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# XLA

An optimizing compiler for Machine Learning (ML)

# XLA: ACCELERATED LINEAR ALGEBRA

AN OPTIMIZING COMPILER FOR ML

- ✓ Eliminates operations (op) dispatch overhead
- ✓ Fuses ops to avoid round trips to memory:
  - instead of storing the result of op1 and loading it for op2, fuse op1 and op2
- √ does analysis and choices adjusted to the hardware constraints
  - unrolls and vectorizes via known dimensions

JAX: SHORT OVERVIEW Main Components

# JAX Python + NumPy + FUNCTIONAL PROGRAMMING

"JAX is an extensible system for **composable function transformations** of *Python* + *NumPy* code." – as defined by its developers.

- NumPy based Python library that supports automatic differentiation
- Just-in-time (jit) compilation to run efficiently on an accelerator via XLA
- math-like programming:
  - Modular functions which map input to output, that do not affect global variables
- uses asynchronous execution by default<sup>1</sup>
- main execution does not halt until the result is returned by a processing unit, unless needed (e.g. to print it or to use it), instead JAX returns DeviceArray
- DeviceArray is a "result from the future" array whose dimensions we can inspect
- Its developers aim at making it easy to use and focus on reproducibility:
  - minimal & expressive API (based on *NumPy*)
  - same API for CPU/GPU/TPU
  - reproducible results: JAX's seed fixing slightly differs (will come back to this)

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<sup>&</sup>lt;sup>1</sup> Use *block\_until\_ready* when benchmarking, as without it we would measure the time needed to dispatch the commands to the GPU/TPU, rather then executing them.

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# A BIT MORE ON DEVICE ARRAY (JAX ABSTRACT TYPES)

#### ABSTRACT VALUES = SETS OF POSSIBLE INPUTS

- One key idea: Instead of compiling the code for any possible value, compile it for an **abstract** value, *i.e.* set of possible values.
- E.g. we can say the input will be of a particular shape (e.g. ShapedArray(float32[1,64])), without giving the exact values.
- JAX produces a "view" of the Python code valid for many different argument values, by tracing such abstract values.
- JAX uses multiple different levels of abstraction, and different transformations use different abstraction levels.
- Classes in *jax/abstrac\_arrays.py* (all inherit from an *AbstractValue* class):

UnshapedArray level 2
ShapedArray level 1
ConcreteArray level 0
AbstractToken

- Note the <u>trade-off</u>: abstraction Vs. being specific in the code, leading to reduced number of re-compilations and "argument specific" functions (contrary to *Python*'s paradigm where inputs can be anything), respectively.
- Both of best worlds: Avoid re-compilations and still use traceable control flows  $\to$  use "Structured control flow primitives".

# IMPORTS & CREATING JAX DEVICE ARRAY

- Note (convention): use "jnp" and "np" for jax.numpy and original numpy, resp.

```
import jax.numpy as jnp # JAX numpy (will run on GPU if available)
import numpy as np # original CPU-backed NumPy
```

Print available devices:

```
import jax
jax.devices()
```

Make your multiple CPUs visible to JAX<sup>2</sup> (no need to do so for GPU/TPU):

- Creating JAX device array (similar to numpy)

```
x = jnp.asarray([.1, -.1]) # [ 0.1 -0.1], <class 'jax.interpreters.xla.DeviceArray'>
y = jnp.array(x>=0, dtype=jnp.float32) # [1. 0.], <class 'jax.interpreters.xla.DeviceArray'>
```

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<sup>&</sup>lt;sup>2</sup>Required to test *pmap* if you don't have GPU/TPU on your laptop.

