Problem 1:

$$y = [-4, 8, 7, -15, 12]$$
$$\hat{y} = [2, 9, -1, -16, 18]$$

$$MAE = \frac{1}{n}\sum|y_i - \hat{y}_i|$$
$$MAE = \frac{1}{5}([-4, 8, 7, -15, 12] - [2, 9, -1, -16, 18])$$
$$\boldsymbol{MAE = 4.4}$$

$$MSE = \frac{1}{n}\sum(y_i - \hat{y}_i)^2$$
$$MSE = \frac{1}{5}([-4, 8, 7, -15, 12] - [2, 9, -1, -16, 18])^2$$
$$\boldsymbol{MSE = 27.6}$$

$$MAPE = \frac{1}{n}\sum\frac{|y_i - \hat{y}_i|}{|y_i|}$$
$$MAPE = \frac{1}{5}\frac{([-4, 8, 7, -15, 12] - [2, 9, -1, -16, 18])}{[-4, 8, 7, -15, 12]}$$
$$\boldsymbol{MAPE = 0.39}$$

Problem 2:

- Matrix 1

Problem 3:

- 4

M9-HW1

November 11, 2023

1 Problem 1:

Once again consider the plane-strain compression problem shown in "data/plane-strain.png". In this problem you are given node features for 100 parts. These node features have been extracted by processing each part shape using a neural network. You will train a neural network to von Mises stress at each node given its 60 features. Then you will analyze R^2 for the training and testing data, both for the full dataset and for individual shapes within each dataset.

Summary of deliverables

- Neural network model definition
- Training function
- Training loss curve
- Overall R^2 on training and testing data
- Predicted-vs-actual plots for training and testing data
- Histograms of R^2 distributions on training and testing shapes
- Median R^2 values across training and testing shapes

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.metrics import r2_score

import torch
from torch import nn, optim

def plot_shape(dataset, index, model=None, lims=None):
    x = dataset["coordinates"][index][:,0]
    y = dataset["coordinates"][index][:,1]

    if model is None:
        c = dataset["stress"][index]
    else:
        c = model(torch.tensor(dataset["features"][index])).detach().numpy().
 ↪flatten()

    if lims is None:
        lims = [min(c),max(c)]
```

```python
    plt.scatter(x,y,s=5,c=c,cmap="jet",vmin=lims[0],vmax=lims[1])
    plt.colorbar(orientation="horizontal", shrink=.75, pad=0,ticks=lims)
    plt.axis("off")
    plt.axis("equal")

def plot_shape_comparison(dataset, index, model, title=""):
    plt.figure(figsize=[6,3.2], dpi=120)
    plt.subplot(1,2,1)
    plot_shape(dataset,index)
    plt.title("Ground Truth",fontsize=9,y=.96)
    plt.subplot(1,2,2)
    c = dataset["stress"][index]
    plot_shape(dataset, index, model, lims = [min(c), max(c)])
    plt.title("Prediction",fontsize=9,y=.96)
    plt.suptitle(title)
    plt.show()

def load_dataset(path):
    dataset = np.load(path)
    coordinates = []
    features = []
    stress = []
    N = np.max(dataset[:,0].astype(int)) + 1
    split = int(N*.8)
    for i in range(N):
        idx = dataset[:,0].astype(int) == i
        data = dataset[idx,:]
        coordinates.append(data[:,1:3])
        features.append(data[:,3:-1])
        stress.append(data[:,-1])
    dataset_train = dict(coordinates=coordinates[:split], features=features[:
 ↪split], stress=stress[:split])
    dataset_test = dict(coordinates=coordinates[split:],␣
 ↪features=features[split:], stress=stress[split:])
    X_train, X_test = np.concatenate(features[:split], axis=0), np.
 ↪concatenate(features[split:], axis=0)
    y_train, y_test = np.concatenate(stress[:split], axis=0), np.
 ↪concatenate(stress[split:], axis=0)
    return dataset_train, dataset_test, X_train, X_test, y_train, y_test

def get_shape(dataset,index):
    X = torch.tensor(dataset["features"][index])
    Y = torch.tensor(dataset["stress"][index].reshape(-1,1))
    return X, Y

def plot_r2_distribution(r2s, title=""):
    plt.figure(dpi=120,figsize=(6,4))
```

```
    plt.hist(r2s, bins=10)
    plt.xlabel("$R^2$")
    plt.ylabel("Number of shapes")
    plt.title(title)
    plt.show()
```

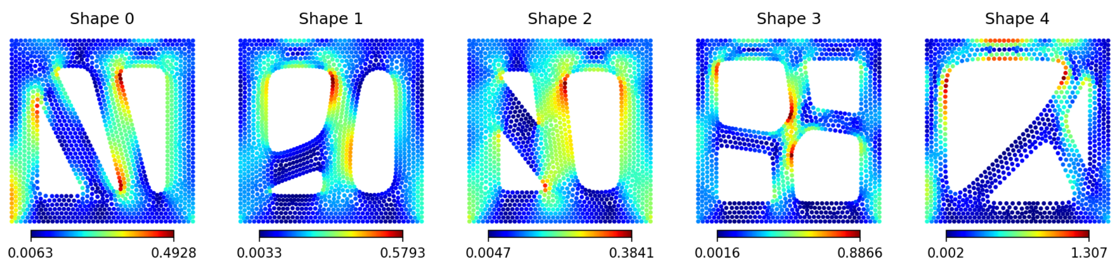
1.1 Loading the data

First, complete the code below to load the data and plot the von Mises stress fields for a few shapes. You'll need to input the path of the data file, the rest is done for you.

All training node features and outputs are in `X_train` and `y_train`, respectively. Testing nodes are in `X_test`, `y_test`.

`dataset_train` and `dataset_test` contain more detailed information such as node coordinates, and they are separated by shape.
Get features and outputs for a shape by calling `get_shape(dataset,index)`. `N_train` and `N_test` are the number of training and testing shapes in each of these datasets.

