NN_Jax_PDE7

June 15, 2022

1 Solving PDEs with Jax

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

We will try to solve the PDE :
$\Delta\psi(x,y) + \psi(x,y) \cdot \frac{\partial\psi(x,y)}{\partial y} = f(x,y)$ on $\Omega = [0,1]^2$
(Problem 7 of the article https://ieeexplore.ieee.org/document/712178)

With mixeds boundary conditions :
$\psi(0,y) = \psi(1,y) = \psi(x,0) = 0$ and $\frac{\partial\psi}{\partial y}(x,1) = 2\sin(\pi x)$
$f(x,y) = \sin(\pi x) \cdot (2 - \pi^2 y^2 + 2y^3 \sin(\pi x))$

The loss to minimize here is $\mathcal{L} = ||\Delta\psi(x,y) + \psi(x,y) \cdot \frac{\partial\psi(x,y)}{\partial y} - f(x)||_2$
The true function ψ should be $\psi(x,y) = y^2 sin(\pi x)$

We want find a solution $\psi(x,y) = A(x,y) + F(x,y)N(x,y)$ s.t:
$A = y\sin(\pi x)$
$F(x,y) = \sin(x-1)\sin(y-1)\sin(x)\sin(y)$

2 Importing libraries

[14]:
```
# 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

[15]:
```
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 weigths 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

[16]:
```
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

[17]:
```
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.multiply(inputY,jnp.sin(jnp.pi*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)).
↪reshape((-1,1))
        F2=jnp.multiply(jnp.sin(inputY),jnp.sin(inputY-jnp.ones_like(inputY))).
↪reshape((-1,1))
        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 jnp.multiply(jnp.sin(jnp.pi*inputs[:,0]),2-jnp.pi**2*inputs[:
↪,1]**2+2*inputs[:,1]**3*jnp.sin(jnp.pi*inputs[:,0])).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)

    # Compute the loss function
    @partial(jit, static_argnums=(0,))
    def loss_function(self,params,batch,targets):
        targets=self.target_function(batch)
        laplacian=self.laplacian(params,batch).reshape(-1,1)
        dsol_dy_values=self.dsol_dy(params,batch)[:,0].reshape((-1,1))
        preds=laplacian+jnp.multiply(self.solution(params,batch[:,0],batch[:
↪,1]),dsol_dy_values).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

[18]:
```
# 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

[19]:
```
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

[20]:
```
opt_init, opt_update, get_params = jax_opt.adam(0.001)

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

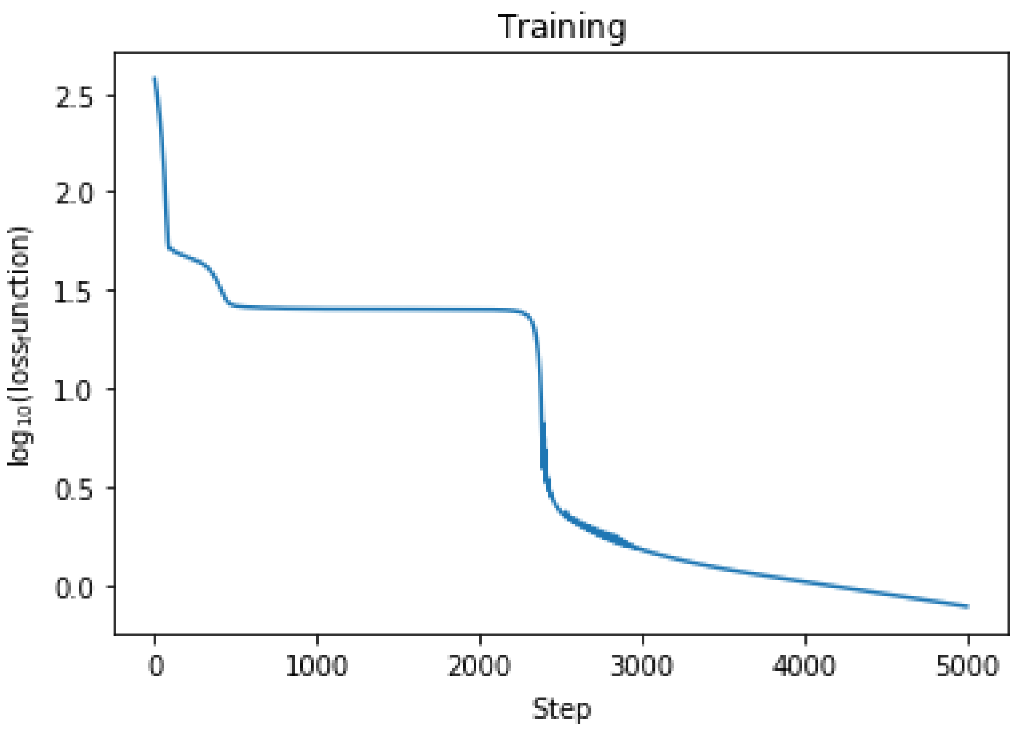
[21]:
```
# Main loop to solve the PDE
for ibatch in range(0,num_batches):
    ran_key, batch_key = jran.split(key)
    XY_train = jran.uniform(batch_key, shape=(batch_size, n_features), minval=0,␣
 ↪maxval=1)