# MAIN JAX COMPONENTS

jit, grad & vmap

jit – for speeding up your code (sequential functions are compiled together with XLA)

grad – for taking derivatives

*vmap* – for automatic vectorization or batching.

from jax import jit, grad, vmap

# QUICK DIVE-IN EXAMPLE

```
import jax.numpy as jnp
from jax import jit, grad, vmap

def predict(params, inputs):
    for W, b in params:
        outputs = jnp.dot(inputs, W) + b
        inputs = jnp.tanh(outputs)
    return outputs

def loss(params, batch):
    inputs, targets = batch
    preds = predict(params, inputs)
    return jnp.sum((preds - targets) ** 2)

gradient_fun = jit(grad(loss))
```

# jit: XLA COMPILATION

# FORCES COMPILATION WITH XLA THE FIRST TIME A FUNCTION IS CALLED, AND IS CACHED THEREAFTER

- JAX uses XLA to compile and run the programs on CPUs/GPUs/TPUs.
- By default, jit traces the code on the ShapedArray abstraction level (abstraction level 1);
   also possible on UnshapedArray (level 2).
- *jit* enforces tracing with abstract value, and *print* within *jit*-ed function looks like this:

```
Traced<ShapedArray(int32[]):JaxprTrace(level=-1/1)>
Traced<ShapedArray(int32[]):JaxprTrace(level=-1/1)>
```

 jit-decorated function is typically called only once to trace its behavior and the resulting computation graph is cached for future calls.

How would this affect:

- print-s in jit-ed function?
- branching/conditioning (if s), loops (for, while)?
- (will revisit this)

```
def selu(x, alpha=1.67, lmbda=1.05):
    return lmbda * np.where(x > 0, x, alpha * np.exp(x) - alpha)
x = random.normal(key, (1000000,))
%timeit selu(x).block_until_ready()
# to speed-up with jit:
selu_jit = jit(selu)
%timeit selu_jit(x).block_until_ready()
```

You can also use **@***jit* as a function decorator:

# *jit*: XLA compilation

#### jit + BRANCHING REQUIRES SPECIFYING 'STATIC\_ARGNUMS'

The tracing of *jit* requires precise value, instead of abstract one *i.e.* the set of all possible values for a Boolean,  $bool = \{true, false\}$ , hence the error:

```
TypeError: Abstract value passed to 'bool', which requires a concrete value. The function to be transformed can't be traced at the required level of abstraction. If using 'jit', try using 'static_argnums' or applying 'jit' to smaller subfunctions instead.
```

#### Example:

```
def f(x, y):
    return (3. * y ** 2) if x < 3 else (-4 * y)

fjit = jit(f)
fjit_static_argnums = jit(f, static_argnums=(0,))
fjit_static_argnums_wrong_index = jit(f, static_argnums=(1,))
fjit(5, 5)  # This will fail!
fjit_static_argnums(s, 5)  # This won't!
fjit_static_argnums_wrong_index(5, 5)  # Fails!</pre>
```

# jit: XLA COMPILATION

#### jit + BRANCHING REQUIRES SPECIFYING 'STATIC\_ARGNUMS'

Example: jit with for loop and 'static\_argnums' (default is None):

```
def sum first n(x, n):
 sum = 0.
 for i in range(n):
   sum += x[i]
 return sum
sum first n = iit(sum first n, static argnums=(0,)) # won't work: "TypeError: 'JaxprTracer' object
      cannot be interpreted as an integer"
sum first n = jit(sum first n, static argnums=(1,)) # works!
# or: ---
def sum first n(x, n):
 return jnp.sum(x[:n])
sum first n = jit(sum first n) # won't work: IndexError: Array slice indices must have static
      start/stop/step to be used with Numpy indexing syntax. ...
sum first n = jit(sum first n, static argnums=(1,)) # works!
# e.g. test:
sum first n(jnp.array([1., 2., 3., 4., 5.]), 2) # if it works, returns: DeviceArray(3.,
      dtype=float32)
```

# grad: JAX'S AUTOMATIC DIFFERENTIATION grad(function\_name)

- grad(f, argnums = 0)
- By default, the gradient is taken with respect to the first argument of the function f;
- use argnums to specify w.r.t. which input argument (int) of f the gradient should be computed;
- e.g. if our loss function has inputs: loss(params, x, y), the gradient w.r.t. params is grad(loss).