```
[ ]: data_path = "/Users/judsonvankyle/Dropbox/My Mac (MacBook Pro (2))/Desktop/CMU/
      ↪AI-ML/HW9/data/stress_nodal_features.npy"
     dataset_train, dataset_test, X_train, X_test, y_train, y_test =␣
      ↪load_dataset(data_path)
     N_train = len(dataset_train["stress"])
     N_test = len(dataset_test["stress"])

     plt.figure(figsize=[15,3.2], dpi=150)
     for i in range(5):
         plt.subplot(1,5,i+1)
         plot_shape(dataset_train,i)
         plt.title(f"Shape {i}")
     plt.show()
```



1.2 Neural network to predict stress

Create a PyTorch neural network class `StressPredictor` below. This should be an MLP with 60 inputs (the given features) and 1 output (stress). The hidden layer sizes and activations are up to you.

[ ]:
```python
class StressPredictor(nn.Module):
    def __init__(self):
        super().__init__()
        self.seq = nn.Sequential(
            nn.Linear(60,100),
        )
        self.seq.append(nn.ReLU())
        self.seq.append(nn.Linear(100,100))
        self.seq.append(nn.ReLU())
        self.seq.append(nn.Linear(100,150))
        self.seq.append(nn.ReLU())
        self.seq.append(nn.Linear(150, 1))
    def forward(self, x):
        return self.seq(x)
```

1.3 Training function

Below, you should define a function `train(model, dataset, lr, epochs)` that will train `model` on the data in `dataset` with the Adam optimizer for `epochs` epochs with a learning rate of `lr`.

Because there are so many total nodes, you should treat each shape as a batch of nodes – each epoch of training will require you to loop through each shape in the dataset in a random order, performing a step of gradient descent for each shape encountered. Your function should automatically generate a plot of the loss curve on training data.

- You can use the provided `get_shape` to access feature and output tensors for each shape.
- Use MSE as a your loss function.
- Look into `np.random.permutation()` for generating a random index order

[ ]:
```python
def train(model, dataset, lr, epochs):
    train_hist = []

    loss_fcn = nn.MSELoss()

    opt = optim.Adam(params = model.parameters(), lr=lr)

    for epoch in range(epochs):
        idxs = np.random.permutation(len(dataset_train["stress"]))

        loss = 0

        for idx in idxs:
            x, y = get_shape(dataset, idx)

            model.train()
            x_out = model(x)
            loss_train = loss_fcn(x_out, y)
            loss += loss_train
```

```
            opt.zero_grad()
            loss_train.backward()
            opt.step()

        train_hist.append(loss.item())

        if epoch % int(epochs / 25) == 0:
            print(f"Epoch {epoch:>4} of {epochs}:   Train Loss = {loss_train.
↪item():.6f}")

    plt.figure(figsize=(15,3),dpi=250)
    plt.plot(train_hist,label="Training")
    plt.title("Training Loss")
    plt.xlabel("Epochs")
    plt.ylabel("Loss")
    plt.show()
    return
```

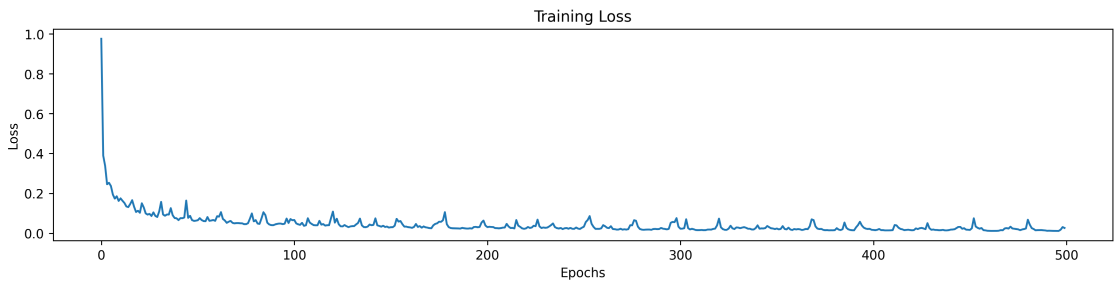
1.4 Training your Neural Network

Now, create your neural network model and run your train function on the training dataset `dataset_train`.
Determining the right number of epochs and learning rate are up to you. The training loss curve should be shown.

[ ]:
```
model = StressPredictor()

lr = 0.001
epochs = 500

train(model, dataset_train, lr, epochs)
```

```
Epoch    0 of 500:   Train Loss = 0.004535
Epoch   20 of 500:   Train Loss = 0.000718
Epoch   40 of 500:   Train Loss = 0.000716
Epoch   60 of 500:   Train Loss = 0.001873
Epoch   80 of 500:   Train Loss = 0.001032
Epoch  100 of 500:   Train Loss = 0.000547
Epoch  120 of 500:   Train Loss = 0.000714
Epoch  140 of 500:   Train Loss = 0.000313
Epoch  160 of 500:   Train Loss = 0.000263
Epoch  180 of 500:   Train Loss = 0.000191
Epoch  200 of 500:   Train Loss = 0.000250
Epoch  220 of 500:   Train Loss = 0.000203
Epoch  240 of 500:   Train Loss = 0.000294
Epoch  260 of 500:   Train Loss = 0.000356
Epoch  280 of 500:   Train Loss = 0.000181
```

