Neural Network for computing damping functions in a $k-\varepsilon$ Turbulence Model

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- The ML will then be some form of regression method.

Machine Learning

In this part you will use Neural Network (NN) to model damping functions in the AKN turbulence model which reads [1]

$$\begin{aligned}
\frac{\partial k}{\partial t}+\frac{\partial \bar{v}_j k}{\partial x_j} &= \frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right]+P_k-\varepsilon \qquad (1)\\
\frac{\partial \varepsilon}{\partial t}+\frac{\partial \bar{v}_j \varepsilon}{\partial x_j} &= \frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{\varepsilon 1}P_k\frac{\varepsilon}{k}-C_{\varepsilon 2}f_2\frac{\varepsilon^2}{k}\\
\nu_t &= C_\mu f_\mu \frac{k^2}{\varepsilon}, \quad P_k=\nu_t\left(\frac{\partial \bar{v}_i}{\partial x_j}+\frac{\partial \bar{v}_j}{\partial x_i}\right)\frac{\partial \bar{v}_i}{\partial x_j}\\
C_{\varepsilon 1} &= 1.5, \quad C_{\varepsilon 2}=1.9, \quad C_\mu=0.09, \quad \sigma_k=1.4, \quad \sigma_\varepsilon=1.4
\end{aligned}$$

where k and ε denote the modeled turbulent kinetic energy and its dissipation, respectively. The damping functions are defined as

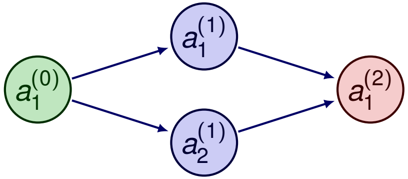
$$f_2 = \left[1-\exp\left(-\frac{y^*}{3.1}\right)\right]^2\left\{1-0.3\exp\left[-\left(\frac{R_t}{6.5}\right)^2\right]\right\}$$

Crash course on Neural Network (NN)

Below I give you some useful links for NN and PyTorch.

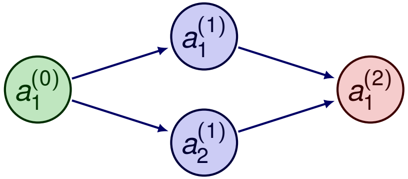
- Good YouTube lectures
  - 3Blue1Brown: But what is a neural network
  - 3Blue1Brown: gradient descent, how neural network learn
  - 3Blue1Brown: backpropagation, intuitively
  - 3Blue1Brown: backpropagation, calculus
  - Sebastian Lague: how to create a neural network
- Celsius to Fahrenheit with PyTorch NN
- Building a Regression Model in PyTorch
- Multi-Target Predictions with Multilinear Regression in PyTorch

NEURAL NETWORK (NN). PYTHON'S PYTORCH. CRASH COURSE



- I create a NN that finds a damping function, $Y \equiv f$, as a function of input $X \equiv y^+$
- 1 input ($X = a_1^{(0)}$), 1 hidden layer with 2 neurons ($a_1^{(1)}, a_2^{(1)}$) and 1 output ($Y = a_1^{(2)}$)

Neural Network (NN). Python's pytorch. Crash Course



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```
class NN(nn.Module):
 def super-__init__(self):
  self.layer_1=nn.Linear(1, 2) # Connection 0-1
  self.layer_2=nn.Linear(2, 1) # Connection 1-2
 def forward(self, x):
  y = torch.nn.functional.sigmoid(self.layer_1(x)) # a_1^{(1)}, a_2^{(1)}, hidden-layer
  output = torch.nn.functional.sigmoid(self.layer_2(y)) # a_1^{(2)}, output-layer
```

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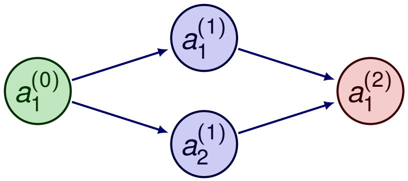

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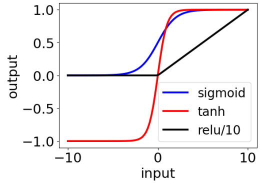

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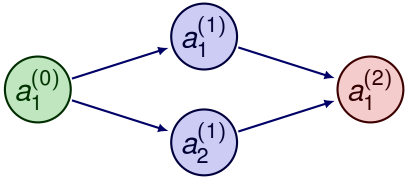
NEURAL NETWORK (NN). FORWARD



Activation 1: $a_1^{(1)} = s_1^{(1)}\left(w_1^{(0)}a_1^{(0)} + b_1^{(0)}\right)$

Activation 2: $a_2^{(1)} = s_2^{(1)}\left(w_2^{(0)}a_2^{(0)} + b_2^{(0)}\right)$

Output: $a_1^{(2)} = s_1^{(2)}\left(w_1^{(1)}a_1^{(1)} + b_1^{(1)} + w_2^{(1)}a_2^{(1)} + b_2^{(1)}\right) \equiv Y$

- *s* is an activation function (`linear`, `sigmoid`, `tanh`, ...)

NEURAL NETWORK (NN). BACKWARD

The Python code for the simple NN model is given in the listing below

