DeepMind

# JAX at DeepMind

NeurIPS 2020

Matteo Hessel, David Budden, Mihaela Rosca, Junhyuk Oh, Fabio Viola, Theophane Weber, Paige Bailey

### DeepMind

# 1. Why JAX?

Matteo Hessel (@matteohessel)



JAX is a Python library designed for high-performance numerical computing Among its key ingredients it supports:

- Differentiation:
  - Forward and reverse mode automatic differentiation of arbitrary numerical functions,
  - E.g: grad, hessian, jacfwd and jacrev.
- Vectorisation:
  - SIMD programming via automatic vectorisation,
  - E.g: vmap, pmap.
- JIT-compilation:
  - XLA is used to just-in-time (JIT)-compile and execute JAX programs,
  - faster CPU code, and transparent GPU and Cloud TPU acceleration..



All these are implemented as **composable program transformations** 



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Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y



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Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y

The value fn is evaluated like any python function

fn(1., 2.) # (1\*\*2 + 2) = 3



All these are implemented as **composable program transformations** 

Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y

The **gradient** df\_dx = grad(fn) is also a function

 $df_dx(1., 2.) \# df_dx = 2*x = 2*1 = 2$ 



All these are implemented as **composable program transformations** 

Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y

The **second-order gradient** df2\_dx = grad(grad(fn)) is also a function

```
df2_dx(1., 2.) \# df2_dx = d(2*x)_dx = 2
```



All these are implemented as **composable program transformations** 

Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y

The **compiled second-order gradient** df2\_dx = jit(grad(grad(fn))) is also a function

df2\_dx(1., 2.) # 2, also traces the code and compiles it



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Consider a numerical function:

def fn(x,y):
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The **compiled second-order gradient** df2\_dx = jit(grad(grad(fn))) is also a function

df2\_dx(1., 2.) # 2, also traces the code and compiles it df2\_dx(1., 2.) # 2, executes the XLA pre-compiled code

But a much faster one after the first execution :)



All these are implemented as **composable program transformations** 

Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y

The **batched compiled second-order gradient** df2\_dx = vmap(jit(grad(grad(fn)))) is also a function

```
xs = jnp.ones((batch_size,))
df2_dx(xs, 2 * xs) # [2, 2], if batch_size=2
```



All these are implemented as **composable program transformations** 

Consider a numerical function:

def fn(x,y):
 return x\*\*2 + y

So is its multi-gpu batched compiled second-order gradient df2\_dx = pmap(vmap(jit(grad(grad(fn)))))

```
xs = jnp.ones((num_gpus, batch_size,))
df2_dx(xs, 2 * xs) # [[2, 2], [2, 2]], if batch_size=2 and num_gpus=2
```



# Why JAX?

JAX is simple but very flexible

- API for numerical functions is fully consistent with NumPy,
- Both Python and NumPy are widely used and familiar,
- Few abstractions (grad, jit, vmap, pmap) but powerful and composable!
- The functional programming style helps writing code that "looks like the math"
- Not a vertically integrated but with a rich ecosystem and community around it
- Battle tested extensively in the past year on projects ranging from Optimisation, SL, GANs, RL, ...

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# 2. Our JAX Ecosystem

David Budden (@davidmbudden)



# Why an Ecosystem?

### DeepMind Researchers have had great initial success with JAX

• How can we continue to support and accelerate their work?

### Considerations

- JAX is not a vertically integrated ML framework (this is a good thing!)
- Needs to support rapidly evolving DeepMind Research requirements
- Where possible, strive for consistency + compatibility with
  - Our TF ecosystem (Sonnet, TRFL, ...)
  - Our research frameworks (Acme, ...)

