JAX

Lecture 25

Dr. Colin Rundel

JAX

JAX is NumPy on the CPU, GPU, and TPU, with great automatic differentiation for high-performance machine learning research.

- JAX provides a NumPy-inspired interface for convenience (jax.numpy),
 can often be used as drop-in replacement
- All JAX operations are implemented in terms of operations in XLA (Accelerated Linear Algebra compiler)
- Supports sequential execution or JIT compilation
- Updated autograd which can be used with native Python and NumPy functions

JAX & NumPy

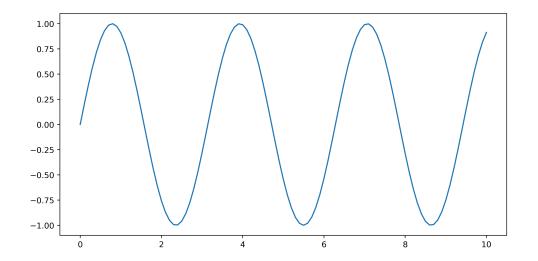
```
1 import numpy as np
2
3 x_np = np.linspace(0, 10, 101)
4 y_np = 2 * np.sin(x_np) * np.cos(x_np)
5 plt.plot(x_np, y_np)
```

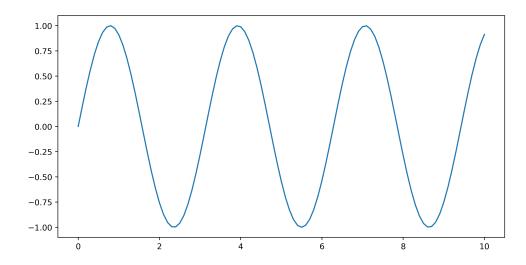
```
import jax.numpy as jnp

x_jnp = jnp.linspace(0, 10, 101)

y_jnp = 2 * jnp.sin(x_jnp) * jnp.cos(x_jnp)

plt.plot(x_jnp, y_jnp)
```





```
1 type(x_np)
```

numpy.ndarray

```
1 type(x_jnp)
```

jaxlib.xla_extension.ArrayImpl

```
1 \times jnp
 1 x_np
array([ 0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0. Array([ 0. , 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.
                                                     0.8, 0.9, 1., 1.1, 1.2, 1.3, 1.4, 1.5
      0.8, 0.9, 1., 1.1, 1.2, 1.3, 1.4, 1.
      1.6, 1.7, 1.8, 1.9, 2., 2.1, 2.2, 2.3
                                                     1.6, 1.7, 1.8, 1.9, 2., 2.1, 2.2, 2.3
      2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3., 3.
                                                     2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3., 3.1
      3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9
                                                     3.2, 3.3, 3.4, 3.5, 3.6, 3.7, 3.8, 3.9
      4., 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.
                                                     4. , 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7
      4.8, 4.9, 5., 5.1, 5.2, 5.3, 5.4, 5.
                                                     4.8, 4.9, 5., 5.1, 5.2, 5.3, 5.4, 5.5
      5.6, 5.7, 5.8, 5.9, 6., 6.1, 6.2, 6.3
                                                     5.6, 5.7, 5.8, 5.9, 6., 6.1, 6.2, 6.3
      6.4, 6.5, 6.6, 6.7, 6.8, 6.9, 7., 7.
                                                     6.4, 6.5, 6.6, 6.7, 6.8, 6.9, 7., 7.1
      7.2, 7.3, 7.4, 7.5, 7.6, 7.7, 7.8, 7.9
                                                     7.2, 7.3, 7.4, 7.5, 7.6, 7.7, 7.8, 7.9
      8. , 8.1, 8.2, 8.3, 8.4, 8.5, 8.6, 8.
                                                     8. , 8.1, 8.2, 8.3, 8.4, 8.5, 8.6, 8.7
      8.8, 8.9, 9., 9.1, 9.2, 9.3, 9.4, 9.5
                                                     8.8, 8.9, 9., 9.1, 9.2, 9.3, 9.4, 9.5
      9.6, 9.7, 9.8, 9.9, 10.])
                                                     9.6, 9.7, 9.8, 9.9, 10. ], dtype=float32)
                                                1 x jnp.dtype
 1 x np.dtype
```

dtype('float64')

dtype('float32')