```
Epoch  300 of 500:   Train Loss = 0.000244
Epoch  320 of 500:   Train Loss = 0.000302
Epoch  340 of 500:   Train Loss = 0.000384
Epoch  360 of 500:   Train Loss = 0.000215
Epoch  380 of 500:   Train Loss = 0.000317
Epoch  400 of 500:   Train Loss = 0.000167
Epoch  420 of 500:   Train Loss = 0.000168
Epoch  440 of 500:   Train Loss = 0.000163
Epoch  460 of 500:   Train Loss = 0.000146
Epoch  480 of 500:   Train Loss = 0.000292
```



1.5 R^2 Score

Compute the R^2 Score on the training dataset. You will have to convert between tensors and arrays versions to use sklearn functions, or you can write your own function.

[ ]:
```
y_pred = model(torch.tensor(X_train))
r2_train = r2_score(y_train.reshape(-1,1), y_pred.detach().numpy())
print(f"R^2 Train: {r2_train}")
```

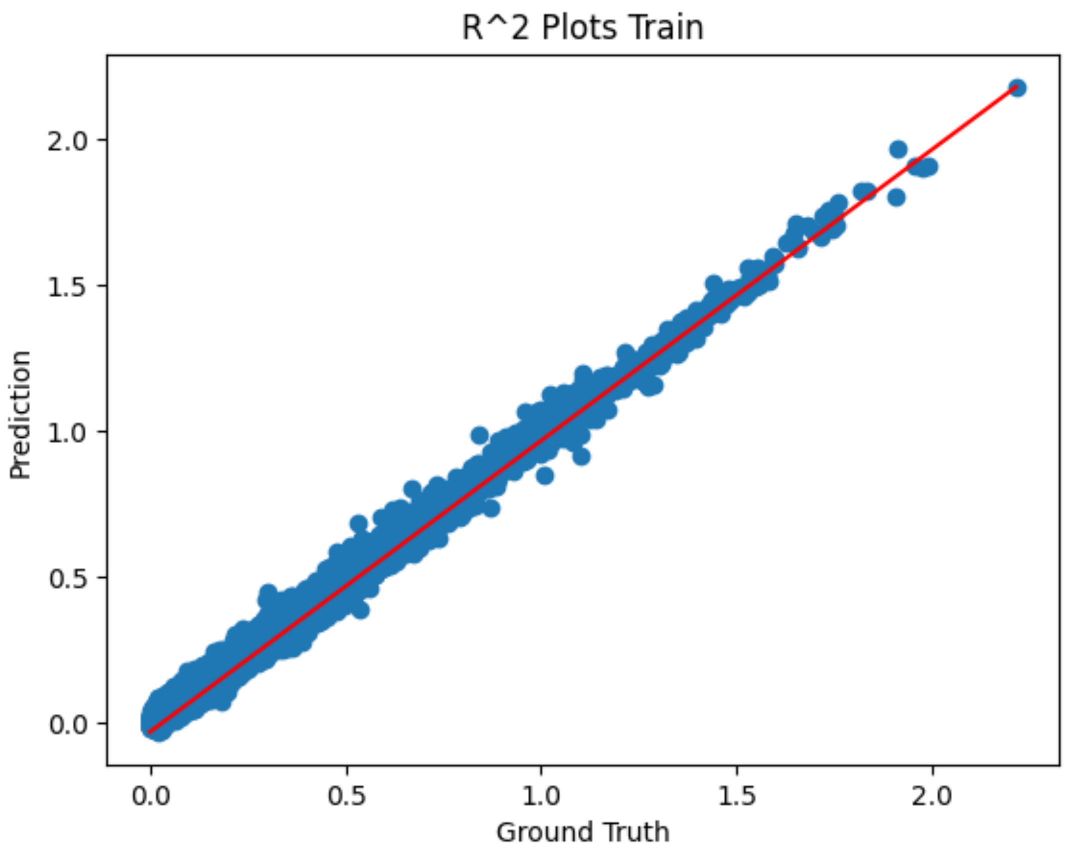
```
R^2 Train: 0.9890267435233027
```

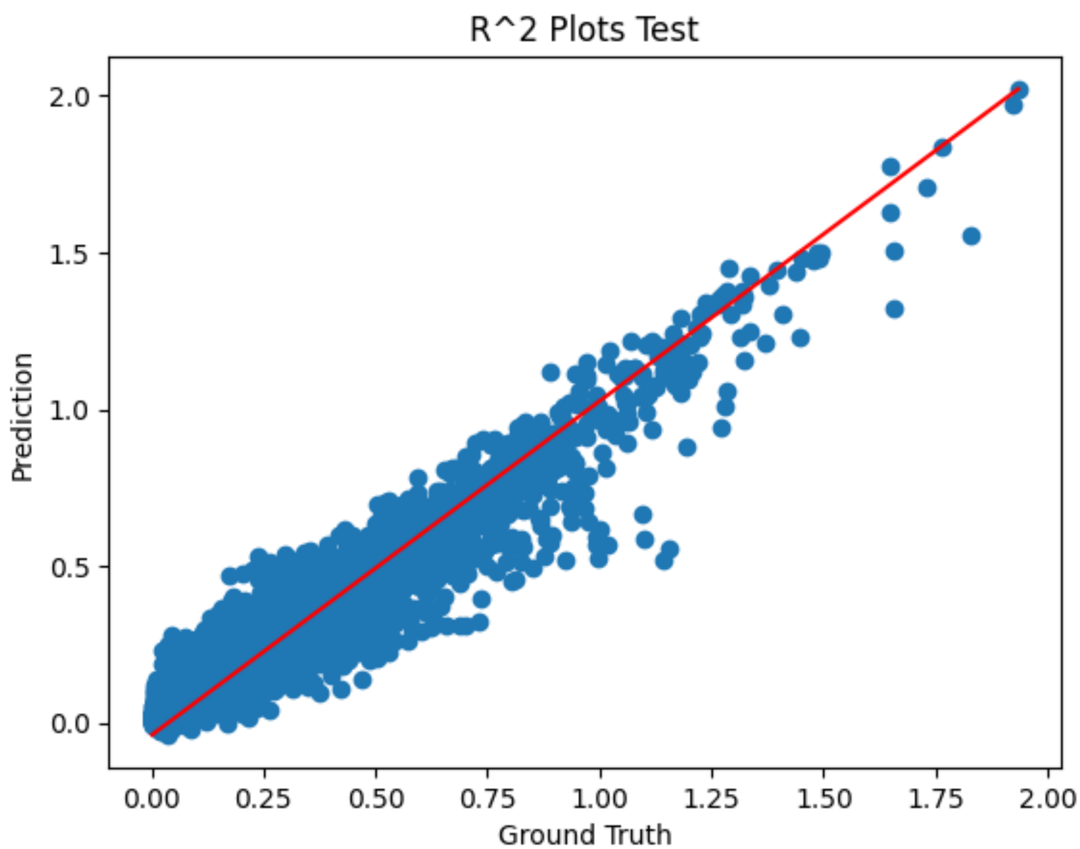
1.6 R^2 Plots

Now, generate predicted-vs-actual plots that display both data and a theoretical best fit line. Make 2 such plots - one for training data and one for testing.

[ ]:
```
plt.figure()
y_pred = model(torch.tensor(X_train))
plt.scatter(y_train.reshape(-1,1), y_pred.detach().numpy(), label=f"Model {i}")
plt.plot([np.min(y_train), np.max(y_train)], [np.min(y_pred.detach().numpy()),
    np.max(y_pred.detach().numpy())], label="Best Fit", color="r")
plt.title("R^2 Plots Train")
plt.xlabel("Ground Truth")
plt.ylabel("Prediction")
plt.show()
```