Can also be combined with jit:

jit(grad(some\_function(input)))

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c.f. jax.vip & jax.jvp for more advanced autodiff for reverse–mode vector-Jacobian products and forward-mode Jacobian–vector products, resp.

# grad: JAX'S AUTOMATIC DIFFERENTIATION grad(function\_name)

```
import jax.numpy as jnp
from jax import grad
def test fun(x, v):
 return x**2 + x*v + v**2
grad x test fun = grad(test fun, argnums=0) # default
grad v test fun = grad(test fun, argnums=1)
\# df/dx = 2x + v: f'(0, 1) = 1
print('df/dx (0, 1) = {}'.format(grad x test fun(inp.float32(0), inp.float32(1))))
\# d^2f/dx^2 = 2; f'(0, 1) = 2
print('d^2 f/dx^2 (0, 1) = {}'.format(grad(grad x test fun)
    (jnp.float32(0), jnp.float32(1))))
print('d^2 f/dx^2 (3, 3) = {}'.format(grad(grad_x_test_fun)
    (jnp.float32(3), jnp.float32(3))))
\# df/dv = x + 2v; f'(0, 1) = 2
print('df/dy (0, 1) = {}'.format(grad y test fun(jnp.float32(0), jnp.float32(1))))
def g(x, v):
 """g=3*df/dx = 3*(2x+y)."""
 grad x = grad_x_test_fun(x, y)
 return 3 * grad x
print(grad(g)(jnp.float32(0), jnp.float32(1))) # prints 6, Default is w.r.t. first arg
```

# vmap: AUTO-VECTORIZATION vmap(some\_function, in\_axes = (None, 0))

Vectorizes the operations inside the function:

- √ runs faster, as the operations are "vectorized"
- √ useful for gradients

Most common use is for handling minibatches:

- 1. Write your function for one sample;
- 2. Wrap your function *f* with:

```
batched_f = vmap(f, in_axes=(None, 0), out_axes=0)
```

#### The argument *in\_axes*:

- specifies over which axes the function's arguments should be parallelized
- it's a tuple of length equal to the number of the function's arguments if there are more than one, otherwise it's one integer
- e.g. (0,1, None): parallelize over 0-th and 1-st dimension of first and second argument, resp; and don't parallelize over third argument.

The argument  $out\_axes$  is analogous to  $in\_axes$  but refers to axes of the function's output to parallelize over. As loss functions map to  $\mathbb{R}$  it is often 0.

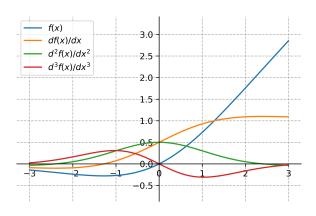
# EXAMPLE FOR jit, grad & vmap

THE SWISH NON-LINEARITY [RAMACHANDRAN ET AL., 2017]

```
import jax.numpy as jnp
from jax import grad, jit, vmap
@iit
def sigmoid(x):
 """Computes Sigmoid."""
 return 1 / (1 + inp.exp(-x))
@jit
def swish(x):
 """Computes the Swish non-linearity: 'x * sigmoid(x)'.
 Source: "Searching for Activation Functions" (Ramachandran et al. 2017)
 https://arxiv.org/abs/1710.05941
 return x * sigmoid(x)
batch swish = vmap(swish, in axes=0, out axes=0)
first derv swish = vmap(grad(swish), in axes=0, out axes=0)
second dery swish = vmap(grad(grad(swish)), in axes=0, out axes=0)
third dery swish = vmap(grad(grad(grad(swish))), in axes=0, out axes=0)
x = jnp.arange(-3, 3, .005) # (1200,)
dx = first derv swish(x)
d2x = second derv swish(x)
d3x = third derv swish(x)
```

# EXAMPLE FOR jit, grad & vmap

THE SWISH NON-LINEARITY [RAMACHANDRAN ET AL., 2017]



```
# ...
plt.plot(x, batch_swish(x), label='$f(x)$')
plt.plot(x, dx, label='$df(x)/dx$')
plt.plot(x, d2x, label='$d^2f(x)/dx^2$')
plt.plot(x, d3x, label='$d^3f(x)/dx^3$')
```