### DeepMind JAX Ecosystem

- Libraries of reusable and un-opinionated JAX components
- Each library does one thing well and supports incremental buy-in
- Open source everything to enable research sharing + reproducibility



### Haiku

Haiku is a tool For building neural networks Think: "Sonnet for JAX"

### **Motivation**

- JAX programs are functional
- NN params/state better fit the OO paradigm

import jax
import haiku as hk

#### @hk.transform

def loss\_fn(images, labels):
 model = hk.nets.MLP([1000, 100, 10])
 logits = model(images)
 labels = one\_hot(labels, 1000)
 return losses.softmax\_cross\_entropy(logits, labels)

images, labels = next(dataset)
params = loss\_fn.init(rng\_key, images, labels)
loss = loss\_fn.apply(params, images, labels)

### Haiku (github.com/deepmind/dm-haiku)

- Converts stateful modules to pure functions
- API-matches Sonnet, porting from TF is trivial
  - Have reproduced AlphaGo, AlphaStar, AlphaFold, ...
- Mature API and widely adopted



## **Optax**

The artist formerly known as jax.experimental.optix

### **Motivation**

- Gradient processing is fundamental to ML Research
- Like NNs, optimizers are stateful

### Optax (github.com/deepmind/optax)

- Gradient processing and optimization library
- Comprehensive library of popular optimizers
- Simplifies gradient-based updates of NN params
  - Compatible with all popular JAX NN libraries
- Mature API and widely adopted

```
import jax
import optax
```

params = ... // a JAX tree

opt = optax.adam(learning\_rate=1e-4)
state = opt.init(params)

```
@jax.jit
def step(state, params, data):
    dloss_dparams = jax.grad(loss_fn)(*data)
    updates, state = opt.update(dloss_dparams, state)
    params = optax.apply_updates(params, updates)
    return state, params
```

```
for data in dataset:
    state, params = step(state, params, data)
```



### **RLax**

### "RLax is the best RL textbook I've read!"

- Anonymous

### Motivation

- Reinforcement Learning is hard, getting it wrong is easy
- Want a common substrate for *sharing* new ideas

### RLax (github.com/deepmind/rlax)

- Library of mathematical operations related to RL
- Emphasis on readability
- Building blocks rather than complete algorithms
  - But, lots of full agent examples available
- Widely adopted for RL research

# import jax import optax import rlax

#### def loss\_fn(params, o\_tm1, a\_tm1, r\_t, d\_t, o\_t):

q\_tm1 = network.apply(params, o\_tm1)
q\_t = network.apply(params, o\_t)
td\_error = rlax.q\_learning(q\_tm1, a\_tm1, r\_t, d\_t, q\_t)
return rlax.l2\_loss(td\_error)

#### @jax.jit

### def learn(state, params, transition): dloss\_dparams = jax.grad(loss\_fn)(\*transition)

updates, state = opt.update(dloss\_dparams, state)
params = optax.apply\_updates(params, updates)
return state, params



### **The Future**

### Our ecosystem is evolving rapidly

- Graph neural networks (github.com/deepmind/jraph)
- Testing & reliability (<u>github.com/deepmind/chex</u>)
- ... plus others coming soon!

### Checkout examples using DeepMind's JAX ecosystem

- Supervised Learning (<u>github.com/deepmind/jaxline</u>)
- Reinforcement learning (<u>github.com/deepmind/acme</u>)

### Others are also building great stuff with JAX

- Neural Networks (<u>github.com/google/flax</u>)
- Molecular Dynamics
- Chemical Modelling
- (github.com/google/jax-md)
- (github.com/deepchem/jaxchem)