Compatibility

```
1 y mix = 2 * np.sin(x jnp) * jnp.cos(x_np); y_mix
Array([ 0.
              , 0.19867, 0.38942, 0.56464, 0.71736,
        0.84147, 0.93204, 0.98545, 0.99957, 0.97385,
       0.9093 , 0.8085 , 0.67546 , 0.5155 , 0.33499 ,
       0.14112, -0.05837, -0.25554, -0.44252, -0.61186,
      -0.7568 , -0.87158 , -0.9516 , -0.99369 , -0.99616 ,
      -0.95892, -0.88345, -0.77276, -0.63127, -0.4646,
       -0.27942, -0.08309, 0.11655, 0.31154, 0.49411,
       0.65699, 0.79367, 0.89871, 0.96792, 0.99854,
       0.98936, 0.94073, 0.8546, 0.7344, 0.58492,
       0.41212, 0.22289, 0.02478, -0.17433, -0.36648,
      -0.54402, -0.69987, -0.82783, -0.92278, -0.98094,
       -0.99999, -0.97918, -0.91933, -0.82283, -0.69353,
       -0.53657, -0.35823, -0.1656, 0.03362, 0.23151,
       0.42017, 0.59207, 0.74038, 0.85916, 0.9437,
       0.99061, 0.99803, 0.96566, 0.89479, 0.78825,
       0.65029, 0.4864, 0.30312, 0.10775, -0.09191,
       -0.2879 , -0.47242 , -0.63811 , -0.77835 , -0.88757 ,
       -0.9614 , -0.9969 , -0.99266 , -0.94885 , -0.8672 ,
       -0.75099, -0.60483, -0.43457, -0.24698, -0.04954,
       0.14988, 0.34331, 0.52307, 0.68196, 0.81367,
       0.91295], dtype=float32)
```

```
1 type(y_mix)
```

Aside - PRNG

JAX vs NumPy

Pseudo random number generation in JAX is a bit different than with NumPy - the latter depends on a global state that is updated each time a random function is called.

NumPy's PRNG guarantees something called sequential equivalence which amounts to sampling N numbers sequentially is the same as sampling N numbers at once (e.g. a vector of length N).

```
1    np.random.seed(0)
2    print("individually:", np.stack([np.random.uniform() for i in range(5)]))
individually: [0.54881 0.71519 0.60276 0.54488 0.42365]

1    np.random.seed(0)
2    print("all at once: ", np.random.uniform(size=5))
all at once: [0.54881 0.71519 0.60276 0.54488 0.42365]
```

Parallelization & Sequential equivalence

Sequantial equivalence can be problematic in light of parallelization, consider the following code:

```
1  np.random.seed(0)
2
3  def bar():
4    return np.random.uniform()
5  def baz():
6    return np.random.uniform()
7
8  def foo():
9    return bar() + 2 * baz()
```

How do we guarantee that we get consistent results if we don't know the order that bar() and baz() will run?

PRNG keys

JAX makes use of 'random keys' which are just a fancier version of random seeds - all of JAX's random functions require that a key be passed in.

```
1 key = jax.random.PRNGKey(1234); key
Array([ 0, 1234], dtype=uint32)

1 jax.random.normal(key)
Array(-0.5402, dtype=float32)

1 jax.random.normal(key)
Array(-0.5402, dtype=float32)

1 jax.random.normal(key, shape=(3,))
Array([-0.01978, -0.0731, -1.07825], dtype=float32)
```

Note that JAX does not provide a sequential equivalence guarantee - this is so that it can support vectorization for the generation of PRN.

