Contents

1	Main function	1
2	Neuralnet initialize	9
3	Xavier Initialization	10
4	Neuralnet code	11
5	Supervised neuralnet	12
6	Unsupervised neuralnet	13
7	Callback	16
8	Adam optimizer	17
9	BGFS Optimizer	19
10	Predict	21

1 Main function

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:54:01 2020
5 @author: nastavirs
8 import tensorflow as tf
9 import numpy as np
10 import time
import scipy.io
12 np.random.seed(1234)
tf.set_random_seed(1234)
14 class NSPINN:
15
      # notational conventions
      # _tf: placeholders for input/output data and points used to
16
      regress the equations
      # _pred: output of neural network
# _data: input-output data
17
      # _star: preditions
19
20
      from init_NN import initialize_NN
      from Xavi_init import xavier_init
21
22
      from NN import neural_net
      from Sup_NN import net_NS
23
      from Unsup_NN import net_f_NS
24
      from Callback import callback
      from Adam_train import Adam_train
26
from BGFS_train import BFGS_train
```

```
from predict import predict
28
      def __init__(self, xi, yi, zi, ti, ui, vi, wi, xb, yb, zb, tb,
      ub, vb, wb, x, y, z, t, layers):
           xyzt_i = np.concatenate([xi, yi, zi, ti], 1)
30
           xyzt_b = np.concatenate([xb, yb, zb, tb], 1)
31
           xyzt = np.concatenate([x, y, z, t], 1)
32
33
           self.lowb = xyzt_b.min(0)
34
           self.upb = xyzt_b.max(0)
35
36
           self.xyzt_i = xyzt_i
37
           self.xyzt_b = xyzt_b
38
           self.xyzt = xyzt
39
40
           self.xi = xyzt_i[:, 0:1]
41
           self.yi = xyzt_i[:, 1:2]
42
           self.zi = xyzt_i[:, 2:3]
43
           self.ti = xyzt_i[:, 3:4]
44
45
           self.xb = xyzt_b[:, 0:1]
46
           self.yb = xyzt_b[:, 1:2]
47
           self.zb = xyzt_b[:, 2:3]
48
           self.tb = xyzt_b[:, 3:4]
49
50
           self.x = xyzt[:, 0:1]
51
52
           self.y = xyzt[:, 1:2]
           self.z = xyzt[:, 2:3]
53
           self.t = xyzt[:, 3:4]
54
55
           self.ui = ui
56
57
           self.vi = vi
           self.wi = wi
58
59
           self.ub = ub
60
           self.vb = vb
61
62
           self.wb = wb
63
64
           self.layers = layers
65
66
           self.weights, self.biases = self.initialize_NN(layers)
67
           self.learning_rate = tf.placeholder(tf.float32, shape=[])
68
69
           self.sess = tf.Session(config=tf.ConfigProto(
70
       allow_soft_placement=True,
71
      log_device_placement=True))
72
           self.x_ini_tf = tf.placeholder(tf.float32, shape=[None,
73
       self.xi.shape[1]])
           self.y_ini_tf = tf.placeholder(tf.float32, shape=[None,
       self.yi.shape[1]])
           self.z_ini_tf = tf.placeholder(tf.float32, shape=[None,
       self.zi.shape[1]])
           self.t_ini_tf = tf.placeholder(tf.float32, shape=[None,
       self.ti.shape[1]])
          self.u_ini_tf = tf.placeholder(tf.float32, shape=[None,
```

