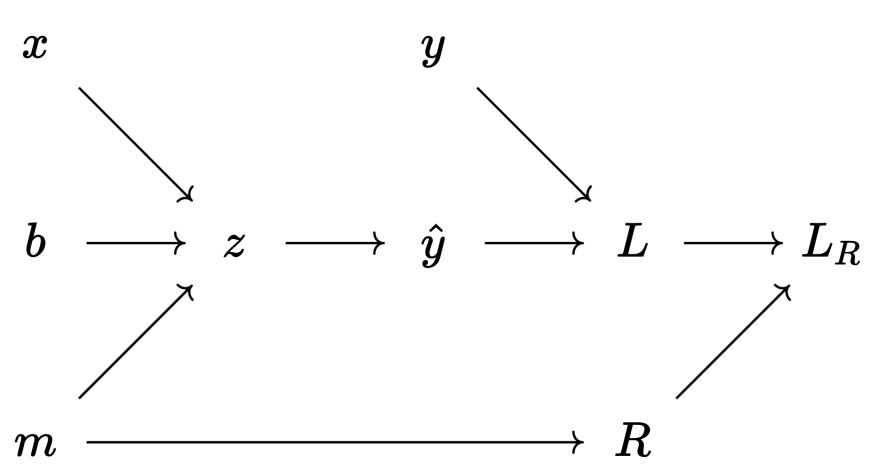
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$$D_{m} = D_{z} \frac{dz}{dm} + D_{R} \frac{dR}{dm}$$

$$= D_{z} x + D_{R} m$$

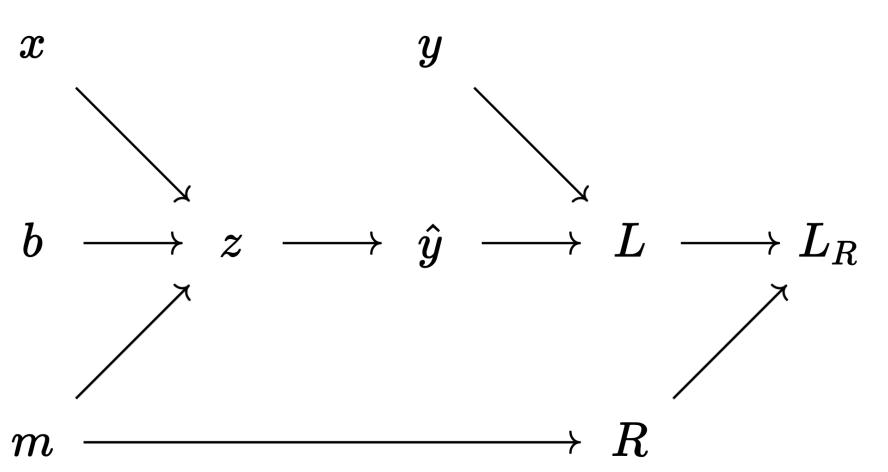
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$$\begin{split} D_z &= D_{\hat{y}} \frac{d\hat{y}}{dz} = D_{\hat{y}} \sigma'(z) \\ D_m &= D_z \frac{dz}{dm} + D_R \frac{dR}{dm} \\ &= D_z x + D_R m \end{split}$$
 etc...

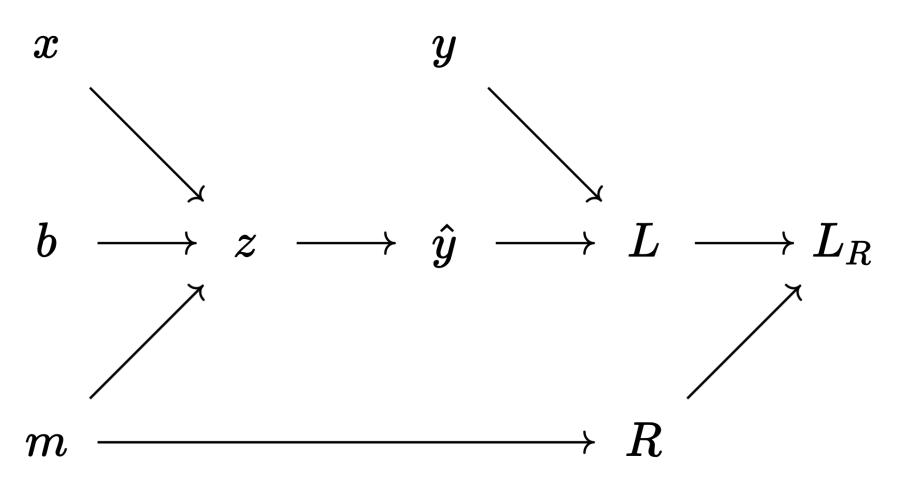
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etc...