Splitting keys

Since a key is essentially a seed we do not want to reuse them (unless we want an identical output). Therefore to generate multiple different PRN we can split a key to deterministically generate two (or more) new keys.

```
1 new_key2, sub_key2 = jax.random.split(key)
  1 new key1, sub key1 = jax.random.split(key)
  2 print(f"key : {key}")
                                                        2 print(f"key : {key}")
  3 print(f"new key1: {new key1}")
                                                        3 print(f"new key2: {new key2}")
  4 print(f"sub key1: {sub_key1}")
                                                        4 print(f"sub key2: {sub key2}")
key
    : [ 0 1234]
                                                      key
                                                             : [ 0 1234]
new key1: [2113592192 1902136347]
                                                      new key2: [2113592192 1902136347]
sub key1: [603280156 445306386]
                                                      sub key2: [603280156 445306386]
  1 new key3, *sub keys3 = jax.random.split(key, num=3)
  2 sub keys3
[Array([1047329699, 140093922], dtype=uint32),
 Array([2907975018, 3484112841], dtype=uint32)]
```

JAX performance & jit

JAX performance

```
1 key = jax.random.PRNGKey(1234)
  2 \times jnp = jax.random.normal(key, (1000, 1000))
  3 \times np = np.array(x jnp)
  1 type(x np)
                                                             1 type(x jnp)
numpy.ndarray
                                                          jaxlib.xla extension.ArrayImpl
  1 x np.shape
                                                             1 x jnp.shape
(1000, 1000)
                                                           (1000, 1000)
  1 %timeit y = x np @ x np
                                                             1 %timeit y = 3*x np + x np
8.7 ms \pm 360 \mus per loop (mean \pm std. dev. of 7 runs, 536 \mus \pm 33.5 \mus per loop (mean \pm std. dev. of 7 runs
  1 %timeit y = x jnp @ x jnp
                                                             1 %timeit y = 3*x jnp + x jnp
4.19 ms \pm 516 \mus per loop (mean \pm std. dev. of 7 runs 529 \mus \pm 36 \mus per loop (mean \pm std. dev. of 7 runs,
  1 %timeit y = (x jnp @ x jnp).block until ready()
                                                             1 %timeit y = (3*x jnp + x jnp).block until ready(
3.92 ms \pm 215 \mus per loop (mean \pm std. dev. of 7 runs
                                                          496 \mus ± 39 \mus per loop (mean ± std. dev. of 7 runs,
```

```
1 def SELU np(x, \alpha=1.67, \lambda=1.05):
     "Scaled Exponential Linear Unit"
     return \lambda * np.where(x > 0, x, \alpha * np.exp(x) -
```

```
1 SELU np jit = jax.jit(SELU np)
```

```
1 def SELU jnp(x, \alpha=1.67, \lambda=1.05):
     "Scaled Exponential Linear Unit"
     return \lambda * jnp.where(x > 0, x, \alpha * jnp.exp(x)
```

```
1 SELU jnp jit = jax.jit(SELU jnp)
```

```
1 \times = np.arange(1e6)
2 %timeit y = SELU np(x)
```

4.38 ms \pm 127 μ s per loop (mean \pm std. dev. of 7 runs 1.78 ms \pm 85.7 μ s per loop (mean \pm std. dev. of 7 runs

```
1 %timeit y = SELU_np_jit(x).block_until_ready()
```

TracerArrayConversionError: The numpy.ndarray convers The error occurred while tracing the function SELU na See https://jax.readthedocs.io/en/latest/errors.html;

```
1 x = jnp.arange(1e6)
2 %timeit y = SELU jnp(x).block until ready()
```

```
1 %timeit y = SELU_jnp_jit(x).block_until_ready()
```

370 μ s \pm 20.5 μ s per loop (mean \pm std. dev. of 7 runs

jit limitations

When it works the jit tool is fantastic, but it does have a number of limitations,