```
self.ui.shape[1]])
                        self.v_ini_tf = tf.placeholder(tf.float32, shape=[None,
               self.vi.shape[1]])
                        self.w_ini_tf = tf.placeholder(tf.float32, shape=[None,
               self.wi.shape[1]])
 80
                        self.x_boundary_tf = tf.placeholder(tf.float32, shape=[None
               , self.xb.shape[1]])
                        self.y_boundary_tf = tf.placeholder(tf.float32, shape=[None
                  self.yb.shape[1]])
                        self.z_boundary_tf = tf.placeholder(tf.float32, shape=[None
 83
                , self.zb.shape[1]])
                        self.t_boundary_tf = tf.placeholder(tf.float32, shape=[None
 84
                , self.tb.shape[1]])
                        self.u_boundary_tf = tf.placeholder(tf.float32, shape=[None
 85
                , self.ub.shape[1]])
                        self.v_boundary_tf = tf.placeholder(tf.float32, shape=[None
 86
                , self.vb.shape[1]])
                        self.w_boundary_tf = tf.placeholder(tf.float32, shape=[None
                , self.wb.shape[1]])
                        self.x_tf = tf.placeholder(tf.float32, shape=[None, self.x.
 89
               shape [1]])
                        self.y_tf = tf.placeholder(tf.float32, shape=[None, self.y.
 90
               shape [1]])
                        self.z_tf = tf.placeholder(tf.float32, shape=[None, self.z.
               shape[1]])
 92
                       self.t_tf = tf.placeholder(tf.float32, shape=[None, self.t.
               shape [1]])
                        self.u_ini_pred, self.v_ini_pred, self.w_ini_pred, self.
               p_ini_pred = \
                                 self.net_NS(self.x_ini_tf, self.y_ini_tf, self.z_ini_tf
                , self.t_ini_tf)
                        self.u_boundary_pred, self.v_boundary_pred, self.
 96
               w_boundary_pred, self.p_boundary_pred = \
                                 self.net_NS(self.x_boundary_tf, self.y_boundary_tf,
 97
               self.z_boundary_tf, self.t_boundary_tf)
 98
                        \verb|self.u_pred|, \verb|self.v_pred|, \verb|self.w_pred|, \verb|self.p_pred|, \verb|self.w_pred|, \end{|self.w_pred}, \end
               f_u_pred, self.f_v_pred, self.f_w_pred, self.f_e_pred = \
                                 self.net_f_NS(self.x_tf, self.y_tf, self.z_tf, self.
               t_tf)
100
                        alpha = 100
                        beta = 100
103
                        self.loss = alpha * tf.reduce_mean(tf.square(self.u_ini_tf
104
               - self.u_ini_pred)) + \
                                                   alpha * tf.reduce_mean(tf.square(self.v_ini_tf
               - self.v_ini_pred)) + \
                                                  alpha * tf.reduce_mean(tf.square(self.w_ini_tf
106
               - self.w_ini_pred)) + \
                                                  beta * tf.reduce_mean(tf.square(self.
               u_boundary_tf - self.u_boundary_pred)) + \
108
                                                  beta * tf.reduce_mean(tf.square(self.
               v_boundary_tf - self.v_boundary_pred)) + \
                                                  beta * tf.reduce_mean(tf.square(self.
109
```

```
w_boundary_tf - self.w_boundary_pred)) + \
                        tf.reduce_mean(tf.square(self.f_u_pred)) + \
                        tf.reduce_mean(tf.square(self.f_v_pred)) + \
111
                        tf.reduce_mean(tf.square(self.f_w_pred)) + \
112
                        tf.reduce_mean(tf.square(self.f_e_pred))
113
114
           self.optimizer = tf.contrib.opt.ScipyOptimizerInterface(
       self.loss,
       method='L-BFGS-B',
       options={'maxiter': 50000,
118
             'maxfun': 50000,
119
             'maxcor': 50,
             'maxls': 50,
121
             'ftol': 1.0 * np.finfo(float).eps})
           self.optimizer_Adam = tf.train.AdamOptimizer(self.
123
       learning_rate)
124
           self.train_op_Adam = self.optimizer_Adam.minimize(self.loss
125
           init = tf.global_variables_initializer()
126
           self.sess.run(init)
127
128
129
130
  if __name__ == "__main__":
131
132
       N \text{ train} = 10000
134
135
       layers = [4, 10, 10, 10, 10, 10, 10, 10, 10, 10, 4]
136
137
       def data_generate(x, y, z, t):
138
           a, d = 1, 1
139
           u = -a * (np.exp(a * x) * np.sin(a * y + d * z) + np.exp(a
140
        * z) * np.cos(a * x + d * y)) * np.exp(- d * d * t)
           v = -a * (np.exp(a * y) * np.sin(a * z + d * x) + np.exp(a
141
        * x) * np.cos(a * y + d * z)) * np.exp(- d * d * t)
                 a * (np.exp(a * z) * np.sin(a * x + d * y) + np.exp(a
142
        * y) * np.cos(a * z + d * x)) * np.exp(- d * d * t)
           p = -0.5 * a * a * (np.exp(2 * a * x) + np.exp(2 * a * y)
143
       + np.exp(2 * a * z) +
                                 2 * np.sin(a * x + d * y) * np.cos(a *
144
        z + d * x) * np.exp(a * (y + z)) +
                                 2 * np.sin(a * y + d * z) * np.cos(a *
145
        x + d * y) * np.exp(a * (z + x)) +
146
                                 2 * np.sin(a * z + d * x) * np.cos(a *
        y + d * z) * np.exp(a * (x + y))) * np.exp(
147
                -2 * d * d * t)
148
          return u, v, w, p
149
```

