AA 203 Recitation #1: Automatic Differentiation with JAX

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1 JAX

JAX follows the *functional programming* paradigm. That is, JAX provides tools to transform a function into another function. Specifically, JAX can automatically compute the *derivative* of a function or composition of functions.

As an example, for $f(x) = \frac{1}{2}\|x\|_2^2$, JAX computes $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$ where $\nabla f(x) = x$.

[ ]:
```python
import jax
import jax.numpy as jnp

def f(x):
    return jnp.sum(x**2)/2    # identical to numpy syntax

grad_f = jax.grad(f)          # compute the gradient function

x = jnp.array([0., 1., 2.])  # use JAX arrays!
print('x:         ', x)
print('f(x):      ', f(x))
print('grad_f(x):', grad_f(x))
```

```
WARNING:jax._src.lib.xla_bridge:No GPU/TPU found, falling back to CPU. (Set
TF_CPP_MIN_LOG_LEVEL=0 and rerun for more info.)
```

```
x:         [0. 1. 2.]
f(x):      2.5
grad_f(x): [0. 1. 2.]
```

2 Automatic Differentation

Automatic Differentiation (AD, autodiff) uses pre-defined derivatives and the chain rule to compute derivatives of more complex functions.

Consider the function $f : \mathbb{R}^n \to \mathbb{R}^m$. The Jacobian of f evaluated at the point $x \in \mathbb{R}^n$ is the matrix

$$\partial f(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x) & \frac{\partial f_1}{\partial x_2}(x) & \cdots & \frac{\partial f_1}{\partial x_n}(x) \\ \frac{\partial f_2}{\partial x_1}(x) & \frac{\partial f_2}{\partial x_2}(x) & \cdots & \frac{\partial f_2}{\partial x_n}(x) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(x) & \frac{\partial f_m}{\partial x_2}(x) & \cdots & \frac{\partial f_m}{\partial x_n}(x) \end{bmatrix} = \left[\frac{\partial f_i}{\partial x_j}(x)\right]_{i=1,j=1}^{m,n} \in \mathbb{R}^{m\times n}.$$

As for any matrix, the Jacobian $\partial f(x) : \mathbb{R}^n \to \mathbb{R}^m$ is a linear map $v \mapsto \partial f(x)v$ defined by the usual matrix-vector multiplication rules.

AD can be used to compute the *Jacobian-Vector Product (JVP)*

$$\begin{aligned}\partial f(x) : \mathbb{R}^n &\to \mathbb{R}^m \\ v &\mapsto \partial f(x)v\end{aligned}$$

and the *Vector-Jacobian Product (VJP)*

$$\begin{aligned}\partial f(x)^\top : \mathbb{R}^m &\to \mathbb{R}^n \\ w &\mapsto \partial f(x)^\top w\end{aligned}$$

The maps $v \mapsto \partial f(x)v$ and $w \mapsto \partial f(x)^\top w$ are also known as the *pushforward* and *pullback*, respectively, of f at x. The vector x is referred to as the primal, while the vectors v and w are termed *seeds* in AD literature.

Consider the function composition

$$h(x) = (f_N \circ f_{N-1} \circ \cdots \circ f_1)(x) = f_N(f_{N-1}(\cdots f_1(x) \cdots)),$$

where each $f_k : \mathbb{R}^{d_k} \to \mathbb{R}^{d_{k+1}}$ is some differentiable map.

We can write this recursively as

$$y_0 = x \in \mathbb{R}^n, \quad y_{k+1} = f_{k+1}(y_k) \in \mathbb{R}^{d_{k+1}}, \quad y_N = h(x) \in \mathbb{R}^{d_N}.$$

By the chain rule, we have

$$\partial h(x) = \partial f_N(y_{N-1}) \partial f_{N-1}(y_{N-2}) \cdots \partial f_1(y_0).$$

This sequence of matrix multiplications that can get quickly get expensive for complicated functions!