# JAX: THE GOTCHAS

# IN-PLACE UPDATES REQUIRE FUNCTION CALLS

#### Modifying *DeviceArray* throws error:

```
import jax.numpy as jnp
import numpy as np

np_arr = np.zeros((2,2), dtype=np.float32)
jnp_arr = jnp.zeros((2,2), dtype=jnp.float32)

np_arr[0, :] = 1  # ok
jnp_arr[0, :] = 1  # TypeError: '<class 'jax.lax.lax._FilledConstant'>' object does not support item assignment.
```

#### Solution: use index, index\_update & index\_add from jax.ops:

```
from jax.ops import index, index_update, index_add
jnp_arr_updated = index_update(jnp_arr, index[0, :], 1)
jnp_arr_added = index_add(jnp_arr, index[0, :], 1)
print(jnp_arr) # unchanged, all zeros
print(jnp_arr_updated) # changed, first row ones
print(jnp_arr_added) # changed, first row ones
```

# Pseudo Random Number Genertors (PRNGs)

SPLITTING STATE OF PRNG FOR IMPROVED REPRODUCIBILITY

Drawbacks of standard PRNGs (e.g. NumPy's Mersenne Twister PRNG):

- shared among processes/threads → reduced reproducibility
- large state size  $\rightarrow$  memory ( $\sim$  2.5 KB)
- can have initialization issues
- slow in general
- e.g. NumPy's Mersenne Twister PRNG fails modern BigCrush tests (c.f. TestU01)

JAX uses a modern Three-fry counter-based PRNG that's **splittable**. The random state is described by two unsigned-*int*32s called **key**.

# PSEUDO RANDOM NUMBER GENERTORS (PRNGS)

SPLITTING STATE OF PRNG FOR IMPROVED REPRODUCIBILITY

```
from jax import random
kev = random.PRNGKev(0)
                          # DeviceArray([0, 0], dtype=uint32)
# don't:
n 1 = random.normal(key, shape=(1,))
n_2 = random.normal(key, shape=(1,)) # same as n 1 !!!
# do·
new key, subkey = random.split(key)
n1 = random.normal(subkey, shape=(1,))
new key 2, subkey 2 = random.split(new key)
n2 = random.normal(subkey 2, shape=(1,)) # good: n2 != n1
# or:
key, *subkeys = random.split(key, 5)
for subkey in subkeys:
 print(random.normal(subkey. shape=(1,))[0])
 # or: print(random.randint(subkey, shape=(1,), minval=0, maxval=10)[0])
# or:
key = random.PRNGKey(10)
for in range(5):
 key, subkey = random.split(key)
 n = random.randint(subkey, shape=(1,), minval=0, maxval=10)[0]
 print(n)
```

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#### CONTROL FLOW

#### *jit* WHEN BRANCHING REQUIRES SPECIFYING *static\_argnums*, *grad* IS OK

It is recommended to use *jit* + *static\_argnums* only if the argument that is specified with it rarely changes.

Current structured control flow primitives (allow for *jit*-ing functions that have conditioning and/or loops):

- lax.cond, will be differentiable soon;
- lax.while\_loop, non-differentiable;
- *lax.fori\_loop*, non-differentiable;
- *lax.scan*, differentiable.

# **Print** IN **jit**-ED FUNCTION

WE CANNOT PRINT THINGS IN COMPILED CODE (OPERANDS ARE ABSTRACT TYPES)

```
Example<sup>3</sup>:
from jax import jit
@jit
def cube(x):
  print('[cube] input: {}'.format(x))
 v = x**3
  print('[cube] result: {}'.format(y))
  return v
print('2^3={}'.format(cube(2)))
print('3^3={}'.format(cube(3)))
Outputs:
[cube] input: Traced<ShapedArray(int32[], weak type=True):JaxprTrace(level=-1/1)>
[cube] result: Traced<ShapedArray(int32[]):JaxprTrace(level=-1/1)>
2^3=8
3^3=27
```

<sup>&</sup>lt;sup>3</sup>For more information see this explanation.