```
150
       xdata = np.linspace(-1, 1, 31)
       ydata = np.linspace(-1, 1, 31)
152
       zdata = np.linspace(-1, 1, 31)
153
       tdata = np.linspace(0, 1, 11)
154
       b0 = np.array([-1] * 900)
155
156
       b1 = np.array([1] * 900)
157
      #boundary values
158
159
       xr1 = np.tile(xdata[0:30], 30)
       yr1 = np.tile(ydata[0:30], 30)
160
161
       zr1 = np.tile(zdata[0:30], 30)
       xr2 = np.tile(xdata[1:31], 30)
162
       yr2 = np.tile(ydata[1:31], 30)
       zc2 = np.tile(zdata[1:31], 30)
164
165
166
       xc1 = xdata[0:30].repeat(30)
       yc1 = ydata[0:30].repeat(30)
167
       zc1 = zdata[0:30].repeat(30)
168
       xc2 = xdata[1:31].repeat(30)
169
       yc2 = ydata[1:31].repeat(30)
       zr1 = zdata[1:31].repeat(30)
       trainx = np.concatenate([b1, b0, xr2, xr1, xr2, xr1], 0).repeat
173
       (tdata.shape[0])
       trainy = np.concatenate([yr1, yr2, b1, b0, yc2, yc1], 0).repeat
174
       (tdata.shape[0])
       trainz = np.concatenate([zc1, zr1, zc1, zr1, b1, b0], 0).repeat
       (tdata.shape[0])
       traint = np.tile(tdata, 5400)
176
177
       trainub, trainvb, trainwb, trainpb = data_generate(trainx,
178
       trainy, trainz, traint)
179
       xb_train = trainx.reshape(trainx.shape[0], 1)
180
       yb_train = trainx.reshape(trainy.shape[0], 1)
181
       zb_train = trainx.reshape(trainz.shape[0], 1)
182
183
       tb_train = trainx.reshape(traint.shape[0], 1)
       ub_train = trainx.reshape(trainub.shape[0], 1)
184
       vb_train = trainx.reshape(trainvb.shape[0], 1)
185
       wb_train = trainx.reshape(trainwb.shape[0], 1)
186
       pb_train = trainx.reshape(trainpb.shape[0], 1)
187
188
       # inital values
189
       x_0 = np.tile(xdata, 31 * 31)
190
       y_0 = np.tile(ydata.repeat(31), 31)
191
       z_0 = zdata.repeat(31 * 31)
193
       t_0 = np.array([0] * x_0.shape[0])
194
       u_0, v_0, w_0, p_0 = data_generate(x_0, y_0, z_0, t_0)
195
196
       ui_train = u_0.reshape(u_0.shape[0], 1)
197
       vi_train = v_0.reshape(v_0.shape[0], 1)
198
       wi_train = w_0.reshape(w_0.shape[0], 1)
200
       p0\_train = p\_0.reshape(p\_0.shape[0], 1)
       xi_train = x_0.reshape(x_0.shape[0], 1)
201
       yi_train = y_0.reshape(y_0.shape[0], 1)
202
```

```
zi_train = z_0.reshape(z_0.shape[0], 1)
203
204
       ti_train = t_0.reshape(t_0.shape[0], 1)
205
       # xyzt data
206
       xx = np.random.randint(31, size=10000) / 15 - 1
207
       yy = np.random.randint(31, size=10000) / 15 - 1
208
       zz = np.random.randint(31, size=10000) / 15 - 1
209
       tt = np.random.randint(11, size=10000) / 10
210
211
212
       uu, vv, ww, pp = data_generate(xx, yy, zz, tt)
213
214
       x_train = xx.reshape(xx.shape[0], 1)
       y_train = yy.reshape(yy.shape[0], 1)
215
216
       z_train = zz.reshape(zz.shape[0], 1)
       t_train = tt.reshape(tt.shape[0], 1)
217
218
219
       model = NSPINN(xi_train, yi_train, zi_train, ti_train,
                         ui_train, vi_train, wi_train,
220
221
                         xb_train, yb_train, zb_train, tb_train,
                         ub_train, vb_train, wb_train,
222
                         x_train, y_train, z_train, t_train, layers)
223
       model.Adam_train(5000, 1e-3)
225
226
       model.Adam_train(5000, 1e-4)
       model.Adam_train(50000, 1e-5)
227
       model.Adam_train(50000, 1e-6)
228
       model.BFGS_train()
229
230
       x_star = (np.random.rand(1000, 1) - 1 / 2) * 2
231
       y_star = (np.random.rand(1000, 1) - 1 / 2) * 2
232
       z_{star} = (np.random.rand(1000, 1) - 1 / 2) * 2
       t_star = np.random.randint(11, size=(100, 1)) / 10
234
235
236
       u_star, v_star, w_star, p_star = data_generate(x_star, y_star,
       z_star, t_star)
237
238
239
       u_pred, v_pred, w_pred, p_pred = model.predict(x_star, y_star,
       z_star, t_star)
240
241
       # Error
       error_u = np.linalg.norm(u_star - u_pred, 2) / np.linalg.norm(
242
       u_star, 2)
       error_v = np.linalg.norm(v_star - v_pred, 2) / np.linalg.norm(
243
       v_star, 2)
244
       error_w = np.linalg.norm(w_star - w_pred, 2) / np.linalg.norm(
       w_star, 2)
       error_p = np.linalg.norm(p_star - p_pred, 2) / np.linalg.norm(
       p_star, 2)
       print('Error u: %e' % error_u)
247
       print('Error v: %e' % error_v)
248
       print('Error v: %e' % error_w)
249
       print('Error p: %e' % error_p)
250
251
       scipy.io.savemat('../NS3D_beltrami_%s.mat' %(time.strftime('%d_
252
       %m_%Y')),
```

