helmholtz

December 28, 2022

1 Numerical solution of the Helmholtz equation

1.1 Description

1.1.1 PDE

We will try to solve the following pde:

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

1.1.2 Boundary conditions

$$\psi(0,y) = e^{jky}$$
, $\psi(1,y) = e^{jk(1+y)}$, $\psi(x,0) = e^{jkx}$ and \$ $(x,1)=e^{(x+1)}$ \$

1.1.3 Loss function

The loss to minimize here is $\mathcal{L} = \frac{1}{N}||\Delta\psi(x,y) + k^2\psi(x,y) + f(x,y)||_2^2$, where N is the size of the training data

1.1.4 Analytical solution

The solution ψ_{th} should be $\psi_{th}(x,y)=e^{jk(x+y)}$

1.1.5 Approximated solution

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

$$\begin{split} F(x,y) &= \sin(x)\sin(y)\sin(x-1)\sin(y-1) \\ A(x,y) &= (1-x)e^{jky} + xe^{jk(1+y)} + (1-y)\{e^{jkx} - [(1-x) + xe^{jk}]\} + y\{e^{jk(x+1)} - [(1-x)e^{jk} + xe^{j2k}]\} \end{split}$$

2 Libraries

```
[1]: import jax, optax
import pickle
import functools
import matplotlib.pyplot
import numpy
%matplotlib inline
```

```
# Set and verify device
jax.config.update('jax_platform_name', 'gpu')
jax.config.update("jax_enable_x64", True)
print(jax.lib.xla_bridge.get_backend().platform)
```

gpu

3 Parameters

```
[2]: # Neural network parameters
     parameters = {}
     parameters['seed'] = 351
     parameters['n_features'] = 2
                                       # Input dimension (x1, x2)
     parameters['n_targets'] = 2
                                        # Output dimension. It's a complex number
      \hookrightarrow (y1 + j*y2)
     parameters['hidden_layers'] = [50, 50, 50, 50, 50] # Hidden layers structure
     parameters['layers'] = [parameters['n_features']] + parameters['hidden_layers']_
      # Training parameters
     parameters['learning_rate'] = optax.linear_schedule(0.005, 0.00001, 0.00001)
      stransition_steps = 50, transition_begin = 5000)
     parameters['optimizer'] = optax.adam(parameters['learning_rate'])
     parameters['maximum_num_epochs'] = 50000
     parameters['report_steps'] = 1000
     parameters['options'] = 1
                                         # 1: we start a new training. 2: We_
      ⇔continue the last training.
                                         # Other cases: We just load the last
      \hookrightarrow training
     # Data parameters
     parameters['batch_size'] = 100
     parameters['domain_bounds'] = jax.numpy.column_stack(([0.0, 0.0], [1.0, 1.0]))
      \hookrightarrow # minimal and maximal value of each axis (x, y)
```

4 Neural network

```
self.keys = jax.random.split(self.key,len(layers))
       self.layers = layers
       self.params = []
  def MLP_create(self):
       11 11 11
       Initialize the MLP weigths and bias
       Parameters
       Returns
       params : list of parameters[[w1,b1],...,[wn,bn]]
           -- weights and bias
       for layer in range(0, len(self.layers)-1):
           in_size,out_size = self.layers[layer], self.layers[layer+1]
           weights = jax.nn.initializers.glorot_normal()(self.keys[layer],__
→(out_size, in_size), jax.numpy.float32)
           bias = jax.nn.initializers.lecun_normal()(self.keys[layer],_
→(out_size, 1), jax.numpy.float32).reshape((out_size, ))
           self.params.append((weights, bias))
      return self.params
  @functools.partial(jax.jit, static_argnums=(0,))
  def NN_evaluation(self, params, inputs):
       n n n
       Evaluate a position (x,y) using the neural network
       Parameters
       params: list of parameters[[w1,b1],...,[wn,bn]]
           -- weights and bias
       inputs : jax.numpy.ndarray[[batch_size,batch_size]]
           -- points in the domain
       Returns
       output : jax.numpy.array[batch_size]
           -- neural network output
       11 11 11
       for layer in range(0, len(params)-1):
           weights, bias = params[layer]
           inputs = jax.nn.tanh(jax.numpy.add(jax.numpy.dot(inputs, weights.
\hookrightarrowT), bias))
      weights, bias = params[-1]
       real_and_imaginary_layers = jax.numpy.dot(inputs, weights.T)+bias #_
The first output of the NN is the real part, the second is the imaginary part
```

```
output = jax.lax.complex(real_and_imaginary_layers[0], u

→real_and_imaginary_layers[1])

return output
```

