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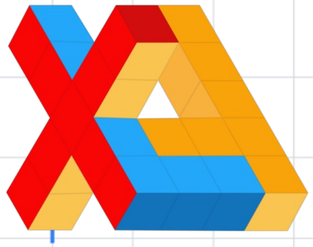


Introduction to JAX with Flax

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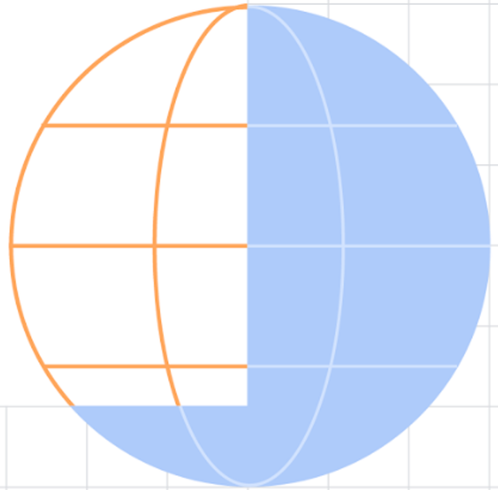
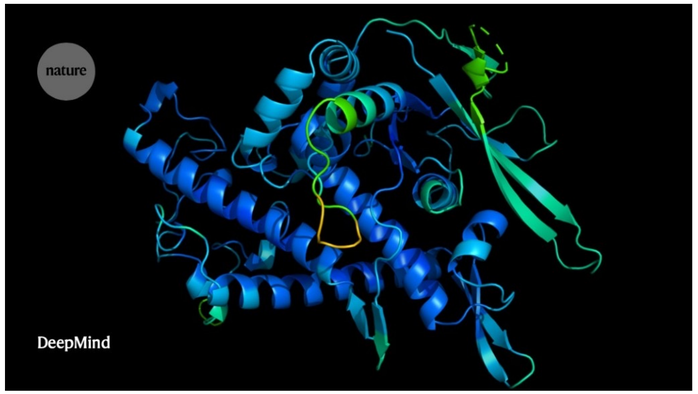


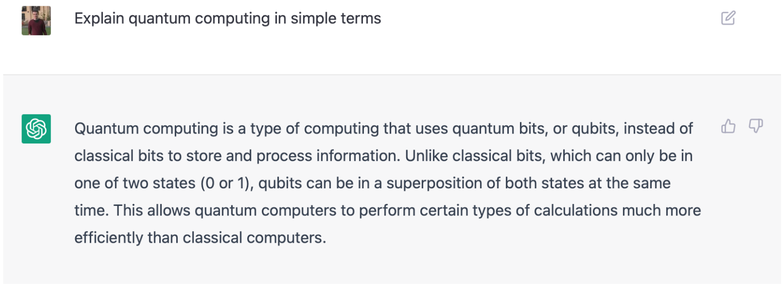
Goals of this talk

1) What features are we looking for in an ML/DL framework?
2) What is JAX?
3) What sets JAX apart from other frameworks?
4) How can train Neural Networks in JAX with Flax?
5) Where can I continue my learning journey into JAX with Flax?

Successes of Machine and Deep Learning



AlphaFold

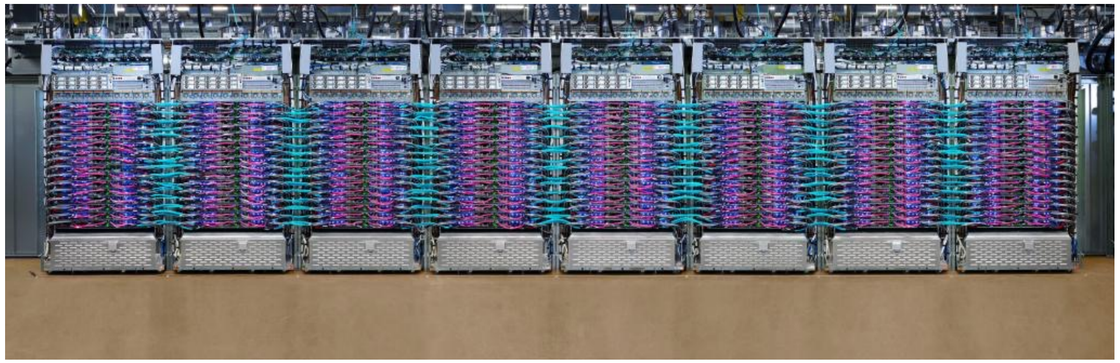


ChatGPT

Sprouts in the shape of text 'Imagen' coming out of a fairytale book.