```
#  initiate the NN model
model = NN()
# define input, X
X=np.zeros(nj,1))
X[:,0] = scaler_yplus.fit_transform(yplus)[:,0]
# define output, Y (f is known)
Y = f
# Training loop
for epoch in range(max_no_epoch):
# Compute prediction and loss, L
    o = model(X) #prediction
    L = loss_fn(o, Y)  # L=|o-Y|_2
    L.backward()
```

- `loss.backward()` computes $dL/dw_1, dL/db_1, dL/ds_1, \ldots$
- They are used to get new improved $w_1, b_1, \ldots$

The Assignment. Appendix Q4 in the eBook

- Download the data Python scripts here.
- The damping functions f_μ and f_2 are used in the AKN model, see Eq. 1. They are functions of y^* and Re_t.
- In this assignment you will create new f_μ and f_2 using NN.
- You will first make them as functions of y^* and y^+.
- The created NN model will be saved to disk, and then you will load the NN model into the Python CFD code, `rans-k-eps-NN.py` (available here)
- The Python script `NN-f2-5200-no-batch.py` uses PyTorch to train a f_2 damping function in the NN model on 80% of the DNS data (randomly chosen) and then test (predict) on the remaining 20%.

Random initial weights and biases

- Study `NN-f2-5200-no-batch.py` carefully.
- Note that the initial weights and biases are randomized in Pytorch.
- If you want to make sure that you get the same results every time you run the script you can save the initial weights and biases, i.e.

```
        if epoch == 0 and batch == 0:
# Define checkpoint
          checkpoint = {
            'epoch': epoch,
            'model_state_dict': model.state_dict(),
            'optimizer_state_dict': optimizer.state_dict(),
            'loss': loss,
           }
          torch.save(checkpoint, 'checkpoint-f2.ct')
```

from one run that converged well.

- Then you load the initial data in a subsequent run (see next slide)

Random initial weights and biases

```
for epoch in range(N_epochs):
    if epoch == 0:
       print('checkpoint loaded')
       checkpoint = torch.load('checkpoint-f2.ct',weights_only=True)

# Apply the state_dict to model and optimizer
       NN = MyNet()
       NN.load_state_dict(checkpoint['model_state_dict'])

       optimizer = torch.optim.SGD(NN.parameters(), lr=learning_rate)
       optimizer.load_state_dict(checkpoint['optimizer_state_dict'])

# Retrieve the training epoch
#           epoch = checkpoint['epoch']
       loss = checkpoint['loss']

       NN.train()  # For training mode (resuming training)
```

INPUT DATA

- The input data, y^* and y^+, are taken from DNS and they are scaled and then assigned to `X`. i.e.

```
# we choose two inputs: yplus_DNS and ystar_DNS
# re-shape
yplus= y_plus_DNS.reshape(-1,1)
ystar= y_star_DNS.reshape(-1,1)
# use scaling, One for each input
scaler_yplus = MinMaxScaler()
scaler_ystar = MinMaxScaler()
# X = input matrix
X=np.zeros((len(yplus_DNS),2))
X[:,0] = scaler_yplus.fit_transform(yplus)[:,0]
X[:,1] = scaler_ystar.fit_transform(ystar)[:,0]
```

- The NN model will try to find suitable weights and biases to fit the input parameters to the output (the **target**), which is f_2 (also taken from DNS). It is assigned to `Y` (next slides)

The Model

```
# current model of f_2
f_2=((1.-np.exp(-y_star_DNS/3.1))**2)*(1.-0.3*np.exp(-(re_t/6.5)**2))