5 Operators

```
[4]: class PDE_operators:
             Class with the operators used to solve the PDE
         Input:
             A function that we want to compute the respective operator
         .....
         def __init__(self, function):
             self.function = function
         @functools.partial(jax.jit, static_argnums=(0,))
         def laplacian_2d(self, params, inputs):
             Compute the two dimensional laplacian.
             Parameters
             _____
             params: list of parameters[[w1,b1],...,[wn,bn]]
                 -- weights and bias
             inputs : jax.numpy.ndarray[[batch_size,batch_size]]
                 -- coordinates (x, y)
             Returns
             laplacian : jax.numpy.ndarray[batch_size]
                 -- numerical values of the laplacian applied to the inputs
             fun = lambda params,x, y: self.function(params, x, y)
             @functools.partial(jax.jit)
             def action(params,x, y):
                 u_xx = jax.jacfwd(jax.jacfwd(fun, 1), 1)(params,x, y)
                 u_yy = jax.jacfwd(jax.jacfwd(fun, 2), 2)(params,x, y)
                 return u_xx + u_yy
             vec_fun = jax.vmap(action, in_axes = (None, 0, 0))
             laplacian = vec_fun(params, inputs[:,0], inputs[:,1]).flatten()
             return laplacian
```

6 Physics Informed Neural Network

```
[5]: class PINN:
         11 11 11
         Solve a PDE using Physics Informed Neural Networks
             The evaluation function of the neural network and the optimizer ____
      ⇔selected to do gradient descent
         def __init__(self, NN_evaluation, optimizer):
             self.NN_evaluation = NN_evaluation
             self.optimizer = optimizer
             self.operators = PDE_operators(self.spatial_solution2d)
             self.laplacian2d = self.operators.laplacian_2d
             self.k_coeff = 0.5 # Wavenumber
         @functools.partial(jax.jit, static argnums = (0, ))
         def spatial_solution2d(self, params, inputX, inputY):
             Compute the complex solution of the PDE on the points (x, y)
             Parameters
             params: list of parameters[[w1,b1],...,[wn,bn]]
                 -- weights and bias
             inputX : jax.numpy.array[batch_size]
                 -- points on the x-axis of the domain
             inputY : jax.numpy.array[batch_size]
                 -- points on the y-axis of the domain
             Returns
             applied_solution : jax.numpy.array[batch_size]
                 -- PINN solution applied to inputs. return F NN plus A, a complex,
      ⇔array
             inputs = jax.numpy.column_stack((inputX, inputY))
             NN = jax.vmap(functools.partial(jax.jit(self.NN_evaluation),
      →params))(inputs)
             F = self.F_function(inputX,inputY)
             A = self.A_function(inputX,inputY)
             F_NN_plus_A = jax.numpy.add(jax.numpy.multiply(F, NN), A).reshape(-1)
             return F_NN_plus_A
         # Definition of the function A(x, y) mentioned above
```

```
@functools.partial(jax.jit, static_argnums = (0, ))
  def A_function(self, inputX, inputY):
       Compute A(x, y) on the inputs
       Parameters
       inputX : jax.numpy.ndarray[batch_size]
           -- points in the axis x
       inputY : jax.numpy.ndarray[batch size]
           -- points in the axis y
       Returns
       A_output : jax.numpy.array[batch_size]
           -- A(x, y) applied to inputs
      j_number = jax.lax.complex(0.0,1.0)
      A1 = (1-inputX)*jax.numpy.exp(j_number*self.k_coeff*inputY) +_
→inputX*jax.numpy.exp(j_number*self.k_coeff*(1+inputY))
       A2 = (1-inputY)*(jax.numpy.exp(j_number*self.k_coeff*inputX) -_
→((1-inputX) + inputX*jax.numpy.exp(j_number*self.k_coeff)))
       A3 = inputY*(jax.numpy.exp(j_number*self.k_coeff*(inputX + 1)) -__