- Must use pure functions (no side effects)
- Must primarily use JAX functions
 - e.g. use jnp.minimum() not np.minimum() or min()
- Must generally avoid conditionals / control flow
- Issues around concrete values when tracing (static values)
- Check performance there are not always gains + there is the initial cost of compilation

autograd

Basics

Like with torch, the grad() function takes a numerical function returning a scalar and returns a function for calculating the gradient of that function.

```
1 def g(x):
  1 \text{ def } f(x):
                                                                           1 def h(x):
      return x**2
                                           return jnp.exp(-x)
                                                                               return jnp.maximum(0,x)
  1 f(3.)
                                      1 g(1.)
                                                                           1 h(-2.)
9.0
                                    Array(0.36788, dtype=float32, weak Array(0., dtype=float32, weak type
    jax.grad(f)(3.)
                                        jax.grad(g)(1.)
                                                                           1 h(2.)
Array(6., dtype=float32, weak type Array(-0.36788, dtype=float32, wea Array(2., dtype=float32, weak type
  jax.grad(jax.grad(f))(3.)
                                      1 jax.grad(jax.grad(g))(1.)
                                                                           1 jax.grad(h)(-2.)
Array(2., dtype=float32, weak type Array(0.36788, dtype=float32, weak Array(0., dtype=float32, weak type
                                                                           1 jax.grad(h)(2.)
                                                                         Array(1., dtype=float32, weak type
```

Aside - vmap()

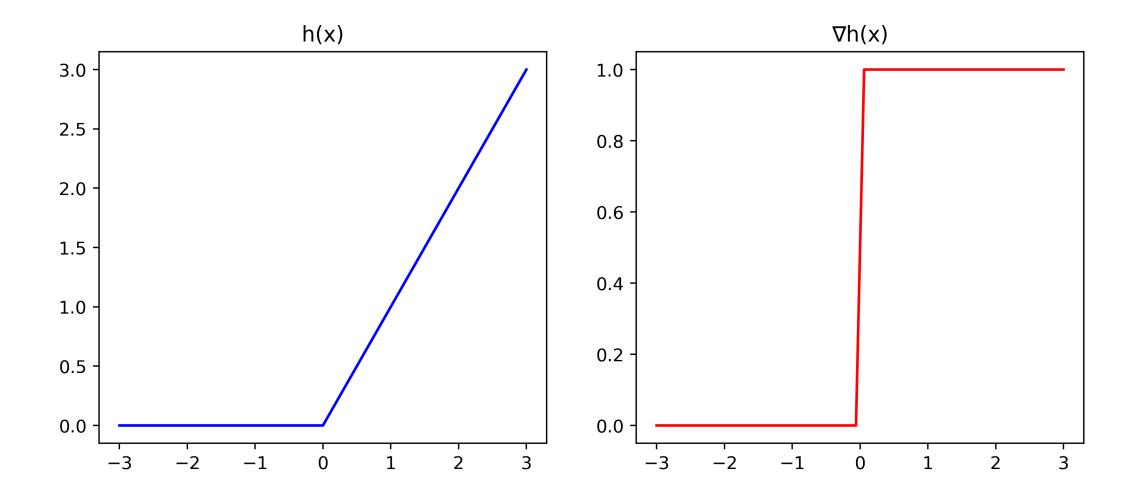
I would like to plot h() and jax.grad(h)() - lets see what happens,

```
1  x = jnp.linspace(-3,3,101)
2  y = h(x)
3  y_grad = jax.grad(h)(x)
```

TypeError: Gradient only defined for scalar-output functions. Output had shape: (101,).

As mentiond on the previous slide - in order to calculate the gradient we need to apply it to a scalar valued function. We can transform our scalar function into a vectorized function using vmap().

```
1 y_grad = jax.vmap(
2  jax.grad(h)
3 )(x)
```



Regession example

```
1 d = pd.read_csv("https://sta663-sp23.github.io/slides/data/ridge.
```

```
x1
                             x2
                                       x3
                                                x4 x5
           У
   -0.151710 0.353658 1.633932
                                 0.553257
                                          1.415731 A
    3.579895 1.311354 1.457500 0.072879
                                          0.330330 B
    0.768329 -0.744034 0.710362 -0.246941 0.008825 B
3
    7.788646 0.806624 -0.228695 0.408348 -2.481624 B
    1.394327 0.837430 -1.091535 -0.860979 -0.810492 A
495 -0.204932 -0.385814 -0.130371 -0.046242
   0.541988 0.845885 0.045291 0.171596 0.332869 A
497 -1.402627 -1.071672 -1.716487 -0.319496 -1.163740 C
498 -0.043645 1.744800 -0.010161 0.422594 0.772606 A
499 -1.550276 0.910775 -1.675396 1.921238 -0.232189 B
[500 rows x 6 columns]
```

```
1  X = jnp.array(
2  pd.get_dummies(
3     d.drop("y", axis=1)
4     ).to_numpy(dtype = np.float:
5  )
6  X.shape

(500, 8)

1  y = jnp.array(
2     d.y.to_numpy(dtype = np.float:
3  )
4  y.shape
```