```
{'U_pred':u_pred, 'V_pred':v_pred, 'W_pred':
     w_pred, 'P_pred':p_pred})
                                     Listing 1: nain
Line 8-11: Import tensorflow, numpy, time, scipy.io to load, calculate and save data.
Line : Initialize seed for pseudo random number generator.
Line 14 : Define class NSPINN to initialize variables.
Line 20-28: Import necessary functions into the class for solver calculations.
Line 29 : Define function _init_ to initialize tensor flow variables with initial, boundary and
Line 30-32 : Concatenate values to create a single array for data manipulation.
Line 34-35 : Assign boundary values.
Line 37-64: Assign input dataset values to local class variables.
Line 66: Initialize weight and biases according to the no of layers.
Line 68: Initialize tensor variable for learning rate.
Line 70 : Initialize session variable.
Line 73-92: Initialize tensor variables for class variables.
Line 94-100 : Calculate pred values from the data set using neuralnet.
Line 104 : Define loss function.
Line 115-124 : Define Optimizer wrapper and input loss parameter.
Line 126-127: Initialize session for calculation.
Line 131 : Define main function.
Line 133 : No of training loops.
Line 135 : No of layers.
Line 137 : Define function data generate to create dataset for beltrami flow.
Line 151-156 : input Dataset.
Line 159-178 : Data manipulation to generate more points.
Line 180-187: Assign boundary values to variables.
Line 190-195 : Data manipulation for initial values.
Line 197-204: Assign initial values to variables.
Line 207-212 : Data manipulation for dataset values.
Line 214-217 : Assign dataset values to variables.
Line 219: Pass initial, boundary, and dataset values to model to predict values.
Line 225-229: Train the model for the given iterations and learning rate.
Line 231-234 : Predict values for x,y,z,t.
```

dataset values.

Line 236 : Generate dataset with the predicted values.

Line 239 : Generated values from neural network.

Line 242-245 : Calculate error value.

Line 247-250 : Print error values.

Line 252: Save data as an .mat file for output.

2 Neuralnet initialize

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:54:44 2020
5 @author: nastavirs
7 import tensorflow as tf
8 import numpy as np
p np.random.seed(1234)
tf.set_random_seed(1234)
def initialize_NN(self, layers):
          weights = []
12
          biases = []
          num_layers = len(layers)
14
          for l in range(0, num_layers - 1):
15
              W = self.xavier_init(size=[layers[1], layers[1 + 1]])
16
              b = tf.Variable(tf.zeros([1, layers[1 + 1]], dtype=tf.
      float32), dtype=tf.float32)
              weights.append(W)
18
19
              biases.append(b)
          return weights, biases
20
```

Listing 2: Neural net

Line 7-8: import numpy and tensorflow for calculations

Line 9 : initialize_NN function is used to initialize and return weights and biases of a NN with layers size and solver type as arguments

Line 10-11 : initialize empty list for weights and biases

Line 12 : assign the size of the layers variable to num_layers by using the len function

Line 13: loop around from to layers-1 to calculate weights and biases for each layer.

Line 14: xavier initialize the weights value by passing size as a list layer 1, layer 1+1

Line 15 : assign a tensorflow variable with zero matrix of size 1, layers 1+i to the variable b

Line 16-17 : append the values created during each loop to the list weights and biases

Line 18: return weights and biases

3 Xavier Initialization

```
# -*- coding: utf-8 -*-
2 """

Created on Sun Nov 8 14:54:56 2020

duthor: nastavirs
6 """

import tensorflow as tf
import numpy as np
np.random.seed(1234)

tf.set_random_seed(1234)

def xavier_init(self, size):
    in_dim = size[0]
    out_dim = size[1]
    xavier_stddev = np.sqrt(2 / (in_dim + out_dim))
    return tf.Variable(tf.truncated_normal([in_dim, out_dim], stddev=xavier_stddev), dtype=tf.float32)
```

Listing 3: Xavier init

Line 11: initialize the xavier_init function definition with arguments class and size

Line 12 : in_dim is the number of input nodes into each output and is assigned 1st value from arg size

 $\hbox{Line 13: out_dim is the number of output nodes for each input and is assigned 2nd value from arg size} \\$

Line 14: calculate the standard deviation.