Key insight: modular! No need to recompute things!

Jacobians

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$$Jf(x) = \begin{bmatrix} \frac{\partial f}{\partial x_{ij}} \end{bmatrix}_{ij} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_j} \\ \vdots & \vdots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \dots & \frac{\partial f_m}{\partial x_j} \end{bmatrix}$$

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- Functional analyst: linear operator from $\mathbb{R}^n \to \mathbb{R}^m$
- Differential geometer: a map from the tangent bundle of \mathbb{R}^n to \mathbb{R}^m

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 - Tangent space to a manifold is the vector space best approximating that manifold
 - Tangent vectors v and domain vectors x are different types of objects
- Similarly, the range of Jf(x) is the tangent space to the range of f at f(x), denoted $T_{f(x)}\mathbb{R}^m$



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Thinking about Jacobians like a Differential Geometer

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JAX's jvp()

$$f(x,y) = (x + 2y, \sin(x)e^y, y^3), f: \mathbb{R}^2 \to \mathbb{R}^3$$

$$Jf(x,y) = \begin{bmatrix} 1 & 2 \\ \cos(x)e^y & \sin(x)e^y \\ 0 & 3y^2 \end{bmatrix} \in \mathbb{R}^{3\times 2}$$

```
from jax import jvp
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  def Jf_manual(x):
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      [1, 2],
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  # compute the jvp manually
  def jvp_manual(x, v):
    return Jf_manual(x) @ v
  x = jnp.array([1., 2.])
  v = jnp.array([2., 3.])
  print(f"manually computed jvp: {jvp_manual(x, v)}")
  # compute the jvp using jax.jvp():
  func_value, jvp_JAX = jvp(f, (x,), (v,)) # jvp returns both the function value and the jvp
  print(f"JAX computed jvp: {jvp_JAX}")
✓ 0.3s
                                                                                        Python
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   print(f"JAX computed jvp: {jvp_JAX}")
 ✓ 0.3s
                                                                                         Python
manually computed jvp: [ 8.
                                  26.637676 36.
JAX computed jvp: [ 8.
                             26.637676 36.
```

But what if we want the full Jacobian matrix?

Post-multiplying a matrix with the *j*th standard basis vector reveals the *j*th column of the matrix, so can construct the full $m \times n$ Jacobian matrix with n JVPs:

```
def Jf_JVPs(x): # compute the full Jacobian at x using JVPs
    Jf = np.zeros(shape = (3, 2))
    for j in range(2):
        # compute the jth basis vector
        ej = np.zeros(shape = 2)
        ej[j] = 1

        # set the jth column equal to JVP with v = ej
        Jf[:, j] = jvp(f, (x,), (ej,))[1] # remember jvp returns function value and jvp

    return Jf

x = jnp.array([2., 3.])

print(f"Jf with JVPs: \n {Jf_JVPs(x)}")
    print(f"Jf manual: \n {Jf_manual(x)}")

> 0.7s

Python
```

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✓ 0.7s
                                                                               Python
Jf with JVPs:
[[ 1.
[-8.35853291 18.26372719]
            27.
Jf manual:
[[ 1. 2. ]
[-8.358533 18.263727]
[ 0. 27. ]]
```

Forward-mode differentiation: jacfwd()

```
from jax import jacfwd
   print(f"Jf with jacfwd(): \n {jacfwd(f)(x)}")
 ✓ 0.3s
                                            Python
Jf with jacfwd():
[[ 1. 2.
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 [ 0. 27. ]]
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- But often more interested in short and fat Jacobians (a lot of variables mapping to a few variables), e.g., loss functions
- If only we could reconstruct a Jacobian matrix one row at a time...

• If $Jf(x) \in \mathbb{R}^{m \times n}$ is a Jacobian matrix, then premultiplying with the basis vector $e_i^T \in \mathbb{R}^m$ will reveal the *i*th row of the Jacobian matrix

