

COL 774: Assignment 3

Semester I, 2023-24

[Part A: Decision Trees]. Total Points: 44

[Part B: Neural Networks]. Total Points: 38

Due Date (for both parts): Tuesday Oct 31st, 11:50 pm.

Notes:

- This assignment has two implementation questions.
- You should submit all your code (including any pre-processing scripts written by you) and any graphs that you might plot.
- Do not submit the datasets. Do not submit any code that we have provided to you for processing.
- Include a **write-up (pdf) file**, one (consolidated) for each part, which includes a brief description for each question explaining what you did. Include any observations and/or plots required by the question in this single write-up file (one for each of the parts A and B).
- You should use Python as your programming language. ~~For Decision tree question (only), we may allow using C/C++/Java but you need to confirm with us first.~~
- Your code should have appropriate documentation for readability.
- You will be graded based on what you have submitted as well as your ability to explain your code.
- Refer to the [course website](#) for assignment submission instructions.
- This assignment is supposed to be done individually. You should carry out all the implementation by yourself.
- We plan to run Moss on the submissions. We will also include submissions from previous years since some of the questions may be repeated. Any cheating will result in a zero on the assignment, a penalty of -10 points and possibly much stricter penalties (including a **fail grade** and/or a **DISCO**).

1. (44 points) Decision Trees (and Random Forests):

Imagine you've been hired by the BCCI as a data analyst due to your machine-learning expertise. Your initial assignment is to construct a decision tree-based classifier(s) to forecast the result of a white ball cricket match using various attributes obtained after the first innings is over, e.g., score, as well as meta-information about the match, such as countries playing, who won the toss etc. Your work will revolve around data obtained from the [StatsGuru](#) repository which has been scraped for this purpose. You've been provided with predefined sets of test, train, and validation datasets available for download from the course website. To gain a comprehensive understanding of the dataset, be sure to read the detailed information in the accompanying readme file. Please refrain from making the data publicly accessible and solely utilize it for the purposes of this assignment.

You've also been given a starter code that facilitates file reading and basic tree data structure definition. However, it's worth noting that you have the flexibility to create your code from scratch, as the use of the starter code is not obligatory. Your primary task is to implement the decision tree algorithm for predicting cricket match outcomes based on a variety of features. Additionally, you'll explore the application of Random Forests in the later stages of this problem.