```
plt.figure()
y_pred = model(torch.tensor(X_test))
plt.scatter(y_test.reshape(-1,1), y_pred.detach().numpy(), label=f"Model {i}")
plt.plot([np.min(y_test), np.max(y_test)], [np.min(y_pred.detach().numpy()), np.
↪max(y_pred.detach().numpy())], label="Best Fit", color="r")
plt.title(f"R^2 Plots Test")
plt.xlabel("Ground Truth")
plt.ylabel("Prediction")
plt.show()
```





1.7 Individual Shape R^2

Because we have a unique problem where groups of nodes in a dataset form a single shape, we can compute an R^2 score for an individual shape. For each shape in the training set, compute an R^2 score. Then create a histogram of the values with the function `plot_r2_hist(r2s)`. Repeat for the testing set.

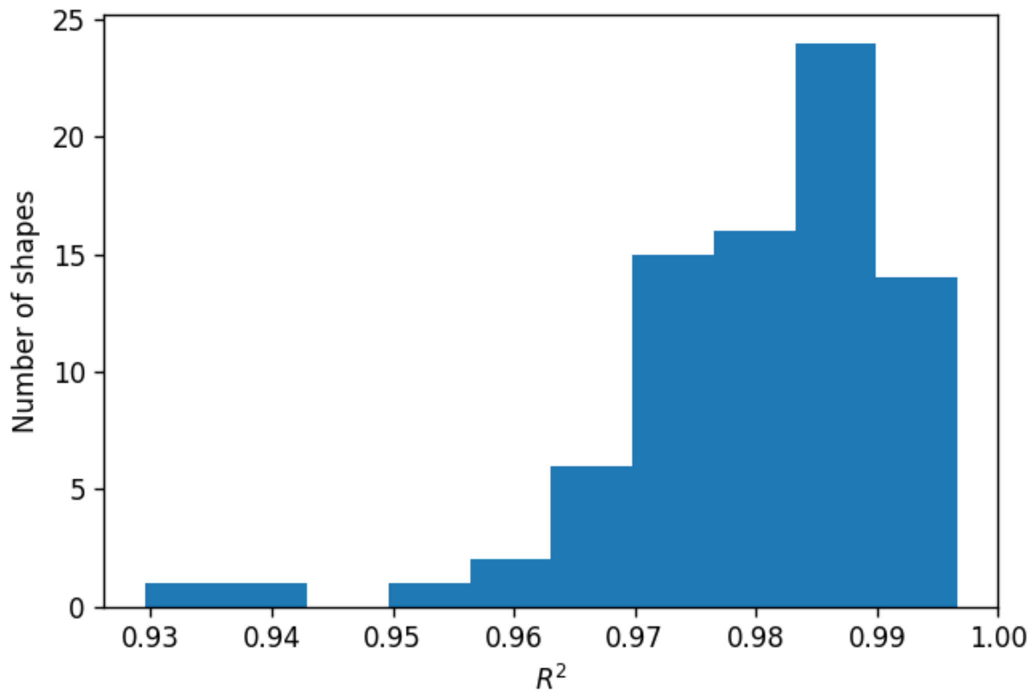
Report the median R^2 score across all training shapes, and the median across all testing shapes.

If your test median is below 0.85, try and tune your network size/training hyperparameters until it reaches this threshold.

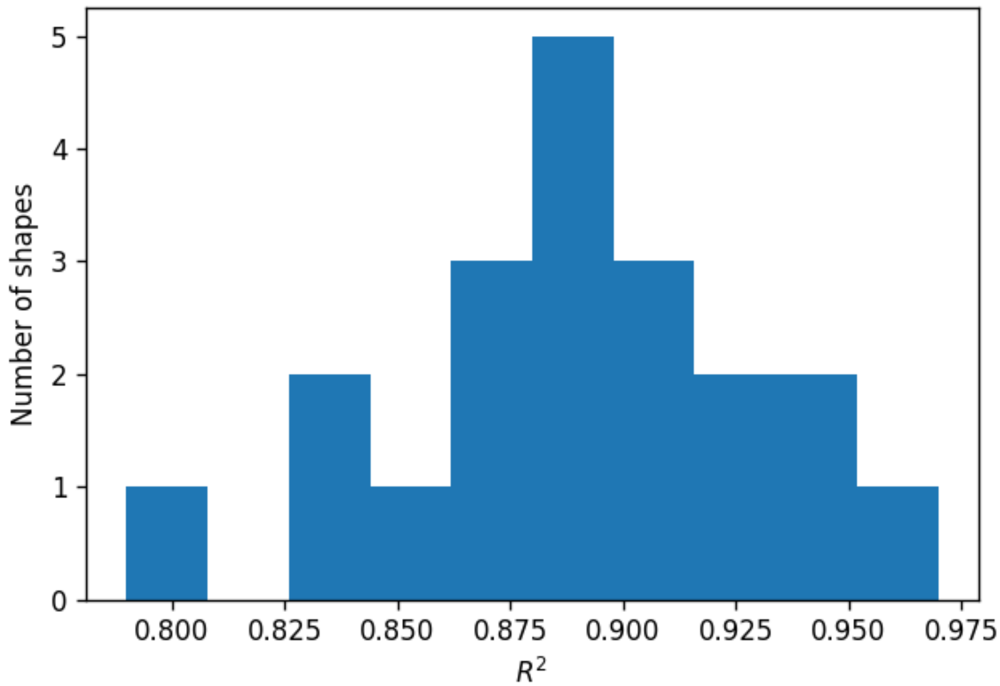
[ ]:
```
r2s_train = []
for i in range(len(dataset_train["stress"])):
    x, y = get_shape(dataset_train, i)
    y_pred = model(x)
    r2s_train.append(r2_score(y.detach().numpy(), y_pred.detach().numpy()))
print(f"Mean R^2 Value: {np.mean(r2s_train)}")
plot_r2_distribution(r2s_train)