Model & loss functions

```
def model(b, X=X):
    return X @ b

def reg_loss(b, \lambda=0., X=X, y=y, model=model):
    return jnp.mean((y - model(b,X).squeeze())**2)

def ridge_loss(b, \lambda=0., X=X, y=y, model=model):
    return jnp.mean((y - model(b,X).squeeze())**2) + \lambda * jnp.sum(b**2)

def lasso_loss(b, \lambda=0., X=X, y=y, model=model):
    return jnp.mean((y - model(b,X).squeeze())**2) + \lambda * jnp.sum(jnp.abs(b))
```

grad() of a multiargument function will take the gradient with respect to the first argument.

```
grad_reg_loss = jax.grad(reg_loss)
grad_ridge_loss = jax.grad(ridge_loss)
grad_lasso_loss = jax.grad(lasso_loss)
```

```
1 key = jax.random.PRNGKey(1234)
  2 b = jax.random.normal(key, (X.shape[1],1))
                                                          1 grad_ridge_loss(b, \lambda = 1)
  1 grad_reg_loss(b)
                                                        Array([-5.8394],
Array([-4.02278],
       [-4.46708],
                                                                [-5.74791],
       [ 0.08748],
                                                                [ 0.68661],
       [ 5.57939],
                                                                [ 5.13631],
       [-1.13703],
                                                               [-4.59595],
       [ 0.03037],
                                                               [-0.35854],
       [ 1.11083],
                                                                [ 3.54811],
       [-0.30304]], dtype=float32)
                                                                [-0.61224]], dtype=float32)
   1 grad_lasso_loss(b, \lambda = 1)
 Array([-5.02278],
        [-5.46708],
        [ 1.08748],
        [ 4.57939],
        [-2.13703],
        [-0.96963],
        [ 2.11083],
        [-1.30304]], dtype=float32)
```

sklearn

```
1 from sklearn.linear_model import LinearRegression
2
3 lm = LinearRegression(fit_intercept=False).fit(X,y)
4 lm.coef_
array([ 0.99505,  2.00762,  0.00232, -3.00088,  0.49329,
```

0.10193, -0.29413, 1.00856], dtype=float32)

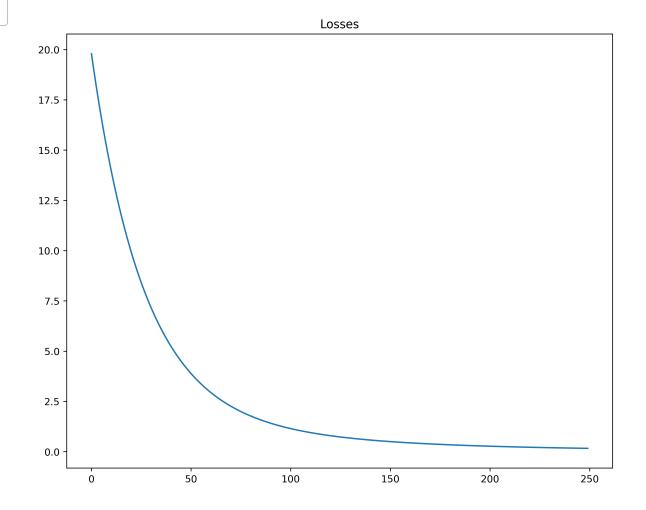
Fit implementation

```
1 def fit(b, loss, λ=0., n=250, lr=0.01, X=X, y=y, model=model):
2  val_grad = jax.value_and_grad(loss)
3
4  losses = []
5  for i in range(n):
6   val, grad = val_grad(b, λ)
7  losses.append(val.item())
8
9  b -= lr * grad
10
11  return (b, losses)
```