Line 15: return a tensorflow variable with from a truncated normal distribution

4 Neuralnet code

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:55:07 2020
5 @author: nastavirs
7 import tensorflow as tf
8 import numpy as np
p np.random.seed(1234)
tf.set_random_seed(1234)
def neural_net(self, X, weights, biases):
          num_layers = len(weights) + 1
12
          H = 2.0 * (X - self.lowb) / (self.upb - self.lowb) - 1.0
14
          for 1 in range(0, num_layers - 2):
15
              W = weights[1]
16
              b = biases[1]
17
              H = tf.tanh(tf.add(tf.matmul(H, W), b))
          W = weights[-1]
19
          b = biases[-1]
20
          Y = tf.add(tf.matmul(H, W), b)
21
          return Y
22
```

Listing 4: NN

```
Line 7-8: import numpy and tensorflow for calculations

Line 9: define function neural net with arguments, class, data set X, weights and biases calculated earlier.

Line 10: assign the length of weights + 1 to the variable num_layers

Line 12: the right hand size of the equation represents the assumed hypothesis function/representation

Line 13: for loop to loop around layers from 0 to n-2 layers

Line 14-15: initialize and assign Weights and biases of layer 1 to W and b

Line 16: we use forward propagation to calculate the H, where we first matrix multiply hypothesis function and weights and add then add the biases. finally pass this to the tanh activation fuction tanh(H*W+b)

Line 17-19: finally we do the same step for the final output layer

Line 20: return Y
```

5 Supervised neuralnet

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:55:15 2020
5 @author: nastavirs
7 import tensorflow as tf
8 import numpy as np
p np.random.seed(1234)
tf.set_random_seed(1234)
def net_NS(self, x, y, z, t):
12
           u_v_w_p = self.neural_net(tf.concat([x, y, z, t], 1), self.
      weights, self.biases)
           u = u_v_w_p[:, 0:1]
v = u_v_w_p[:, 1:2]
14
15
           w = u_v_w_p[:, 2:3]
16
           p = u_v_w_p[:, 3:4]
17
           return u, v, w, p
18
```

Listing 5: supervised NN

```
Line 11 : Define function net_NS with class,x,y,z,t as variables.

Line 13 : Concat x,y,z,t and pass it to the neural net as an argument.

Line 14-17 : assign values from the results of the neural net to variables.

Line 18 : Return u,v,w,p
```

6 Unsupervised neuralnet

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:55:30 2020
5 @author: nastavirs
7 import tensorflow as tf
8 import numpy as np
9 np.random.seed(1234)
tf.set_random_seed(1234)
def net_f_NS(self, x, y, z, t):
12
           Re = 1
13
14
           u_v_w_p = self.neural_net(tf.concat([x, y, z, t], 1), self.
15
      weights, self.biases)
          u = u_v_w_p[:, 0:1]
16
17
          v = u_v_w_p[:, 1:2]
          w = u_v_w_p[:, 2:3]

p = u_v_w_p[:, 3:4]
18
19
20
          u_t = tf.gradients(u, t)[0]
21
           u_x = tf.gradients(u, x)[0]
22
          u_y = tf.gradients(u, y)[0]
23
24
           u_z = tf.gradients(u, z)[0]
          u_xx = tf.gradients(u_x, x)[0]
25
           u_yy = tf.gradients(u_y, y)[0]
26
          u_zz = tf.gradients(u_z, z)[0]
27
28
           v_t = tf.gradients(v, t)[0]
29
          v_x = tf.gradients(v, x)[0]
30
          v_y = tf.gradients(v, y)[0]
31
          v_z = tf.gradients(v, z)[0]
32
          v_xx = tf.gradients(v_x, x)[0]
33
          v_yy = tf.gradients(v_y, y)[0]
34
          v_zz = tf.gradients(v_z, z)[0]
35
36
37
          w_t = tf.gradients(w, t)[0]
           w_x = tf.gradients(w, x)[0]
38
           w_y = tf.gradients(w, y)[0]
39
          w_z = tf.gradients(w, z)[0]
40
41
          w_x = tf.gradients(w_x, x)[0]
          w_yy = tf.gradients(w_y, y)[0]
42
43
           w_zz = tf.gradients(w_z, z)[0]
44
          p_x = tf.gradients(p, x)[0]
45
46
           p_y = tf.gradients(p, y)[0]
47
          p_z = tf.gradients(p, z)[0]
          f_u = u_t + (u * u_x + v * u_y + w * u_z) + p_x - 1/Re * (
49
      u_xx + u_yy + u_zz
          f_v = v_t + (u * v_x + v * v_y + w * v_z) + p_y - 1/Re * (
50
       v_x x + v_y y + v_z z
          f_w = w_t + (u * w_x + v * w_y + w * w_z) + p_z - 1/Re * (
      w_x + w_y + w_z
```

