Due on October 20, 2016

Please refer to <u>homework 1</u> and the class mechanics web page for homework policies and formatting/submission instructions. The submission checklist for this assignment is as follows:

hw4.pdf, bags.m, trainForest.m, forestValue.m, oobError.m

plus any other functions you wrote to run your experiments, as explained in problem 5. Keep in mind that your code must also show up in hw4.pdf.

Classification and Regression Forests

The MATLAB files provided with this assignment follow the class notes to implement a recursive version of classification trees. To streamline this assignment, the following main changes are made with respect to the notes:

- In classification problems, all labels are integers starting at 1, for easier compatibility with MATLAB indexing.
- Training and test data are stored into arrays with one data point per *row* rather than per column. For instance, a labeled classification set T with N samples (\mathbf{x}, y) where features \mathbf{x} are d-dimensional is represented by a data structure T with an $N \times d$ field T.X and an $N \times 1$ field T.Y. We will also look at regression problems, in which the values are real numbers.¹ Those are stored by rows in T.Y as well, so T.Y is a column vector.
- Since we are not interested in classification or regression confidence values in this assignment, the leaves of a classification or regression tree contain the values (discrete labels for classification, real values for regression), rather than their distribution.
- Functions that compute impurity values for training take the set T.y of values as input, rather than all of T (the features are irrelevant for impurity).
- The top-level function treeClassify is renamed treeValue, so the same function can be used for both classification and regression.
- All the parameters and hyper-parameters of a tree are encapsulated into a single data structure that is returned by the provided function treeClassifierDefaults, which in turn calls treeCommonDefaults. This structure is passed to the tree for both training and classification. The call

parms = treeClassifierDefaults(L);

where L is a positive integer (the number of possible label values, which are then $\{1, \ldots, L\}$) returns a structure parms with the following fields:

- parms.maxDepth is the maximum allowed tree depth and is set to Inf by default.
- parms.minSetSize is the minimum allowed set size in any tree node and is set to 1 by default.
- parms.doRandomSplit is a Boolean flag that specifies whether the split dimension at each node is to be chosen at random (true) or optimally. This flag is set to true by default.
- parms.classifier is a Boolean flag that is true for classifiers and false for regressors.
- parms.nLabels is set to L.
- parms.value is a function that takes a vector of labels and returns a plurality label in the vector (that is, a label that has the most representatives in the vector).
- parms.impurity is a function that takes a vector of labels and returns the empirical classification error of parms.value on that vector.
- parms.error is a function that takes an array (not necessarily a vector) fx of computed labels and an equally-sized array y of true labels and returns an equally-sized array of error indicators (a double number that is 1 where fx and y differ and 0 where they coincide).
- parms.aggregateError is a function that takes an array (not necessarily a vector) of error indicators as computed by parms.error and returns the mean error (the fraction of array values that are equal to 1).

The first three fields above are set in treeCommonDefaults and are used for both classification and regression. Leave these fields unchanged. You may want to study these functions to understand more concretely what they do.

¹They could also be vectors of real numbers, but we keep things simple here.

Coding Tips

The code provided with this assignment is recursive, and is both simple and slow. Because of this, first test and debug your code on small inputs, and write a single MATLAB script that computes all you need to solve the problems below. Go full size only once everything works.

If you need to run the same code multiple times with different inputs or parameters, it would be very error-prone to replicate code by cutting and pasting. Instead, write a small number of functions that take the necessary inputs and parameters and call them multiple times. Keep in mind that wrong conclusions are not given credit, even if they are reached through correct reasoning from wrong data. So it's in your interest to program in an orderly and modular way.

When you test a classifier on, say, all the pixels in an image, the provided recursive functions can only process one data point at a time, so it's OK to loop over data (including images) when using treeValue or forestValue. However, it is still bad form (and a waste of your time, and grounds for credit deductions) to use explicit for loops on images when more efficient MATLAB constructs are available.

