Math6373. 02/16/2022 . Robert Azencott

HW2 due date = Sunday February 27 midnight

Automatic Classification by MLP: one dataset per group (your choice) available Datasets at UC Irvine, Kaggle, ...pre-validate choice by email to RA Exclude classical tutorial setups (such as "10 digits recognition" ...)

Q0 brief dataset description

```
# of classes (must be ≥ 6)
Size & practical meaning of each class
# of cases (must be > 6000); explain what is a typical case
# of features (must be > 50); meaning of each feature
# numerical features, # discrete features
Encoding modality for discrete features
```

HW2: Q1: implement 3 layers MLP

```
Xn = training input vectors dim Xn = k features
6 classes (or more) CL1 CL2 ... CL6
MLP: Input Xn \rightarrow hidden layer H \rightarrow OUTn \rightarrow softmax \rightarrow Pn
dim(OUTn) = 6; dim(hidden layer H) = h is unknown
trueOUTn = one-hot encoding for true class(case n)
Xn \rightarrow Hn \rightarrow OUTn \rightarrow P(n)
P(n) = softmax(OUTn) = [P1(n), ..., P6(n)]
Pj(n) = MLP estimate for probability {case n is in class CLj}
Final MLP decision:
{ case n is in CLj } if P_i(n) = max [P1(n), ..., P6(n)]
```

HW2: Q1: CrossEntropy loss function

For case n in CL4 for instance, MLP+softmax → Pn = [P1(n), ..., P6(n)

trueOUTn = $[0\ 0\ 0\ 1\ 0\ 0]$ is transformed by softmax into the true "probability" Qn = $[0\ 0\ 0\ 1\ 0\ 0]$ on $\{1\ 2\ 3\ 4\ 5\ 6\}$ Loss for case n = CrossEntropy(Qn, Pn) = $-\log[P4(n)]$ Loss(n) = CRE(n) = $-\log[Pj(n)]$ if case n is in class CLj

average CrossEntropy on training set of size N trainAVCRE = [CRE(1) + ... + CRE(N)] / N similar definition for testAVCRE

HW2: Q1: CrossEntopy loss function

if case n is in class CLj

```
we have CRE(n) = - log[Pj(n)]
```

- → if MLP + SFT yields a bad estimate like Pj(n) = 1/100 then CRE(n) = log (100) = 4.6 = high loss
- \rightarrow if MLP + SFT yields a very good estimate like Pj(n) = 98% then CRE(n) = log (0.98) = 0.02 = very small loss

If average CRE(n) on class CLj = a(j)

 \rightarrow expect Pj(n) to be of the order of exp[- a(j)])

HW2: Q1: CrossEntropy loss function

Fix optimizer = ADAMS, batch size = N/50, N= training set size, Response function = RELU, # epochs = 10, random initial weights Fix h = k or k/2. Launch a short training of 10 epochs for instance Monitor AVCRE(m) epoch per epoch on training set and test set Display two monitoring curves versus m= 1... 10 on same graph Transform the 10 values AVCRE(m) as explained above in terms of associated estimated probabilities Display the two transformed monitoring curves. Interpret the results Fix the weights & thresholds at end of last epoch Compute then the AVCRE(class CLj) on each class CLj. Interpret results

HW2: Q2: test "low value" h_{low} for h = dim(hidden H)

```
Xn = input vectors dim Xn = k features 6 classes CL1 ... CL6
PCA analysis of set Centered & Rescaled input vectors Xn
Display PEV = percent. explained variance vs #principal components
Compute h_{low} such that PEV(h_{low}) = 90%
Launch automatic learning for h= h<sub>low</sub> using
batchsize = 100, #epochs = 50, loss function = cross-entropy
Plot curves AVCRE(m) on testset & trainset for epochs m= 1... 50
```

then select the best "m" by following criterion; testAVCRE should be as small as possible but inferior to trainAVCRE

HW2: Q2: test "low value" h_{low} for h = dim(hidden H)

