

NN_Jax_Poisson

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1 Solving PDEs with Jax - Poisson

1.1 Description

This file contains our first approach to solve PDEs with neural networks on Jax Library.

Average time of execution # Average time of execution Between 2 and 3 minutes on GPU

1.1.1 PDE

We will try to solve the poisson Equation :

$$-\Delta\psi(x,y) = f(x,y) \text{ on } \Omega = [0,1]^2$$

1.1.2 Boundary conditions

$$\psi|_{\partial\Omega} = 0 \text{ and } f(x,y) = 2\pi^2 \sin(\pi x) \sin(\pi y)$$

1.1.3 Loss function

The loss to minimize here is $\mathcal{L} = \|\Delta\psi(x,y) + f(x,y)\|_2$

1.1.4 Analytical solution

The true function ψ should be $\psi(x,y) = \sin(\pi x) \sin(\pi y)$

1.1.5 Approximated solution

We want find a solution $\psi(x,y) = F(x,y)N(x,y) + A(x,y)$ s.t:

$$F(x,y) = \sin(x-1) \sin(y-1) \sin(x) \sin(y)$$

$$A(x,y) = 0$$

2 Importing libraries

```
[1]: # Jax libraries
from jax import value_and_grad, vmap, jit, jacfwd
from functools import partial
from jax import random as jran
from jax.example_libraries import optimizers as jax_opt
from jax.nn import tanh
from jax.lib import xla_bridge
import jax.numpy as jnp
```

```

# Others libraries
from time import time
import matplotlib.pyplot as plt
import numpy as np
import os
import pickle
print(xla_bridge.get_backend().platform)

```

3 Multilayer Perceptron

```

[2]: class MLP:
    """
        Create a multilayer perceptron and initialize the neural network
        Inputs :
            A SEED number and the layers structure
    """

    # Class initialization
    def __init__(self, SEED, layers):
        self.key = jran.PRNGKey(SEED)
        self.keys = jran.split(self.key, len(layers))
        self.layers = layers
        self.params = []

    # Initialize the MLP weights and bias
    def MLP_create(self):
        for layer in range(0, len(self.layers)-1):
            in_size, out_size = self.layers[layer], self.layers[layer+1]
            std_dev = jnp.sqrt(2/(in_size + out_size))
            weights = jran.truncated_normal(self.keys[layer], -2, 2,
            ↪ shape=(out_size, in_size), dtype=np.float32)*std_dev
            bias = jran.truncated_normal(self.keys[layer], -1, 1, shape=(out_size,
            ↪ 1), dtype=np.float32).reshape((out_size,))
            self.params.append((weights, bias))
        return self.params

    # Evaluate a position XY using the neural network
    @partial(jit, static_argnums=(0,))
    def NN_evaluation(self, new_params, inputs):
        for layer in range(0, len(new_params)-1):
            weights, bias = new_params[layer]
            inputs = tanh(jnp.add(jnp.dot(inputs, weights.T), bias))
        weights, bias = new_params[-1]
        output = jnp.dot(inputs, weights.T) + bias
        return output

```

```

# Get the key associated with the neural network
def get_key(self):
    return self.key

```

4 PDE operators

```

[3]: class PDE_operators:
    """
        Class with the most common operators used to solve PDEs
        Input:
            A function that we want to compute the respective operator
    """

    # Class initialization
    def __init__(self,function):
        self.function=function

    # Compute the two dimensional laplacian
    def laplacian_2d(self,params,inputs):
        fun = lambda params,x,y: self.function(params, x,y)
        @partial(jit)
        def action(params,x,y):
            u_xx = jacfwd(jacfwd(fun, 1), 1)(params,x,y)
            u_yy = jacfwd(jacfwd(fun, 2), 2)(params,x,y)
            return u_xx + u_yy
        vec_fun = vmap(action, in_axes = (None, 0, 0))
        laplacian = vec_fun(params, inputs[:,0], inputs[:,1])
        return laplacian

    # Compute the derivative in x
    @partial(jit, static_argnums=(0,))
    def du_dx(self,params,inputs):
        fun = lambda params,x,y: self.function(params, x,y)
        @partial(jit)
        def action(params,x,y):
            u_x = jacfwd(fun, 1)(params,x,y)
            return u_x
        vec_fun = vmap(action, in_axes = (None, 0, 0))
        return vec_fun(params, inputs[:,0], inputs[:,1])

    # Compute the derivative in y
    @partial(jit, static_argnums=(0,))
    def du_dy(self,params,inputs):
        fun = lambda params,x,y: self.function(params, x,y)
        @partial(jit)