It is more efficient and usually sufficient in practice to compute JVPs via the recursion

$$\begin{aligned}\partial h(x)v_0 &= \partial f_N(y_{N-1}) \partial f_{N-1}(y_{N-2}) \cdots \partial f_1(y_0)v_0 \\ &= v_N \\ v_k &= \partial f_k(y_{k-1})v_{k-1}\end{aligned},$$

and VJPs via the recursion

$$\begin{aligned}\partial h(x)^\top w_0 &= \partial f_1(y_0)^\top \cdots \partial f_{N-1}(y_{N-2})^\top \partial f_N(y_{N-1})^\top w_0 \\ &= w_N \\ w_k &= \partial f_{N-k+1}(y_{N-k})^\top w_{k-1}\end{aligned}.$$

VJPs require more memory than JVPs, since $\{y_k\}_{k=1}^{N-1}$ must be computed and stored first (i.e., the *forward pass*) before recursing (i.e., the *backward pass*).

2.1 Example: VJP as a gradient

For a scalar function $f : \mathbb{R}^n \to \mathbb{R}$, the Jacobian at x is $\underline{\partial f(x) \in \mathbb{R}^{1\times n}}$, so

$$\nabla f(x) = \partial f(x)^\top 1.$$

E.g., if $f(x) = \frac{1}{2}\|x\|_2^2$, then $\nabla f(x) = x \cdot 1$.

[ ]:
```python
f = lambda x: jnp.sum(x**2)/2  # anonymous functions work as well
x = jnp.array([0., 1., 2.])
f_x, dfxT = jax.vjp(f, x)      # compute forward pass and VJP function
dfxT_1 = dfxT(1.)

print('x:       ', x)
print('f(x):    ', f_x)
print('dfxT(1):', dfxT_1)
```

```
x:       [0. 1. 2.]
f(x):    2.5
dfxT(1): (DeviceArray([0., 1., 2.], dtype=float32),)
```

2.2 Example: JVP as a directional derivative

The directional derivative of $f : \mathbb{R}^n \to \mathbb{R}$ at $x \in \mathbb{R}^n$ along $v \in \mathbb{R}^n$ is

$$\nabla f(x)^\top v = \partial f(x) v.$$

E.g., if $f(x) = \frac{1}{2}\|x\|_2^2$, then $\nabla f(x)^\top v = x^\top v$.

[ ]:
```python
f = lambda x: jnp.sum(x**2)/2
x = jnp.array([0., 1., 2.])
v = jnp.array([1., 1., 1.])

# use tuples to separate inputs from seeds
f_x, dfx_v = jax.jvp(f, (x,), (v,))

print('x:     ', x)
print('f(x):  ', f_x)
print('dfx(v):', dfx_v)
```

f(x)

$\partial f(x) v$

```
x:      [0. 1. 2.]
f(x):   2.5
dfx(v): 3.0
```

2.3 Example: Multi-input, multi-output VJP

Let's try something more complicated:

$$
\begin{aligned}
f : \mathbb{R}^n \times \mathbb{R}^n &\to \mathbb{R} \times \mathbb{R} \\
(x, y) &\mapsto \left(\underbrace{\frac{1}{2}\|x\|_2^2 + \frac{1}{2}\|y\|_2^2}_{f_1(x,y)}, \underbrace{\sum_{i=1}^{n} x_i}_{f_2(x,y)} \right)
\end{aligned}
$$

$f = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$

```
[ ]: def f(x, y):
         f1 = jnp.sum(x**2)/2 + jnp.sum(y**2)/2
         f2 = jnp.sum(x)
         return f1, f2

     x = jnp.array([0., 1., 2.])
     y = jnp.array([0., 1., 2.])
     f_xy, dfT = jax.vjp(f, x, y)

     print('x,y:      ', x, y)
     print('f(x,y):   ', f_xy)
     print('dfT(1,1):', dfT((1., 1.)))   # provide tuple as input
```

$\partial_x f(x,y)\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $\partial_y f(x,y)\begin{bmatrix} 1 \\ 1 \end{bmatrix}$

```
x,y:      [0. 1. 2.] [0. 1. 2.]
f(x,y):   (DeviceArray(5., dtype=float32), DeviceArray(3., dtype=float32))
dfT(1,1): (DeviceArray([1., 2., 3.], dtype=float32), DeviceArray([0., 1., 2.],
dtype=float32))
```