    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:  51.43021774291992
Epoch n°200:  46.608707427978516
Epoch n°300:  42.7242546081543
Epoch n°400:  33.08360290527344
Epoch n°500:  26.27277183532715
Epoch n°600:  25.79522705078125
Epoch n°700:  25.579057693481445
Epoch n°800:  25.45096778869629
Epoch n°900:  25.371774673461914
Epoch n°1000:  25.321613311767578
Epoch n°1100:  25.28913116455078
Epoch n°1200:  25.267547607421875
Epoch n°1300:  25.252656936645508
Epoch n°1400:  25.241756439208984
Epoch n°1500:  25.232988357543945
Epoch n°1600:  25.224929809570312
Epoch n°1700:  25.21621322631836
Epoch n°1800:  25.205018997192383
Epoch n°1900:  25.188005447387695
Epoch n°2000:  25.1571102142334
Epoch n°2100:  25.086633682250977
Epoch n°2200:  24.853960037231445
Epoch n°2300:  23.273897171020508
Epoch n°2400:  4.551088333129883
Epoch n°2500:  2.347841739654541
Epoch n°2600:  2.106163740158081
Epoch n°2700:  1.8725926876068115
Epoch n°2800:  1.6912328004837036
Epoch n°2900:  1.5889019966125488
Epoch n°3000:  1.5024032592773438
Epoch n°3100:  1.4266735315322876
Epoch n°3200:  1.3593132495880127
Epoch n°3300:  1.301129937171936
Epoch n°3400:  1.250550627708435
Epoch n°3500:  1.2060681581497192
Epoch n°3600:  1.1661580801010132
Epoch n°3700:  1.1299446821212769
Epoch n°3800:  1.0965420007705688
Epoch n°3900:  1.0653166770935059
Epoch n°4000:  1.0356481075286865
Epoch n°4100:  1.007233738899231
Epoch n°4200:  0.9798058271408081
Epoch n°4300:  0.9529896378517151
Epoch n°4400:  0.9269103407859802
Epoch n°4500:  0.901094913482666
Epoch n°4600:  0.875564694404602
Epoch n°4700:  0.8502098321914673
Epoch n°4800:  0.8249480724334717
Epoch n°4900:  0.7997944951057434
Epoch n°5000:  0.774591863155365
```

10 Plot loss function

[22]:
```
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
```

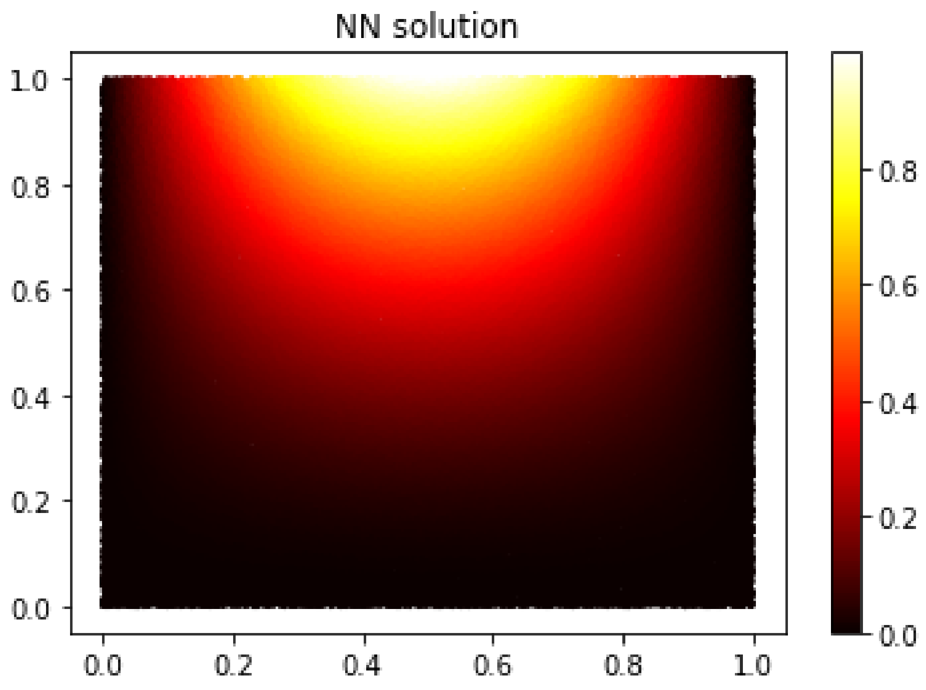
[22]:
```
<function matplotlib.pyplot.show(close=None, block=None)>
```



11 Approximated solution

We plot the solution obtained with our NN

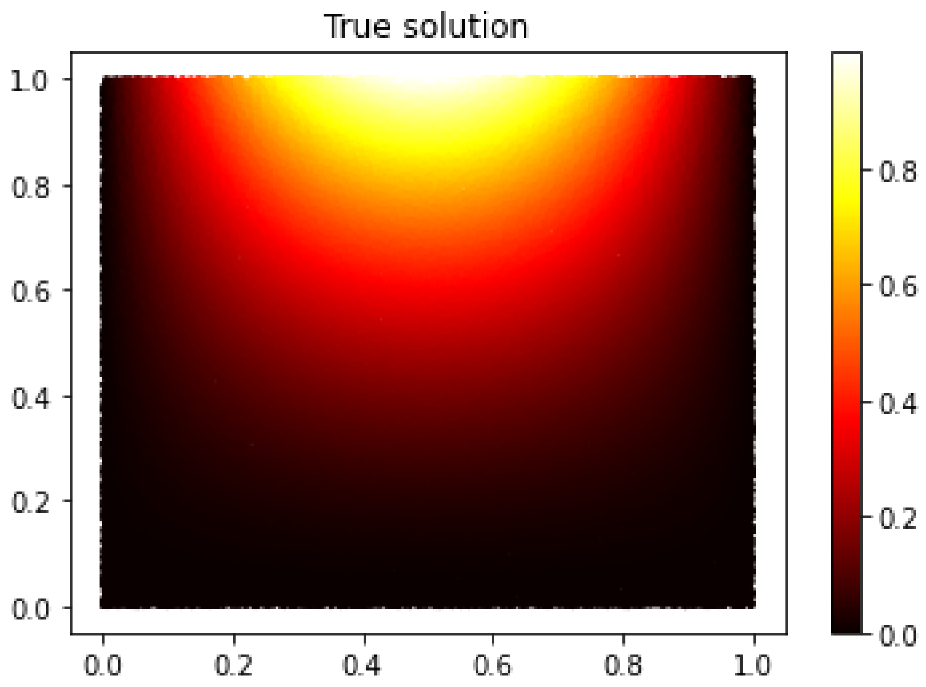
[23]:
```
plt.figure()
params=get_params(opt_state)
n_points=100000
ran_key, batch_key = jran.split(key)
XY_test = jran.uniform(batch_key, shape=(n_points, n_features), minval=0,␣
 ↪maxval=1)