1. As a reference for later problems, you will first use provided code to compute the gradient of two images by convolution with appropriate derivatives of a Gaussian, as we learned in class. The two images are produced by the functions rings and waves. Specifically, the call

$$[I, gI, qI] = rings(L, n)$$

where both L and n are positive integers makes an $n \times n$ image I that shows some rings. The function used to produce the image is known analytically, so it is possible to compute its gradient by exact calculus. The result is in gI, with gI(:, :, 1) containing the x derivative and gI(:, :, 2) containing the y derivative. Here and elsewhere in this assignment, we revert to the more natural convention of an x axis pointing to the right and a y axis pointing up, so that it is easier to visualize what is going on.

The output image qI is a version of gI quantized to L levels, and you will use this image in later problems. If you are interested in seeing how quantization is done, look at the provided function quantize.

You can make a numerical approximation ngI of gI by using the provided function gradient, whose output is in the same format as gI.

Run rings (6, 64) and make a single, full-page figure with a 4 by 2 array of images (four rows and two columns) in your PDF file. The rows show respectively the two components of gI,ngI, abs(ngI - gI), and qI. Use the MATLAB colorbar command to put a color bar next to each of these four images, to make it possible to interpret the values of the gray levels. Make the color bar values legible by setting their font size to 36 points as follows:

cb = colorbar; set(cb, 'FontSize', 36);

Do not show I and do not show your code. Also, do not show the result of running waves. We will use that later. Use imagesc to display the images and put meaningful captions under each.

2. Write a MATLAB function with header

function b = bags(n, k)

that takes positive integers n and k and returns a $n \times k$ matrix b. Each column of b is a random bag out of $A = \{1, ..., n\}$, that is, a set of n values drawn out of A with replacement.

Hand in your code (both in the PDF file and as a separate MATLAB file), as well as the array resulting from the call

bags(5, 3)

Do not use any explicit loops.

3. The function trainForest provided with this assignment takes a training set T, a desired number M of trees, and a parameter structure parms as described above. This function currently ignores M and just calls trainTree to make a forest with a single tree. The resulting forest phi has field phi.tau, which contains the single tree, and a field phi.used that is set to a Boolean column vector with N true values, where N is the number of samples in T. This vector is currently set to all true values to signify that all samples in T were used to train the tree. This will change in your version.

Rewrite trainForest so that it calls trainTree repeatedly and returns a forest phi with M trees in phi.tau. Column j of the Boolean array phi.used should flag the samples in T that were used to train phi.tau(j). Hand in your code (both in the PDF file and as a separate MATLAB file). No output yet.

[Hints: The call unique (b) where b is a column vector returns a unique, sorted list of the items in b. Do not delete the statement that prints out a progress message. This will be useful later, as trainForest is slow.]

4. The function forestValue provided with this assignment just calls treeValue once and returns its result. So calling either function returns the same result.

Rewrite forestValue so that it returns the value computed by the whole forest phi. Hand in your code (both in the PDF file and as a separate MATLAB file). No outputs yet.

5. Let us pretend that we do not know how to compute the gradient of an image. Since we just studied classification trees, it occurs to us that we could at least estimate the values of the gradient quantized to L = 6 values. Specifically, we can train two classification forests (one for I_x and one for I_y) with M trees on the image I and quantized gradients qI you computed earlier, and then use the resulting forest on new images for which we want to compute the gradient.

For training features, we simply take the 5×5 window around each pixel in the image I produced by rings (with the same arguments used earlier), reshape the 25 values into a 25-dimensional row vector, and use the provided functions PCA and compress to shorten these features to, say, 8 components.

For training labels, we use the exact labels in qI.

Of course, we can only compute features and labels for the central 60×60 part of the 64×64 image, for a total of 3600 training samples.

The provided function

function T = features(data, nFeatures, winSize)

computes these samples. The first argument is a data structure with fields data.X and data.Y. In the example, these are 64 by 64 images, and data.y is either the x or the y component of the true quantized gradient. The value of nFeatures is Inf if all the pixels in the image are to be used for training. Otherwise, nFeatures pixels chosen at random are used.² The value of winSize is the side length of the square feature window (5 in the example). The function features does *not* do PCA. It returns a training set in the format described earlier.

Train two forests (one for I_x and one for I_y) with M = 10 trees using all the 3600 valid pixels in images I and qI from problem 1, and compute six images. The first two images show the true labels. The second two show the labels resulting from running your classifiers on the 64×64 training image produced by rings. The third two images show the binary training classification error on each component of the gradient of I. In the error images, a pixel is black if there is no error and white if there is.