→((1-inputX)*jax.numpy.exp(j_number*self.k_coeff) + inputX*jax.numpy.
→exp(j_number*2*self.k_coeff)))
      A output = A1 + A2 + A3
      return A_output
   # Definition of the function F(x, y) mentioned above
  @functools.partial(jax.jit, static_argnums = (0, ))
  def F_function(self, inputX, inputY):
       n n n
       Compute F(x, y) on the inputs
       Parameters
       inputX : jax.numpy.ndarray[batch_size]
           -- points in the axis x
       inputY : jax.numpy.ndarray[batch_size]
           -- points in the axis y
      Returns
       F_output : jax.numpy.array[batch_size]
           -- F(x, y) applied to inputs
      F1 = jax.numpy.multiply(jax.numpy.sin(inputX), jax.numpy.sin(inputX -_u
→1))
      F2 = jax.numpy.multiply(jax.numpy.sin(inputY), jax.numpy.sin(inputY -__
→1))
```

```
F_output = jax.numpy.multiply(F1, F2)
      return F_output
  # Definition of the function f(x, y) mentioned above
  @functools.partial(jax.jit, static_argnums = (0, ))
  def exact_function(self, inputs):
      11 11 11
      Compute f(x, y) on the inputs
      Parameters
      _____
      inputs : jax.numpy.ndarray[[batch_size, batch_size]]
          -- (x, y) points from the domain
      Returns
      exact_output : jax.numpy.array[batch_size]
          -- f(x, y) applied to inputs
      j_number = jax.lax.complex(0.0,1.0)
      exact_output = self.k_coeff**2*jax.numpy.exp(j_number*self.

¬k_coeff*(inputs[:,0] + inputs[:,1]))
      return exact output
  # Definition of the pde mentioned above
  @functools.partial(jax.jit, static_argnums = (0, ))
  def pde_function(self, params, inputs):
      11 11 11
      Compute the pde on the inputs
      Parameters
      _____
      params : list of parameters[[w1,b1],...,[wn,bn]]
          -- weights and bias
      inputs : jax.numpy.ndarray[[batch_size, batch_size]]
          -- (x, y) points from the domain
      Returns
      pde_value : jax.numpy.array[batch_size]
          -- pde applied to inputs
      pde_value = self.laplacian2d(params, inputs) + self.k_coeff**2*self.
spatial_solution2d(params, inputs[:,0], inputs[:,1])
      return pde_value
  # Definition of the loss function mentioned above
  @functools.partial(jax.jit, static_argnums = (0, ))
```

```
def loss_function(self, params, inputs):
      Compute the loss of the pde inside the domain
      Parameters
       _____
      params: list of parameters[[w1,b1],...,[wn,bn]]
          -- weights and bias
      inputs : jax.numpy.ndarray[[batch_size, batch_size]]
          -- (x, y) points from the domain
      Returns
       loss_value : a float64
          -- loss function applied to inputs
      residual = self.pde_function(params, inputs) + self.
→exact_function(inputs)
      loss_value = (jax.numpy.linalg.norm(residual)**2)/inputs.shape[0]
      return loss_value
  # Make one train step
  @functools.partial(jax.jit, static_argnums = (0, ))
  def train_step(self, params, opt_state, inputs):
      Make just one step of the training
      Parameters
      params: list of parameters[[w1,b1],...,[wn,bn]]
          -- weights and bias
      opt_state : a tuple given by optax library
          -- state(hystorical) of the gradient descent
       inputs : jax.numpy.ndarray[[batch_size, batch_size]]
          -- (x, y) inputs from the domain
      Returns
       loss: a float64
          -- loss function applied to inputs
      new_params : list of parameters[[w1,b1],...,[wn,bn]]
          -- weights and bias updated
       opt_state : a tuple given by optax
          -- update the state(hystorical) of the gradient descent
      loss, gradient = jax.value_and_grad(self.loss_function)(params, inputs)
      updates, new_opt_state = self.optimizer.update(gradient, opt_state)
      new_params = optax.apply_updates(params, updates)
      return loss, new_params, new_opt_state
```

