

Google JAX

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Code

In this lecture series we will code in Python

Favorite libraries

- Google JAX
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- Google JAX...

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Topics

- Scientific computing: history and background
- JIT compilation
- Autodiff
- Array operations
- Functional programming

History: Setting the stage

Before we can understand JAX, we need to know a bit about the history of scientific computing

Let's recall some of the major paradigms and ideas:

- Languages and compilers
- Dynamic and static types
- Background on vectorization / JIT compilers

Fortran / C — static types and AOT compilers

Example. Suppose we want to compute the sequence

$$k_{t+1} = sk_t^\alpha + (1 - \delta)k_t$$

from some given k_0

Let's write a function in C that

1. implements the loop
2. returns the last k_t

```
int main() {  
    double k = 0.2;  
    double alpha = 0.4;  
    double s = 0.3;  
    double delta = 0.1;  
    int i;  
    int n = 1000;  
    for (i = 0; i < n; i++) {  
        k = s * pow(k, alpha) + (1 - delta) * k;  
    }  
    printf("k = %f\n", k);  
}
```

First we compile the whole program (ahead-of-time compilation):

```
>> gcc solow.c -o out -lm
```

Now we execute:

```
>> ./out
```

```
x = 6.240251
```


Pros

- fast arithmetic
- fast loops

Cons

- slow to write
- lack of portability
- hard to debug
- hard to parallelize
- low interactivity

For comparison, the same operation in Python:

```
 $\alpha$  = 0.4  
s = 0.3  
 $\delta$  = 0.1  
n = 1_000  
k = 0.2  
  
for i in range(n-1):  
    k = s * k** $\alpha$  + (1 -  $\delta$ ) * k  
  
print(k)
```

Python is **interpreted** rather than compiled

- code is executed statement by statement
- data types are queried on the fly
- arithmetic operations require method resolution

Pros

- easy to write
- high portability
- immediate feedback — high interactivity
- easy to debug

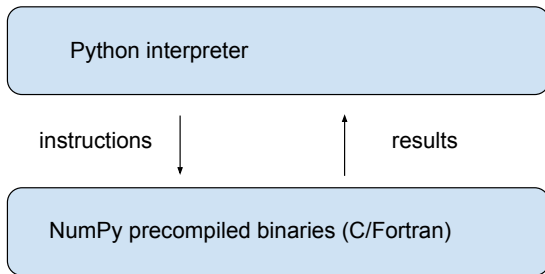
Cons

- slow

So how can we get

good execution speeds **and** high productivity / interactivity?

Python + NumPy



```
import numpy
```

```
A = ((2.0, -1.0),  
      (5.0, -0.5))
```

```
b = (0.5, 1.0)
```

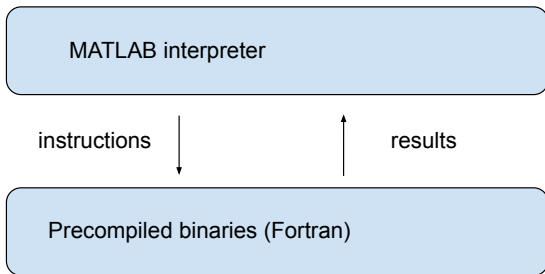
```
A, b = np.array(A), np.array(b)
```

```
x = np.inv(A) @ b
```

1. Arrays defined with high-level commands
 - (Python / NumPy API)
2. Execution takes place in an efficient low-level environment
 - Efficient machine code (compiled C / Fortran)
3. Results are returned to the high-level interface

MATLAB

NumPy is similar to and borrows from the older MATLAB programming environment



```
A = [2.0, -1.0  
      5.0, -0.5];
```

```
b = [0.5, 1.0]';
```

```
x = inv(A) * b
```

Advantages of NumPy / MATLAB

- Operations are passed to specialized machine code
- Type-checking is paid per array, not per array element

Disadvantages

- Can be highly memory intensive (intermediate arrays)
- Fails to specialize on array **shapes**
- Limited — how would you accelerate the Solow code using NumPy?

Julia — rise of the JIT compilers

Can do MATLAB / NumPy style vectorized operations

```
A = [2.0  -1.0  
     5.0  -0.5]
```

```
b = [0.5  1.0]'
```

```
x = inv(A) * b
```

But also has fast loops via an efficient JIT compiler

Example. Suppose, again, that we want to compute

$$k_{t+1} = sk_t^\alpha + (1 - \delta)k_t$$

from some given k_0

- Iterative, not easily vectorized

```
function solow(k0, α=0.4, δ=0.1, n=1_000)
    k = k0
    for i in 1:(n-1)
        k = s * k^α + (1 - δ) * k
    end
    return k
end

solow(0.2) # JIT-compiled at first call
```

Julia accelerates solow at runtime via a JIT compiler

Pros:

- fast execution — assuming correct type inference
- dynamically typed...(but compiler wants type stability)
- close to the maths

Cons:

- Everything compiled might not be optimal
 - debugging is more challenging
 - slow first runs
- Package instability
- Repeated breaking changes

Python + Numba — same architecture, same speed

```
from numba import jit

@jit(nopython=True)
def solow(k0,  $\alpha=0.4$ ,  $\delta=0.1$ , n=1_000):
    k = k0
    for i in range(n-1):
        k = s * k** $\alpha$  + (1 -  $\delta$ ) * k
    return k

solow(0.2)
```

Runs at same speed as Julia / C / Fortran

OK, let's talk about the next generation...