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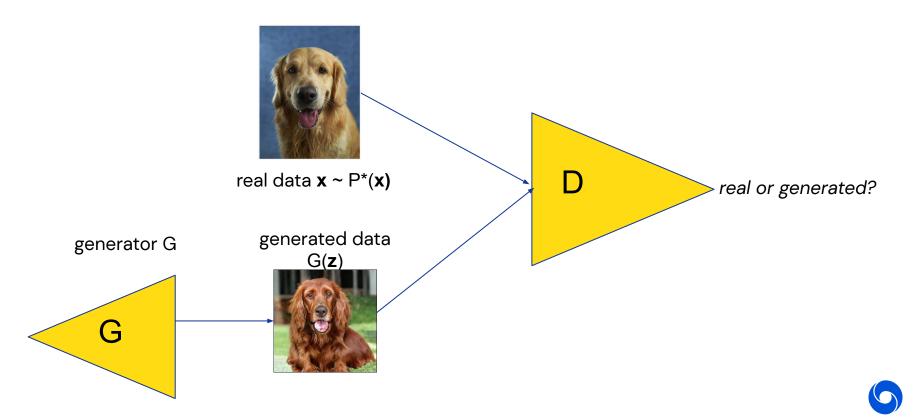
# 3. Generative Models & GANs

Mihaela Rosca



Slide thanks to Jeff Donahue.

### **GAN intro**



Join the discussion on Twitter (#JAXecosystem)

# **GANs - Gradients as first order citizens**

for \_ in range(num\_disc\_updates):

rng, rng\_disc = jax.random.split(rng, 2)

disc\_grads = jax.grad(gan.disc\_loss)(params.disc, params.gen, data\_batch, rng\_disc)
disc\_update, disc\_opt\_state = optimizers.disc.update(disc\_grads, opt\_state.disc)
new\_disc\_params = optax.apply\_updates(params.disc, disc\_update)

for \_ in range(num\_gen\_updates):

```
rng, rng_gen = jax.random.split(rng, 2)
gen_grads = jax.grad(gan.gen_loss)(params.gen, new_disc_params, data_batch, rng_gen)
gen_update, gen_opt_state = optimizers.gen.update(gen_grads, opt_state.gen)
new_gen_params = optax.apply_updates(params.gen, gen_update)
```

# Gradient as first order citizens - easy tracking

for \_ in range(num\_disc\_updates):

```
rng, rng_disc = jax.random.split(rng, 2)
```

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disc\_update, disc\_opt\_state = optimizers.disc.update(disc\_grads, opt\_state.disc)

new\_disc\_params = optax.apply\_updates(params.disc, disc\_update)

Direct access to gradients (not hidden inside the optimizer)! Can easily track gradients at different layers, effect of regularizers on gradients, etc.

With haiku, disc\_grads is a dictionary from module name to variables:



### Having more control - easier to make the right decisions

def disc\_loss(self, disc\_params, gen\_params, state, data\_batch, rng):
 samples, gen\_state = self.sample(gen\_params, state.gen, rng, data\_batch.shape[0])

disc\_inputs = jnp.concatenate((data\_batch, samples), axis=0)
disc\_outpus, disc\_state = self.disc.apply(disc\_params, state.disc, disc\_inputs)
data\_disc\_output, samples\_disc\_output = jnp.split(disc\_outpus, [data\_batch.shape[0],], axis=0)

loss = cross\_entropy\_disc\_loss(data\_disc\_output, samples\_disc\_output)

state = (disc\_state, gen\_state)

return loss, state



## Having more control - easier to make the right decisions

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## Functional approach makes code close to math

Reparametrization trick (GANs, VAEs, etc):

$$\nabla_{\theta} \mathbb{E}_{p_{\theta}(\mathbf{x})} f(\mathbf{x}) = \mathbb{E}_{p(\epsilon)} \nabla_{\theta} f(g_{\theta}(\epsilon)), \qquad \mathbf{x} = g_{\theta}(\epsilon)$$

def reparametrized\_jacobians(function, params, dist\_builder, rng, num\_samples):
 def surrogate(params):

dist = dist\_builder(\*params)

return jax.vmap(function)(dist.sample((num\_samples,), seed=rng))

return jax.jacfwd(surrogate)(params)

6

> Bonus! Easily to get jacobians - grad for each batch element!