A photo of a Shiba Inu dog with a backpack riding a bike. It is wearing sunglasses and a beach hat.

Imagen



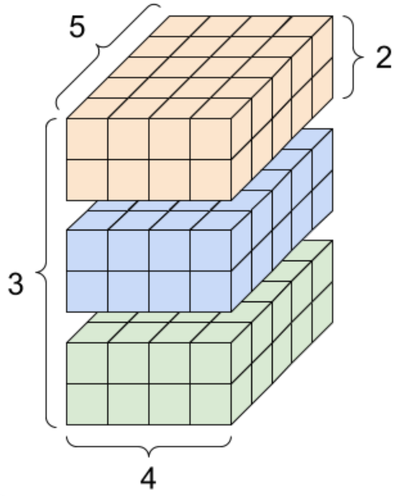
TPU Data Center

Secret sauce:
Enormous compute power

How can we make efficient use of the compute power? => DL frameworks

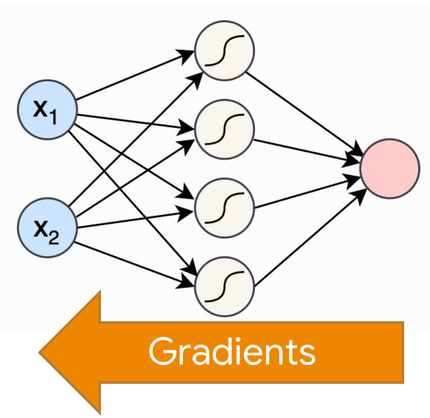
Basic Requirements on a Deep Learning Framework

Matrix operations

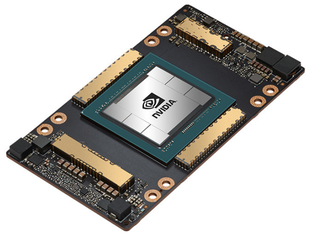


NumPy

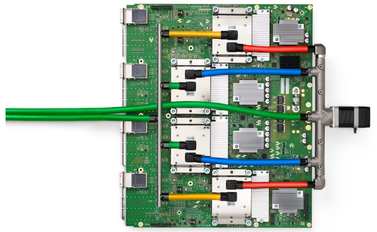
Automatic Differentiation



Accelerator support



GPUs (NVIDIA A100)



TPU v4

JAX: Accelerated NumPy with Autograd

- **Matrix Operations**: JAX shares the same basic API with NumPy

```
import jax
import jax.numpy as jnp
print("Using jax", jax.__version__)
```

```
Using jax 0.3.25
```

```
a = jnp.zeros((2, 5), dtype=jnp.float32)
print(a)
```

```
[[0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0.]]
```

JAX: Accelerated NumPy with Autograd

- **Accelerator Support**: JAX supports operations on various backends, e.g. GPUs

```
b = jnp.arange(6)
print(b)
```

```
[0 1 2 3 4 5]
```

```
b.__class__
```

```
jaxlib.xla_extension.DeviceArray
```

Tensor by default on accelerator (here GPU)
JAX arrays on CPU are NumPy arrays

JAX: Accelerated NumPy with Autograd

- **Automatic Differentiation**: JAX allows to *transform* functions, such as taking the gradient of a function via `jax.grad`

```
def mse_loss(preds, labels):
    return ((preds - labels) ** 2).mean()

print('Loss', mse_loss(jnp.array([1.0, 2.0]),
                       jnp.array([0.0, 1.5])))
```

```
Loss 0.625
```

```
mse_grad_fn = jax.grad(mse_loss)
print('Loss gradient', mse_grad_fn(jnp.array([1.0, 2.0]),
                                   jnp.array([0.0, 1.5])))
```

```
Loss gradient [1.  0.5]
```