<https://jax.readthedocs.io/en/latest/>

A high-performance numerical computing library

- Developed by [Google Research](#) (prev. Google Brain)
- NumPy-style API for array operations
- GPU/TPU acceleration
- Automatic differentiation
- Math-centric library semantics
- Rising popularity among ML researchers

“The JAX compiler aims to enable researchers to write Python programs...that are automatically compiled and scaled to leverage accelerators and supercomputers”

Example. AlphaFold3 is built with Google JAX

google-deepmind / alphafold3

<> Code Issues 18 Pull requests Actions Projects Security Insights

alphafold3 Public Watch 65

main 1 Branch 2 Tags Go to file Add file <> Code

Δ **Augustin-Zidek** and **copybara-github** Validate bonded atoms against th... 6207434 - 13 hours ago 156 Commits

.github/workflows	Do not test ref_pos which depends on a specific RDKit ve...	4 months ago
docker	Do not limit parallelism of make when building HMMER	4 days ago
docs	Save embeddings as float16 instead of float32 to make t...	last week
legal	Add translations of legal terms	3 months ago
src/alphafold3	Validate bonded atoms against the CCD	13 hours ago
CMakeLists.txt	Initial release of AlphaFold 3	6 months ago
LICENSE	Initial release of AlphaFold 3	6 months ago

Highly accurate protein structure prediction with AlphaFold

John Jumper, Richard Evans, Alexander Pritzel, Tim Green,
Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool,...

Nature Vol. 596 (2021)

- Citation count = 35K
- Nobel Prize in Chemistry 2024

“The acronym JAX stands for **Just After eXecution**”

- monitor function execution once and then compile

Another acronym:

- **J**ust-in-time compilation
- **A**utomatic differentiation
- **X**LA (accelerated linear algebra)

Familiar NumPy-style array API

```
import jax.numpy as jnp

A = ((2.0, -1.0),
      (5.0, -0.5))

b = (0.5, 1.0)

A, b = jnp.array(A), jnp.array(b)

x = jnp.inv(A) @ b
```

Accelerated linear algebra (XLA)

Array operations are

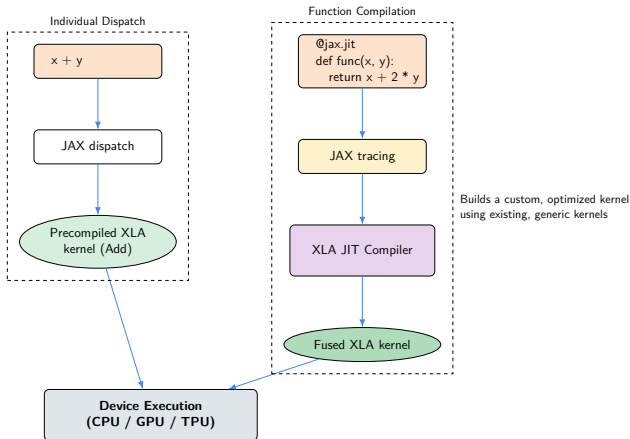
- sent to precompiled XLA device code that takes array shapes as a parameter
- automatically parallelized
- automatically optimized for and deployed to available hardware

Explicit just-in-time compilation

```
@jax.jit
def f(x):
    term1 = 2 * jnp.sin(3 * x) * jnp.cos(x/2)
    term2 = 0.5 * x**2 * jnp.cos(5*x) / (1 + 0.1 * x**2)
    term3 = 3 * jnp.exp(-0.2 * (x - 4)**2) * jnp.sin(10*x)
    return term1 + term2 + term3
```

- Compiles at first call (e.g., `result = f(x)`)
- Compiler specializes on **both** shape and data type

Precompiled vs compiled in JAX:



JIT compiler tools for optimization

- Operations combined into fused kernels for GPU/TPU
- Eliminate intermediate buffers / memory writes and reads
- Loop unrolling
- Specialized algorithms
- Memory layout optimization for multi-dimensional arrays

“JAX’s JIT compiler acts like a master engineer”