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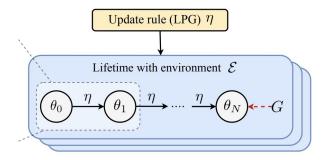
# 4. Meta-gradients

Junhyuk Oh (@junh\_oh)



# **Discovering RL Algorithms (Oh et al., NeurIPS 2020)**

Goal: Meta-learn a RL update rule from a distribution of agents and environments.



### **Technical Challenges**

- Parallel: Simulate independent learning agents, each of which is interacting with its own environment.
- Synchronous: Apply the same update rule (i.e., meta-learner) to all learning agents.
- Meta-gradient: Calculate meta-gradient over the update procedure.
- Scalability: Increase the number of learning agents without introducing extra cost.



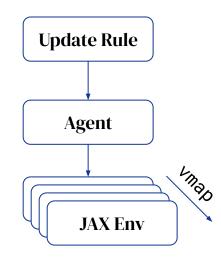
[Step 1] Implement a single update rule / single agent / single JAX environment interactions.



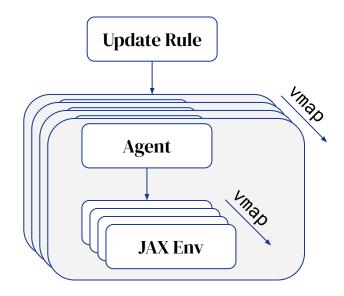


[Step 1] Implement a single update rule / single agent / single JAX environment interactions.

[Step 2] Add vmap to implement a single update rule / single agent / multi JAX environment interactions.

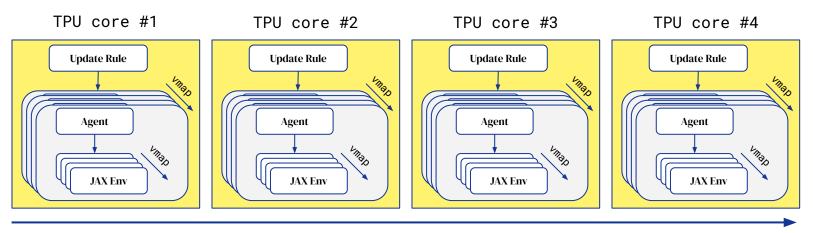


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[Step 3] Add vmap to implement a single update rule / multi agent / multi JAX environment interactions.





[Step 1] Implement a single update rule / single agent / single JAX environment interactions.
[Step 2] Add vmap to implement a single update rule / single agent / multi JAX environment interactions.
[Step 3] Add vmap to implement a single update rule / multi agent / multi JAX environment interactions.
[Step 4] Add pmap to implement multiple copies of them across TPU cores with a shared update rule.



### pmap

## **Pseudocode and Result**

```
def inner_update(params, meta_params, rng, env_state):
 def inner_loss(params, meta_params, rng, env_state):
   # Generate rollout and apply update rule.
    rollout = jax.vmap(do_rollout, in_axes=(None, 0, 0))(
        params, rng, env_state)
    return jax.vmap(apply_update_rule, in_axes=(None, 0))(
        meta_params, rollout)
 # Calulate gradient and update parameters.
  g = jax.grad(inner_loss)(params, rollout, meta_out)
 new_params = jax.tree_multimap(lambda p, g: p - g, params, g)
  return new_params
def meta_grad(meta_params, params, rng, env_state):
 def outer_loss(meta_params, params, rnq, env_state):
    new_params = jax.vmap(inner_update, in_axes=(0, None, 0, 0))(
        params, meta_params, rng, env_state)
    return jax.vmap(validate, in_axes=(0, None))(new_params, meta_params)
 # Calulate meta-gradient.
 meta_g = jax.grad(outer_loss)(meta_params, params, rng, env_state)
 return jax.lax.pmean(meta_g, 'i')
```

