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#______
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#The files contain code and data associated with the paper titled
#"A Deep Learning Approach to Estimate Stress Distribution: A Fast and
#Accurate Surrogate of Finite Element Analysis".
#The paper is authored by Liang Liang, Minliang Liu, Caitlin Martin,
#and Wei Sun, and published at Journal of The Royal Society Interface, 2018.
#The file list: ShapeData.mat, StressData.mat, DLStress.py, im2patch.m,
#UnsupervisedLearning.m, ReadMeshFromVTKFile.m, ReadPolygonMeshFromVTKFile.m,
#WritePolygonMeshAsVTKFile.m, Visualization.m, TemplateMesh3D.vtk, TemplateMesh2D.vtk.
#Note: *.m and *.py files were converted to pdf files for documentation purpose.
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#INCLUDING, WITHOUT LIMITATION, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS
#FOR A PARTICULAR PURPOSE.
# % %
# go to cmd and follow the instructions to setup matlab python engine
#https://www.mathworks.com/help/matlab/matlab external/install-the-matlab-engine-for-python.html
# 응 응
from keras.models import Sequential
from keras.layers import Dense, Conv2DTranspose
import numpy
from numpy.random import RandomState
import scipy.io as sio
import time
import matlab.engine
#%% Unsupervised Learning is done in Matlab
def UnsupervisedLearning (DataFile, ShapeDataFile, StressDataFile, IdxList train, IdxList test):
idx train mat=matlab.double(list(IdxList train+1)) #+1 to matlab index
idx test mat=matlab.double(list(IdxList test+1))  #+1 to matlab index
DataFlag = eng.UnsupervisedLearning(DataFile, ShapeDataFile, StressDataFile, idx train mat,
   idx test mat)
MatData=sio.loadmat(DataFile)
X=MatData['ShapeCode train']
X=numpy.asmatrix(X)
X=X.transpose()
S=MatData['Stress train']
S=numpy.asmatrix(S)
Y = MatData['Y2n train']
Y = numpy.array([])
Y.resize((len(IdxList train),64))
for k in range(0, len(IdxList train)):
Y[k,:,]=Y [:,:,:,k]
#end
Y=numpy.asmatrix(Y)
X t=MatData['ShapeCode test']
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X t=numpy.asmatrix(X t)
X t=X t.transpose()
S t=MatData['Stress test']
S t=numpy.asmatrix(S t)
Y t = MatData['Y2n test']
Y t = numpy.array([])
Y t.resize((len(IdxList test),64))
for k in range(0, len(IdxList test)):
Y_t[k,:,]=Y_t_[:,:,:,k]
#end
Y t=numpy.asmatrix(Y t)
#
L=MatData['L2']
W1=MatData['W1']
W2=MatData['W2']
. . . . #
Proj=MatData['Proj']
MeanShape=MatData['MeanShape']
. . . . #
return X, X t, Y, Y t, S, S t, L, W1, W2, Proj, MeanShape
#-----
#%% S11/S22/S12: 5000xN, S all=[S11; S22; S12]
def ComputeVonMisesStress all (S all):
N=S all.shape[1]
VM all=numpy.array([])
VM all.resize(5000, N)
S11 all=S all[0:5000,:]
S22 all=S all[5000:10000,:]
S12 all=S all[10000:15000,:]
for n in range (0,N):
for k in range (0, 5000):
S11=S11 all[k,n]
S22=S22 all[k,n]
S12=S12 \text{ all}[k,n]
    VM=S11*S11+S22*S22-S11*S22+3*S12*S12
VM=numpy.sqrt(VM)
VM all[k,n]=VM
#end
#end
return VM all;
#----- A is ground truth, A[:,n] is vector of stress values; B is the reonstructed
version of A
def ComputeError(A, B):
MAE=numpy.zeros(A.shape[1])
NMAE=numpy.zeros(A.shape[1])
for n in range(0, A.shape[1]):
a=A[:,n]
b=B[:,n]
c=numpy.absolute(a-b)
a abs=numpy.absolute(a)
a_max=numpy.max(a_abs[301:4700])
```

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MAE[n]=numpy.mean(c)
NMAE[n]=MAE[n]/a max
#end
return MAE, NMAE
#end
#-----
def ComputeError peak(A, B):
AE=numpy.zeros(A.shape[1])
APE=numpy.zeros(A.shape[1])
for n in range(0, A.shape[1]):
a=A[:,n]
b=B[:,n]
a abs=numpy.absolute(a)
b abs=numpy.absolute(b)
a_max=numpy.max(a_abs[301:4700])
b max=numpy.max(b abs[301:4700])
AE[n]=numpy.absolute(a max-b max)