r2s_test = []
```

```python
for i in range(len(dataset_test["stress"])):
    x, y = get_shape(dataset_test, i)
    y_pred = model(x)
    r2s_test.append(r2_score(y.detach().numpy(), y_pred.detach().numpy()))
print(f"Mean R^2 Value: {np.mean(r2s_test)}")
plot_r2_distribution(r2s_test)
```

```
Mean R^2 Value: 0.9798640564099863
```




```
Mean R^2 Value: 0.8902756460598569
```



Number of shapes
0
1
2
3
4
5
0.800
0.825
0.850
0.875
0.900
0.925
0.950
0.975
R^2

M9-L1-P1

November 7, 2023

1 M9-L1 Problem 1

Here, you will implement three loss functions from scratch in numpy: MAE, MSE, and MAPE.

```
[ ]: import numpy as np

     y_gt1 = np.array([1,2,3,4,5,6,7,8,9,10])
     y_pred1 = np.array([1,1.3,3.1,4.6,5.9,5.9,6.4,9.2,8.1,10.5])

     y_gt2 = np.array([-3.23594765, -3.74125693, -2.3040903 ,  0.         ,  0.
      ↪30190142, -1.68434859,  1.10160357,  0.8587438 ,  1.76546802,  3.13787123, 3.
      ↪72990216,  5.89871795,  6.06406803,  6.28329118,  7.46406525, 8.21246221, 10.
      ↪23145281,  9.39080133, 10.76761316, 10.45903557, 9.61872736, 13.68392163, 14.
      ↪75332509, 14.00530973, 17.87581523, 15.01028079, 17.36899084, 17.99463433,␣
      ↪20.57318325, 21.36834867, 20.91252318, 21.99432414, 21.58696173, 21.
      ↪35253687, 23.84400704, 25.20685402, 27.13938159, 27.97005662, 27.23893581,␣
      ↪28.18254573, 28.29488138, 28.78200226, 29.35433587, 33.86996731, 32.2681256␣
      ↪, 33.19828933, 33.24215413, 36.13102571, 34.59822336, 36.85796679, 37.
      ↪03382637, 39.17478129, 39.13565951, 39.32441832, 41.33545414, 42.65055409,␣
      ↪43.1473253 , 44.24186584, 44.1636577 , 45.29382449, 45.84269107, 47.
      ↪01418421, 47.41917695, 47.36462649, 50.12692109, 50.40629987, 50.03646832,␣
      ↪52.98803478, 52.47654002, 54.29436964, 55.83010066, 56.08857887, 57.9575825␣
      ↪, 56.44194186, 58.93769518, 58.7091293 , 59.3817281 , 60.53226145, 61.
      ↪65814444, 62.88444817, 62.52171885, 65.44628103, 65.86970284, 64.72638258,␣
      ↪68.60946432, 69.87568716, 70.01716341, 69.51704486, 69.48480293, 72.
      ↪46859314, 71.86955033, 74.3537582 , 74.19817397, 75.82512388, 76.0634371 ,␣
      ↪77.27222973, 77.43474244, 80.06869878, 79.26832623, 80.40198936])
```