```
return u, v, w, p, f_u, f_v, f_w, f_e
                               Listing 6: unsupervised NN
Line 7-8: import numpy and tensorflow for calculations
Line 9 : define net_f_NS function with arguments class x,y,z,t
Line 11 : Initialize Reynolds number.
Line 13 : define variable u_v_w_p as the return of the function neuralnet with tensorflow variable
          which is the result of concatenation of x,y and t and 1 implies along column axis, weights,
          biases which are passed as arguments for the class
Line 14-17 : slice u_v_p columns wise and assign it to u,v,w,p.
Line 19 : calculating the gradient of u wrt t and assign it to u_t
Line 20 : calculating the gradient of u wrt x and assign it to u\_x
Line 21 : calculating the gradient of u wrt y and assign it to u\_y
Line 22 : calculating the gradient of u wrt z and assign it to u\_z
Line 23 : calculating the gradient of u_x wrt x and assign it to u_xx
Line 24 : calculating the gradient of u_y wrt y and assign it to u_y
Line 25 : calculating the gradient of u_y wrt y and assign it to u_y
Line 27 : calculating the gradient of v wrt t and assign it to v_t
Line 28 : calculating the gradient of v wrt x and assign it to v_x
Line 29 : calculating the gradient of v wrt y and assign it to v_y
Line 30 : calculating the gradient of v wrt z and assign it to v_z
Line 31 : calculating the gradient of v_x wrt x and assign it to v_xx
Line 32: calculating the gradient of v_y wrt y and assign it to v_yy
Line 33 : calculating the gradient of v_z wrt z and assign it to v_zz
Line 35 : calculating the gradient of w wrt t and assign it to w_t
Line 36 : calculating the gradient of w wrt x and assign it to w_x
Line 37 : calculating the gradient of w wrt y and assign it to w_y
Line 38 : calculating the gradient of w wrt z and assign it to \text{w\_z}
Line 39 : calculating the gradient of w_x wrt x and assign it to w_x
Line 40 : calculating the gradient of w_y wrt y and assign it to w_y
Line 41 : calculating the gradient of w_z wrt z and assign it to w_zz
Line 43 : calculating the gradient of p wrt x and assign it to p_x
Line 44: calculating the gradient of p wrt y and assign it to p_y
Line 45: calculating the gradient of p wrt z and assign it to p_z
Line 47: calculate the nonlinear partial differentiation equation (N-S) f as
            u\_t + (u*u\_x + v*u\_y + w*u\_z) + p\_x - 1/Re*(u\_xx + u\_yy + u\_zz) \ \ and \ \ assign \ \ it \ \ to \ \ variable \ f\_u = 1/Re*(u\_xx + u\_yy + u\_zz)
```

 $f_e = u_x + v_y + w_z$

52

```
Line 48 : calculate the nonlinear partial differentiation equation (N-S) f as v\_t+(u*v\_x+v*v\_y+w*v\_z)+p\_y-1/Re*(v\_xx+v\_yy+v\_zz) \ and \ assign \ it \ to \ variable \ f\_v
```

- Line 50 : calculate the nonlinear partial differentiation equation (N-S) f as $(u_x+v_y+w_z)$ and assign it ti variable f_e
- Line 52 : returns u,v,w,p,f_u,f_v,f_w.f_e as the result of function net_NS

7 Callback

Listing 7: callback

```
Line 7-8: import numpy for calculations  \mbox{Line 9: define function callback with parameter class,loss} \\ \mbox{Line 10: print loss.}
```

8 Adam optimizer

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:56:19 2020
5 @author: nastavirs
7 import tensorflow as tf
8 import numpy as np
9 import time
np.random.seed(1234)
tf.set_random_seed(1234)
def Adam_train(self, nIter=5000, learning_rate=1e-3):
13
           tf_dict = {self.x_ini_tf: self.xi, self.y_ini_tf: self.yi,
14
      self.z_ini_tf: self.zi, self.t_ini_tf: self.ti,
                      self.u_ini_tf: self.ui, self.v_ini_tf: self.vi,
      self.w_ini_tf: self.wi,
                      self.x_boundary_tf: self.xb, self.y_boundary_tf:
16
       self.yb, self.z_boundary_tf: self.zb,
                      self.t_boundary_tf: self.tb, self.u_boundary_tf:
       self.ub, self.v_boundary_tf: self.vb,
                      self.w_boundary_tf: self.wb, self.x_tf: self.x,
      self.y_tf: self.y, self.z_tf: self.z,
                      self.t_tf: self.t, self.learning_rate:
19
      learning_rate}
20
          start_time = time.time()
21
          for it in range(nIter):
22
               self.sess.run(self.train_op_Adam, tf_dict)
23
24
25
               if it % 10 == 0:
26
                   elapsed = time.time() - start_time
27
28
                  loss_value = self.sess.run(self.loss, tf_dict)
                  print('It: %d, Loss: %.3e, Time: %.2f' %
29
                         (it, loss_value, elapsed))
30
                   start_time = time.time()
31
33
           self.optimizer.minimize(self.sess,
                                   feed_dict=tf_dict,
34
                                   fetches=[self.loss],
35
                                   loss_callback=self.callback)
```