Linear regression

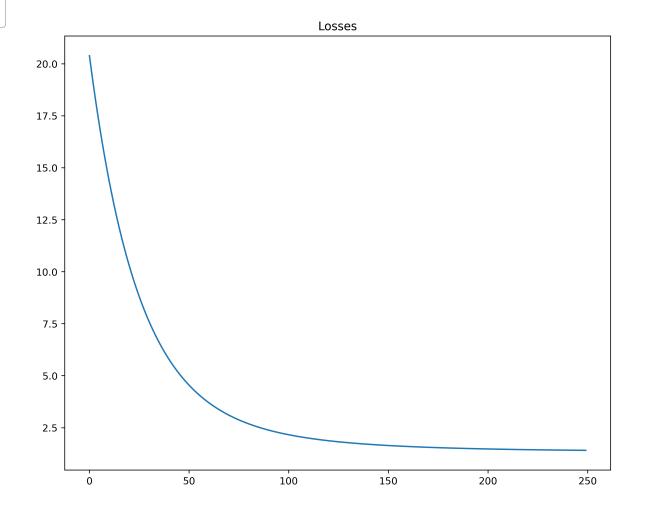
```
1 b = jax.random.normal(key, (X.shape[1],1))
2 b_hat, losses = fit(b, reg_loss)
```

1 b_hat



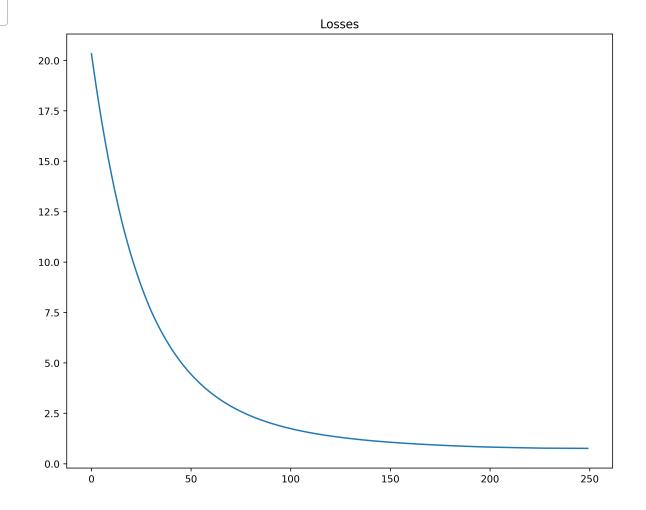
Ridge regression

```
1 b = jax.random.normal(key, (X.shape[1],1))
2 b_hat, losses = fit(b, ridge_loss, \lambda=0.1)
```



Lasso regression

```
1 b = jax.random.normal(key, (X.shape[1],1))
2 b_hat, losses = fit(b, lasso_loss, \lambda=0.1)
```



Jitting fit?

```
1 fit_jit = jax.jit(fit)
2 b_hat, losses = fit_jit(b, reg_loss, λ=0.1)
```

TypeError: Cannot interpret value of type <class 'function'> as an abstract array; it does not have a dtype

```
1 fit_jit = jax.jit(fit, static_argnames=["loss","λ","n","X","y","model"])
2 b_hat = fit_jit(b, reg_loss)
```

ConcretizationTypeError: Abstract tracer value encountered where concrete value is expected: Traced<ShapedAr The problem arose with the `float` function. If trying to convert the data type of a value, try using `x.ast The error occurred while tracing the function fit at /var/folders/ds/8sqz2v4d355btthn6r88kdc00000gn/T/ipyker

Simpler fit

```
1 def fit_simple(b, loss, λ=0., n=250, lr=0.01, X=X, y=y, model=model):
2    grad = jax.grad(loss)
3
4    for i in range(n):
5        b -= lr * grad(b, λ)
6
7    return b
8
9    b_hat = fit_simple(b, reg_loss)
```

```
1 fit_jit = jax.jit(fit_simple, static_argnames=["loss","λ","n","X","y","model"])
2 b_hat_jit = fit_jit(b, reg_loss)
```