Using 16-core TPUv2

1K parallel learning agents

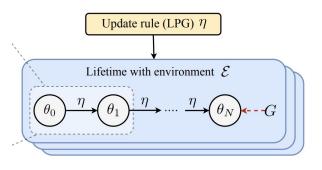
60K parallel environments

1 shared update rule

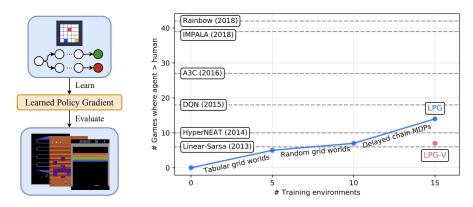
3M steps per second



# Summary



### Goal: Meta-learn a RL update rule from a distribution of agents and environments.



### **Technical Challenges**

- **Parallel**: Simulate independent learning agents, each of which is interacting with its own environment.
- **Synchronous**: Apply the same update rule (i.e., meta-learner) to all learning agents.
- Meta-gradient: Calculate meta-gradient over the update procedure.
- Scalability: Increase the number of learning agents without introducing extra cost.

### $\rightarrow$ JAX + TPU helped address the above without requiring much engineering effort.



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# 5. Search

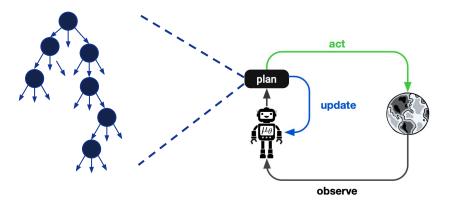
{Fabio Viola (@fabiointheuk), Theophane Weber(@theophaneweber)}



# Shifting gears a bit: search and model-based RL in jax

So far, we have mostly looked at applications of Jax which leverage its gradient computation capabilities. Is this all we can use Jax for?

Here we showcase another application where Jax enables fast research iteration:



Monte-Carlo Tree Search in a model-based RL setting, as seen in alphazero/muzero

Challenges:

- Integration of control logic and neural network machinery (tricky to debug!)
- Scalability and parallelism



# Why implement a model/search-based RL algorithm?

"Model-free algorithms are in turn far from the state of the art in domains that require *precise and sophisticated lookahead*, such as chess and Go" *-Schrittwieser et al. (2019)* 

"By employing search, we can find strong move sequences potentially *far away* from the apprentice policy, accelerating learning in complex scenarios" *–Anthony et al. (2017)* 

"....predictive models can enable a real robot to manipulate *previously unseen* objects and solve new tasks" *-Ebert et al. (2018)*  "Model-based planning is an essential ingredient of human intelligence, enabling *flexible adaptation* to new tasks and goals"

-Lake et al. (2016)

"...a flexible and general strategy such as mental simulation allows us to reason about a wide range of scenarios, even *novel* ones..." –Hamrick (2017)

"...[models] enable better *generalization* across states, remain valid across tasks in the same environment, and exploit additional unsupervised learning signals..." *-Weber et al.* (2017) Abraham (2020). The Cambridge Handbook of the Imagination.