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 - So v^T is a *linear functional* on the tangent space of \mathbb{R}^m : $v^T \in (T_{f(x)}\mathbb{R}^m)^* \cong \mathbb{R}^m$
- The n-dimensional vector $v^T J f(x)$ is a row vector, making it a linear opeartor on \mathbb{R}^n , so it lives in the cotangent space of \mathbb{R}^n : $v^T J f(x) \in (T_x \mathbb{R}^n)^* \cong \mathbb{R}^n$

$$(T_x\mathbb{R}^n)^* \leftarrow T_{f(x)}\mathbb{R}^m)^*$$

$$T_x\mathbb{R}^n \xrightarrow{\mathsf{jvp}} T_{f(x)}\mathbb{R}^m$$

$$\mathbb{R}^n \xrightarrow{f} \mathbb{R}^m$$

vjp() example

$$f(x,y) = (x + 2y, \sin(x)e^y, y^3), f: \mathbb{R}^2 \to \mathbb{R}^3$$

$$Jf(x,y) = \begin{bmatrix} 1 & 2 \\ \cos(x)e^y & \sin(x)e^y \\ 0 & 3y^2 \end{bmatrix} \in \mathbb{R}^{3\times 2}$$

```
from jax import vjp
  def f(x):
    return jnp.array([x[0] + 2 * x[1], jnp.sin(x[0]) * jnp.exp(x[1]), x[1]**3])
  def Jf_manual(x):
    return jnp.array([
      [1, 2],
      [jnp.cos(x[0]) * jnp.exp(x[1]), jnp.sin(x[0]) * jnp.exp(x[1])],
      [0, 3 * x[1] **2]
  # compute the vjp manually
  def vjp_manual(x, v):
    return v @ Jf_manual(x)
  x = jnp.array([1., 2.])
  v = jnp.array([2., 3., 4.])
  print(f"manually computed jvp: {vjp_manual(x, v)}")
  # compute the jvp using jax.jvp():
  func_value, vjp_JAX = vjp(f, x) # vjp signature is a bit different from jvp
  print(f"JAX computed jvp: {vjp_JAX(v)}")
✓ 0.2s
                                                                                       Python
```

vjp() example

$$f(x,y) = (x + 2y, \sin(x)e^y, y^3), f: \mathbb{R}^2 \to \mathbb{R}^3$$

$$Jf(x,y) = \begin{vmatrix} 1 & 2 \\ \cos(x)e^y & \sin(x)e^y \\ 0 & 3y^2 \end{vmatrix} \in \mathbb{R}^{3\times 2}$$

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 ✓ 0.2s
                                                                                        Python
manually computed jvp: [13.976972 70.65303 ]
JAX computed jvp: (DeviceArray([13.976972, 70.65303], dtype=float32),)
```

Computing a full Jacobian matrix using vjp()

Post-multiplying a matrix with the ith standard basis vector reveals the ith column of the matrix, so can construct the full $m \times n$ Jacobian matrix with m VJPs:

```
def Jf_VJPs(x): # compute the full Jacobian at x using VJPs
    Jf = np.zeros(shape = (3, 2))
    for i in range(3):
        # compute the ith basis vector
        ei = np.zeros(shape = 3)
        ei[i] = 1

        # set the ith column equal to JVP with v = ej
        Jf[i] = vjp(f, x)[1](ei)[0]
    return Jf

x = jnp.array([2., 3.])

print(f"Jf with VJPs: \n {Jf_VJPs(x)}")
    print(f"Jf manual: \n {Jf_manual(x)}")
```

Computing a full Jacobian matrix using vjp()

Post-multiplying a matrix with the ith standard basis vector reveals the ith column of the matrix, so can construct the full $m \times n$ Jacobian matrix with m VJPs:

