Training a neural network to replace "dataset projections" in d-refinement

This notebook is a companion to "Mesh d-refinement: a data-based computational framework to account for complex material response". The neural network referred to in the appendix is devised herein.

```
J. Garcia-Suarez, 2023
All rights reserved
```

Prepare data for training

Dataset

```
We use exactly the same data that was used for DDCM d-refinement (section 4), these data were obtained from sampling the octet-truss unit cell (section 3.2.).

numLoadSteps = 29;(*number of steps per trajectory*)

SetDirectory [NotebookDirectory []];

dataNL = Import["dataset.csv"];(*make sure that the file
  "dataset.csv" is in the same directory as the notebook, or add path*)

Save per-element stress-strain evolution:

numElements = Dimensions [dataNL][[1]] / numLoadSteps;
```

Characteristic values

These are necessary to normalize the values the NN handles, as it will be much more efficient if there are no units and everything is O(1)

```
Ec = 3591851.;

\sigmac = 16. * 10<sup>4</sup>; (*pressure *)

\epsilonc = \sigmac/Ec;
```

Save trajectories

Prepare data for the NN: reshape and add the origin for each trajectory

```
elementTrajectories = ConstantArray[, {numElements}];
lod
 data = dataNL[[1+(ii-1)*numLoadSteps ;; numLoadSteps *ii, All]];
 data = PrependTo [data, {0., 0., 0., 0., 0., 0.}];
 elementTrajectories [[ii]] = data;
 , {ii, 1, numElements}]
Separate strain and stress, and normalize
allStrain = \frac{1}{-} * (Take[#, 3] & /@ Flatten[elementTrajectories , 1]);
allStress = \frac{1}{\sigma c} * (Drop[#, 3] & /@ Flatten[elementTrajectories , 1]);
Put data in correct input form and separate batches (training validation and verification):
nTraining = Floor[0.7 * numElements];(*70% data training*)
nValidation = Floor[0.9 * numElements] - nTraining;
(*10% to run validation during training*)
nVerification = numElements - (nTraining + nValidation);
(*last 10% to test after training*)
trainingData = Table[allStrain[[ii]] → allStress[[ii]], {ii, 1, nTraining}];
testData = Table[allStrain[[ii]] → allStress[[ii]], {ii, 1+nTraining, numElements}];
```

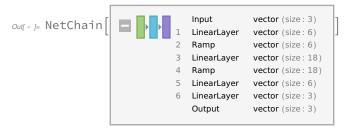
Neural Network

Define architecture

```
This simple architecture is made by:
- Input (3 neurons, one per strain component -- \epsilon_{xx}, \epsilon_{yy} and \gamma_{xy})
- Linear layer (6 neurons)
- Non-linear ReLu layer (6 neurons)
- Linear layer (18 neurons)
- Non-linear ReLu layer (18 neurons)
- Linear layer (6 neurons)
- Output (linear layer w/ 3 neurons, one per stress component -- \sigma_{xx}, \sigma_{yy} and \tau_{xy})
net = NetChain[{6, Ramp, 18, Ramp, 6, 3}, "Input" → 3];
Initialize weights
initializedNet = NetInitialize [net, Method → "Xavier"];
Training
```

trainedNet =

NetTrain[initializedNet , trainingData , ValidationSet → testData , Method → "ADAM"]



Final test

Compute the verification error (%):

$$verAvError = \frac{100}{nVerification} *$$

$$\label{thm:constraint} \begin{split} &\text{Total@Table[Norm[}\sigma\text{c*trainedNet} \text{ /@}\left(\frac{\text{elementTrajectories [[ii, All, 1 ;; 3]]}}{\epsilon\text{c}}\right) - \\ &\text{elementTrajectories [[ii, All, 4 ;; 6]]]/ Norm[elementTrajectories [[ii, All, 4 ;; 6]]], {ii, numElements - nVerification, numElements}] \end{split}$$

Out[•]= 0.959105

Less than 1%