# MNIST CLASSIFICATION USING JAX AND PYTORCH [PASZKE ET AL., 2017] See full code on GitHub Based on this jax tutorial

# Using MLP with 2 hidden layers, and 10 output layers (10 digits/classes):

```
layer_sizes = [784, 512, 512, 10]
step_size = 0.0001
num_epochs = 8
batch_size = 128
n targets = 10
```

## Initialize the parameters of the MLP:

#### Other helper functions:

```
@jit
def predict(params, image):
 """ Per-sample predictions. """
 activations = image
 for w, b in params[:-1]:
   outputs = np.dot(w, activations) + b
   activations = relu(outputs)
 final w, final b = params[-1]
 logits = np.dot(final w, activations) + final b
 return logits - logsumexp(logits) # for numerical stability
# Make a batched version of the 'predict' function
batched predict = vmap(predict, in axes=(None, 0))
@iit
def accuracy(params, images, targets):
 target class = np.argmax(targets, axis=1)
 predicted class = np.argmax(batched predict(params, images), axis=1)
 return np.mean(predicted_class == target_class)
```

#### Other helper functions:

## Training function:

# MNIST EXAMPLE JAX

## Training:

# MNIST EXAMPLE JAX

#### Output:

Epoch 0 in 5.99 sec Training set accuracy 0.9594333171844482 Test set accuracy 0.9560999870300293 Epoch 1 in 2.97 sec Training set accuracy 0.97843337059021 Test set accuracy 0.9702000021934509 Epoch 2 in 2.98 sec Training set accuracy 0.9874666929244995 Test set accuracy 0.976699948310852 Epoch 3 in 2.93 sec Training set accuracy 0.9911167025566101 Test set accuracy 0.9785999655723572 Epoch 4 in 2.94 sec Training set accuracy 0.9934166669845581 Test set accuracy 0.9788999557495117 Epoch 5 in 2.97 sec Training set accuracy 0.9956166744232178 Test set accuracy 0.9799000024795532 Epoch 6 in 3.15 sec Training set accuracy 0.996399998664856 Test set accuracy 0.9799999594688416 Epoch 7 in 2.99 sec Training set accuracy 0.9974666833877563

Test set accuracy 0.9810999631881714

#### **PyTorch**

## Imports & helper functions to convert data:

```
import numpy as onp
import torch.nn as nn
# jax -> pytorch
torch.from_jax = lambda x: torch.from_numpy(onp.asarray(x))
# pytorch -> jax
np.astensor = lambda x: np.asarray(x.numpy())
```

#### Loss function:

```
def criterion(x, y):
   return - torch.sum(x * y)
```

#### **PyTorch**

#### Class MLP:

```
class MLP(nn.Module):
 def __init__(self, layer_sizes, non_lin=nn.ReLU):
   super(). init ()
   lavers = []
   for i in range(1, len(layer sizes)-1):
      layers.append(nn.Linear(layer_sizes[i-1], layer sizes[i]))
      layers.append(non lin())
   layers.append(nn.Linear(layer sizes[-2], layer sizes[-1]))
   self.main = nn.Sequential(*layers)
   self.n param layers = len(list(self.main.named parameters())) // 2
 def forward(self, x):
   x = self.main(x) # bsize x n labels
   y = torch.logsumexp(x, dim=1)
   return x.sub(y.view(-1, 1))
 def cp params(self, cp params):
   if type(cp params) is not list:
      raise TypeError("Expected list. Got {}".format(type(cp params)))
   if self.n param layers != len(cp params):
      raise ValueError("Expected equal len. Got {} and {}.".format(
          len(self.main.named parameters()), len(cp params)))
    modules = list(self.main.modules())[0]
   with torch.no grad():
      for i, (w, b) in enumerate(cp params):
        modules[i*2].weight.copy (torch.from numpy(onp.asarray(w)).float())
       modules[i*2].bias.copy (torch.from numpy(onp.asarray(b)).float())
```