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

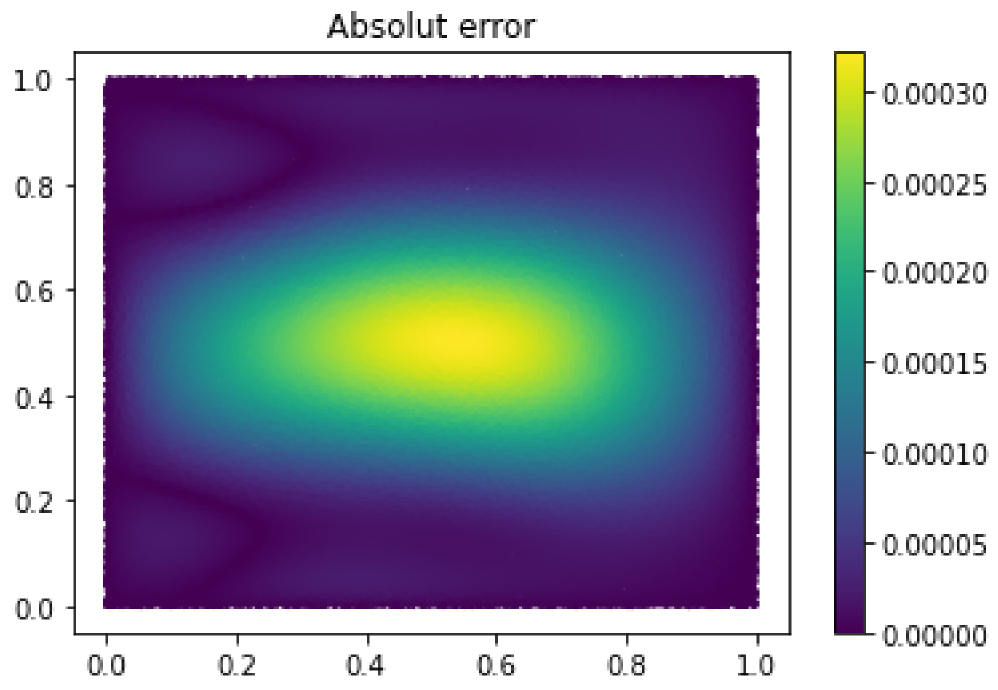
[27]:
```
def true_solution(X):
    return jnp.multiply(X[:,1]**2,jnp.sin(jnp.pi*X[:,0]))

plt.figure()
n_points=100000
ran_key, batch_key = jran.split(key)
XY_train = 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 |true solution - neural network output|

[25]:
```
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(predictions-true_sol)

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

[26]:
```
trained_params = jax_opt.unpack_optimizer_state(opt_state)
pickle.dump(trained_params, open("./NN_saves/NN_jax_params.pkl", "wb"))
```