Listing 8: adam

```
Line 7,8,9: Import tensorflow, numpy and time for run time.

Line 10-11: Set seed for pseudo random number generator.

Line 12: Define function adam train with input variables of class, no of Iterations and learning rate

Line 14: Initiate tf.dict with all the required variables

Line 21: Initiate variable start.time to start time counter.

Line 22: Start for loop to loop for nIter.

Line 23: Run session to initialize tensor variables
```

Line 26-31: Print Loss and time for every ten iterations

Line 33: Use Wrapper to minimize the loss function in $\mathsf{tf.dict}$

9 BGFS Optimizer

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:56:32 2020
5 @author: nastavirs
7 import tensorflow as tf
8 import numpy as np
9 import time
np.random.seed(1234)
tf.set_random_seed(1234)
def BFGS_train(self):
           tf_dict = {self.x_ini_tf: self.xi, self.y_ini_tf: self.yi,
14
      self.z_ini_tf: self.zi, self.t_ini_tf: self.ti,
                      self.u_ini_tf: self.ui, self.v_ini_tf: self.vi,
      self.w_ini_tf: self.wi,
                      self.x_boundary_tf: self.xb, self.y_boundary_tf:
       self.yb, self.z_boundary_tf: self.zb,
                      self.t_boundary_tf: self.tb, self.u_boundary_tf:
       self.ub, self.v_boundary_tf: self.vb,
                      self.w_boundary_tf: self.wb, self.x_tf: self.x,
18
      self.y_tf: self.y, self.z_tf: self.z,
                      self.t_tf: self.t}
19
20
           self.optimizer.minimize(self.sess,
22
                                   feed_dict=tf_dict,
                                   fetches=[self.loss],
23
                                   loss_callback=self.callback)
24
25
      # mini-batch to be implemented
26
      # def train(self, epoch=10, nIter=150, learning_rate=1e-3):
27
28
            for ep in range(epoch):
      #
29
30
      #
                 batch_size1 = len(self.x0) // nIter
      #
31
                batch_size2 = len(self.xb) // nIter
32
      #
      #
                batch_size3 = len(self.x) // nIter
33
34
                arr1 = np.arange(batch_size1 * nIter)
35
      #
                arr2 = np.arange(batch_size2 * nIter)
36
37
                arr3 = np.arange(batch_size3 * nIter)
38
                permu1 = np.random.permutation(arr1).reshape((nIter,
      batch_size1))
                permu2 = np.random.permutation(arr2).reshape((nIter,
40
      batch_size2))
                permu3 = np.random.permutation(arr3).reshape((nIter,
41
      batch_size3))
42
                start_time = time.time()
43
      #
                for it in range(nIter):
44
      #
                     tf_dict = {self.x_ini_tf: self.x0[permu1[it, :],
45
      :],
                               self.y_ini_tf: self.y0[permu1[it, :],
46
```

```
:],
                                  self.z_ini_tf: self.z0[permu1[it, :],
       :],
                                  self.t_ini_tf: self.t0[permu1[it, :],
       :],
       #
                                  self.u_ini_tf: self.u0[permu1[it, :],
49
       :],
                                  self.v_ini_tf: self.v0[permu1[it, :],
       #
       :],
                                  self.w_ini_tf: self.w0[permu1[it, :],
       #
       :],
                                  self.x_boundary_tf: self.xb[permu2[it,
        :], :],
                                  self.y_boundary_tf: self.yb[permu2[it,
       #
53
        :], :],
                                  self.z_boundary_tf: self.zb[permu2[it,
54
       :], :],
                                  self.t_boundary_tf: self.tb[permu2[it,
        :], :],
       #
                                  self.u_boundary_tf: self.ub[permu2[it,
56
       :], :],
                                  self.v_boundary_tf: self.vb[permu2[it,
        :], :],
                                  self.w_boundary_tf: self.wb[permu2[it,
58
        :], :],
                                  self.x_tf: self.x[permu3[it, :], :],
       #
59
                                  self.y_tf: self.y[permu3[it, :], :],
       #
60
       #
                                  self.z_tf: self.z[permu3[it, :], :],
61
                                  self.t_tf: self.t[permu3[it, :], :],
       #
62
                                  self.learning_rate: learning_rate}
       #
63
64
       #
                      self.sess.run(self.train_op_Adam, tf_dict)
65
       #
66
       #
                      # Print
67
       #
                      if it % 10 == 0:
68
69
       #
                          elapsed = time.time() - start_time
                          loss_value = self.sess.run(self.loss, tf_dict
       #
70
      )
      #
                          print('epoch: %d, It: %d, Loss: %.3e, Time:
71
       %.2f' %
                                 (ep, it, loss_value, elapsed))
73
                          start_time = time.time()
74
       #
       #
             self.optimizer.minimize(self.sess,
75
       #
                                       feed_dict=tf_dict,
76
                                       fetches=[self.loss],
77
       #
                                      loss_callback=self.callback)
78
```

Listing 9: BGFS

learning rate

Line 7,8,9: Import tensorflow, numpy and time for run time.

Line 10-11: Set seed for pseudo random number generator.

Line 12: Define function BGFS train with input variables of class, no of Iterations and

Line 14: Initiate tf.dict with all the required variables

Line 21: Use Wrapper to minimize the loss function in tf.dict

10 Predict