```

```

def action(params,x,y):
    u_y = jacfwd(fun, 2)(params,x,y)
    return u_y
vec_fun = vmap(action, in_axes = (None, 0, 0))
return vec_fun(params, inputs[:,0], inputs[:,1])

```

5 Physics Informed Neural Networks

```

[4]: class PINN:
    """
    Solve a PDE using Physics Informed Neural Networks
    Input:
        The evaluation function of the neural network
    """

    # Class initialization
    def __init__(self, NN_evaluation):
        self.operators=PDE_operators(self.solution)
        self.laplacian=self.operators.laplacian_2d
        self.NN_evaluation=NN_evaluation
        self.dsol_dy=self.operators.du_dy

    # Definition of the function A(x,y) mentioned above
    @partial(jit, static_argnums=(0,))
    def A_function(self, inputX, inputY):
        return jnp.zeros_like(inputX).reshape(-1,1)

    # Definition of the function F(x,y) mentioned above
    @partial(jit, static_argnums=(0,))
    def F_function(self, inputX, inputY):
        F1=jnp.multiply(jnp.sin(inputX),jnp.sin(inputX-jnp.ones_like(inputX)))
        F2=jnp.multiply(jnp.sin(inputY),jnp.sin(inputY-jnp.ones_like(inputY)))
        return jnp.multiply(F1,F2).reshape((-1,1))

    # Definition of the function f(x,y) mentioned above
    @partial(jit, static_argnums=(0,))
    def target_function(self, inputs):
        return (2*jnp.pi**2*jnp.sin(jnp.pi*inputs[:,0])*jnp.sin(jnp.pi*inputs[:,
→,1])).reshape(-1,1)

    # Compute the solution of the PDE on the points (x,y)
    @partial(jit, static_argnums=(0,))
    def solution(self, params, inputX, inputY):
        inputs=jnp.column_stack((inputX, inputY))
        NN = vmap(partial(jit(self.NN_evaluation), params))(inputs)
        F=self.F_function(inputX, inputY)

```

```

        A=self.A_function(inputX,inputY)
        return jnp.add(jnp.multiply(F,NN),A).reshape(-1,1)

    # Compute the loss function
    @partial(jit, static_argnums=(0,))
    def loss_function(self,params,inputs,targets):
        preds=self.laplacian(params,inputs).reshape(-1,1)
        return jnp.linalg.norm(preds+targets)

    # Train step
    @partial(jit, static_argnums=(0,))
    def train_step(self,i, opt_state, inputs, pred_outputs):
        params = get_params(opt_state)
        loss, gradient = value_and_grad(self.loss_function)(params,inputs,
↪pred_outputs)
        return loss, opt_update(i, gradient, opt_state)

```

6 Initialize neural network

```

[5]: # Neural network parameters
SEED = 351
n_features, n_targets = 2, 1          # Input and output dimension
layers = [n_features,30,30,n_targets] # Layers structure

# Initialization
NN_MLP=MLP(SEED,layers)
params = NN_MLP.MLP_create()          # Create the MLP
NN_eval=NN_MLP.NN_evaluation          # Evaluate function
solver=PINN(NN_eval)
key=NN_MLP.get_key()

```

7 Train parameters

```

[6]: batch_size = 10000
num_batches = 5000
report_steps=100
loss_history = []

```

8 Adam optimizer

It's possible to continue the last training if we use options=1

```

[7]: opt_init, opt_update, get_params = jax_opt.adam(0.0005)

```

```

options=0
if options==0: # Start a new training
    opt_state=opt_init(params)

else:          # Continue the last training
    # Load trained parameters for a NN with the layers [2,30,30,1]
    best_params = pickle.load(open("./NN_saves/NN_jax_params.pkl", "rb"))
    opt_state = jax_opt.pack_optimizer_state(best_params)
    params=get_params(opt_state)

```

9 Solving PDE

```

[8]: # Main loop to solve the PDE
for ibatch in range(0,num_batches):
    ran_key, batch_key = jran.split(key)
    XY_train = jran.uniform(batch_key, shape=(batch_size, n_features), minval=0,
    ↪maxval=1)

    targets = solver.target_function(XY_train)
    loss, opt_state = solver.train_step(ibatch,opt_state, XY_train,targets)
    loss_history.append(float(loss))

    if ibatch%report_steps==report_steps-1:
        print("Epoch n°{}: ".format(ibatch+1), loss.item())
    if ibatch%5000==0:
        trained_params = jax_opt.unpack_optimizer_state(opt_state)
        pickle.dump(trained_params, open("./NN_saves/NN_jax_checkpoint.pkl",
    ↪"wb"))