```
def Jf_VJPs(x): # compute the full Jacobian at x using VJPs
     Jf = np.zeros(shape = (3, 2))
     for i in range(3):
       # compute the ith basis vector
       ei = np.zeros(shape = 3)
       ei[i] = 1
       # set the ith column equal to JVP with v = ej
       Jf[i] = vjp(f, x)[1](ei)[0]
     return Jf
   x = jnp.array([2., 3.])
   print(f"Jf with VJPs: \n {Jf_VJPs(x)}")
   print(f"Jf manual: \n {Jf_manual(x)}")
 ✓ 0.1s
                                                            Python
Jf with VJPs:
               2.
[[ 1.
 [-8.35853291 18.26372719]
 [ 0.
             27.
Jf manual:
[[ 1.
             2.
[-8.358533 18.263727]
 [ 0.
           27.
```

Reverse-mode differentiation: jacrev()

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...better for short and fat Jacobians

Forward vs. Reverse Mode Performance Comparison

$$f(x) = \left\| \frac{e^x - x^2}{\tan x} \right\|, x \in \mathbb{R}^n$$

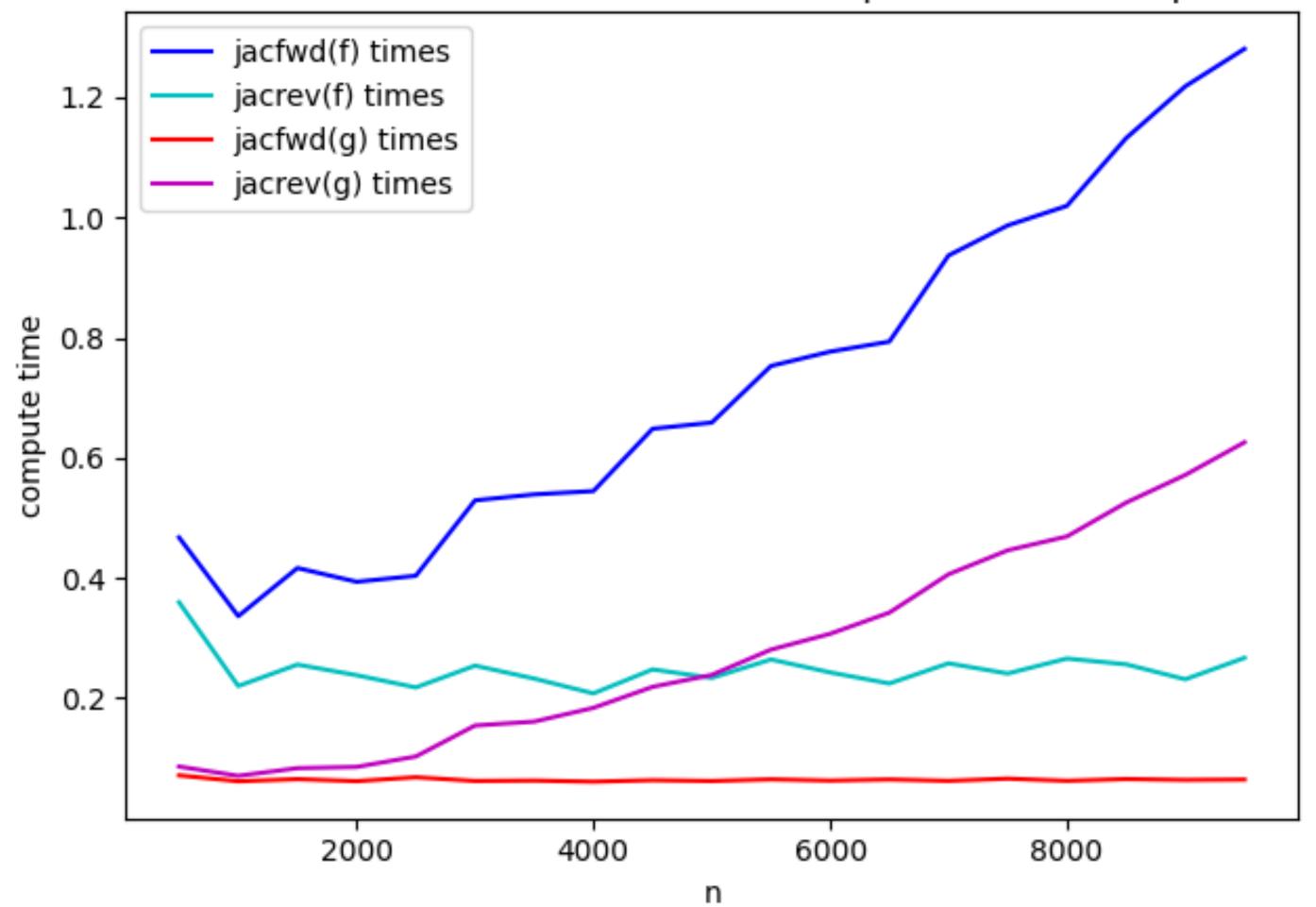
$$g(t) = t^{\sin(1, t, t^2, \dots, t^{n-1})}, t \in \mathbb{R}$$

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Forward and reverse mode differentiation performance comparison



Performance

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 - Control flow must be agnostic to valued of traced variables
 - Requires array shapes of functions to be known ahead of time

JIT example, simple function

$$f(x) = \sigma\left(\left\|\hat{I} - I\right\|_{2}^{2}\right), I \in \mathbb{R}^{128 \times 128}$$

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def f_np(Ihat, I):
    diff = np.linalg.norm(Ihat - I) **2 / 2
    return 1 / (1 + np.exp(-diff))

def f_jnp(Ihat, I):
    diff = jnp.linalg.norm(Ihat - I) **2 / 2
    return 1 / (1 + jnp.exp(-diff))

f_jnp_jitted = jit(f_jnp)
```