To **select a stopping epoch mSTOP**: first evaluate visually **StabTrain** = epoch of stabilization for trainAVCRE(m) improvement of trainAVCRE(m) should be small for m > StabTrain MinTest = epoch when testAVCRE(m) reaches a global minimum and then starts roughly increasing for most m > MinTest **SafeZone** = all epochs m such that testAVCRE(m) > trainAVCRE(m) this is the zone of **no overfit SafeMinTest** = epoch m* in SafeZone where testAVCRE(m) reaches its minimum on SafeZone & starts increasing on SafeZone m* is often a good mSTOP, but compare it to StabTrain

HW2: Q2: test "low value" h_{low} for h = dim(hidden H)

- Fix m= mSTOP after preceding analysis
- Fix the corresponding MLP classifier denoted MLP_{low}
- For each case #n, this classifier outputs probabilities P1(n) ... P6(n)

- Apply the decision rule
- Predicted class (case n) = class CLj when Pj(n) = max[P1(n) ... P6(n)]
- Run all cases through this MLP_{low} classifier

Compute the 6x6 confusion matrix (in % of accurate classification) interpret the confusion matrix on test set and trainset

HW2 : Q3 : evaluate h_{high} for h = dim(hidden layer)

Separately for each class CLj , of sizeN(j)

Launch PCA analysis for all the N(j) inputs Xn belonging to class CLj Display curve PEVj = % explained variance vs # principal components Compute hj such that PEVj(hj) = 90%

Define $h_{high} = h1 + h2 + ... + h6$

Implement the approach of Q2 for this new value of h

Then select the best of the two sizes h_{high}, h_{low}

Q4: start DEEP LEARNING by AutoEncoder construction

```
Xn = input vector dim <math>Xn = k h= dim H= h<sub>high</sub>
MLP: INP \rightarrow H \rightarrow OUT \rightarrow softmax \rightarrow P(n) = [P1(n), ..., P6(n)]
Goal: Improve this MLP= MLP<sub>high</sub>
Xn → vector Zn (read on Hidden layer H); dim Zn = h
Zn is computed using the weights and thresholds of MLP<sub>high</sub>
Construct an auto encoder L1 -> L2 -> L3 to encode /decode Zn
Zn on L1 => Kn on L2 = encoding Zn => Z'n on L3 = decoding Kn
Z'n should be close to Zn; dim (hidden layer L2) = h2
First step: Compute h2 by PCA analysis of the new inputs Zn
h2= # principal components to get 95% of explained variance
```

Q4: AutoEncoder construction

Construct an auto encoder L1 \Rightarrow L2 \Rightarrow L3 to encode /decode Zn Xn \Rightarrow vector Zn (read on Hidden layer H); dim Zn = h
Zn on L1 => Kn on L2 = encoding Zn => Z'n on L3 = decoding Kn dim (hidden layer L2) = h2; dimL1 = dimL3 = h = h_{high}
Z'n should be close to Zn \Rightarrow Loss function = MSE(Zn,Z'n)

Train auto encoder using batches of size 100
Monitor training by display of the two curves
TrainMSE(m) and TestMSE(m) versus m (epoch per epoch)
Plot also the rescaled TrainRMSE(m) and TestRMSE(m)
Select the best m and fix the corresponding weights/thresholds

Q5: MLP with 3 hidden layers

Keep only weights /thresholds for first half L1 -> L2 of autoencoder Zn computed from Xn using the weights and thresholds of MLP_{high} Zn has become a typical input for L1 The weights /thresholds of autocoder L1 >> L2 transform Zn into a new input vector Kn on L2 Train new short classifier with only 1 hidden layer H3 and inputs Kn Kn on L2 \rightarrow H3 \rightarrow OUT \rightarrow softmax \rightarrow new probability vector P(n) select dimH3 by PCA analysis of the set of all Kn Use cross-entropy as loss function

Q6: MLP_{long} with three hidden layers

Using Q3, Q4 and Q5 we now have a long MLP = MLP_{long} inputXn \Rightarrow H = L1 \Rightarrow L2 \Rightarrow H3 \Rightarrow OUT \Rightarrow softmax \Rightarrow 6 probabilities Xn => Zn => Kn => Un => On => softmax => P(n) weights /thresholds for Xn => Zn were obtained in Q3 weights /thresholds for Zn => Kn were obtained in Q4 weights /thresholds for Kn => Un => On => P(n) were obtained in Q5

Compare performances between all constructed MLP classifiers MLP_{low} MLP_{high} MLP_{long}