Performance

```
1 %timeit b hat = fit simple(b, reg loss)
442 ms \pm 2.07 ms per loop (mean \pm std. dev. of 7 runs, 1 loop each)
  1 %timeit b hat jit = fit jit(b, reg loss)
307 \mus \pm 2.44 \mus per loop (mean \pm std. dev. of 7 runs, 1,000 loops each)
  1 %timeit b hat jit = fit jit(b, reg loss).block until ready()
310 \mus \pm 2.88 \mus per loop (mean \pm std. dev. of 7 runs, 1,000 loops each)
  1 b hat
                                                            1 b hat jit
Array([[ 0.99112],
                                                          Array([[ 0.99112],
       [ 1.9805 ],
                                                                 [ 1.9805 ],
       [ 0.01186],
                                                                 [ 0.01186],
       [-2.97414],
                                                                 [-2.97414],
       [-0.04457],
                                                                 [-0.04457],
       [ 0.0032 ],
                                                                 [ 0.0032 ],
       [-0.00745],
                                                                 [-0.00745],
       [ 0.24779]], dtype=float32)
                                                                 [ 0.24779]], dtype=float32)
```

Pytrees

What is a pytrees?

a pytree is a container of leaf elements and/or more pytrees. Containers include lists, tuples, and dicts. A leaf element is anything that's not a pytree, e.g. an array. In other words, a pytree is just a possibly-nested standard or user-registered Python container. If nested, note that the container types do not need to match. A single "leaf", i.e. a non-container object, is also considered a pytree.

Why do we need them?

In machine learning, some places where you commonly find pytrees are:

- Model parameters
- Dataset entries

This helps us avoid functions with large argument lists and make it possible to vectorize / map more operations.

tree_map

JAX provides a number of built-in tools for working with / iterating over pytrees, tree_map() being the most commonly used,

```
1 list_of_lists = [
2    [1, 2, 3],
3    [1, 2],
4    [1, 2, 3, 4]
5 ]
```

```
1 jax.tree_map(
2 lambda x: x**2,
3 list_of_lists
4 )
```

```
[[1, 4, 9], [1, 4], [1, 4, 9, 16]]
```

```
1 jax.tree_map(
2 lambda x,y: x+y,
3 list_of_lists, list_of_lists
4 )
```

```
[[2, 4, 6], [2, 4], [2, 4, 6, 8]]
```

```
1 d = {
2   'W': jnp.array([[1.,2.],[3.,4.],[5.,6.]]),
3   'b': jnp.array([-1.,1.])
4 }
```

```
1 jax.tree_map(
2 lambda p: (p-jnp.mean(p))/jnp.std(p),
3 d
4 )
```

Nested trees

tree_map() will iterate and apply the desired function over *all* of the leaf elements while maintaining the structure of the pytree (similar to rapply() in R).

```
1 example_trees = [
2    [1, 'a', object()],
3    (1, (2, 3), ()),
4    [1, {'k1': 2, 'k2': (3, 4)}, 5],
5    {'a': 2, 'b': (2, 3)},
6    jnp.array([1, 2, 3]),
7  ]
8
9 jax.tree_map(type, example_trees)
```

```
[[int, str, object],
  (int, (int, int), ()),
  [int, {'kl': int, 'k2': (int, int)}, int],
  {'a': int, 'b': (int, int)},
  jaxlib.xla_extension.ArrayImpl]
```

FNN example - Parameter setup

```
1 def init params(layer widths, key):
     params = []
     for n in, n out in zip(layer widths[:-1], layer widths[1:]):
       key, new key = jax.random.split(key)
 4
      params.append(
 6
         dict(
           W = jax.random.normal(new key, shape=(n in, n_out)) * np.sqrt(2/n_in),
 7
           b = jnp.ones(shape=(n out,))
 8
 9
1.0
11
     return params
12
   key = jax.random.PRNGKey(1234)
14 params = init params([1, 128, 128, 1], key)
```

```
1 jax.tree_map(lambda x: x.shape, params)

[{'W': (1, 128), 'b': (128,)},
    {'W': (128, 128), 'b': (128,)},
    {'W': (128, 1), 'b': (1,)}]
```