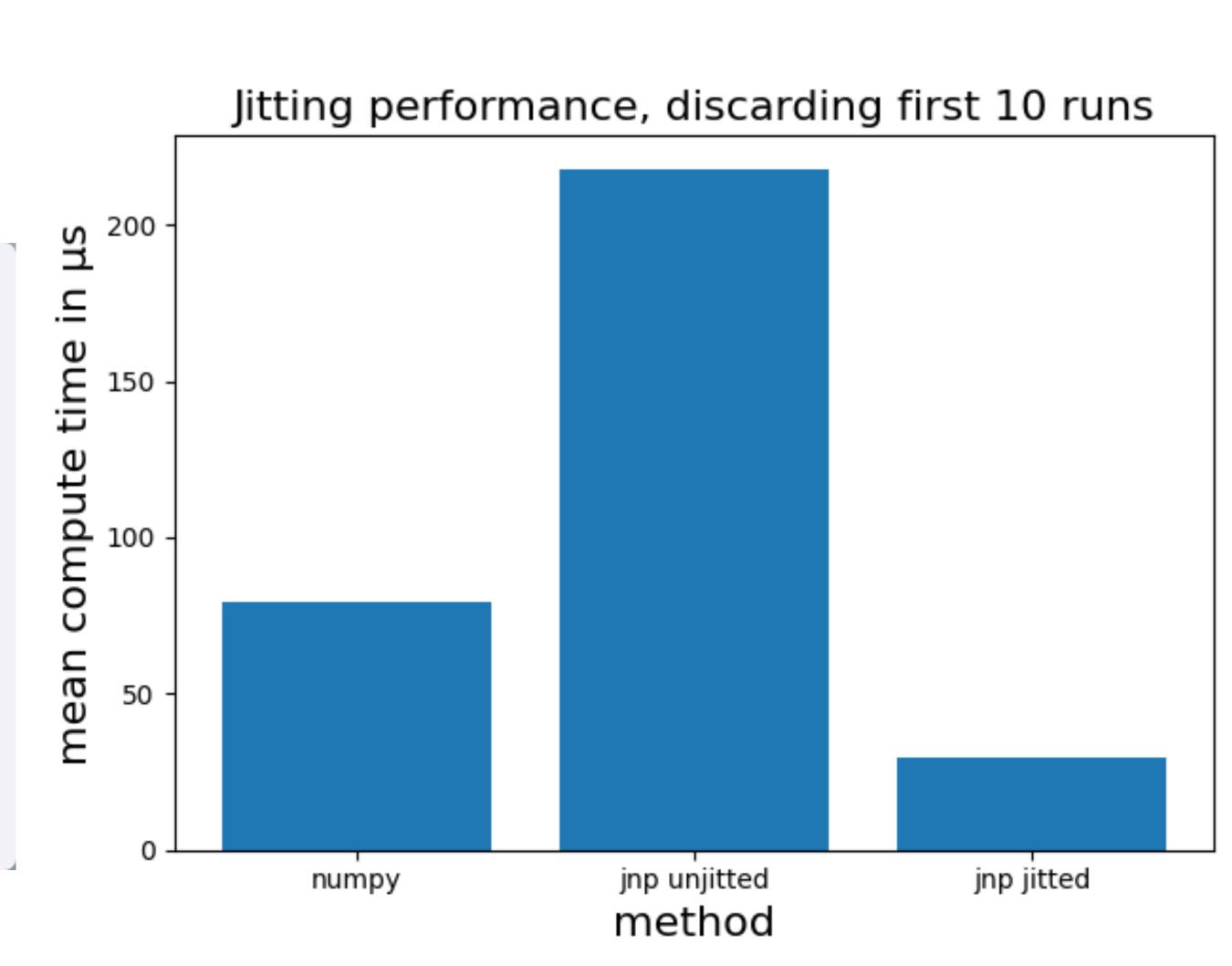
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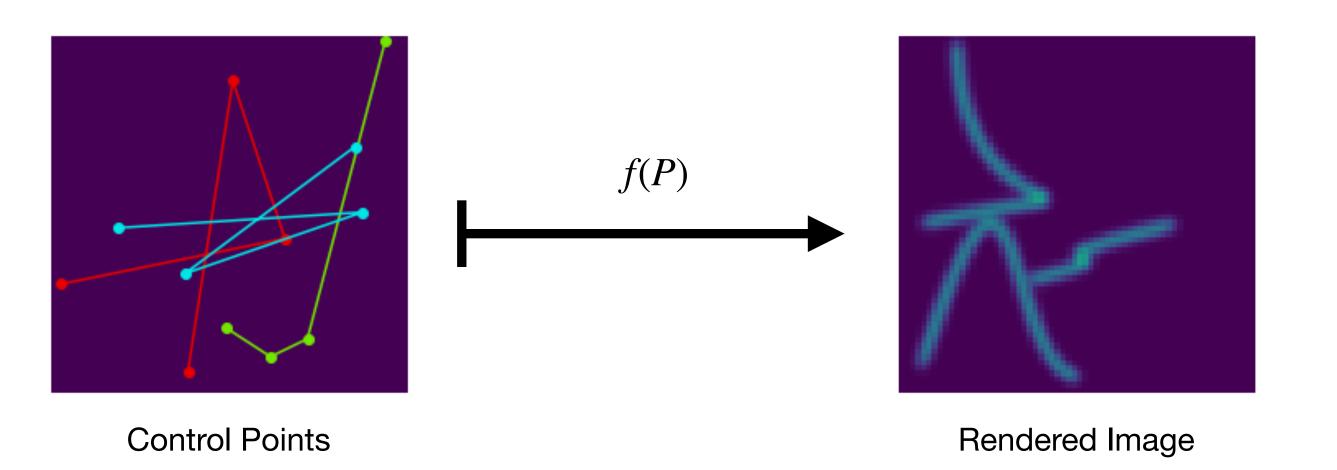