Amos et al (24

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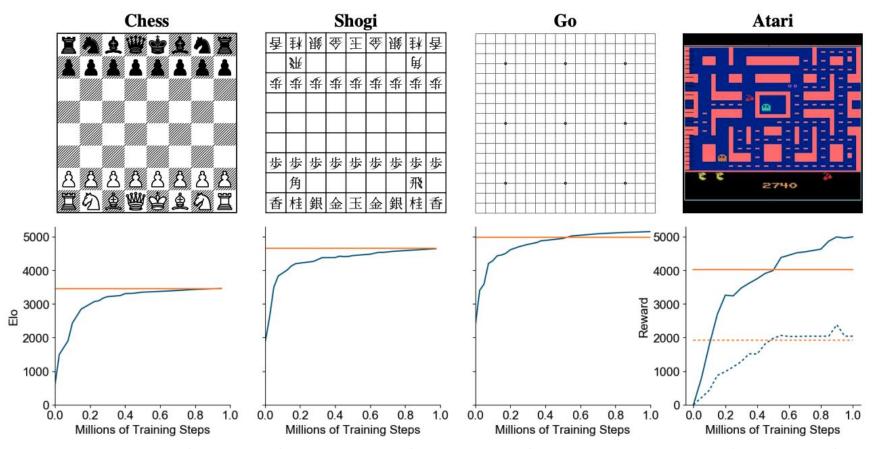
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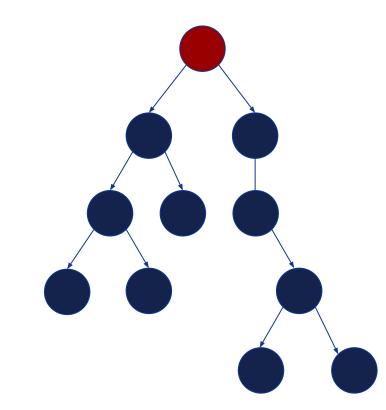
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#### MuZero (Schrittwieser et al., 2019)

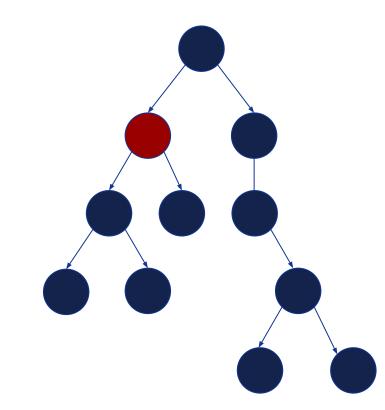




#### Neurally-guided MCTS:

1. Traverse tree using chosen heuristic In (alpha/mu)-zero, we use PUCT, which picks nodes with highest score, where the score combines policy prior, action values, and exploration bonus (derived from visit counts)

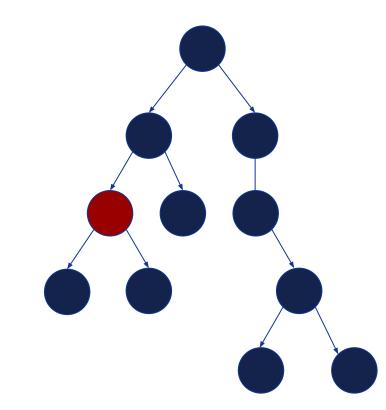




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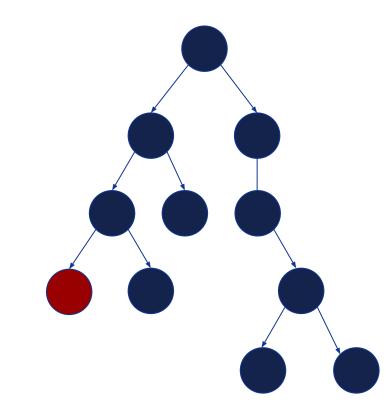




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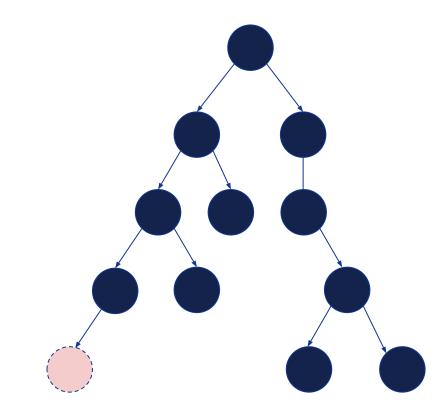




