NN_Jax_PDE5

June 21, 2022

1 Solving PDEs with Jax - Problem 5

1.1 Description

1.1.1 Average time of execution

Between 2 and 3 minutes on GPU

1.1.2 PDE

We will try to solve the problem 5 of the article https://ieeexplore.ieee.org/document/712178

$\Delta\psi(x,y) = f(x,y)$ on $\Omega = [0,1]^2$
with $f(x,y) = e^{-x}(x-2+y^3+6y)$

1.1.3 Boundary conditions

$\psi(0,y) = y^3$,$\psi(1,y) = (1+y^3)e^{-1}$,$\psi(x,0) = xe^{-x}$ and $\psi(x,1) = e^{-x}(x+1)$

1.1.4 Loss function

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

1.1.5 Analytical solution

The true function ψ should be $\psi(x,y) = e^{-x}(x+y^3)$

1.1.6 Approximated solution

We want find a solution $\psi(x,y) = A(x,y) + F(x,y)N(x,y)$ s.t:
$F(x,y) = \sin(x-1)\sin(y-1)\sin(x)\sin(y)$
$A(x,y) = (1-x)y^3 + x(1+y^3)e^{-1} + (1-y)x(e^{-x}-e^{-1}) + y[(1+x)e^{-x} - (1-x+2xe^{-1})]$

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)
```

gpu

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 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 Two dimensional PDE operators

[3]:
```
class PDE_operators2d:
    """
        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 partial 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 partial 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_operators2d(self.solution)
        self.laplacian=self.operators.laplacian_2d
        self.NN_evaluation=NN_evaluation

    # Definition of the function A(x,y) mentioned above
    @partial(jit, static_argnums=(0,))
    def A_function(self,inputX,inputY):
        A1=jnp.add(jnp.multiply((1-inputX),inputY**3),jnp.
↪multiply(inputX,(1+inputY**3)*jnp.exp(-1)))
        A2=jnp.multiply(jnp.multiply((1-inputY),inputX),jnp.exp(-inputX)-jnp.
↪exp(-1))
        A3=jnp.multiply(jnp.multiply(inputY,(1+inputX)),jnp.exp(-inputX))
        A4=jnp.multiply(inputY,-1+inputX-2*inputX*jnp.exp(-1))
        return jnp.add(jnp.add(A1,A2),jnp.add(A3,A4)).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):
```

```python
        t_f1=jnp.add(jnp.add(inputs[:,0]-2,inputs[:,1]**3),6*inputs[:,1])
        return jnp.multiply(jnp.exp(-inputs[:,0]),t_f1).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,batch):
        targets=self.target_function(batch)
        preds=self.laplacian(params,batch).reshape(-1,1)
        return jnp.linalg.norm(preds-targets)

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

6 Initialize neural network

[5]:
```python
# Neural network parameters
SEED = 351
n_features, n_targets = 2, 1            # Input and output dimension
layers = [n_features,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 = 50
num_batches = 100000
report_steps=1000
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(0.00005)

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 [2,30,1]
    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)

    loss, opt_state = solver.train_step(ibatch,opt_state, XY_train)
    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°1000:  1.4161701202392578
Epoch n°2000:  0.508507251739502
Epoch n°3000:  0.3503561019897461
Epoch n°4000:  0.33535873889923096
Epoch n°5000:  0.3159961700439453
```