JIT example, Bezier rendering function

$$\mathbf{B}(t) = (1-t)^3 \mathbf{P_0} + 3(1-t)^2 t \mathbf{P_1} + 3(1-t)t^2 \mathbf{P_2} + t^3 \mathbf{P_3}, \quad \mathbf{P_i} \in \mathbb{R}^2, \text{ control points}$$

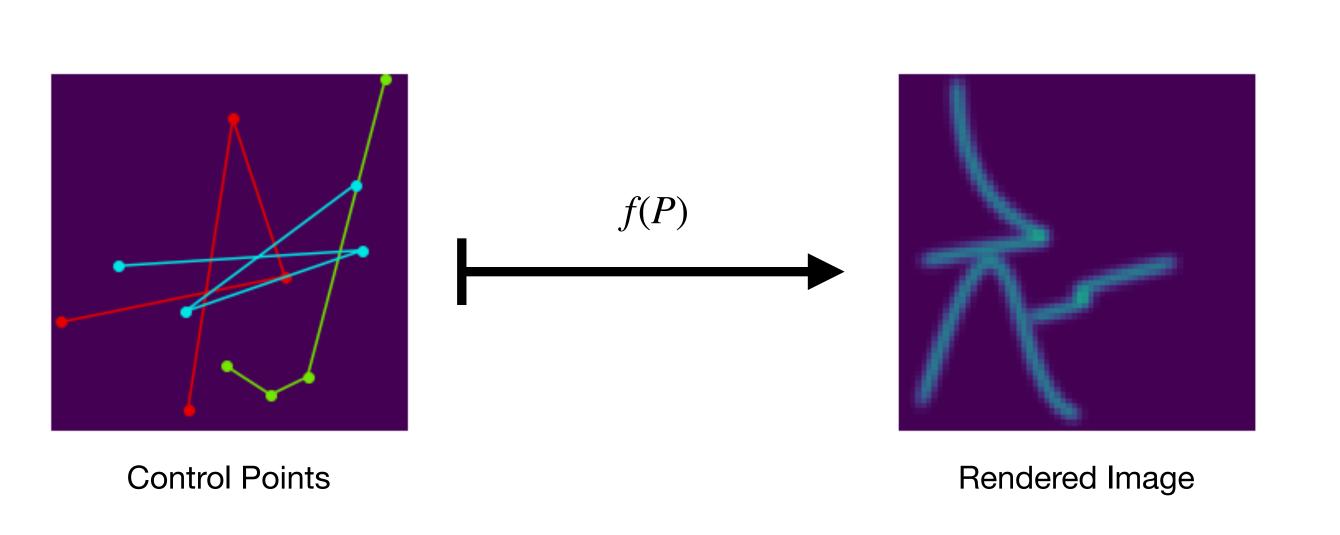
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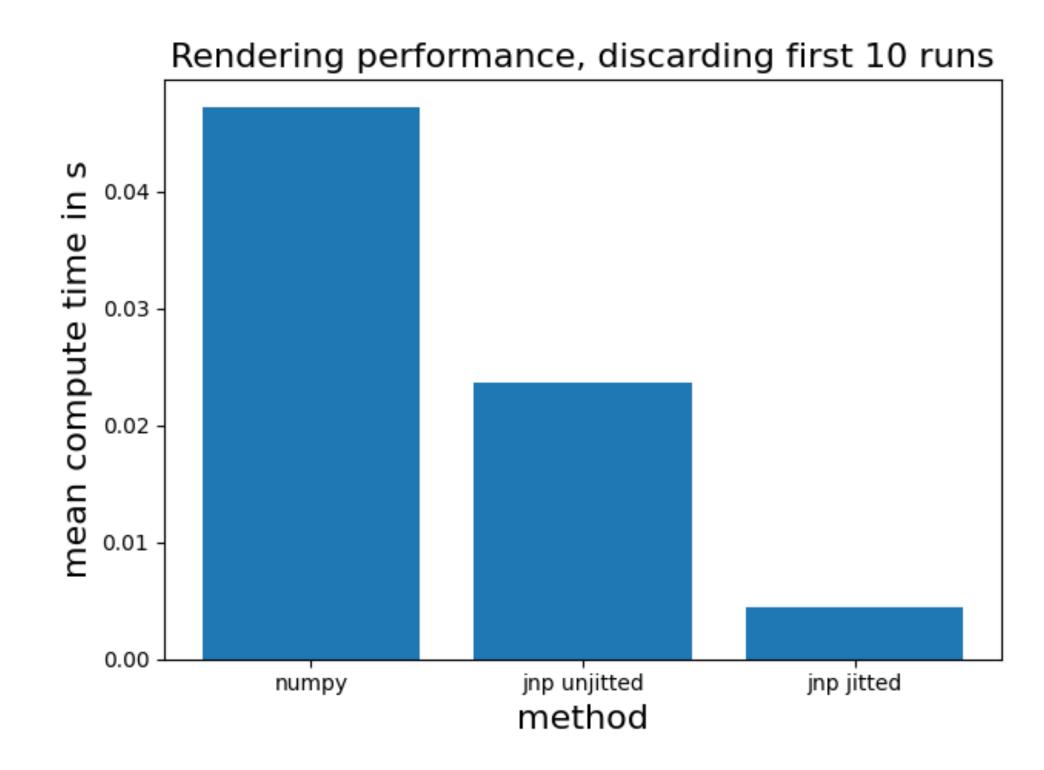
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Control flow can't depend on values of inputs