2.4 Example: VJP and JVP for a Matrix Input

We can generalize VJPs and JVPs to non-vector inputs as well:

$$
\begin{aligned}
f : \mathbb{R}^{n \times n} &\to \mathbb{R} \\
X &\mapsto a^\top X b
\end{aligned}
$$

```
[ ]: def f(X):
         a, b = jnp.array([0., 1., 2.]), jnp.array([0., 1., 2.])
         return a @ (X @ b)

     X = jnp.ones((3, 3))
     f_x = f(X)
     w, V = jnp.array(1.), jnp.eye(3)
     f_x, dfT = jax.vjp(f, X)
     f_x, df_v = jax.jvp(f, (X,), (V,))

     print('X:\n', X, '\n', 'f(X): ', f_x, '\n', sep='')
     print('dfT(1):\n', dfT(w), '\n', 'df(I): ', df_v, sep='')
```

```
X:
[[1. 1. 1.]
 [1. 1. 1.]
```

```
 [1. 1. 1.]]
f(X): 9.0

dfT(1):
(DeviceArray([[0., 0., 0.],
              [0., 1., 2.],
              [0., 2., 4.]], dtype=float32),)
df(I): 5.0
```

3 Auto-Vectorizing Functions with `jax.vmap`

For some complicated function $f : \mathbb{R}^n \to \mathbb{R}^m$, we want to calculate $f(x)$ for *many* different values of x without looping.

This is known as *vectorizing* a function. JAX can do this automatically!

[ ]:
```python
f = lambda x: jnp.array([jnp.sum(x**2)/2, jnp.linalg.norm(x, jnp.inf)])
f = jax.vmap(f)

batch_size, n = 100, 3
x = jnp.ones((batch_size, n))  # dummy values with desired shape

print(x.shape)
print(f(x).shape)
```

in axis = 0

```
(100, 3)
(100, 2)
```

for row in x:
store f(row)

3.1 Example: Batch Evaluation of a Neural Network

[ ]:
```python
def f(x, W, b):
    return W[1] @ jnp.tanh(W[0] @ x + b[0]) + b[1]
f = jax.vmap(f, in_axes=(0, None, None))
f = jax.vmap(f, in_axes=(0, None, None))

n, m = 3, 5
batch_size = 100
hdim = 32

W = (jnp.ones((hdim, n)), jnp.ones((m, hdim)))
b = (jnp.ones(hdim), jnp.ones(m))
x = jnp.ones((40, batch_size, n))

print(x.shape)
print(f(x, W, b).shape)
```

x → 3D
batch → 2D

for batch in x:
→ for vec in batch:
store f(vec, W, b)

```
(40, 100, 3)
(40, 100, 5)
```

3.2 Example: Jacobian Matrix from JVPs and VJPs

Let $e_k^{(d)} \in \{0,1\}^d$ denote the k^{th} coordinate vector in d dimensions.

$n \gg 1$

For $f : \mathbb{R}^n \to \mathbb{R}^m$, we can compute the full Jacobian $\partial f(x) \in \mathbb{R}^{m\times n}$ with either n JVPs

$x \in \mathbb{R}^n$

$$\partial f(x) = \partial f(x) I_n = \begin{bmatrix} \partial f(x) e_1^{(n)} & \partial f(x) e_2^{(n)} & \cdots & \partial f(x) e_n^{(n)} \end{bmatrix},$$

$f(x) = L(x)$

$f: \mathbb{R}^n \to \mathbb{R}$

or m VJPs

$$\partial f(x)^\top = \partial f(x)^\top I_m = \begin{bmatrix} \underbrace{\partial f(x)^\top}_{\mathbb{R}^n} e_1^{(m)} & \partial f(x)^\top e_2^{(m)} & \cdots & \partial f(x)^\top e_m^{(m)} \end{bmatrix}.$$

$\partial f(x) \in \mathbb{R}^{1\times n}$

This is what the source code for `jax.jacfwd` and `jac.jacrev` does.

```
f = lambda x: jnp.array([x[0], x[0]**2 + x[2]**2])

def df(x, v):
    fx, dfx_v = jax.jvp(f, (x,), (v,))
    return dfx_v

def dfT(x, w):
    fx, dfxT = jax.vjp(f, x)
    return dfxT(w)[0]  # need to index into tuple

n, m = 3, 2
x = jnp.ones(n)
Jx = jax.vmap(df, in_axes=(None, 0))(x, jnp.eye(n))
JxT = jax.vmap(dfT, in_axes=(None, 0))(x, jnp.eye(m))
print('Jacobian (forward AD):')
print(Jx)
print('\nJacobian (reverse AD):')
print(JxT)
```