Analytical gradient:
`(preds - labels)`

JAX: Function Transformations

- JAX is based on **transformations of pure functions**
  - Pure functions = functions without any side effects, limited to input and outputs
- For this, JAX lifts functions into an intermediate language called `jaxpr`

```
exmp_preds = jnp.array([1.0, 2.0])
exmp_labels = jnp.array([0.0, 1.5])
```

```
jax.make_jaxpr(mse_loss)(exmp_preds, exmp_labels)
```

```
{ lambda ; a:f32[2] b:f32[2]. let
    c:f32[2] = sub a b
    d:f32[2] = integer_pow[y=2] c
    e:f32[] = reduce_sum[axes=(0,)] d
    f:f32[] = div e 2.0
  in (f,) }
```

Inputs with evaluated shapes

Basic function operations

Output with evaluated shape

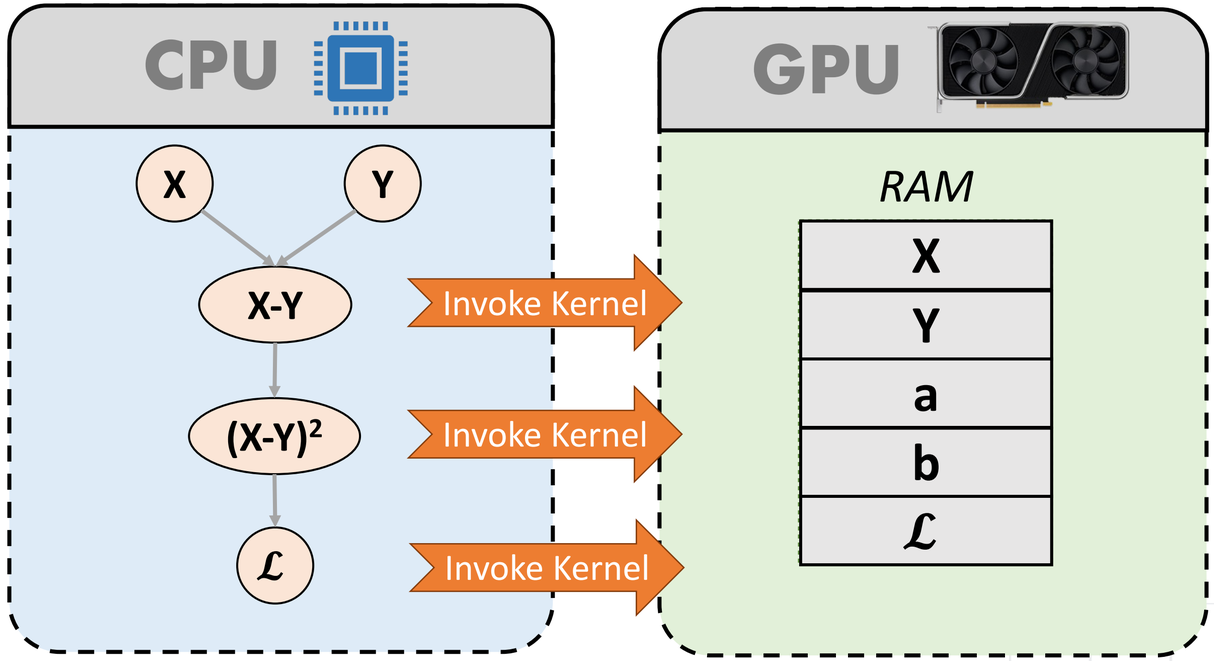
JAX: Function Transformations

- JAX offers several function transformations, most importantly:
  - `jax.grad` – Gradient of a function
  - `jax.jit` – Just-In-Time Compilation
  - `jax.vmap` – Vectorize function
  - `jax.pmap` – Parallelize function on multiple devices

JAX: Just-In-Time Compilation

- Naïve execution of operations can lead to considerable overhead in GPU ↔ CPU communication
- Can we do better?
- Yes, with Just-In-Time Compilation!

```python
def mse_loss(x, y):
    return ((x - y) ** 2).mean()
```



JAX: Just-In-Time Compilation

- Just-In-Time (JIT) compilation allows for very efficient code with little effort
- Transforming a function via `jax.jit` uses XLA (Accelerated Linear Algebra) to compile multiple operations together to improve speed and memory usage

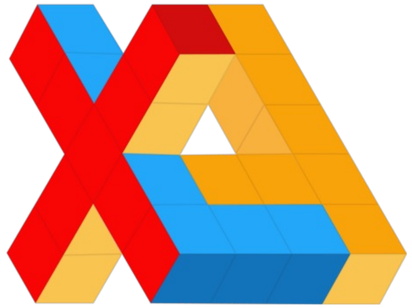
```
mse_jit = jax.jit(mse_loss)
```

```
%timeit mse_loss(x_batch, y_batch).block_until_ready()
```

```
434 µs ± 13.3 µs per loop (mean ± std. dev. of 7 runs, 10
00 loops each)
```

```
%timeit mse_jit(x_batch, y_batch).block_until_ready()
```