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```
from jax import jit
  def add_one_or_two(x, add_one):
    if add_one: # control flow depends on the argument add_one
      return x + 1
    else:
      return x + 2
  add_one_or_two_jitted = jit(add_one_or_two)
  add_one_or_two_jitted(1.0, True)
Python
ConcretizationTypeError
                                         Traceback (most recent call last)
/data/philliplo125/jax-tutorial/tutorial.ipynb Cell 41' in <cell line: 10>()
            return x + 2
      9 add_one_or_two_jitted = jit(add_one_or_two)
---> 10 add_one_or_two_jitted(1.0, True)
    [... skipping hidden 14 frame]
/data/philliplo125/jax-tutorial/tutorial.ipynb Cell 41' in add_one_or_two(x, add_one)
        def add_one_or_two(x, add_one):
     4 if add_one: # control flow depends on the argument add_one
           return x + 1
          else:
    [... skipping hidden 1 frame]
File ~/anaconda3/envs/jax-tutorial/lib/python3.9/site-packages/jax/core.py:1123, in concretization_function_error.<locals>.error(self, arg)
   1122 def error(self, arg):
-> 1123 raise ConcretizationTypeError(arg, fname_context)
ConcretizationTypeError: Abstract tracer value encountered where concrete value is expected: Traced<ShapedArray(bool[], weak_type=True)>with<DynamicJaxprTrace(level=0/1)>
The problem arose with the `bool` function.
While tracing the function add_one_or_two at /tmp/ipykernel_1263005/1343836691.py:3 for jit, this concrete value was not available in Python because it depends on the value of the arg
ument 'add_one'.
See https://jax.readthedocs.io/en/latest/errors.html#jax.errors.ConcretizationTypeError
```

Use static_argnums