$f_1(x)$ $f_2(x)$

(value,)

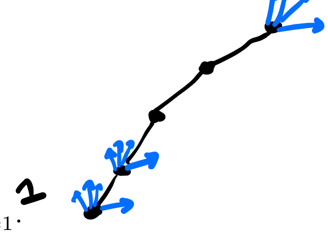
```
Jacobian (forward AD):
[[1. 2.]
 [0. 0.]
 [0. 2.]]

Jacobian (reverse AD):
[[1. 0. 0.]
 [2. 0. 2.]]
```

3.3 Example: Linearizing Dynamics at Many Points

For $\dot{x} = f(x,u)$ with $x \in \mathbb{R}^n$ and $u \in \mathbb{R}^m$, recall the first-order Taylor approximation

$$f(x,u) \approx \underbrace{f(\bar{x}_k, \bar{u}_k)}_{=c_k} + \underbrace{\partial_x f(\bar{x}_k, \bar{u}_k)}_{=A_k} \underbrace{(x - \bar{x})}_{\Delta x_t} + \underbrace{\partial_u f(\bar{x}_k, \bar{u}_k)}_{=B_k} \underbrace{(u - \bar{u})}_{\Delta u_t}.$$

K



We want $A_k \Delta x_t$, $B_k \Delta u_t$, and c_k for $\{(\bar{x}_k, \bar{u}_k)\}_{k=1}^{K}$ and $\{(\Delta x_t, \Delta u_t)\}_{t=1}^{T}$.

This scenario may correspond to evaluating Taylor approximations for T perturbations $(\Delta x_t, \Delta u_t)$ that we want to test at the K points $(\bar{x}_k, \bar{u}_k)$.

[ ]:
```
# Inverted pendulum (with unit mass and unit length)
f = lambda x, u: jnp.array([x[1], 9.81*jnp.sin(x[0]) + u[0]])

def taylor(x̄, ū, Δx, Δu):
    f_x̄ū, AΔx = jax.jvp(lambda x: f(x, ū), (x̄,), (Δx,))
    _, BΔu = jax.jvp(lambda u: f(x̄, u), (ū,), (Δu,))
    return f_x̄ū, AΔx, BΔu

print(type(taylor))

n, m = 2, 1
K, T = 5, 10
x̄, ū = jnp.ones((K, n)), jnp.ones((K, m))
Δx, Δu = jnp.ones((T, n)), jnp.ones((T, m))

taylor = jax.vmap(taylor, in_axes=(None, None, 0, 0))
print(type(taylor))

taylor = jax.vmap(taylor, in_axes=(0, 0, None, None))
print(type(taylor))

c, Ax, Bu = taylor(x̄, ū, Δx, Δu)
print(c.shape)
print(Ax.shape)
print(Bu.shape)
```

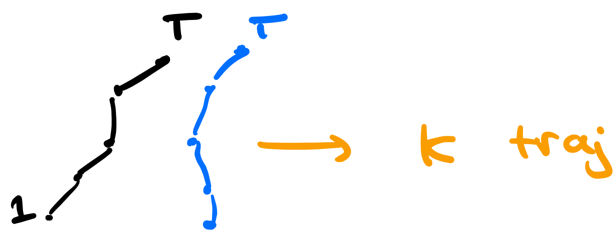
$\partial_x f(\bar{x}_k, \bar{u}_k)\Delta x_t$

$A_k \Delta x_t$

1: $O(K)$

2: $O(T)$

```
<class 'function'>
<class 'function'>
<class 'function'>
(5, 10, 2)
(5, 10, 2)
(5, 10, 2)
```



If, instead, we have $K = 5$ trajectories $\{(\bar{x}_k, \bar{u}_k)\}_{k=1}^{K}$ and each trajectory $\bar{x}_k$ has $T = 10$ timesteps $\{(\bar{x}_{k,t}, \bar{u}_{k,t})\}_{t=1}^{T}$, and similarly for $(\Delta x, \Delta u)$, then we can evaluate Taylor approximations for all these trajectories with two calls to vmap as below.