APE[n]=AE[n]/a max
#end
return AE, APE
#end
#%% Define the Deep Learning Model: shape encoding, nonlinear mapping, stress decoding
def CreateModel ShapeEncoding (NodeCount, Proj):
model = Sequential()
model.add(Dense(3, input dim=NodeCount*3, kernel initializer='normal', activation='linear'))
W0=model.layers[0].get weights()
W0[0]=Proj
model.layers[0].set weights(W0)
model.compile(loss='mean squared error', optimizer='adamax')
return model
#end
def CreateModel NonlinearMapping (Xshape, Yshape):
model = Sequential()
model.add(Dense(128, input dim=Xshape[1], kernel initializer='normal', activation='softplus'
   ))
model.add(Dense(128, kernel initializer='normal', activation='softplus'))
model.add(Dense(Yshape[1], kernel initializer='normal', activation='linear'))
model.compile(loss='mean squared error', optimizer='adamax')
return model
#end
#-----
def CreateModel StressDecoding(W1 in, W2 in):
model = Sequential()
model.add(Conv2DTranspose(filters=256, kernel size=[5,5], strides=(1,1), input shape=(1,1,64)
   ),data format='channels last'))
model.add(Conv2DTranspose(filters=3, kernel size=[10,20], strides=(10,20)))
model.compile(loss='mean squared error', optimizer='adamax')
W0=model.layers[0].get weights()
W1=model.layers[1].get weights()
W0[0]=W2 in
W1<mark>[0]=</mark>W1 in
model.layers[0].set weights(W0)
```

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model.layers[1].set weights(W1)
return model
# % %
ShapeDataFile='ShapeData.mat'
StressDataFile='StressData.mat'
TempDataFile='TempData.mat'
ResultFile='DL Stress result.mat'
MatData shape=sio.loadmat(ShapeDataFile)
ShapeData=MatData shape['ShapeData']
#응응
#make sure you can see DLStress.py in the current directory of spyder
eng = matlab.engine.start matlab()
rng=RandomState(0)
IndexList= numpy.arange(0, 729, 1)
S11MAE=[]; S11NMAE=[];
S22MAE=[]; S22NMAE=[];
S12MAE=[]; S12NMAE=[];
VMMAE=[]; VMNMAE=[];
S11AE=[]; S11APE=[];
S22AE=[]; S22APE=[];
S12AE=[]; S12APE=[];
VMAE=[]; VMAPE=[];
IndexList test=[];
IndexList train=[];
for k in range (0, 100):
#specify traning set and testing set
rng.shuffle(IndexList)
idx train=IndexList[0:656]
idx test=IndexList[656:729]
IndexList train.append(idx train)
IndexList test.append(idx test)
ShapeData train=ShapeData[:,idx train]
ShapeData test=ShapeData[:,idx test]
#unsupervised learning in Matlab
t1=time.clock()
[X, X t, Y, Y t, S, S t, L, W1, W2, Proj, MeanShape]=UnsupervisedLearning(TempDataFile,
   ShapeDataFile, StressDataFile, idx train, idx test)
t2=time.clock()
print(k, 'Unsupervised Learning', t2-t1)
#subtract mean shape
for n in range (0, 656):
ShapeData train[:,n]-=MeanShape[:,0]
#end
for n in range (0, 73):
ShapeData_test[:,n]-=MeanShape[:,0]
#end
#alghouth encoding has been done in Matlab, redo it here
```

```
ShapeEncoder = CreateModel ShapeEncoding(5000, Proj)
X=ShapeEncoder.predict(ShapeData train.transpose(), batch size=100, verbose=0)
X t=ShapeEncoder.predict(ShapeData test.transpose(), batch size=100, verbose=0)
t3=time.clock()
print(k, 'Shape Encoding', t3-t2)
NMapper=CreateModel NonlinearMapping (X.shape, Y.shape)
NMapper.fit(X, Y, epochs=5000, batch size=100, verbose=0)
#test
Yp=NMapper.predict(X t, batch size=idx test.size, verbose=0)
for n in range (0, 64):
Yp[:,n]=Yp[:,n]*L[n]
#end
Ypp = numpy.array([])
Ypp.resize((idx test.size,1,1,64))
for n in range(0, idx test.size):
Ypp[n,0,0,:]=Yp[n,:]
#end
t4=time.clock()
print(k, 'Nonlinear Mapping', t4-t3)
StressDecoder=CreateModel StressDecoding (W1, W2);
Spp=StressDecoder.predict(Ypp);
Sp = numpy.array([])
Sp.resize((15000, idx test.size))
for n in range(0, idx test.size):
tempS11=Spp[n,:,:,0];
tempS11=tempS11.reshape((5000), order='F')
Sp[0:5000,n]=tempS11