```
def stupid_mult(a, b): # multiply two integers a and b in a very dumb way
    bs = b * np.ones(shape = (a,)) # the shape of bs depends on a!
    ab = np.sum(bs)
    return ab
  stupid_mult_jitted = jit(stupid_mult)
  stupid_mult_jitted(3, 4)
Python
TracerIntegerConversionError
                                          Traceback (most recent call last)
/data/philliplo125/jax-tutorial/tutorial.ipvnb Cell 45' in <cell line: 8>()
         return ab
      7 stupid_mult_jitted = jit(stupid_mult)
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[... skipping hidden 14 frame]
/data/philliplo125/jax-tutorial/tutorial.ipynb Cell 45' in stupid_mult(a, b)
       def stupid_mult(a, b): # multiply two integers a and b in a very dumb way
----> \frac{2}{2} bs = b * np.ones(shape = (a,)) # the shape of bs depends on a!
          ab = np.sum(bs)
          return ab
File ~/anaconda3/envs/jax-tutorial/lib/python3.9/site-packages/numpy/core/numeric.py:204, in ones(shape, dtype, order, like)
    201 if like is not None:
           return _ones_with_like(shape, dtype=dtype, order=order, like=like)
--> 204 a = empty(shape, dtype, order)
    205 multiarray.copyto(a, 1, casting='unsafe')
    206 return a
File ~/anaconda3/envs/jax-tutorial/lib/python3.9/site-packages/jax/core.py:519, in Tracer.__index__(self)
    518 def __index__(self):
--> 519 raise TracerIntegerConversionError(self)
TracerIntegerConversionError: The __index__() method was called on the JAX Tracer object Traced<ShapedArray(int32[], weak_type=True)>with<DynamicJaxprTrace(level=0/1)>
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  stupid_mult_jitted = jit(stupid_mult, static_argnums = 0)
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✓ 0.1s
                                                                                                                                                                                    Python
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 ✓ 0.1s
                                                                                                                                                                                    Python
DeviceArray(12., dtype=float32)
```

Automatic vectorization with vmap()

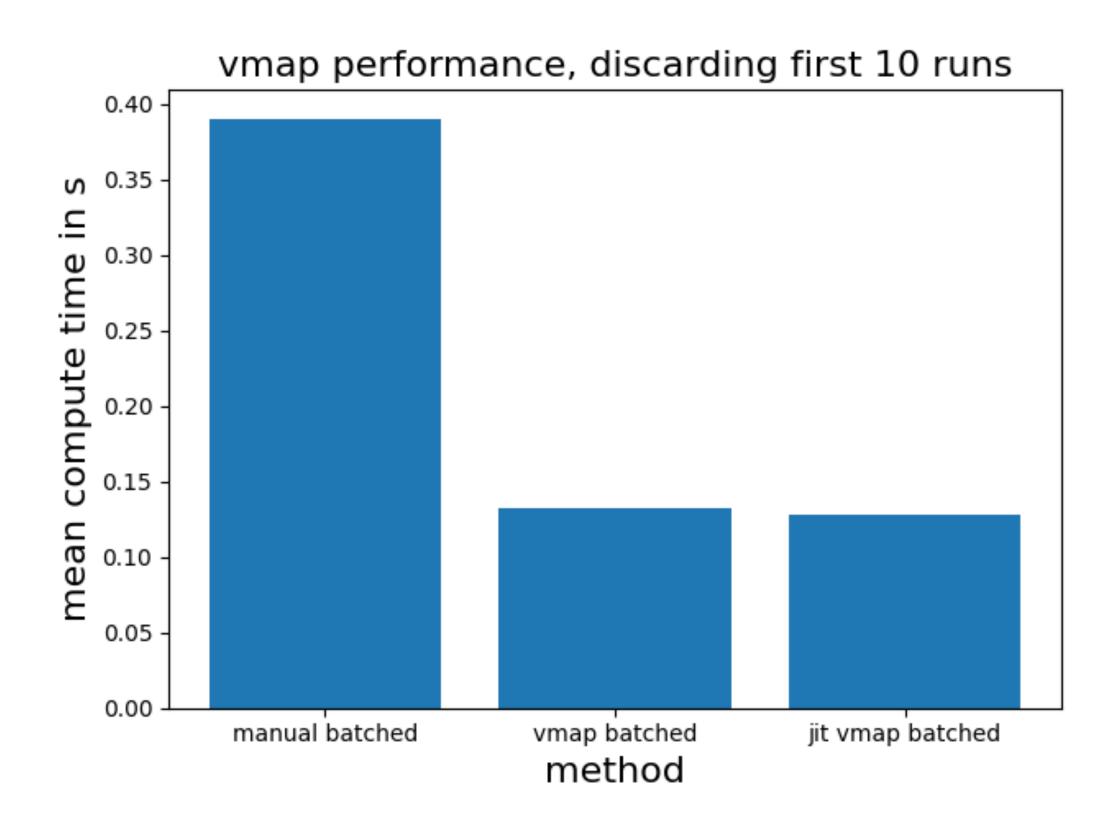
Compute Frobenius norm of one hundred 1000 x 1000 matrices

```
def frob_norm(A):
     Compute the Frobenus norm of a matrix A
     111
     return jnp.linalg.norm(A)
6
   def manual_batched_frob_norm(As):
     n = As.shape[0]
     norms = jnp.zeros(shape = As.shape[0])
     for i in range(n):
       norms = norms.at[i].set(frob_norm(As[i]))
     return norms
   vmap_batched_frob_norm = vmap(frob_norm)
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- Repo: https://github.com/PhillipLo/jax-tutorial