```

```

Epoch n°100: 673.6737060546875
Epoch n°200: 505.8928527832031
Epoch n°300: 394.48870849609375
Epoch n°400: 313.5435791015625
Epoch n°500: 259.1355285644531
Epoch n°600: 229.37533569335938
Epoch n°700: 217.2259521484375
Epoch n°800: 213.3198699951172
Epoch n°900: 212.01670837402344
Epoch n°1000: 211.15426635742188
Epoch n°1100: 209.9100341796875
Epoch n°1200: 207.41326904296875
Epoch n°1300: 201.66140747070312
Epoch n°1400: 193.5465850830078
Epoch n°1500: 187.15386962890625
Epoch n°1600: 184.02920532226562
Epoch n°1700: 181.86134338378906

```

```

Epoch n°1800: 175.73419189453125
Epoch n°1900: 156.1564483642578
Epoch n°2000: 139.15335083007812
Epoch n°2100: 109.80931091308594
Epoch n°2200: 52.870853424072266
Epoch n°2300: 17.989492416381836
Epoch n°2400: 7.996098518371582
Epoch n°2500: 3.72841739654541
Epoch n°2600: 2.632183313369751
Epoch n°2700: 1.995606780052185
Epoch n°2800: 1.59634268283844
Epoch n°2900: 1.372849702835083
Epoch n°3000: 1.2082157135009766
Epoch n°3100: 1.0947226285934448
Epoch n°3200: 0.9832468032836914
Epoch n°3300: 0.8891815543174744
Epoch n°3400: 0.8169487118721008
Epoch n°3500: 0.7565268278121948
Epoch n°3600: 0.7112950682640076
Epoch n°3700: 0.6710832715034485
Epoch n°3800: 0.6246097683906555
Epoch n°3900: 0.5940172672271729
Epoch n°4000: 0.5544905662536621
Epoch n°4100: 0.5367295742034912
Epoch n°4200: 0.5019344091415405
Epoch n°4300: 0.48238810896873474
Epoch n°4400: 0.4735819697380066
Epoch n°4500: 0.44664886593818665
Epoch n°4600: 0.43133780360221863
Epoch n°4700: 0.4237716794013977
Epoch n°4800: 0.40775978565216064
Epoch n°4900: 0.3930644690990448
Epoch n°5000: 0.38667407631874084

```

10 Plot loss function

```

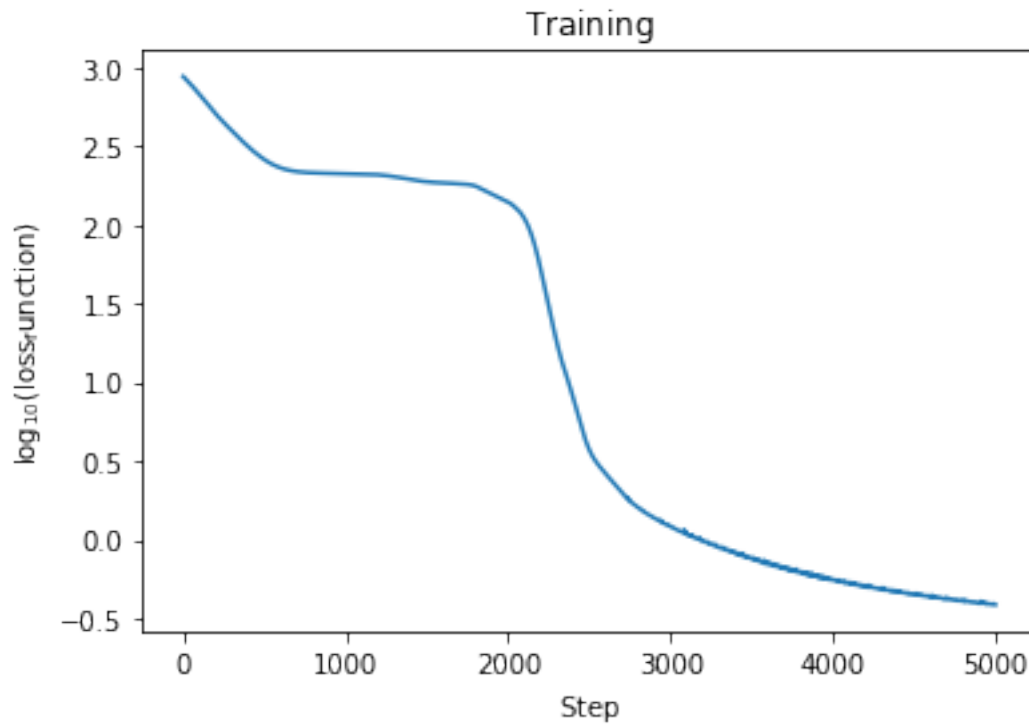
[9]: fig, ax = plt.subplots(1, 1)
    __=ax.plot(np.log10(loss_history))
    xlabel = ax.set_xlabel(r'$\{\rm Step\}$')
    ylabel = ax.set_ylabel(r'$\log_{10}\{\rm (loss\_function)\}$')
    title = ax.set_title(r'$\{\rm Training\}$')
    plt.show