```
y_pred2 = np.array([-3.17886560e+00, -3.72628642e+00, -2.28154027e+00, -2.
↪42424242e-06, 2.96261368e-01, -1.70080838e+00,  1.09113641e+00,  8.
↪60043722e-01, 1.76729042e+00,  3.12498677e+00,  3.72452933e+00,  5.
↪81293300e+00, 6.01791742e+00,  6.27564586e+00,  7.43093457e+00,  8.
↪18505900e+00, 1.00785853e+01,  9.41006754e+00,  1.07339029e+01,  1.
↪05483666e+01, 9.86429504e+00,  1.35944803e+01,  1.46257911e+01,  1.
↪41092530e+01, 1.74700758e+01,  1.52285866e+01,  1.73610430e+01,  1.
↪80283176e+01, 2.02578402e+01,  2.10543695e+01,  2.08801196e+01,  2.
↪19111495e+01, 2.17786086e+01,  2.17754891e+01,  2.39269636e+01,  2.
↪51674432e+01, 2.68054871e+01,  2.76337491e+01,  2.73444399e+01,  2.
↪82677426e+01, 2.85915692e+01,  2.91907133e+01,  2.98552019e+01,  3.
↪32092384e+01, 3.24325813e+01,  3.33437229e+01,  3.36586115e+01,  3.
↪58501097e+01, 3.51566050e+01,  3.69363787e+01,  3.73654528e+01,  3.
↪90232127e+01, 3.93355670e+01,  3.97886962e+01,  4.13471034e+01,  4.
↪24678677e+01, 4.31186248e+01,  4.41080463e+01,  4.44437982e+01,  4.
↪54581242e+01, 4.61509657e+01,  4.71832256e+01,  4.78047650e+01,  4.
↪81822755e+01, 5.00379827e+01,  5.06088232e+01,  5.08521636e+01,  5.
↪27428151e+01, 5.29526597e+01,  5.42661662e+01,  5.54230479e+01,  5.
↪60162341e+01, 5.72972123e+01,  5.71389028e+01,  5.87005639e+01,  5.
↪91111760e+01, 5.98988234e+01,  6.08826528e+01,  6.18502423e+01,  6.
↪28491288e+01, 6.32501917e+01,  6.48567227e+01,  6.55629719e+01,  6.
↪57207391e+01, 6.75883810e+01,  6.85509197e+01,  6.91918142e+01,  6.
↪96421235e+01, 7.02288144e+01,  7.17044458e+01,  7.21593122e+01,  7.
↪34448231e+01, 7.40436375e+01,  7.50845851e+01,  7.57923722e+01,  7.
↪67262442e+01, 7.74266118e+01,  7.86387737e+01,  7.91677250e+01,  8.
↪00787815e+01])
```

1.1 Mean Absolute Error

Complete the definition for `MAE(y_gt, y_pred)` below.

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| = \frac{1}{n}\sum_{i=1}^{n}|e_i|$$

`MAE(y_gt1, y_pred1)` should return 0.560.

[ ]:
```
def MAE(y_gt, y_pred):
    return np.sum(abs(y_gt - y_pred)) / len(y_gt)

print(f"MAE(y_gt1, y_pred1) = {MAE(y_gt1, y_pred1):.3f}")
print(f"MAE(y_gt2, y_pred2) = {MAE(y_gt2, y_pred2):.3f}")
```

```
MAE(y_gt1, y_pred1) = 0.560
MAE(y_gt2, y_pred2) = 0.290
```

1.2 Mean Squared Error

Complete the definition for `MSE(y_gt, y_pred)` below.

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(e_i)^2 = \frac{1}{n}e^T e$$

`MSE(y_gt1, y_pred1)` should return 0.454.

```
[ ]: def MSE(y_gt, y_pred):
         return np.sum(np.power((y_gt - y_pred),2)) / len(y_gt)

     print(f"MSE(y_gt1, y_pred1) = {MSE(y_gt1, y_pred1):.3f}")
     print(f"MSE(y_gt2, y_pred2) = {MSE(y_gt2, y_pred2):.3f}")
```

```
MSE(y_gt1, y_pred1) = 0.454
MSE(y_gt2, y_pred2) = 0.174
```

1.3 Mean Absolute Percentage Error

Complete the definition for `MAPE(y_gt, y_pred, epsilon)` below.

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i - \hat{y}_i|}{|y_i| + \varepsilon} = \frac{1}{n}\sum_{i=1}^{n}\frac{|e_i|}{|y_i| + \varepsilon}$$

`MAPE(y_gt1, y_pred1, 1e-6)` should return 0.112.

```
[ ]: def MAPE(y_gt, y_pred, epsilon=1e-6):
         return np.sum(abs(y_gt - y_pred)/(abs(y_gt) + epsilon)) / len(y_gt)

     print(f"MAPE(y_gt1, y_pred1) = {MAPE(y_gt1, y_pred1):.3f}")
     print(f"MAPE(y_gt2, y_pred2) = {MAPE(y_gt2, y_pred2):.3f}")
```