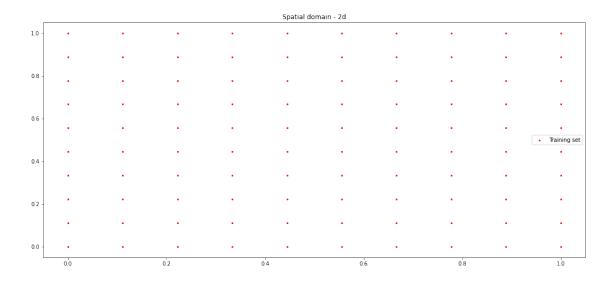
7 Analytical solution

8 Dataset creation

9 Dataset plot

```
[7]: fig, ax = matplotlib.pyplot.subplots()
   fig.set_size_inches(18, 8.0)
   title = ax.set_title('Spatial domain - 2d')
   graph = matplotlib.pyplot.scatter(XY_train[:,0], XY_train[:,1], color = 'red', \( \text{u} \)
   \[ \text{us} = 5)
   \]
  \[ = ax.legend(['Training set'])

matplotlib.pyplot.savefig('./Images/domain2d.png', facecolor = 'white', \( \text{u} \)
  \[ \text{ubox_inches} = 'tight')
  \]
matplotlib.pyplot.show()
```



10 Model initialization

```
[8]: key = jax.random.PRNGKey(parameters['seed'])
    NN_MLP = MLP(key, parameters['layers'])
    params = NN_MLP.MLP_create()  # Create the MLP
    NN_eval = NN_MLP.NN_evaluation  # Evaluation function
    solver = PINN(NN_eval, parameters['optimizer'])
    opt_state = parameters['optimizer'].init(params)
```

11 Training

```
pickle.dump(loss_history, open("./Checkpoints/
 ⇔loss_history_helmholtz", "wb"))
elif parameters['options'] == 2:
                                      # continue the last training
    params = pickle.load(open("./Checkpoints/params_helmholtz", "rb"))
    opt state = pickle.load(open("./Checkpoints/opt state helmholtz", "rb"))
    loss_history = pickle.load(open("./Checkpoints/loss_history_helmholtz",_

¬"rb"))
    iepoch = len(loss_history)
    # Main loop to solve the PDE
    for ibatch in range(iepoch, parameters['maximum num epochs']+1):
        loss, params, opt_state = solver.train_step(params, opt_state, XY_train)
        loss_history.append(float(loss))
        if (ibatch%parameters['report_steps']) == parameters['report_steps']-1:
            print("Epoch n°{}: ".format(ibatch+1), loss.item())
        if loss <= numpy.min(loss_history): # save if the current state is the
 \hookrightarrowbest
            pickle.dump(params, open("./Checkpoints/params_helmholtz", "wb"))
            pickle.dump(opt_state, open("./Checkpoints/opt_state_helmholtz", __
 →"wb"))
            pickle.dump(loss_history, open("./Checkpoints/
 ⇔loss_history_helmholtz", "wb"))
    params = pickle.load(open("./Checkpoints/params_helmholtz", "rb"))
    opt_state = pickle.load(open("./Checkpoints/opt_state_helmholtz", "rb"))
    loss_history = pickle.load(open("./Checkpoints/loss_history_helmholtz",_

"rb"))
```