#### **PyTorch**

## Training function:

```
def train mnist pytorch(net, training generator,
                        tr images, tr labels, te images, te labels,
                        num epochs=10, n targets=10):
 optimizer = optim.SGD(net.parameters(), lr=step size, momentum=0)
 device = torch.device("cuda")
 for epoch in range(num epochs):
   start time = time.time()
   for x, y in training generator: # x: bsize x 784
      labels = one hot(v, n targets) # v: bsize x 10
      labels = torch.from jax(labels).long().to(device)
      inputs = torch.from numpy(x).float().to(device)
      optimizer.zero grad()
      outputs = net(inputs)
      loss = criterion(outputs, labels)
      loss.backward()
      optimizer.step()
   epoch time = time.time() - start time
   train acc = accuracy pytorch(net, tr images, tr labels)
   test acc = accuracy pytorch(net, te images, te labels)
   print("Epoch {} in {:0.2f} sec".format(epoch, epoch time))
   print("Training set accuracy {}".format(train acc))
   print("Test set accuracy {}".format(test acc))
```

#### **PyTorch**

# Training:

#### **PyTorch**

## Output:

Epoch 0 in 3.66 sec Training set accuracy 0.9591833353042603 Test set accuracy 0.9552000164985657 Epoch 1 in 3.38 sec Training set accuracy 0.9778666496276855 Test set accuracy 0.9711000323295593 Epoch 2 in 3.29 sec Training set accuracy 0.9874500036239624 Test set accuracy 0.9777000546455383 Epoch 3 in 3.29 sec Training set accuracy 0.9908833503723145 Test set accuracy 0.9794000387191772 Epoch 4 in 3.29 sec Training set accuracy 0.9940833449363708 Test set accuracy 0.9789000749588013 Epoch 5 in 3.56 sec Training set accuracy 0.9948500394821167 Test set accuracy 0.9787000417709351 Epoch 6 in 3.35 sec Training set accuracy 0.9974166750907898 Test set accuracy 0.9803000688552856 Epoch 7 in 3.29 sec Training set accuracy 0.9975500106811523 Test set accuracy 0.9809000492095947

#### VERIFICATION: VALUES WE GET WITH JAX & PYTORCH IMPLEMENTATIONS

## JAX:

```
loss jax Traced<ConcreteArray(320.86725)>with<JVPTrace(level=2/0)>
loss jax Traced<ConcreteArray(393.53812)>with<JVPTrace(level=2/0)>
loss jax Traced<ConcreteArray(275.22656)>with<JVPTrace(level=2/0)>
loss jax Traced<ConcreteArray(273.5281)>with<JVPTrace(level=2/0)>
loss jax Traced<ConcreteArray(230.26147)>with<JVPTrace(level=2/0)>
loss jax Traced<ConcreteArray(169.82643)>with<JVPTrace(level=2/0)>
loss jax Traced<ConcreteArray(124.452896)>with<JVPTrace(level=2/0)>
```

## PyTorch:

```
loss pytorch 320.8672180175781
loss pytorch 275.2265625
loss pytorch 273.528076171875
loss pytorch 230.26145935058594
loss pytorch 169.82643127441406
loss pytorch 124.45288848876953
```

## CONCLUSIONS

- it's a Python library for ML that builds on NumPy that allows for functional programming, with Automatic Differentiation
- main advantage is speed, and can run on CPU/GPU/TPU
- to make use of its advantages, aim to write code with:
  - functions that map inputs  $\rightarrow$  outputs, which don't impact global variables
  - compositional functions, with smaller nested functions that can be jit-ed



- O Download/Installation & intro
- Read the docs: reference docs & developer docs
- JAX tutorial at NeurIPS '19 @44h26 (video+slides)
- Some cloud colabs
- Colab: Test it out on GPU/TPUs for free: Top menu  $\to$  *Runtime*  $\to$  *Change runtime type*  $\to$  Choose between *None/GPU/TPU*

#### What's next:

- Libraries for Neural Networks: Stax, Flax, Trax

THANKS.

## References I

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