```
MAPE(y_gt1, y_pred1) = 0.112
MAPE(y_gt2, y_pred2) = 0.032
```

M9-L1-P2

November 11, 2023

0.1 M9-L1 Problem 2

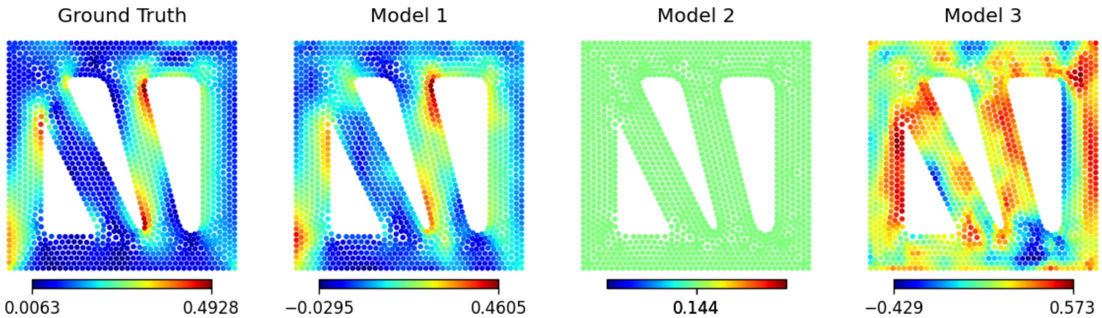
Recall the von Mises stress prediction problem from the module 6 homework. In this problem, you will compute the R^2 score for a few model predictions for a single shape in this dataset. You will also plot the predicted-vs-actual stress for each model.

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.metrics import r2_score

float32 = np.float32
```

[ ]:
```
```

-
-
-
-

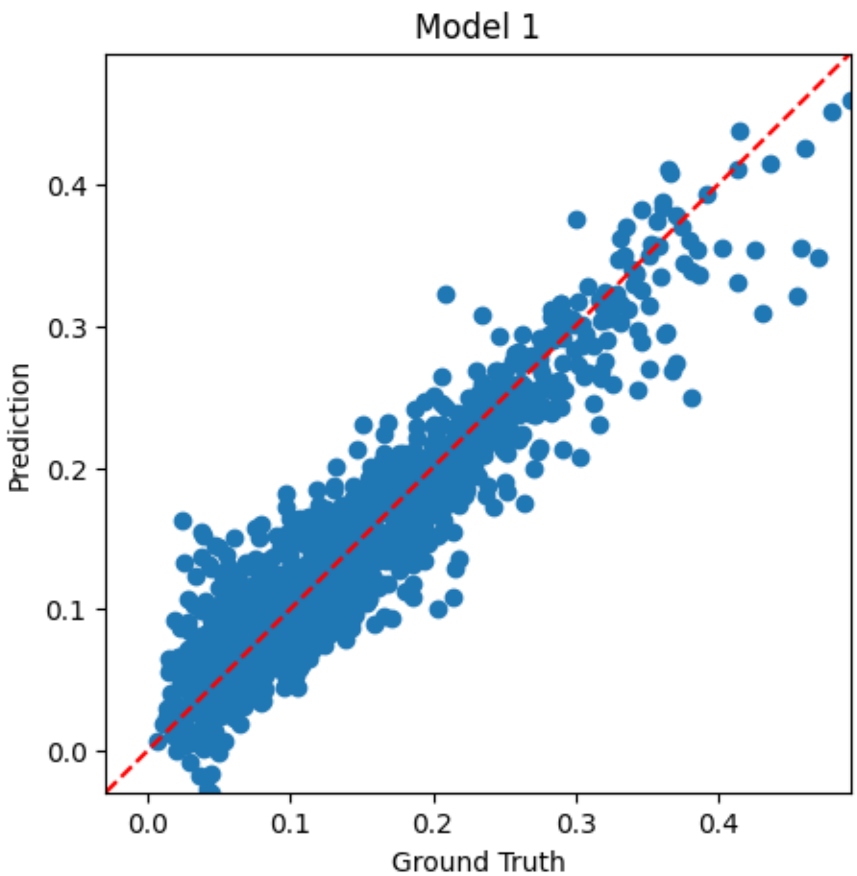
[ ]:
```
def plot_shape(x, y, stress, lims=None):

    if lims is None:
        lims = [min(stress),max(stress)]

    plt.scatter(x,y,s=5,c=stress,cmap="jet",vmin=lims[0],vmax=lims[1])
    plt.colorbar(orientation="horizontal", shrink=.75, pad=0,ticks=lims)
    plt.axis("off")
    plt.axis("equal")

def plot_all(x, y, gt, model1, model2, model3):
    plt.figure(figsize=[12,3.2], dpi=120)
    plt.subplot(141)
    plot_shape(x, y, gt)
    plt.title("Ground Truth")

    plt.subplot(142)
    plot_shape(x, y, model1)
    plt.title("Model 1")

    plt.subplot(143)
    plot_shape(x, y, model2)
    plt.title("Model 2")

    plt.subplot(144)
    plot_shape(x, y, model3)
    plt.title("Model 3")

    plt.show()

plot_all(xs, ys, gt, model1, model2, model3)
```