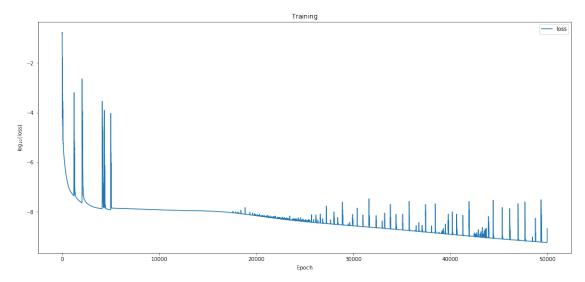
Training start

Epoch n°1000: 5.508144004289995e-08
Epoch n°2000: 2.3492064342453148e-08
Epoch n°3000: 1.712214673089992e-08
Epoch n°4000: 1.3584209498974991e-08
Epoch n°5000: 6.782584311577836e-07
Epoch n°6000: 1.3726638647027041e-08
Epoch n°7000: 1.3330959503670555e-08
Epoch n°8000: 1.292204132239227e-08
Epoch n°9000: 1.2481982923987923e-08
Epoch n°10000: 1.2053273138377728e-08
Epoch n°11000: 1.1713291331651193e-08
Epoch n°12000: 1.1489137949481197e-08
Epoch n°13000: 1.1309575373356905e-08
Epoch n°14000: 1.1089247318201054e-08

```
Epoch n°15000:
                1.077665372165983e-08
Epoch n°16000:
                1.0324800746245108e-08
                9.686227017984392e-09
Epoch n°17000:
Epoch n°18000:
                8.846504053505464e-09
Epoch n°19000:
                7.929729709992478e-09
Epoch n°20000:
                7.032529485325194e-09
Epoch n°21000:
                6.220678566630447e-09
Epoch n°22000:
                5.553653758169135e-09
Epoch n°23000:
                4.931916761029431e-09
Epoch n°24000:
                4.710894492075254e-09
                4.076219021928677e-09
Epoch n°25000:
                3.72667566061403e-09
Epoch n°26000:
                3.4367460096975306e-09
Epoch n°27000:
Epoch n°28000:
                3.1837851237343453e-09
Epoch n°29000:
                2.953595009631633e-09
                2.741923196143276e-09
Epoch n°30000:
Epoch n°31000:
                4.641513257320245e-09
                2.362142943674844e-09
Epoch n°32000:
Epoch n°33000:
                2.947162020402487e-09
Epoch n°34000:
                2.0270427864634136e-09
Epoch n°35000:
                1.876677980376093e-09
Epoch n°36000:
                1.734740948593067e-09
Epoch n°37000:
                1.5955786930573046e-09
Epoch n°38000:
                1.4704999107296139e-09
Epoch n°39000:
                1.3568966503466736e-09
Epoch n°40000:
                1.24363017358315e-09
Epoch n°41000:
                1.1446279565527412e-09
Epoch n°42000:
                1.0963765863613892e-09
Epoch n°43000:
                9.70507006996731e-10
Epoch n°44000:
                9.060656007673109e-10
Epoch n°45000:
                8.261451947135163e-10
Epoch n°46000:
                7.673061995049718e-10
Epoch n°47000:
                1.4628239085135382e-09
                6.666410260233888e-10
Epoch n°48000:
Epoch n°49000:
                6.207587188713992e-10
Epoch n°50000:
                1.8636584057964905e-09
```

12 Loss function plot

```
fig, ax = matplotlib.pyplot.subplots(1, 1)
fig.set_size_inches(18, 8.0)
__ = ax.plot(numpy.log10(loss_history))
xlabel = ax.set_xlabel(r'${\rm Epoch}$')
ylabel = ax.set_ylabel(r'$\log_{10}{\rm (loss)}$')
title = ax.set_title(r'${\rm Training}$')
ax.legend(['loss'])
```