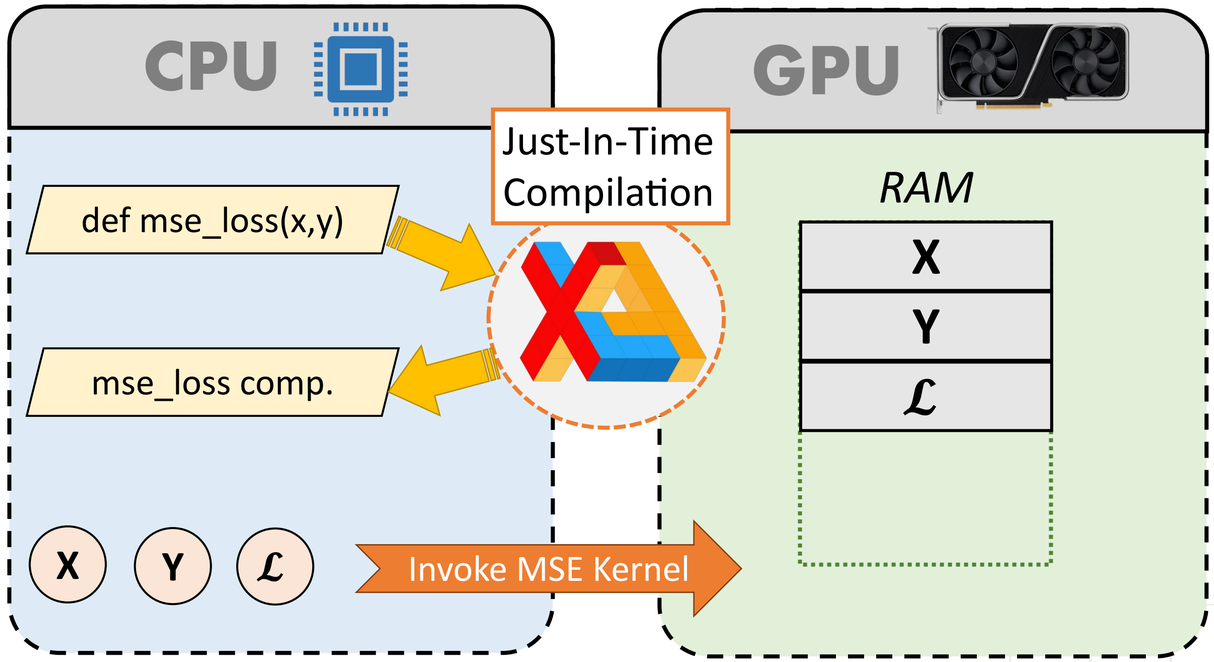
```
58.7 µs ± 1.42 µs per loop (mean ± std. dev. of 7 runs, 1
0000 loops each)
```



JAX: Just-In-Time Compilation

- Improves **execution speed** (operation fusion, specializing for shapes)
- Improves **memory usage** (fewer intermediate variables)
- Improves **portability** (any backend supported in XLA)

```
@jax.jit
def mse_loss(x, y):
    return ((x - y) ** 2).mean()
```