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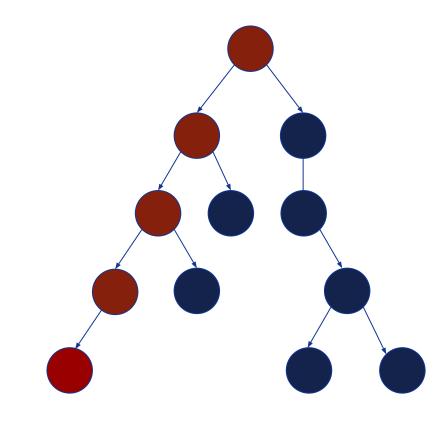




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- 2. Expand node:
  - a. Compute state transition, state value, and policy prior by calling model (neural network)
  - b. Add node to tree





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- 2. Expand node:
  - a. Compute state transition, state value, and policy prior by calling model (neural network)
  - b. Add node to tree
- 3. Backward step: propagate information from new leaf node to all ancestors in tree

# Why is implementing efficient MCTS a challenging task?

- Some researchers don't want to use C++ day-to-day, and prefer higher level languages, like python
- Performing MCTS in batch in plain python can be slow
- Furthermore, vanilla MCTS is a essentially a sequential algorithm each sim depends on the results of the previous sims – putting further constraints on how to parallelize computation\*

One possible approach:

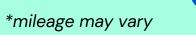
• Rely on just in time compilation to bridge the gap between interpreted and compiled languages – well aligned with the programming paradigm of JAX!



# Why implementing search in JAX?

Expected advantages:

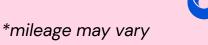
- Still performant once jitted and applied to batched data
- Save costs of moving data in and out of the accelerators
- Allows to easily jit and batch both acting and learning of RL agents
- Easiness to write and modify search components\*
  - it's just JAX numpy
  - write for single batch element, use vmap to vectorize
  - nice to be able to inspect your algorithm with python workflow
- Potentially differentiable all the way through



# Why implementing search in JAX?

Expected disadvantages:

- Likely less efficient if no batches (e.g. if deploying a trained RL agent in a single environment setup)
- Use some of the accelerator compute and memory is used for the search (rather than just reserving all of it for inference)
- Search depth limited by accelerator memory
- Performance of concurrently running multiple searches will be constrained by slowest instance



#### **Code snippets: search**

```
. . .
def search(self, params, rng_key, root, num_simulations, discount):
  def body fun(sim, loop state):
    rng key, params, tree = loop state
    rng_key, simulate_key, expand_key = jax.random.split(rng_key, 3)
    leaf_indices, unexplored_actions = simulate(
        simulate key, tree, self. action selection fn, self. max depth)
    leaf index = sim + 1
    tree = expand(
        params, expand_key, tree, self._recurrent_fn, leaf_indices,
        unexplored actions, leaf index)
    tree = backward(tree, leaf index)
    loop state = rng key, params, tree
    return loop state
  tree = self._init_tree(root, discount)
  rng_key, , tree = jax.lax.fori_loop(
      0, num simulations, body fun, (rng key, params, tree))
  return tree.search result()
. . .
```

#### **Code snippet: node expansion**

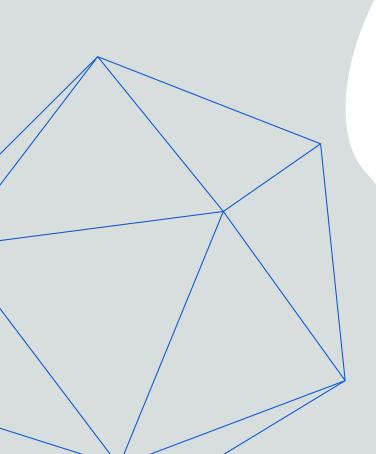
```
...
def expand(
    params, rng_key, tree, recurrent_fn, node_indices, actions, next_node_index):
    embeddings = tree.embeddings[tree.batch_range, node_indices]
    step, embeddings = recurrent_fn(params, rng_key, actions, embeddings)
    tree = update_node(
        tree, next_node_index, step.prior_probs, step.values, embeddings)
...
```

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# 6. Questions & Debate





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