# output is f_2_NN (see below) predicted by the NN. Our target is f_2
# transpose the target vector to make it a column vector
Y = f_2.transpose()
Y= Y.reshape(-1,1)  # makes an array of size [len(Y), 1]
```

The NN model is using 10 neurons and three hidden layers (instead of two and one, respectively, in the example above) and the ReLu actuator is used (instead of Sigmoid above)

```
class MyNet(nn.Module):

    def __init__(self):
        super().__init__()
        self.input   = nn.Linear(2, 10)  #axis 0: number of inputs
        self.hidden1 = nn.Linear(10, 10)
        self.hidden2 = nn.Linear(10, 1)  #axis 1: number of outputs

    def forward(self, x):
        x = nn.functional.relu(self.input(x))
        x = nn.functional.relu(self.hidden1(x))
        x = self.hidden2(x)
```

SAVING MODEL

At the end of `NN-f2-5200-no-batch.py` the NN model is saved to disk

```
# save NN model to disk
filename = 'model-neural-k-omega-f_2.pth'
torch.save(NN, filename)
dump(scaler_yplus,'scaler-yplus-k-omega-f_2.bin')
dump(scaler_ystar,'scaler-ystar-k-omega-f_2.bin')

yplus_min = np.min(yplus_train)
ystar_min = np.min(ystar_train)
f_2_min = np.min(f_2_train)

yplus_max = np.max(yplus_train)
ystar_max = np.max(ystar_train)
f_2_max = np.max(f_2_train)

np.savetxt('min-max-model-f_2.txt', [yplus_min,yplus_max,ystar_min,ystar_max,f_2_min,f_2_max]
```

CFD CODE `RANS-K-EPS-NN.PY`

- The NN model `NN-f2-5200-no-batch.py` is loaded at the beginning.
- I define a 1D grid. `yc`, from wall-to-wall. The location of the cell centers are stored in `yp`.
- First, the $\bar{v}_1$ equation is solved.
- The friction Reynolds number, $Re_\tau \equiv u_\tau \delta/\nu = 5\,200$, where δ is half-channel width. u_τ and δ are set to one and hence $\nu = 1/Re_\tau$.
- We're computing fully-developed channel flow (i.e. $\partial \bar{v}_1/\partial x_1 = 0$) and the driving pressure gradient, $\partial \bar{p}/\partial x_1 = 1$ is prescribed, which is obtained from force balance

CFD CODE RANS-K-EPS-NN.PY

- Next, the k and ε equations are solved.
- You may note that the negative source terms in both equations are included in S_P where the total source is $S = S_U + S_P\Phi$, see p. 16 in my CFD lecture notes. With this procedure, there is no way that k and ε can go negative since all terms in the discretized equation (see Eq. 13 on p, 17) then are positive.
- Recall that $a_P = a_W + a_E - S_P$.

GETTING STARTED

T 1.9. Run the `NN-f2-5200-no-batch.py` script and create the NN model. Then run the CFD code, both using the standard AKN $k-\varepsilon$ model, i.e. `NN_bool = False` and using the NN model, i.e. `NN_bool = True`

1.10. In `NN-f2-5200-no-batch.py` I use y^+ and y^* as input parameters. For example, use only one of them. Or maybe y^* and Re_t, as in the original model. Or P^k, or .... You want your NN model to work also in other flows and/or at other Reynolds numbers. Hence, your input parameters must be non-dimensional. The DNS data are non-dimensionalized with u_τ and ν (i.e. you can regard $u_\tau = \nu = 1$)

1.11. Do one of many of the subtasks below

- Use your NN model at other Reynolds numbers. You find DNS data for $Re_\tau = 550$, $Re_\tau = 2\,000$ and $Re_\tau = 10\,000$, at the course www page. Note that when you increase the Reynolds number in `rans-k-eps-NN.py` you may need to increase the number of cells (i.e. increasing `nj`) so that $y^+ < 1$ for the wall-adjacent cells.
- Include another NN model for f_μ
- Train your NN model(s) at $Re_\tau = 10\,000$ and use it in the CFD code for lower Reynolds numbers.

REFERENCES

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[5] Sudarshana S Rao and Santosh R Desai. Machine learning based traffic light detection and ir sensor based proximity sensing for autonomous cars. In *Proceedings of the International Conference on IoT Based Control Networks & Intelligent Systems – ICICNIS*, 2021.