```

```

[9]: <function matplotlib.pyplot.show(close=None, block=None)>

```

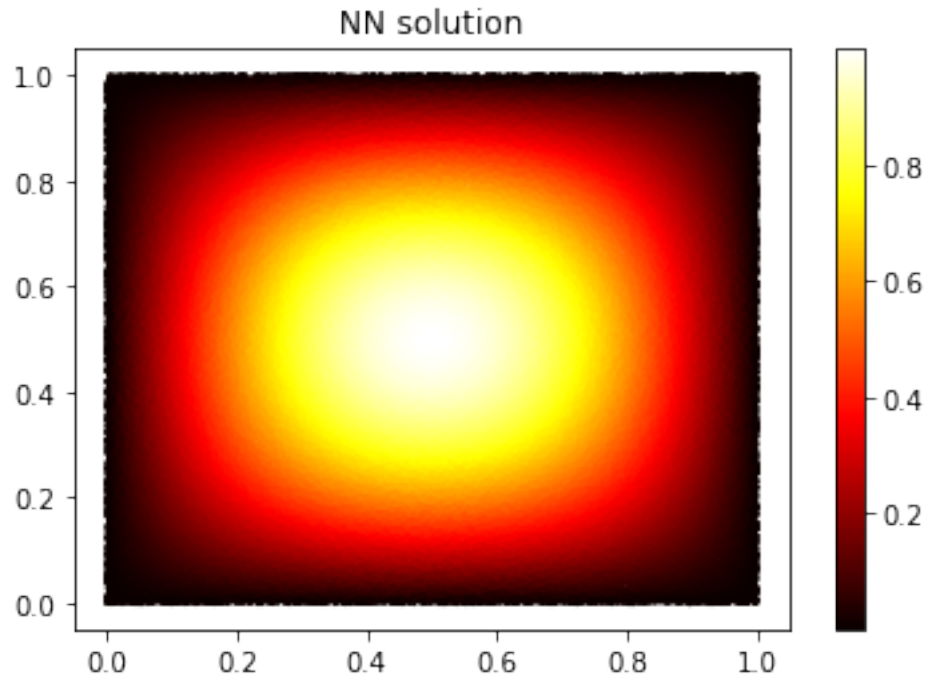


11 Approximated solution

We plot the solution obtained with our NN

```
[10]: plt.figure()
      params=get_params(opt_state)
      n_points=100000
      ran_key, batch_key = jran.split(key)
      XY_test = jran.uniform(batch_key, shape=(n_points, n_features), minval=0,
      ↪maxval=1)

      predictions = solver.solution(params,XY_test[:,0],XY_test[:,1])
      plt.scatter(XY_test[:,0],XY_test[:,1], c=predictions, cmap="hot",s=2)
      plt.clim(vmin=jnp.min(predictions),vmax=jnp.max(predictions))
      plt.colorbar()
      plt.title("NN solution")
      plt.show()
```