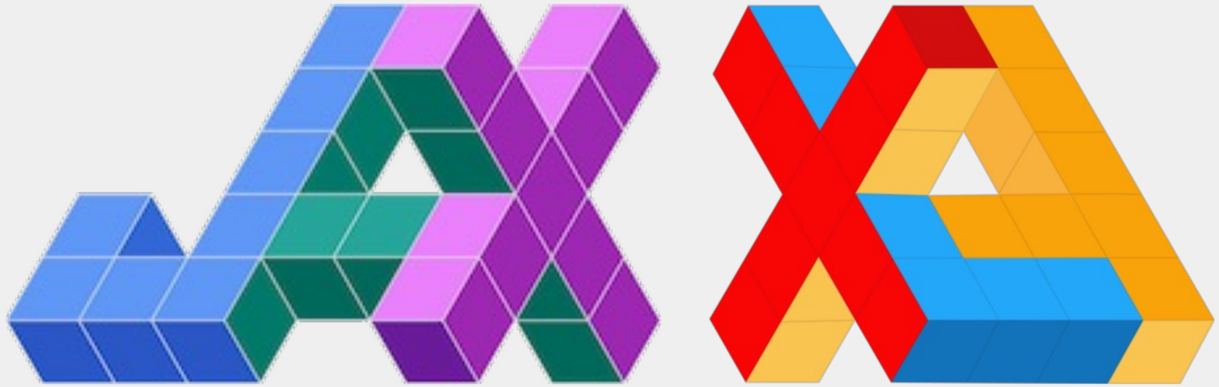


JAX: 🔪 The Sharp Bits 🔪

- JAX relies on pure functions, which requires function-centric programming
  - **Immutable Tensors**: in-place operations could have side-effects (JIT may still use in-place ops)
  - **Pseudo Random Numbers**: seed needs to be passed explicit to functions, no global seed variable
- JIT-Compilation is shape specific, need more care with dynamic shapes (e.g., graphs or natural language – use padding)
- Debugging in JIT-compiled functions more difficult since compiled functions can't throw an error ⟶ potentially undesired side-effects

Summary

- JAX is Accelerated NumPy with Autograd
- Key feature:
  transformations of pure functions
- Just-In-Time compilation for taking full advantage of accelerators



```
exmp_preds = jnp.array([1.0, 2.0])
exmp_labels = jnp.array([0.0, 1.5])
```

```
jax.make_jaxpr(mse_loss)(exmp_preds, exm
```

```
{ lambda ; a:f32[2] b:f32[2]. let
    c:f32[2] = sub a b
    d:f32[2] = integer_pow[y=2] c
    e:f32[] = reduce_sum[axes=(0,)] d
    f:f32[] = div e 2.0
  in (f,) }
```

Neural Networks with JAX

- How can we implement an NN in JAX?
- Several libraries available, such as:
  - Flax – Google Brain, focuses on flexibility and clarity
  - Haiku – DeepMind, focuses on simplicity and compositionality
  - Trax – Google Brain, solutions for common training tasks
  - Equinox – Patrick Kidger and Cristian Garcia, NNs as callable Pytrees

Flax: Neural Networks with JAX

- Main aspects of a Neural Network library in JAX:
  - How can we implement Neural Network layers as functions? Linen API
  - How do we handle parameters (weights, biases, etc.)? Pytrees
  - How do we optimize the model's parameters? Optax
  - How do we put everything together with JIT support? TrainState

Flax: Linen API

- Flax defines layers as **Modules**, acting as an *immutable dataclass*

```
from flax import linen as nn
```

```
class MyModule(nn.Module):
    # Some dataclass attributes, like hidden dimension
    # varname : vartype

    def setup(self):
        # Flax uses "lazy" initialization.
        # In here, define your submodules etc.
        pass

    def __call__(self, x):
        # Function for forward pass
        pass
```

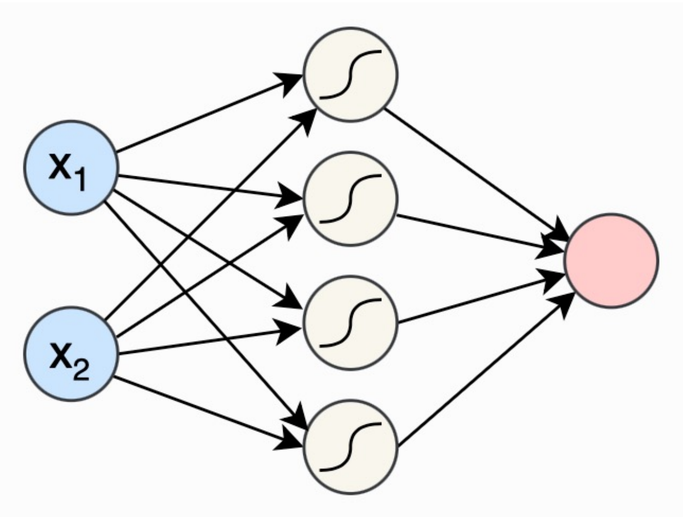
Flax: Linen API

- Flax defines layers as **Modules**, acting as an *immutable dataclass*

```
class SimpleClassifier(nn.Module):
    num_hidden : int   # Number of hidden neurons
    num_outputs : int  # Number of output neurons

    def setup(self):
        # Create the modules we need to build the network
        # nn.Dense is a linear layer
        self.linear1 = nn.Dense(features=self.num_hidden)
        self.linear2 = nn.Dense(features=self.num_outputs)

    def __call__(self, x):
        # Forward pass
        x = self.linear1(x)
        x = nn.tanh(x)
        x = self.linear2(x)
        return x
```