- (a) **(15 points) Decision Tree Construction** Construct a decision tree using the given data to predict whether the team will win or lose the match. You should use mutual information as the criteria for selecting the attribute to split on. At each node, you should select the attribute which results in the maximum decrease in the entropy of the class variable (i.e. has the highest mutual information with respect to the class variable). Remember some attributes are categorical and some are continuous. For handling continuous attributes, you should use the following procedure. At any given internal node of the tree, a numerical attribute is considered for a two-way split by calculating the median attribute value from the data instances coming to that node, and then computing the information gain if the data was split based on whether the numerical value of the attribute is greater than the median or not. For example, if you have 10 instances coming to a node, with values of an attribute being (0,0,0,1,1,2,2,2,3,4) in the 10 instances, then we will split on value 1 of the attribute (median). Note that in this setting, a numerical attribute can be considered for splitting multiple times. At any step, choose the attribute which results in the highest mutual information by splitting on its median value as described above.
- For categorical attributes, you have to perform k way split where k is a number of unique attribute values. For example, if the following instance of training data arrives at a node (*India, India, England, Kenya, Australia, England*) then splitting on this attribute will result in 4 children nodes. While testing if an example coming at this node have a different attribute value (For eg: *Pakistan*) then consider the node as a leaf node and return the prediction.
- Experiment with different maximum depths specifically for {5, 10, 15, 20, 25} and report the accuracy on train and test datasets. Feel free to experiment with other depths for performance gain. Plot the train and test set accuracies against the maximum depth in the tree. On the X-axis you should plot the maximum depth in the tree and the Y-axis should represent the train and test accuracies. Comment on your observations. Also, report the test accuracies for only win prediction and only loss prediction. Comment on your observation.
- (b) **(5 points) Decision Tree One Hot Encoding:** Categorical attributes having more than 2 categories can be encoded using one hot encoding. In one hot encoding, each category of attribute is represented by a new attribute which has 0,1 value depending on the attribute value. Replace the above categorical attributes having more than 2 categories with respective one hot encoding attributes. For example, the attribute *team* has the following categories {*India, Australia, England*} then after replacement the attribute *team* will be replaced with these 3 attributes *team_India, team_Australia, team_England* each having 2 categories 0,1. Repeat part (a) for this transformed dataset with maximum depths for {15, 25, 35, 45}. Compare the results with part (a) and comment on your observations. Feel free to experiment with other depths for performance gain. We will extend this version of the Decision Tree for the part (c) below.
- (c) **(8 points) Decision Tree Post Pruning** One of the ways to reduce overfitting in decision trees is to grow the tree fully and then use post-pruning based on a validation set. In post-pruning, we greedily prune the nodes of the tree (and the sub-tree below them) by iteratively picking a node to prune so that the resultant tree gives a maximum increase in accuracy on the validation set. In other words, among all the nodes in the tree, we prune the node such that pruning it (and the sub-tree below it) results in a maximum increase in accuracy over the validation set. This is repeated until any further pruning leads to a decrease in accuracy over the validation set. Read the following notes on pruning decision trees to avoid overfitting (also available from the course website). Post-prune the trees of different maximum depths obtained in part (b) above using the validation set. Again for each tree plot the training, validation and test set accuracies against the number of nodes in the tree as you successively prune the tree. Comment on your findings.
- (d) **(8 points) Decision Tree sci-kit learn:** As there are number of libraries which provide Decision tree implementation, we would like to compare our own implementation against these. Use the sci-kit learn library to build the decision tree on the dataset provided to you. Change the value of the *criterion* parameter to *entropy*. Next, (i) Vary *max_depth* in range {15, 25, 35, 45}. Keep all other arguments default. Report the train and test accuracies and plot the accuracies against maximum depth. Use the validation set to determine the best value of the depth parameter for your final model. (ii) Next, choose the default value of the depth parameter (which grows the tree fully), and vary value of the pruning parameters *ccp_alpha*, in the range {0.001, 0.01, 0.1, 0.2}. Use default value of all other parameters. Again, plot train and test accuracies against the value of the pruning parameter. Choose the value of the *ccp_alpha* parameter¹ which gives the maximum accuracy on the validation set, and

¹You should read about the semantics of this parameter from Scikit's documentation.

use this as your final model. Now, compare the results obtained using the best model obtained in sub-parts (i) and (ii) above, i.e., with varying *max_depth*, and *ccp_alpha* parameters, with part (b) and (c) and comment on your observations. Note: **Sci-kit's internal implementation uses a one-hot encoding to split multi-valued discrete attributes, so in some sense, results here are comparable to your implementations in parts (b) and (c), respectively.**

- (e) **(8 points) Random Forests:** Random Forests are extensions of decision trees, where we grow multiple decision trees in parallel on bootstrapped samples constructed from the original training data. A number of libraries are available for learning Random Forests over a given training data. In this particular question, you will use the sci-kit learn library of Python to grow a Random Forest. [Click here](#) to read the documentation and the details of various parameter options. Try growing different forests by playing around with various parameter values. Especially, you should experiment with the following parameter values (in the given range): (a) ***n_estimators*** (50 to 350 in range of 100). (b) ***max_features*** (0.1 to 1.0 in range of 0.2) (c) ***min_samples_split*** (2 to 10 in range of 2). You are free to try out non-default settings of other parameters too. Use the out-of-bag accuracy to tune to the optimal values for these parameters. You should perform a grid search over the space of parameters (read the description at the link provided for performing grid search). Report training, out-of-bag, validation and test set accuracies for the optimal set of parameters obtained. How do your numbers, i.e., train, validation and test set accuracies compare with those you obtained in part (c) and part (d) above?
- (f) **Extra Fun: No Credits!:** Read about the XG-boost algorithm which is an extension of decision trees to Gradient Boosted Trees. You can read about gradient boosted trees [here](#) (link 1) and [here](#) (link 2). Try out using XG-boost on the above dataset. Try out different parameter settings, and find the one which does best on the validation set. Report the corresponding test accuracies. How do these compare with those reported for Random Forests?