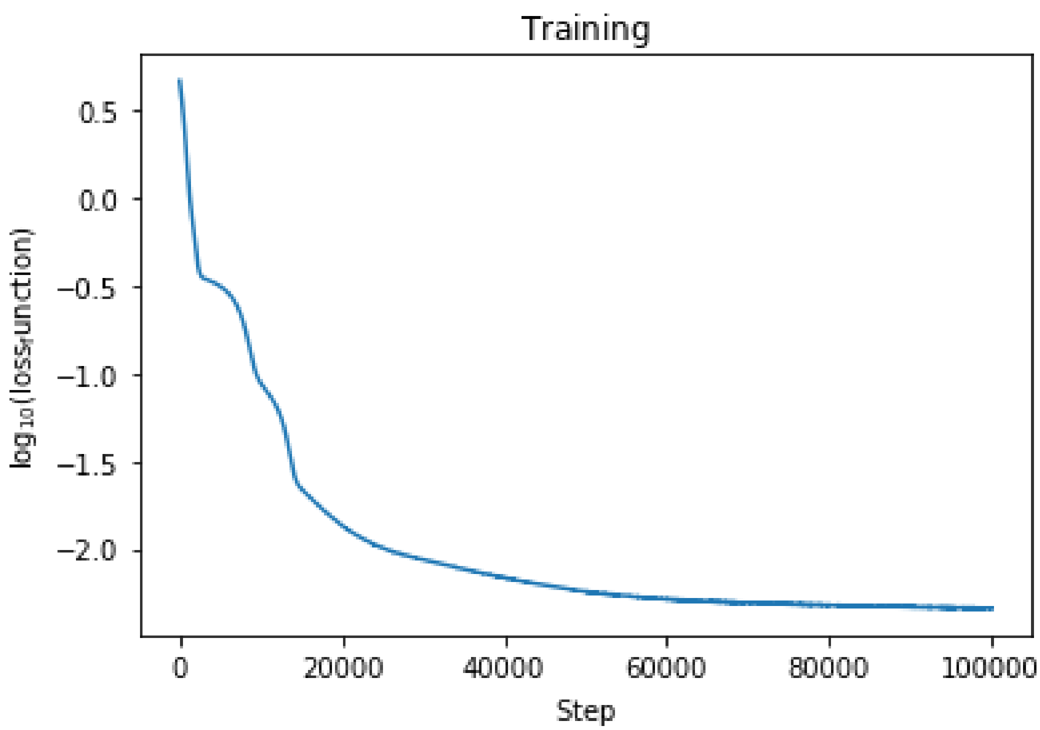
```
Epoch n°6000:  0.2889123558998108
Epoch n°7000:  0.24822157621383667
Epoch n°8000:  0.1858883649110794
Epoch n°9000:  0.11743717640638351
Epoch n°10000:  0.0883866399526596
Epoch n°11000:  0.07638377696275711
Epoch n°12000:  0.06408627331256866
Epoch n°13000:  0.04696416109800339
Epoch n°14000:  0.0279924925416708
Epoch n°15000:  0.02208159863948822
Epoch n°16000:  0.019892903044819832
Epoch n°17000:  0.017964016646146774
Epoch n°18000:  0.01626688614487648
Epoch n°19000:  0.014823420904576778
Epoch n°20000:  0.013621220365166664
Epoch n°21000:  0.012656135484576225
Epoch n°22000:  0.011874306946992874
Epoch n°23000:  0.011211562901735306
Epoch n°24000:  0.010620303452014923
Epoch n°25000:  0.01013614609837532
Epoch n°26000:  0.009762097150087357
Epoch n°27000:  0.009448214434087276
Epoch n°28000:  0.009177767671644688
Epoch n°29000:  0.008931156247854233
Epoch n°30000:  0.008698645979166031
Epoch n°31000:  0.008480792865157127
Epoch n°32000:  0.008273071609437466
Epoch n°33000:  0.008073559030890465
Epoch n°34000:  0.007877359166741371
Epoch n°35000:  0.007690975908190012
Epoch n°36000:  0.007510618772357702
Epoch n°37000:  0.007338885683566332
Epoch n°38000:  0.007172423414885998
Epoch n°39000:  0.007014378439635038
Epoch n°40000:  0.00686219334602356
Epoch n°41000:  0.006718161981552839
Epoch n°42000:  0.00658787228167057
Epoch n°43000:  0.006447346415370703
Epoch n°44000:  0.006322874687612057
Epoch n°45000:  0.0062063317745924
Epoch n°46000:  0.006096957717090845
Epoch n°47000:  0.005994355771690607
Epoch n°48000:  0.005903910845518112
Epoch n°49000:  0.005809021182358265
Epoch n°50000:  0.005726422183215618
Epoch n°51000:  0.005652638152241707
Epoch n°52000:  0.005578850395977497
Epoch n°53000:  0.005513239186257124
```

```
Epoch n°54000:  0.005453368648886681
Epoch n°55000:  0.005397585220634937
Epoch n°56000:  0.0053525641560554504
Epoch n°57000:  0.00529949925839901
Epoch n°58000:  0.005256304517388344
Epoch n°59000:  0.005216503515839577
Epoch n°60000:  0.0051793064922094345
Epoch n°61000:  0.005144989117980003
Epoch n°62000:  0.005113508552312851
Epoch n°63000:  0.00508406525477767
Epoch n°64000:  0.005056595895439386
Epoch n°65000:  0.005033764522522688
Epoch n°66000:  0.0050077978521585464
Epoch n°67000:  0.00498595368117094
Epoch n°68000:  0.004964722320437431
Epoch n°69000:  0.004945378750562668
Epoch n°70000:  0.004926398396492004
Epoch n°71000:  0.004908924922347069
Epoch n°72000:  0.0048911902122199535
Epoch n°73000:  0.0048751914873719215
Epoch n°74000:  0.004860007669776678
Epoch n°75000:  0.004846594296395779
Epoch n°76000:  0.004838292952626944
Epoch n°77000:  0.004817616194486618
Epoch n°78000:  0.004816572647541761
Epoch n°79000:  0.004799532704055309
Epoch n°80000:  0.004779526498168707
Epoch n°81000:  0.00476783886551857
Epoch n°82000:  0.00475620711222291
Epoch n°83000:  0.004745344631373882
Epoch n°84000:  0.004742323886603117
Epoch n°85000:  0.0047234585508704185
Epoch n°86000:  0.004712650086730719
Epoch n°87000:  0.004703030455857515
Epoch n°88000:  0.004692358896136284
Epoch n°89000:  0.004682101774960756
Epoch n°90000:  0.004672268871217966
Epoch n°91000:  0.004669539630413055
Epoch n°92000:  0.004653334617614746
Epoch n°93000:  0.004644602537155151
Epoch n°94000:  0.004634924232959747
Epoch n°95000:  0.004626475740224123
Epoch n°96000:  0.004618755541741848
Epoch n°97000:  0.0046081640757620335
Epoch n°98000:  0.004599463660269976
Epoch n°99000:  0.00459072133526206
Epoch n°100000:  0.004582080990076065
```