```
# -*- coding: utf-8 -*-
3 Created on Sun Nov 8 14:56:40 2020
5 @author: nastavirs
7 import numpy as np
8 import tensorflow as tf
9 def predictNS(self, x_star, y_star, z_star, t_star):
10
           tf_dict = {self.x_tf: x_star, self.y_tf: y_star, self.z_tf:
11
        z_star, self.t_tf: t_star}
           u_star = self.sess.run(self.u_pred, tf_dict)
13
           v_star = self.sess.run(self.v_pred, tf_dict)
w_star = self.sess.run(self.w_pred, tf_dict)
14
15
           p_star = self.sess.run(self.p_pred, tf_dict)
16
17
           return u_star, v_star, w_star, p_star
18
```

Listing 10: Solver

Line 7-8: import numpy and tensorflow for calculations

Line 9 : define function predict with arguments class and x_star,y_star,z_star,t_star predict values for training

Line 11 : define tensorflow dict with x_tf,y_tf,z_tf,t_tf with corresponding input value.

Line 13-16 : sess.run evaluates and returns values after a session for input parameters u.pred,v_pred,v_pred,p_pred and train_dict is also an input because pred values depends on it, assign it to u_star,v_star,v_star,p_star.

Line 16 : return u_star, v_star,w_star, and p_star for function predict

Matlab Code

```
1
  clear
   close all
2
set(0, 'defaulttextinterpreter', 'latex')
   %load Cylinder3D.mat
   load NS3D_beltrami.mat
fig = figure();
  set(fig,'units','normalized','outerposition',[0 0 1 1])
10
   for num = 100:100 %size(t_star,1)
       disp(num)
11
12
13
       clf
14
       subplot(2,2,1)
15
       plot_isosurface_griddata(x_star, y_star, z_star, U_star(:,num),
16
       '$x$','$y$','$z$','Regressed $u(t,x,y,z)$')
       drawnow()
17
18
19
       subplot (2,2,2)
20
       plot_isosurface_griddata(x_star, y_star, z_star, V_star(:,num),
        '$x$','$y$','$z$','Regressed $v(t,x,y,z)$')
21
       drawnow()
22
23
       subplot(2,2,3)
       plot_isosurface_griddata(x_star, y_star, z_star, W_star(:,num),
24
        '$x$','$y$','$z$','Regressed $w(t,x,y,z)$')
       drawnow()
25
26
27
       subplot (2,2,4)
       plot_isosurface_griddata(x_star, y_star, z_star, P_star(:,num),
28
        '$x$','$y$','$z$','Regressed $p(t,x,y,z)$')
       drawnow()
29
30
       %%%
31
32
33
   end
34
   % addpath ~/export_fig
35
36  % export_fig ./Cylinder_3D_results.png -r300
```

Listing 11: plotting

```
12
   nn = 100;
x = linspace(x_1, x_r, nn);
y = linspace(y_l, y_r, nn);
z = linspace(z_l, z_r, nn);
17
   [Xplot, Yplot, Zplot] = meshgrid(x,y,z);
19
   Uplot = griddata(x_star,y_star,z_star, u_star, Xplot,Yplot,Zplot);
^{21}
   idx = linspace(min(u_star),max(u_star),5);
22
isosurface(Xplot, Yplot, Zplot, Uplot, idx(2));
25 hold all
isosurface(Xplot, Yplot, Zplot, Uplot, idx(3));
   hold all
   isosurface(Xplot, Yplot, Zplot, Uplot, idx(4));
29 zlim([idx(1), idx(5)])
30 view(3)
31 xlabel(xlab);
32
   ylabel(ylab);
33 zlabel(zlab);
34 title(tit);
35
36 axis tight
37
   axis equal
38 colormap jet
39 colorbar
40 alpha(0.7)
set(gca,'FontSize',20);
set(gcf, 'Color', 'w');
```

Listing 12: calculate Isosurface