2. (38 points) Neural Networks:

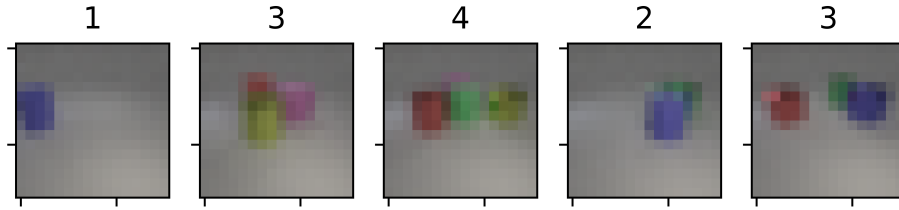
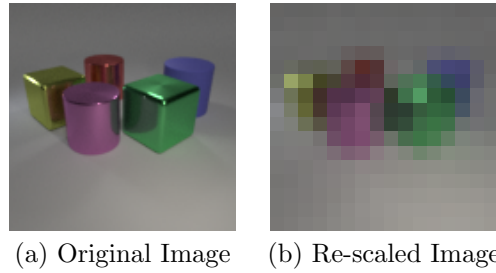


Figure 1: Sample data. The numeric label represents the true number of objects in an image.

In this problem, you will work with the modified version of CLEVR dataset. This is an image dataset consisting of RGBA pixel values of 16×16 size images of objects placed on grey surface. The task is to predict number of objects in an image. The number of objects in an image vary between 1 to 5. Therefore this is a multiclass dataset containing 5 classes. Fig 2 shows some sample examples. The Dataset contains a train and a test set consisting of 10000 and 1000 examples, respectively. Note that the dataset is balanced; i.e. the number of examples is approximately same for all classes in train and test set. Instead of using the standard squared error loss over the logistic function, we will instead use the cross-entropy loss defined over the softmax activation function. Softmax is a generalization of logistic function for the case of multi-valued variables. Given a set of linear inputs $\{net_k^{(L)}\}_{k=1}^r$, applying softmax over it, results in a probability vector of size r , given as $o_1, o_2 \dots o_r$, such that $\sum_k o_k = 1$, and where $o_k = \frac{e^{net_k^{(L)}}}{\sum_{k'} e^{net_{k'}^{(L)}}}$. Given two distributions P and Q , defined over a random variable y , the cross-entropy between them is defined via the expression: $\sum_k P(y = k) \log Q(y = k)$. Then, in our case, the loss $J(\theta)$, is defined as the cross entropy between the true label distribution given as $\tilde{p}(y = k|x) = \mathbb{1}\{k = \tilde{k}\}$, where \tilde{k} , is the true label, and the predicted distribution $\hat{p}(y = k|x) = o_k$ (recall that o_k is simply the probability of outputting label k by the network). Then, the cross entropy loss is defined as:

$$J(\theta) = \sum_{k=1}^r -\mathbb{1}\{k = \tilde{k}\} \log(o_k) \quad (1)$$

The partial derivative of $J(\theta)$, as defined above is given as:

$$\frac{\partial J(\theta)}{\partial net_k^{(L)}} = \begin{cases} (o_k - 1), & \text{if } k = \tilde{k} \\ o_k & \text{otherwise} \end{cases} \quad (2)$$

- (a) **(12 points)** Write a program to implement a generic neural network architecture to learn a model for multi-class classification which outputs probability distribution by using softmax. You will implement the backpropagation algorithm (from first principles) to train your network. You should use mini-batch Stochastic Gradient Descent (mini-batch SGD) algorithm to train your network. Use the Cross Entropy Loss over each mini-batch as your loss function (mentioned above in 1). You will use the sigmoid as activation function for the units in the hidden layer (we will experiment with other activation units in one of the parts below) and softmax at output layer to get final predicted probability distribution. Your implementation(including back-propagation) MUST be from first principles and not using any

pre-existing library in Python for the same. It should be generic enough to create an architecture based on the following input parameters:

