Google JAX

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Topics

- Foo
- Bar

What's JAX?

`https://jax.readthedocs.io/en/latest/`

- Just-in-time compilation
- Automatic differentiation
- Xccelerated linear algebra

Example. AlphaFold3 (Google JAX)

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 = 30K
- Nobel Prize in Chemistry 2024

History: Setting the stage

- Some history of scientific computing
- Dynamic and static types
- Background on vectorization / JIT compilers

Fortran / C — static types and AOT compilers

Example. Suppose we want to compute the sequence

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

from some given k_0

Let's write a function in C that

1. implements the loop
2. returns the last k_t

```c
#include <stdio.h>
#include <math.h>

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);
}
```

```
❯❯ gcc solow.c -o out -lm
❯❯ ./out

x = 6.240251
```

Pros

- fast

Cons

- time consuming to write
- lack of portability
- hard to debug
- hard to parallelize
- low interactivity

For comparison, the same operation in Python:

```
α = 0.4
s = 0.3
δ = 0.1
n = 1_000
k = 0.2

for i in range(n-1):
    k = s * k**α + (1 - δ) * k

print(k)
```

Pros

- easy to write
- high portability
- easy to debug
- high interactivity

Cons

- slow

So how can we get

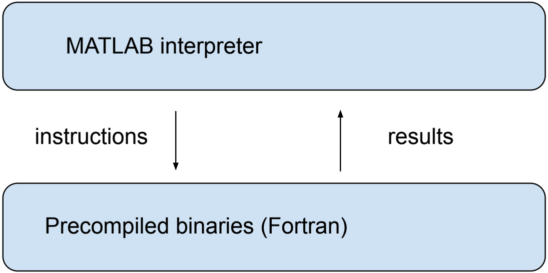
good execution speeds **and** high productivity / interactivity?

MATLAB

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

b = [0.5, 1.0]';

x = inv(A) * b
```



MATLAB interpreter
instructions
results
Precompiled binaries (Fortran)

Python + NumPy

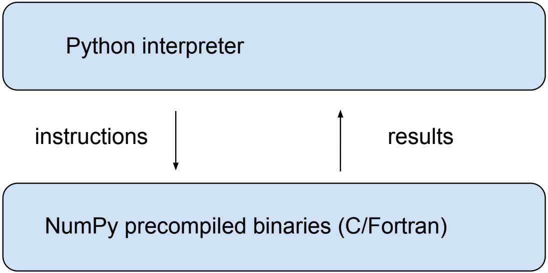
```python
import numpy

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
```


Python interpreter
instructions
results
NumPy precompiled binaries (C/Fortran)

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

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

from some given k_0

- Iterative, not easily vectorized

```julia
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)
```

Julia accelerates `solow` at runtime via a JIT compiler

Python + Numba — same architecture, same speed

```python
from numba import jit

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

solow(0.2)
```

Runs at same speed as Julia / C / Fortran

Back to JAX

- Just-in-time compilation
- Automatic differentiation
- Xccelerated linear algebra

Automatic differentiation

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

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

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

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

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)

A non-pure function

```python
tax_rate = 0.1  # Global
price = 10.0    # Global

def add_tax_non_pure():
    global price
    # The next line both accesses and modifies global state
    price = price * (1 + tax_rate)
    return price
```

A pure function

```
def add_tax_non_pure(price, tax_rate=0.1):
    price = price * (1 + tax_rate)
    return price
```

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 subtle bugs that arise from mutating shared state

Advantages for JAX:

- Functional programming facilitates autodiff because pure functions are more straightforward to differentiate (don't mod external state
- Pure functions are easier to parallelize and optimize for hardware accelerators like GPUs (don't depend on shared mutable state, more independence)
- Transformations can be composed cleanly with multiple transformations yielding predictable results
- Portability across hardware: The functional approach helps JAX create code that can run efficiently across different hardware accelerators without requiring hardware-specific implementations.

JAX PyTrees

A PyTree is a concept in the JAX library that refers to a tree-like data structure built from Python containers.

Examples.

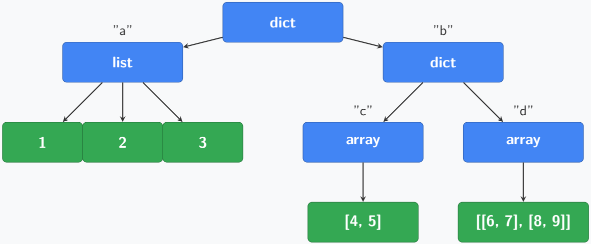
- A dictionary of lists of parameters
- A list of dictionaries of parameters, etc.

JAX can

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

```python
# 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)
```

Advantages over NumPy / MATLAB

- can specialize machine code based on parameter types / shapes
- automatically matches tasks with accelerators (GPU / TPU)
- fuses array operations for speed and memory efficiency

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

- exposes low level functions
- elegant functional programming style – close to maths
- elegant autodiff tools
- array operations follow standard NumPy API
- automatic parallelization
- same code, multiple backends (CPUs, GPUs, TPUs)