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)>
```

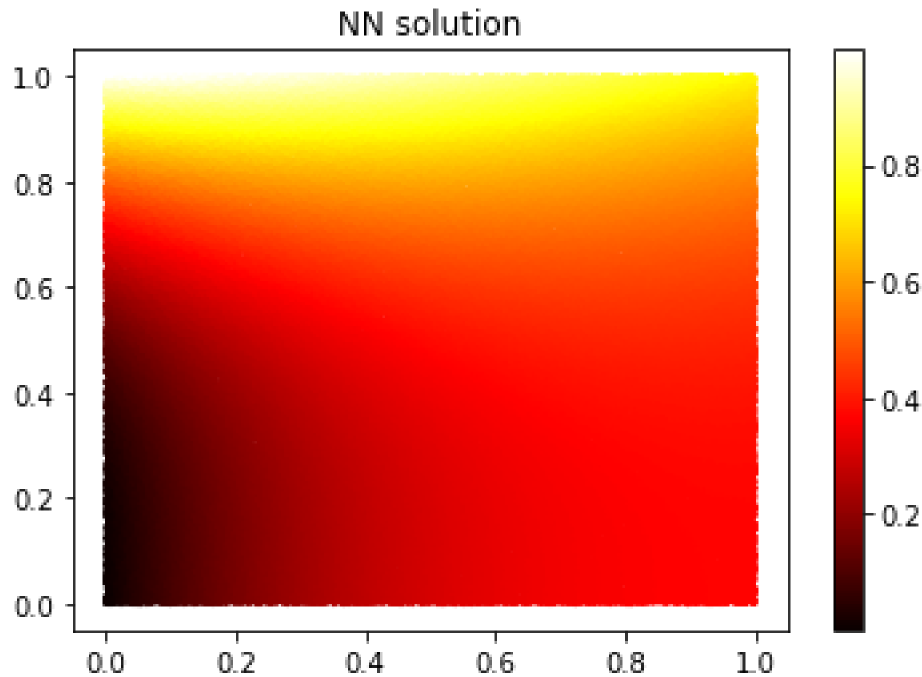


11 Approximated solution

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

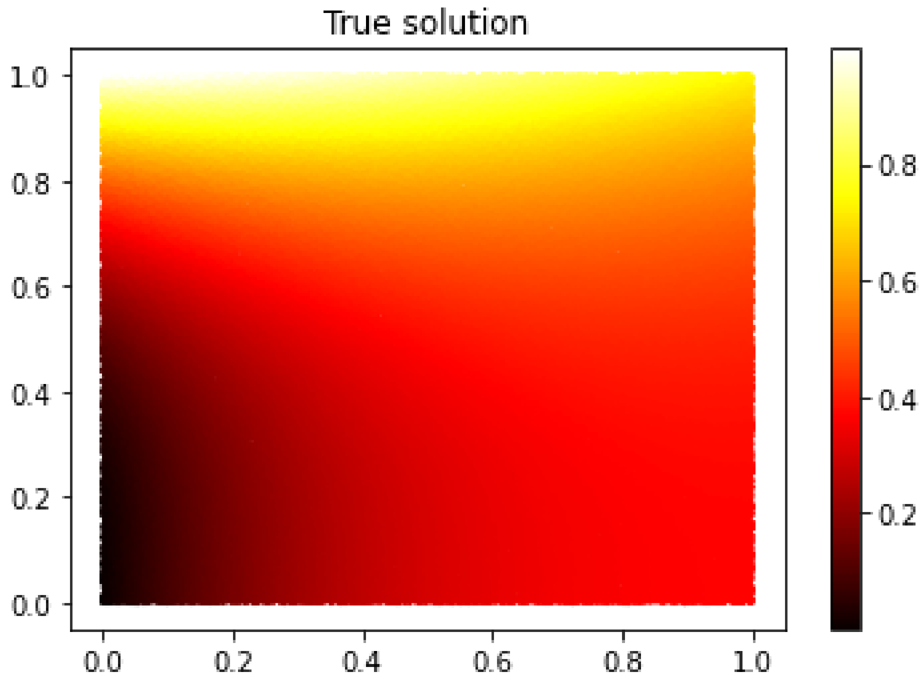
We plot the true solution, its form was mentioned above

[11]:
```
def true_solution(inputs):
    return jnp.multiply(jnp.exp(-inputs[:,0]),inputs[:,0]+inputs[:,1]**3)