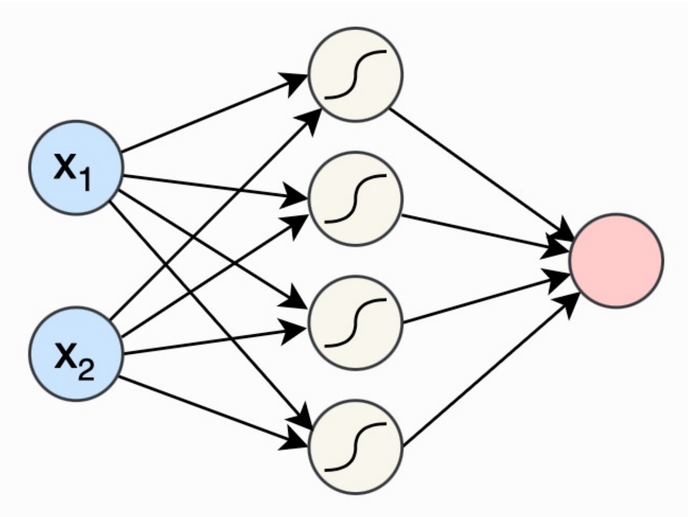


Flax: Linen API

- We can combine sub-module definition and their call via `nn.compact`:

```python
class SimpleClassifierCompact(nn.Module):
    num_hidden : int   # Number of hidden neurons
    num_outputs : int  # Number of output neurons

    @nn.compact
    def __call__(self, x):
        # Forward pass while defining necessary layers
        x = nn.Dense(features=self.num_hidden)(x)
        x = nn.tanh(x)
        x = nn.Dense(features=self.num_outputs)(x)
        return x
```



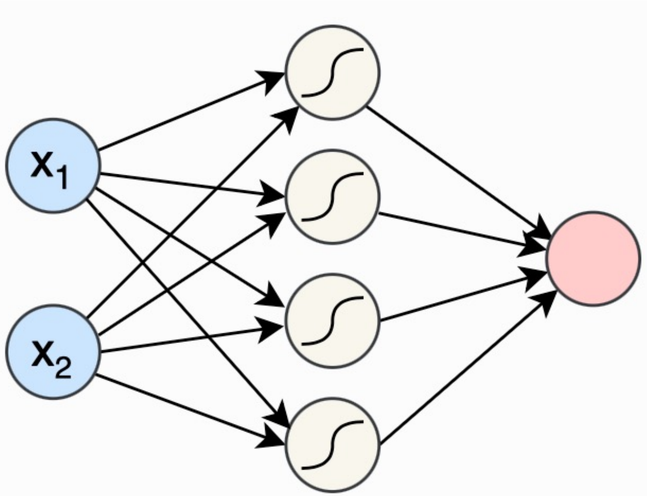
Flax: Linen API

- Parameters cannot be part of the Module since they must be *mutable*
- Solution: parameters act as an additional input to the module
- Create parameters via `module.init` function:

```
example_input = jnp.zeros((16, 2))
```

```
model = SimpleClassifier(num_hidden=4, num_outputs=1)
```

```
params = model.init(jax.random.PRNGKey(42),
                    example_input)
```



Flax: Linen API

- Parameters are stored as **Immutable Pytrees**, a tree-structured container
  - In Flax, Pytrees are mostly nested dictionaries, with leafs being the parameter values
  - Pytrees allow functions to access collections like parameters, and potentially give one as output
- JAX defines several operations on Pytrees, example: print the shapes of the parameters

```
jax.tree_map(lambda p: p.shape, params)
```

```
FrozenDict({
    params: {
        linear1: {
            bias: (4,),
            kernel: (2, 4),
        },
        linear2: {
            bias: (1,),
            kernel: (4, 1),
        },
    },
})
```