Automatic differentiation

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

def f( $\theta$ , x):
    for W, b in  $\theta$ :
        w = x @ W + b
        x = jnp.tanh(w)
    return x

def loss( $\theta$ , x, y):
    return jnp.sum((y - f( $\theta$ , x))**2)

grad_loss = jit(grad(loss))  # Now use gradient descent
```

Features of JAX

Let's review some other features

- Functional programming
- PyTrees

Functional Programming

JAX adopts a functional programming style

Key feature: **functions are pure!**

- Deterministic: same input \implies same output
- Have no side effects (don't modify state outside their scope)

Functional programming usually adopts immutable data

A non-pure function

```
tax_rate = 0.1
prices = [10.0, 20.0]

def add_tax(prices):
    for i, price in enumerate(prices):
        prices[i] = price * (1 + tax_rate)
    print('Modified prices: ', prices)
```

Why is this not pure?

A **pure** function

```
tax_rate = 0.1
prices = [10.0, 20.0]

def add_tax_pure(prices, tax_rate):
    return [price * (1 + tax_rate) for price in prices]
```


General advantages:

- Helps testing: each function can operate in isolation
- Data dependencies are explicit, which helps with understanding and optimizing complex computations
- Promotes deterministic behavior and hence reproducibility
- Prevents bugs that arise from mutating shared state

Advantages for JAX:

- Pure functions are easier to differentiate
- Pure functions are easier to parallelize and optimize (don't depend on shared mutable state)
- Transformations can be composed cleanly (predictable results)

JAX PyTrees

A tree-like data structure built from Python containers

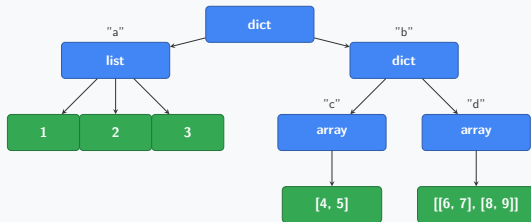
A concept, not a data type


Examples.


- A list of dictionaries, each dictionary contains parameters
- A dictionary of lists
- A dictionary of lists of dictionaries
- etc.

JAX PyTree Structure

```
pytree = {  
  "a": [1, 2, 3],  
  "b": {"c": jnp.array([4, 5]), "d": jnp.array([[6, 7], [8, 9]])}  
}
```



 Container nodes (dict, list, tuple)

 Leaf nodes (arrays, scalars)

JAX can

- apply functions to all leaves in a PyTree structure
- differentiate functions with respect to the leaves of PyTrees
- etc.

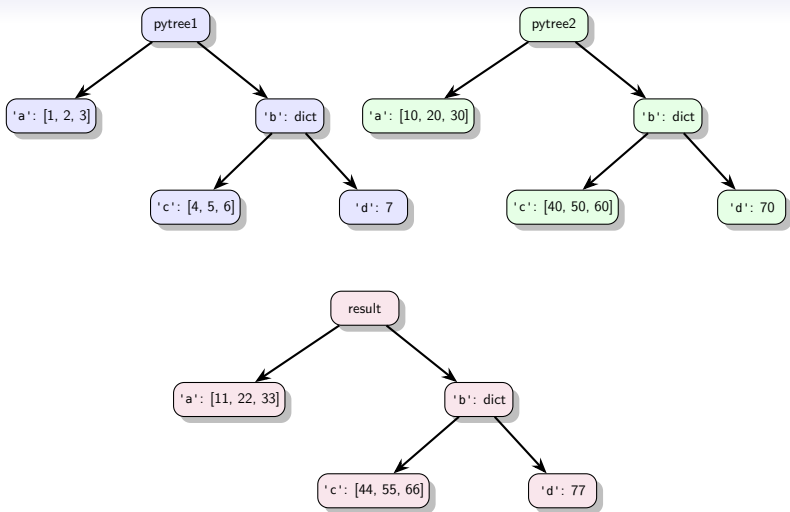


Figure: `jax.tree.map(lambda x, y: x + y, pytree1, pytree2)`

Apply gradient updates to all parameters

```
def sgd_update(params, grads, learning_rate):  
    return jax.tree.map(  
        lambda p, g: p - learning_rate * g,  
        params,  
        grads  
    )
```

Calculate gradients (PyTree with same structure as params)

```
grads = jax.grad(loss_fn)(params, inputs, targets)
```

Update all parameters at once

```
updated_params = sgd_update(params, grads, 0.01)
```

Summary

Advantages over NumPy / MATLAB

- Can specialize machine code to data types **and** shapes!
- Automatically matches tasks with accelerators
- Same code, multiple backends (CPUs, GPUs, TPUs)
- Can fuse array operations for speed and memory efficiency
- Integrated efficient autodiff

Advantages of JAX (vs PyTorch / Tensorflow / etc.) for economists:

- elegant functional programming style – close to maths
- elegant autodiff tools
- array operations follow standard NumPy API

Exposes low level functions / fewer off-the-shelf solutions