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.clim(vmin=jnp.min(true_sol),vmax=jnp.max(true_sol))
plt.colorbar()
plt.title("True solution")
```

```
plt.show()
```

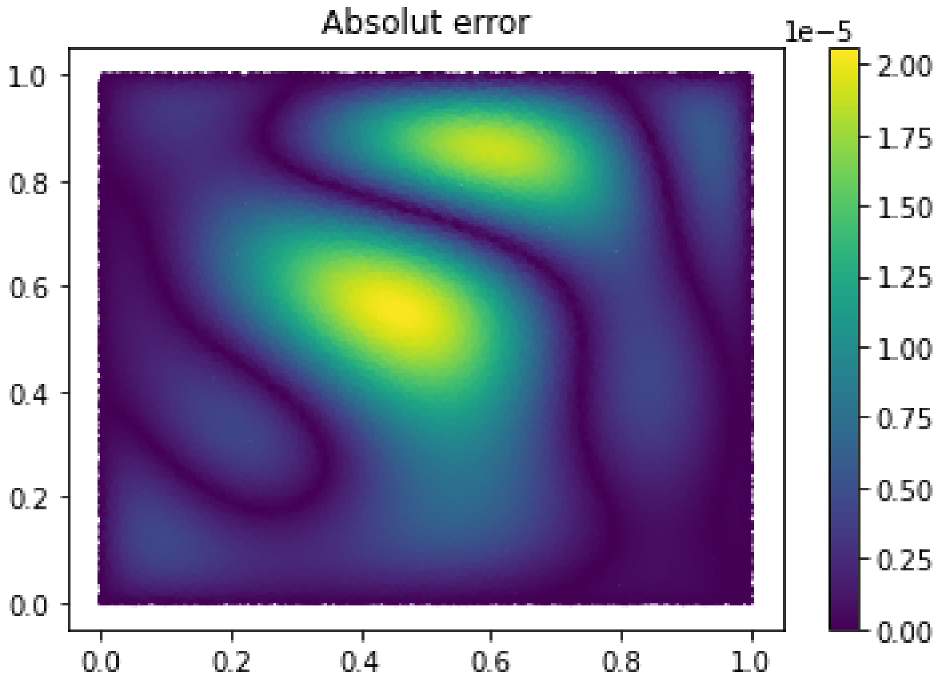


13 Absolut error

We plot the absolut error, it's |true solution - 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(predictions-true_sol)

plt.scatter(XY_test[:,0],XY_test[:,1], c=error, cmap="viridis",s=2)
plt.clim(vmin=0,vmax=jnp.max(error))
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"))
```