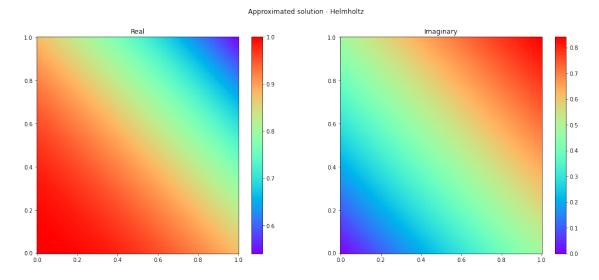


13 Load best params of the training

```
[11]: params = pickle.load(open("./Checkpoints/params_helmholtz", "rb"))
```

14 Approximated solution plot

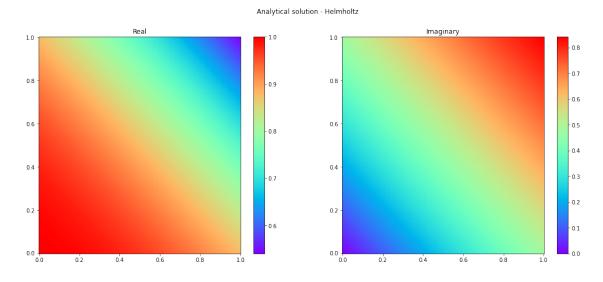
Plotting: 200 out of 200



15 Analytical solution plot

```
fig, ax = matplotlib.pyplot.subplots(1,2)
fig.set_size_inches(18, 7.2)
title = fig.suptitle('Analytical solution - Helmholtz')
for i in range(npoints):
   print("Plotting: {} out of {}".format(i+1, npoints), end='\r')
   real_values[i,:] = jax.numpy.real(functools.
 →partial(analytical_solution)(x[i,:], y[i,:]))
    imag_values[i,:] = jax.numpy.imag(functools.
 →partial(analytical_solution)(x[i,:], y[i,:]))
title = ax[0].set_title('Real')
graph = ax[0].pcolormesh(x, y, real_values, cmap = 'rainbow')
matplotlib.pyplot.colorbar(graph, ax=ax[0])
title = ax[1].set_title('Imaginary')
graph = ax[1].pcolormesh(x, y, imag_values, cmap = 'rainbow')
matplotlib.pyplot.colorbar(graph, ax=ax[1])
matplotlib.pyplot.savefig('./Images/analytical_helmholtz.png', facecolor = u
 ⇔'white', bbox_inches = 'tight')
matplotlib.pyplot.show()
```

Plotting: 200 out of 200



16 Squared error plot

```
[15]: npoints = 200
      values = numpy.zeros((npoints, npoints))
      x, y = numpy.meshgrid(numpy.linspace(parameters['domain_bounds'][0,0],_
       ⇒parameters['domain bounds'][0,1], npoints), numpy.
       ار, اinspace(parameters['domain_bounds'][1,0], parameters['domain_bounds'][1,1], المالية
       ⇔npoints))
      fig, ax = matplotlib.pyplot.subplots()
      fig.set_size_inches(18, 8.0)
      title = ax.set_title('Squared error - Helmholtz')
      for i in range(npoints):
          print("Plotting: {} out of {}".format(i+1, npoints), end='\r')
          real_squared_error = (jax.numpy.real(functools.partial(solver.
       ⇒spatial_solution2d, params)(x[i,:], y[i,:])) - jax.numpy.real(functools.
       →partial(analytical_solution)(x[i,:], y[i,:])))**2
          imag_squared_error = (jax.numpy.imag(functools.partial(solver.
       ⇒spatial_solution2d, params)(x[i,:], y[i,:])) - jax.numpy.imag(functools.
       →partial(analytical_solution)(x[i,:], y[i,:])))**2
          values[i,:] = real_squared_error + imag_squared_error
      print("MSE: ", numpy.mean(values.flatten()))
      graph = matplotlib.pyplot.pcolormesh(x, y, values, cmap = 'rainbow')
      matplotlib.pyplot.colorbar()
      matplotlib.pyplot.savefig('./Images/squared error_helmholtz.png', facecolor = __

    'white', bbox_inches = 'tight')

      matplotlib.pyplot.show()
```

MSE: 2.007965818461194e-14