Model

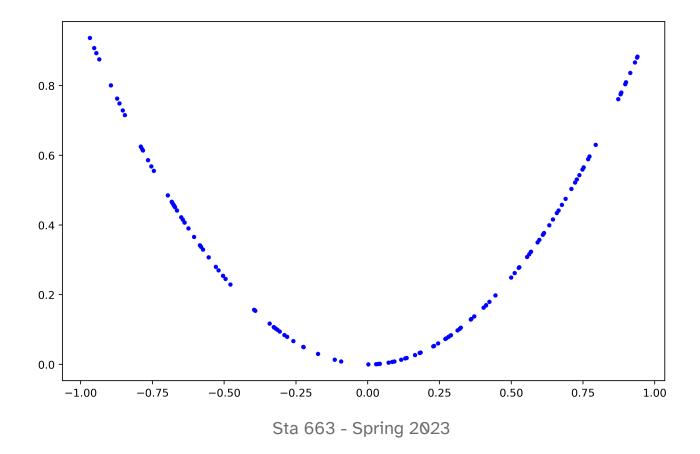
```
1 from functools import partial
 2
   class model:
     def forward(self, params, x):
 4
       *hidden, last = params
 5
       for layer in hidden:
 6
         x = x @ layer['W'] + layer['b']
 7
         x = jax.nn.relu(x)
 8
       return x @ last['W'] + last['b']
 9
10
     def loss fn(self, params, x, y):
11
12
       return jnp.mean((self.forward(params, x) - y) ** 2)
13
     @partial(jax.jit, static argnames=['self', 'lr'])
14
15
     def step(self, params, x, y, lr=0.0001):
16
       grads = jax.grad(self.loss fn)(params, x, y) # Note that since `params` is a pytree so will `grads`
17
       return jax.tree map(
18
         lambda p, g: p - lr * g, params, grads
19
20
21
     def fit(self, params, x, y, n = 1000):
       for i in range(n):
22
23
         params = self.step(params, x, y)
```

Data

```
1 key = jax.random.PRNGKey(12345)
2 x = jax.random.uniform(key, (128, 1), minval=-1., maxval=1.)
3 y = x**2
```

```
1 x.shape, y.shape
```

```
((128, 1), (128, 1))
```



Fitting

```
1  m = model()

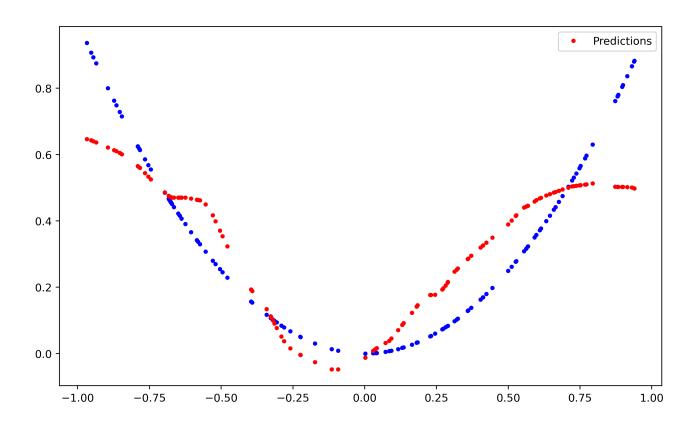
1  m.loss_fn(params, x, y)

Array(5.64001, dtype=float32)

1  params_fit = m.fit(params, x, y, n=1000)
2  m.loss_fn(params_fit, x, y)

Array(0.01788, dtype=float32)

1  y_hat = m.forward(params_fit, x)
```



What next?

Additional Resources

There are a number of other libraries built on top of JAX that provide higher level interfaces for common tasks,

- Neural networks (torch-like interfaces)
 - flax Google brain
 - haiku DeepMind
 - equinox
- Bayesian models
 - BlackJAX samplers for log-probability densities (optional backend for pymc)
- Other
 - Optax gradient processing and optimization library (DeepMind)
 - Awesome-JAX collection of JAX related links and resources