Sub-module names

Parameters within sub-module

Flax: Linen API

- Run a module with parameters via `module.apply`:

```
example_input = jax.random.normal(jax.random.PRNGKey(0),
                                  (4, 2))
```

```
model.apply(params, example_input)
```

```
DeviceArray([[-0.07297172],
             [ 0.22177655],
             [-0.18521681],
             [-0.165456  ]], dtype=float32)
```

Flax: Linen API

- Several common network layers have been predefined in the Linen API, such as:
  - Linear Layers (`nn.Dense`, `nn.DenseGeneral`)
  - Convolutions (`nn.Conv`, `nn.ConvTranspose`, etc.)
  - Normalizations (`nn.BatchNorm`, `nn.LayerNorm`, etc.)
  - Attention mechanisms (`nn.SelfAttention`, etc.)
  - Recurrent Neural Networks (`nn.LSTMCell`, `nn.GRUCell`, etc.)

Flax: Neural Networks with JAX

- Main aspects of a Neural Network library in JAX:
  - How can we implement Neural Network layers as functions? Linen API
  - How do we handle parameters (weights, biases, etc.)? Pytrees
  - How do we optimize the model's parameters? Optax
  - How do we put everything together with JIT support? TrainState

Optax: NN Optimization in JAX

- Optax is a gradient processing and optimization library for JAX based on Pytrees
- Provides building blocks and common optimizers (SGD, Adam, etc.) in a similar function-oriented fashion as Flax

```
optimizer = optax.adam(learning_rate=1e-3)
```

Immutable dataclass

```
opt_state = optimizer.init(params)
```

In Adam, momentum and adaptive learning rate parameters

```
updates, opt_state = optimizer.update(grads,
                                      opt_state,
                                      params)
```

Update momentum etc., and get parameter updates/changes

```
params = optax.apply_updates(params, update)
```

Creates a new Pytree with updated parameters

Flax: Training API

- How can we combine the model execution, gradient calculation, and optimizer step, while allowing for Just-In-Time compilation?
- Flax offers a solution with the flax.training sub-library, in particular: TrainState
  - Immutable dataclass with model forward function, parameters, and optimizer (can be extended)

```
from flax.training.train_state import TrainState

model_state = TrainState.create(apply_fn=model.apply,
                                params=params,
                                tx=optimizer)
```

Flax: Training API

- A TrainState object can be used as input argument to a function, on which we may apply function transformations (`jax.grad`, `jax.jit`, etc.)
- Example: binary classification

```
def calculate_loss(state, params, batch):
    data_input, labels = batch

    logits = state.apply_fn(params, data_input)
    logits = logits.squeeze(axis=-1)

    loss = optax.sigmoid_binary_cross_entropy(logits,
                                              labels)
    loss = loss.mean()
    return loss
```

Obtain model predictions

Calculate loss (error of model)

Flax: Training API

- Combine everything into a function that executes a whole training step:

```
grad_fn = jax.value_and_grad(calculate_loss,
                             argnums=1)
```

Returns both output value (loss) and gradients for second input argument (parameters)

```
@jax.jit
def train_step(state, batch):
    loss, grads = grad_fn(state, state.params, batch)
    state = state.apply_gradients(grads=grads)
    return state, loss
```

Creates new TrainState with updated optimizer state and parameters

Flax: Training API

- To train the model, we can now just write a training loop that calls the training function several times for different input batches

```
def train_model(state, data_loader, num_epochs=100):
    for epoch in range(num_epochs):
        for batch in data_loader:
            state, loss = train_step(state, batch)
    return state
```

```
trained_model_state = train_model(model_state,
                                  train_data_loader,
                                  num_epochs=100)
```

Flax: Neural Networks with JAX

- Main aspects of a Neural Network library in JAX:
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  - How do we handle parameters (weights, biases, etc.)? Pytrees
  - How do we optimize the model's parameters? Optax
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Flax: Neural Networks with JAX

- What we haven't discussed yet:
  - Logging can be done with external libraries (e.g., TensorBoard)
  - Flax supports data loading from any other library (e.g., TensorFlow, PyTorch, etc.)
  - Binding parameters to a specific module for easier evaluation
  - Automatically vectorizing and/or parallelizing via jax.vmap and jax.pmap
  - Writing a research code framework for minimal code overhead
  - And much, much more...