tempS22=Spp[n,:,:,1];
tempS22=tempS22.reshape((5000), order='F')
Sp[5000:10000,n]=tempS22
tempS12=Spp[n,:,:,2];
tempS12=tempS12.reshape((5000), order='F')
Sp[10000:15000,n]=tempS12
#end
Sp=numpy.asmatrix(Sp)
t5=time.clock()
print(k, 'Stress Decoding', t5-t4)
#compare ground-truth S and predicted Sp
[S11MAE k, S11NMAE k]=ComputeError(S t[0:5000,:], Sp[0:5000,:])
S11MAE.append(S11MAE k)
S11NMAE.append(S11NMAE k)
[S22MAE k, S22NMAE k]=ComputeError(S t[5000:10000,:], Sp[5000:10000,:])
S22MAE.append(S22MAE k)
S22NMAE.append(S22NMAE k)
[S12MAE k, S12NMAE k]=ComputeError(S t[10000:15000,:], Sp[10000:15000,:])
S12MAE.append(S12MAE k)
S12NMAE.append(S12NMAE k)
#peak stress error
[S11AE_k, S11APE_k]=ComputeError_peak(S_t[0:5000,:], Sp[0:5000,:])
S11AE.append(S11AE k)
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S11APE.append(S11APE k)
[S22AE k, S22APE k]=ComputeError peak(S t[5000:10000,:], Sp[5000:10000,:])
S22AE.append(S22AE k)
S22APE.append(S22APE k)
[S12AE k, S12APE k]=ComputeError peak(S t[10000:15000,:], Sp[10000:15000,:])
S12AE.append(S12AE k)
S12APE.append(S12APE k)
#compare Von Mises Stress
VM t=ComputeVonMisesStress all (S t)
VMp=ComputeVonMisesStress all (Sp)
[VMMAE k, VMNMAE k]=ComputeError(VM t, VMp)
VMMAE.append(VMMAE k)
VMNMAE.append(VMNMAE k)
#peak stress error
[VMAE k, VMAPE k]=ComputeError peak(VM t, VMp)
VMAE.append(VMAE k)
VMAPE.append(VMAPE k)
#report
t6=time.clock()
print(k, 'ComputeError', t6-t5)
print('VM', numpy.mean(VMMAE), numpy.std(VMMAE), numpy.mean(VMNMAE), numpy.std(VMNMAE))
print('S11', numpy.mean(S11MAE), numpy.std(S11MAE), numpy.mean(S11NMAE), numpy.std(S11NMAE))
print('S22', numpy.mean(S22MAE), numpy.std(S22MAE), numpy.mean(S22NMAE), numpy.std(S22NMAE))
print('S12', numpy.mean(S12MAE), numpy.std(S12MAE), numpy.mean(S12NMAE), numpy.std(S12NMAE))
print('VMpeak', numpy.mean(VMAE), numpy.std(VMAE), numpy.mean(VMAPE), numpy.std(VMAPE))
print('S11peak', numpy.mean(S11AE), numpy.std(S11AE), numpy.mean(S11APE), numpy.std(S11APE))
print('S22peak', numpy.mean(S22AE), numpy.std(S22AE), numpy.mean(S22APE), numpy.std(S22APE))
print('S12peak', numpy.mean(S12AE), numpy.std(S12AE), numpy.mean(S12APE), numpy.std(S12APE))
#end
# 응 응
sio.savemat (ResultFile,
{'DataFile':DataFile,
'IndexList test':IndexList test, 'IndexList train':IndexList train,
    'VMMAE':VMMAE, 'VMNMAE':VMNMAE,
    'S11MAE':S11MAE, 'S11NMAE':S11NMAE,
   'S22MAE':S22MAE, 'S22NMAE':S22NMAE,
'S12MAE':S12MAE, 'S12NMAE':S12NMAE,
'VMAE':VMAE,'APE':VMAPE,
'S11AE':S11AE,'S11APE':S11APE,
'S22AE':S22AE,'S22APE':S22APE,
'S12AE':S12AE,'S12APE':S12APE})
#응응
# to save the predicted stress distribution during cross validation
# insert the function below to the code block of the cross validation
# sio.savemat('StressData pred.mat', {'Sp':Sp, 'idx test':idx test})
#%% show the time cost on the testing set: input shape, output stress
t start=time.clock()
X t=ShapeEncoder.predict(ShapeData test.transpose(), batch size=100, verbose=0)
Yp=NMapper.predict(X t, batch size=idx test.size, verbose=0)
for n in range (0, 64):
Yp[:,n]=Yp[:,n]*L[n]
```

```
#end
Ypp = numpy.array([])
Ypp.resize((idx test.size,1,1,64))
for n in range(0, idx test.size):
Ypp[n,0,0,:]=Yp[n,:]
Spp=StressDecoder.predict(Ypp);
Sp = numpy.array([])
Sp.resize((15000, idx test.size))
for n in range(0, idx test.size):
tempS11=Spp[n,:,:,0];
tempS11=tempS11.reshape((5000), order='F')
Sp[0:5000,n]=tempS11
tempS22=Spp[n,:,:,1];
tempS22=tempS22.reshape((5000), order='F')
Sp[5000:10000,n]=tempS22
tempS12=Spp[n,:,:,2];
tempS12=tempS12.reshape((5000), order='F')
Sp[10000:15000,n]=tempS12
Sp=numpy.asmatrix(Sp)
t end=time.clock()
print('Time Cost Per Testing Sample ', (t end-t start)/73)
```