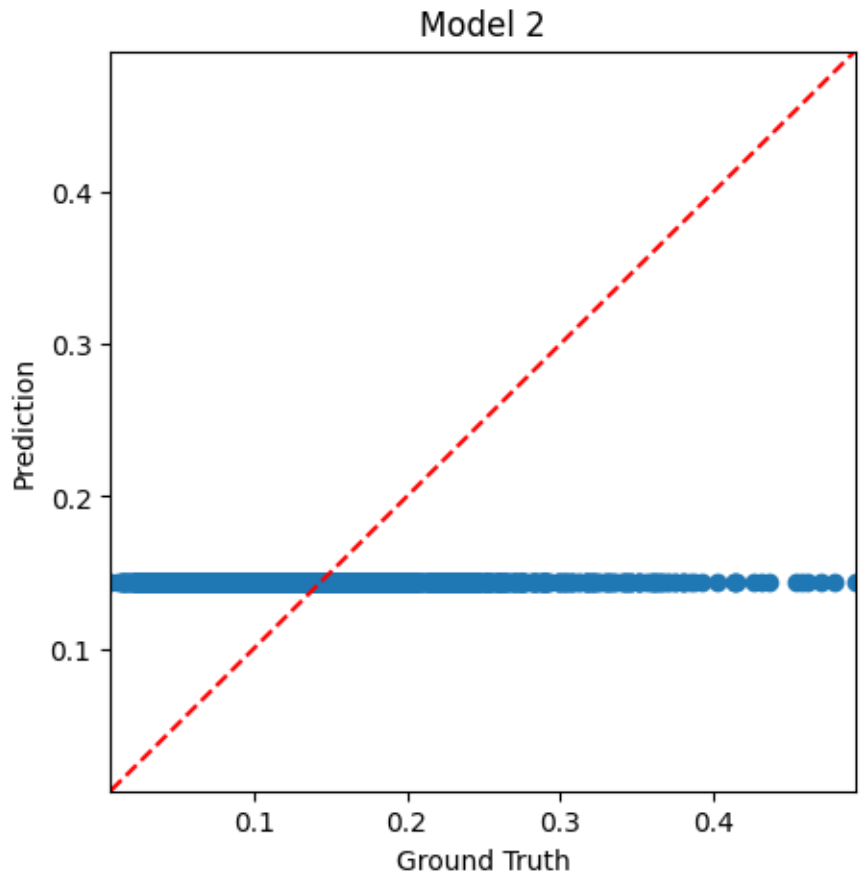


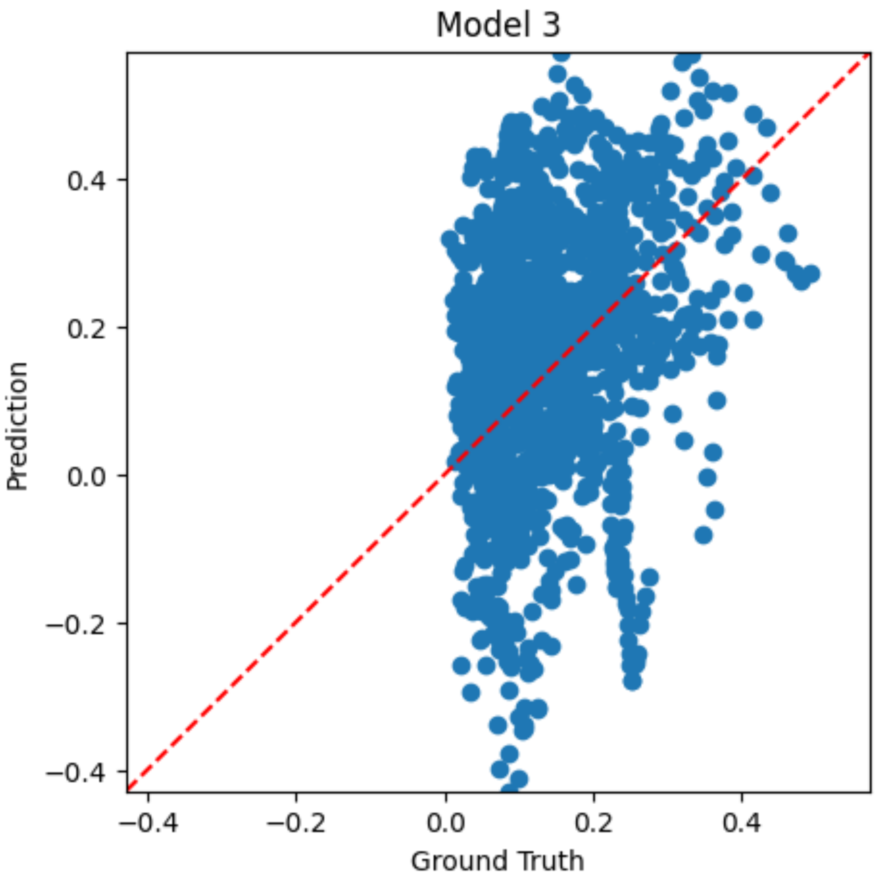
[ ]:
```
def R_Squared(y_gt, y_pred):
    RSS = np.sum(np.power((y_gt - y_pred), 2))
    TSS = np.sum(np.power((y_gt - np.mean(y_gt)),2))
    return 1 - RSS/TSS

model1_r_squared = R_Squared(gt, model1)
model2_r_squared = R_Squared(gt, model2)
model3_r_squared = R_Squared(gt, model3)

print(f"Model 1 R^2: {model1_r_squared}")
print(f"Model 2 R^2: {model2_r_squared}")
print(f"Model 3 R^2: {model3_r_squared}")
```

[ ]:
```
def plot_r2(gt, pred, title):
    plt.figure(figsize=[5,5])

    plt.scatter(gt, pred)

    plt.plot([-1000,1000], [-1000,1000],"r--")

    all = np.concatenate([gt, pred])
    plt.xlim(np.min(all), np.max(all))
```

```
    plt.ylim(np.min(all), np.max(all))
    plt.xlabel("Ground Truth")
    plt.ylabel("Prediction")
    plt.title(title)
    plt.show()

plot_r2(gt, model1,"Model 1")
plot_r2(gt, model2,"Model 2")
plot_r2(gt, model3,"Model 3")
```




Model 2
0.4
0.3
0.2
0.1
Prediction
0.1
0.2
0.3
0.4
Ground Truth



1.

2.