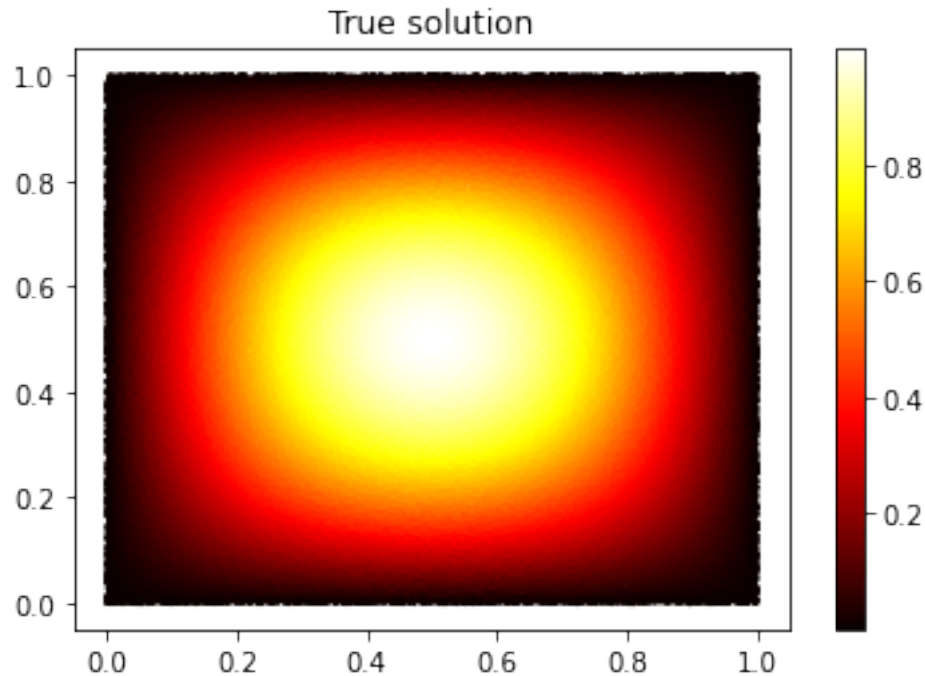
12 True solution

We plot the true solution, its form was mentioned above

```
[11]: def true_solution(inputs):
        return jnp.sin(jnp.pi*inputs[:,0])*jnp.sin(jnp.pi*inputs[:,1])

plt.figure()
n_points=100000
ran_key, batch_key = jran.split(key)
XY_test = jran.uniform(batch_key, shape=(n_points, n_features), minval=0,
    ↪maxval=1)

true_sol = true_solution(XY_test)
plt.scatter(XY_test[:,0],XY_test[:,1], c=true_sol, cmap="hot",s=2)
plt.colorbar()
plt.title("True solution")
plt.show()
```



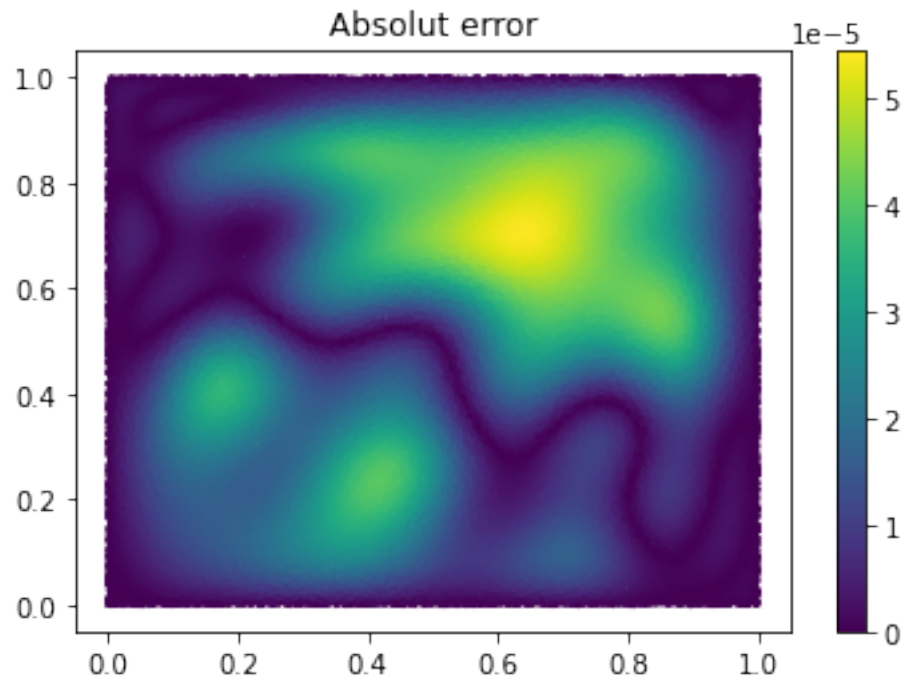
13 Absolut error

We plot the absolut error, it's $|\text{true solution} - \text{neural network output}|$

```
[12]: plt.figure()
      params=get_params(opt_state)
      n_points=100000
      ran_key, batch_key = jran.split(key)
      XY_test = jran.uniform(batch_key, shape=(n_points, n_features), minval=0,
      ↪maxval=1)

      predictions = solver.solution(params,XY_test[:,0],XY_test[:,1])[:,0]
      true_sol = true_solution(XY_test)
      error=abs(true_sol-predictions)

      plt.scatter(XY_test[:,0],XY_test[:,1], c=error, cmap="viridis",s=2)
      plt.colorbar()
      plt.title("Absolut error")
      plt.show()
```



14 Save NN parameters

```
[13]: trained_params = jax_opt.unpack_optimizer_state(opt_state)
      pickle.dump(trained_params, open("./NN_saves/NN_jax_params.pkl", "wb"))
```