- Mini-Batch Size (M)
- Number of features/attributes (n)
- Hidden layer architecture: List of numbers denoting the number of perceptrons in the corresponding hidden layer. Eg. a list $[100\ 50]$ specifies two hidden layers; first one with 100 units and second one with 50 units.
- Number of target classes (r)

Assume a fully connected architecture i.e., each unit in a hidden layer is connected to every unit in the next layer.

- (b) **(5 points)** Use the above implementation to experiment with a neural network having a **single** hidden layer. Vary the number of hidden layer units from the set $\{1, 5, 10, 50, 100\}$. Set the learning rate to 0.01. Use a mini-batch size of 32 examples. This will remain constant for the remaining experiments in the parts below. To be specific you will have following arguments in the generic neural network:

- $M = 32$
- $n = 1024$ ($16 \times 16 \times 4$)
- Hidden layer sizes to be chosen from options
- $r = 5$

Choose a suitable stopping criterion and report it. Read about precision, recall and F (also known as F1) score here. Report the precision, recall and F1 score for each class at different hidden layer units on test data and train data. You could compute these metrics using scikit-learn utility. Plot the average F1 score vs the number of hidden units. Comment your findings.

- (c) **(5 points)** In this part we will experiment with the depth of neural network. Vary the hidden layer sizes as $\{\{512\}, \{512, 256\}, \{512, 256, 128\}, \{512, 256, 128, 64\}\}$. Keep learning rate and batch size same as part b. Use same stopping criteria as before and report the precision, recall and F1 score for all variations on test data and train data. Plot the average F1 score vs the network depth.
- (d) **(5 points)** Use an adaptive learning rate inversely proportional to number of epochs i.e. $\eta_e = \frac{\eta_0}{\sqrt{e}}$ where $\eta_0 = 0.01$ is the seed value and e is the current epoch number² and repeat part c. See if you need to change your stopping criteria. Report your stopping criterion. As before, report the precision, recall and F1 score for each class at different hidden layer depth on test data and train data. Plot the average F1 score vs depth of hidden units. How do your results compare with those obtained in the part above? Does the adaptive learning rate make training any faster? Comment on your observations.
- (e) **(6 points)** Several activation units other than sigmoid have been proposed in the literature such as tanh, and ReLU to introduce non linearity into the network. ReLU is defined using the function: $g(z) = \max(0, z)$. In this part, we will replace the sigmoid activation units by the ReLU for all the units in the hidden layers of the network. You can read about relative advantage of using the ReLU over several other activation units [on this blog](#).

Change your code to work with the ReLU activation unit in the hidden layers. The activations in the final layer still stay softmax. Note that there is a small issue with ReLU that it is non-differentiable at $z = 0$. This can be resolved by making the use of sub-gradients - intuitively, sub-gradient allows us to make use of any value between the left and right derivative at the point of non-differentiability to perform gradient descent see this ([Wikipedia page](#) for more details). Repeat the part d with ReLU activation. Report your training and test set precision, recall and F1 score. Plot the average F1 score vs network depth. Also, make a relative comparison of test set accuracies obtained in part d. What do you observe? Which ones performs better?

- (f) **(5 points)** Use `MLPClassifier` from scikit-learn library to implement a neural network with the same architectures as in part e above. Use Stochastic Gradient Descent as the solver. Note that `MLPClassifier` only allows for Cross Entropy Loss over the final network output. Set the following parameters:
- `hidden_layer_sizes`: to be vary according to part c.
 - `activation`: relu
 - `solver`: sgd

²One epoch corresponds to one complete pass through the data

- `alpha`: 0
- `batch_size`: 32
- `learning_rate`: invscaling

Keep all other parameter as default. You need to decide the stopping criteria accordingly. Now report the same metrics and plots as of part e. Compare the results with part e, and comment on your observations.