Summary

- Flax is a library for NN tools in JAX
- Using immutable dataclasses for more object-oriented programming “feeling”
- Can be combined with several external libraries for optimization, logging, data loading, etc.

```python
def calculate_loss(state, params, batch):
    data_input, labels = batch

    logits = state.apply_fn(params, data_input
    logits = logits.squeeze(axis=-1)

    loss = optax.sigmoid_binary_cross_entropy(

    loss = loss.mean()
    return loss
```

```python
grad_fn = jax.value_and_grad(calculate_loss,
                             argnums=1)
```

```python
@jax.jit
def train_step(state, batch):
    loss, grads = grad_fn(state, state.params,
    state = state.apply_gradients(grads=grads)
    return state, loss
```

When and why to use JAX with Flax?

Benefits

- JAX is extremely fast with Just-In-Time compilation
- Function transformations are powerful tools to easily parallelize and vectorize your code
- Function-oriented programming is helpful in areas like meta-learning, where one needs explicit gradients

Drawbacks

- The code overhead is usually larger than in other frameworks
- Not as user-friendly / fail-safe as other frameworks
- Handling dynamic shapes can be annoying
- Community still considerably smaller than e.g. TensorFlow or PyTorch

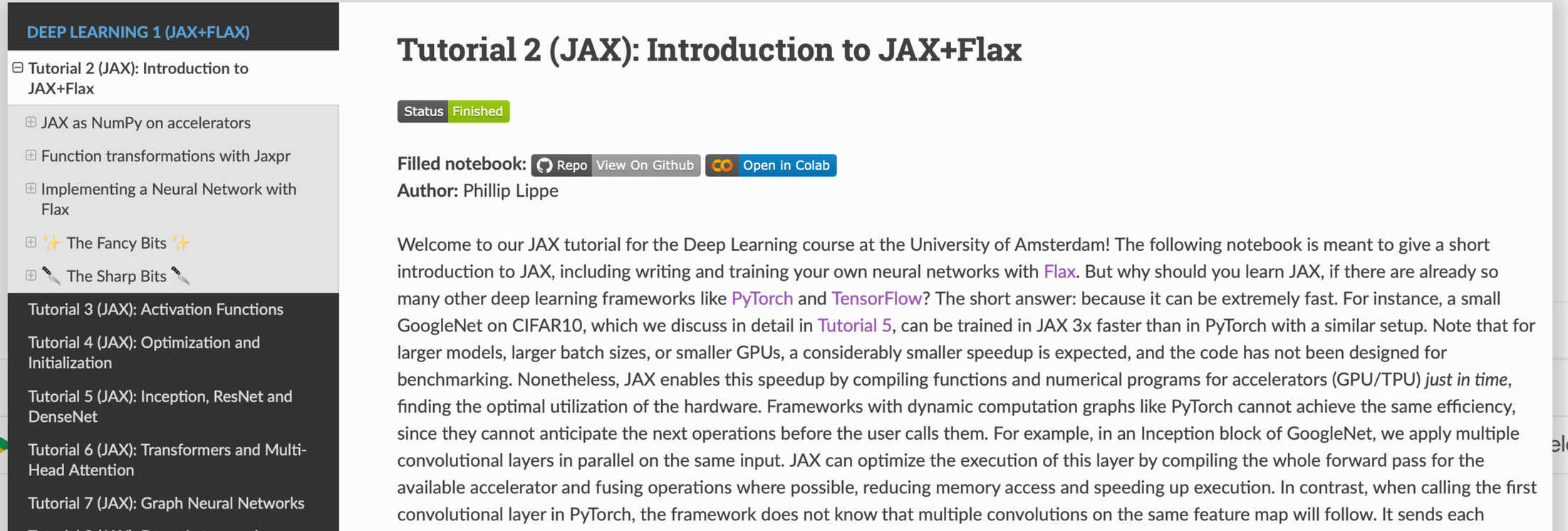
Recommendation: if you are doing research and want to get maximum performance out of your code, give JAX a try!

Goals of this talk

1) What features are we looking for in an ML/DL framework?
2) What is JAX?
3) What sets JAX apart from other frameworks?
4) How can train Neural Networks in JAX with Flax?
5) Where can I continue my learning journey into JAX with Flax?

Further resources on JAX with Flax

- The JAX and Flax documentations have great introduction tutorials
- If you are interested in seeing JAX with Flax used in practice, and learn new methods in Deep Learning, check out our UvA Deep Learning tutorials!



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Experts

Thank You!

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Slides
(personal website)