[ ]:
```
# Inverted pendulum (with unit mass and unit length)
f = lambda x, u: jnp.array([x[1], 9.81*jnp.sin(x[0]) + u[0]])
def taylor(x̄, ū, Δx, Δu):
    f_x̄ū, AΔx = jax.jvp(lambda x: f(x, ū), (x̄,), (Δx,))
    f_x̄ū, BΔu = jax.jvp(lambda u: f(x̄, u), (ū,), (Δu,))
    return f_x̄ū, AΔx, BΔu
```

```
n, m = 2, 1
K, T = 5, 10
x̄ = jnp.ones((K, T, n)) # note the different sizes
ū = jnp.ones((K, T, m))
Δx, Δu = jnp.ones((K, T, n)), jnp.ones((K, T, m))

# two successive calls to vmap:
# we linearize for the K trajectories that each have T timesteps
taylor = jax.vmap(taylor)
taylor = jax.vmap(taylor)

c, Ax, Bu = taylor(x̄, ū, Δx, Δu)
print(c.shape)
print(Ax.shape)
print(Bu.shape)
```

```
(5, 10, 2)
(5, 10, 2)
(5, 10, 2)
```

4 Other Features and Nuances of JAX

See the JAX documentation for more details.

4.1 Just-In-Time (JIT) Compilation

JAX can compile code to run fast on both CPUs and GPUs. The first call to a "jitted" function will compile and cache the function; subsequent calls are then much faster.

[ ]:
```
def selu(x, alpha=1.67, lmbda=1.05):
    return lmbda * jnp.where(x > 0, x, alpha * jnp.exp(x) - alpha)

x = jnp.ones(int(1e7))
%timeit -r10 -n100 selu(x).block_until_ready()

selu_jit = jax.jit(selu)
%timeit -r10 -n100 selu_jit(x).block_until_ready()
```

```
42.5 ms ± 2.95 ms per loop (mean ± std. dev. of 10 runs, 100 loops each)
10.4 ms ± 426 µs per loop (mean ± std. dev. of 10 runs, 100 loops each)
```

4.2 In-Place Updates

JAX arrays are immutable. In keeping with the functional programming paradigm, updates to array values at indices are done via JAX functions.

[ ]:
```
X = jnp.zeros((3,3))
try:
```

```
    X[0, :] = 1.
except Exception as e:
    print("Exception: {}".format(e))
print('\nX:\n', X, sep='')

Y = X.at[0, :].set(1.)
print('\nY:\n', Y, sep='')
```

```
Exception: '<class 'jaxlib.xla_extension.DeviceArray'>' object does not support
item assignment. JAX arrays are immutable. Instead of ``x[idx] = y``, use ``x =
x.at[idx].set(y)`` or another .at[] method:
https://jax.readthedocs.io/en/latest/_autosummary/jax.numpy.ndarray.at.html

X:
[[0. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]]

Y:
[[1. 1. 1.]
 [0. 0. 0.]
 [0. 0. 0.]]
```

4.3 Pseudo-Random Number Generation (PRNG)

JAX does explicit PRNG; after initiailizing a PRNG state, it can be forked into new PRNG states for parallel stochastic generation.

This enables reproducible results; propagate the key and make new subkeys whenever new random numbers are needed.

[ ]:
```
seed = 0
key = jax.random.PRNGKey(seed)
print(jax.random.normal(key, shape=(1,)))
print(jax.random.normal(key, shape=(1,)))  # same value sampled!

print('\nkey', key)
key, *subkeys = jax.random.split(key, 3)
print('|-- SPLIT --> key     ', key)
print('          --> subkeys', subkeys[0],
      '--> normal', jax.random.normal(subkeys[0], shape=(1,)))
print('                     ', subkeys[1],
      '--> normal', jax.random.normal(subkeys[1], shape=(1,)))
```

```
[-0.20584226]
[-0.20584226]

key [0 0]
|-- SPLIT --> key     [2467461003  428148500]
```

```
--> subkeys [3186719485 3840466878] --> normal [0.5781488]
            [2562233961 1946702221] --> normal [0.8535516]
```