Hand in your code (both in the PDF file and as a separate MATLAB file) and show the six resulting images in a single figure with two images per row and with appropriate captions. When you list your code in the PDF, make sure it fits on the page, possibly by breaking longer functions over multiple pages.

[Hints: Organize your code so that it is easy to run additional experiments with different training or test data. I chose to write the following functions to keep things clear, even at the cost of repeating some computation:

- assemble packages all the data (training and testing), plus fields that help me keep track of what experiment I am running into a single data structure data.
- experiment takes the structure computed by assemble plus the other parameters it needs and runs an entire experiment. It outputs a single structure result with all that the function computes. This function also writes images to files with appropriate names, so it is easy to include these into the solution PDF file. Designing appropriate file names take time and care and makes the function somewhat lengthy. However, this is effort well spent, to prevent mistakes when you show your results.

It is likely that you will add to these functions as you solve additional problems below. You may choose to do things differently, but explain clearly what you do as you show your code.]

6. Run the same tests as for the previous problem, but use the files output by waves for testing. Training is still done on the images from rings. No code, just show the usual six-image figure.

[Hint: You should expect significantly worse results for testing than those you obtained for training.]

7. Quantizing gradient values to six levels is a very drastic measure. A much better solution is to modify random forests to they can do regression in addition to classification. Interestingly, all we need to do is to write a new function treeRegressorDefaults to call instead of treeClassifierDefaults as discussed next.

Instead of minimizing the misclassification rate, a regressor minimizes the empirical Root Mean Squared Error (RMSE)

$$\overline{err}(f,T) = \sqrt{\frac{1}{N}\sum_{n=1}^{N} \|f(\mathbf{x}_n) - y_n\|^2}$$

where N is the number of training samples in T and the discrete label is now replaced by a real value y_n .

Instead of a plurality label, the regressor computes the empirical mean of the training values at a leaf of the tree:

$$m(Y) = \frac{1}{|Y|} \sum_{n=1}^{|Y|} y_n$$

²This argument is provided for generality. We will not use it in this assignment, so you can set it to Inf all the time.

where Y is the set of values at a leaf. Instead of the misclassification rate, impurity is the deviation from this mean, as measured by the empirical variance

$$\sigma(Y) = \frac{1}{|Y|} \sum_{n=1}^{|Y|} (y_n - m(Y))^2 .$$

These changes are implemented for you in the provided function treeRegressorDefaults. Note that the function takes no arguments.

If needed, modify any code you wrote for previous problems to also accommodate a regressor. No code in any of the tree or forest computations needs to change, if you wrote things properly (that is, if you used the fields of parms whenever possible and appropriate).

Then, train two random forests with M = 10 trees as regressors for the two components of the gradient. Use the same features as above, but now use as values the two components of gI rather than the labels qI.

There is no code to submit for this problem. Instead, compute six images. As before, the first two show the true values for each component of the gradient of I. The second two show the regression values resulting from running your regressors on the training image itself for each component of the gradient of I. The third two images show the regression error on each component of the gradient of I. Show the six resulting images in a single figure with appropriate captions. Each image should come with a color bar with font size 36, as explained earlier.

8. Repeat the previous problem using the images from rings for training and those from waves for testing. Only hand in the six-image figure. Each image should come with a color bar with font size 36, as explained earlier.

[Hint: Again, test results are worse than results on the training image.]

9. Write a MATLAB function with header

function e = oobError(phi, T, parms)

that computes the out-of-bag error estimate for a random forest phi trained on set T and with tree parameters parms. Your function should use the appropriate fields of the parms data structure returned by either treeClassifierDefaults or treeReqressorDefaults to compute error and aggregate error.

Hand in your code (both in the PDF file and as a separate MATLAB file). Also show a table with four rows and two columns (plus column and row headers) that lists the errors in your regression experiments (the one without label quantization). Specifically, for the x and y components of the gradient, the four rows should show (i) the aggregate numerical RMSE error deriving from computing the gradient with the provided gradient function; (ii) the aggregate empirical RMSE training error; (iii) the aggregate out-of-bag RMSE error estimate; (iv) the aggregate empirical test error. All errors are computed against the true gradient values produced by waves (for the testing errors) or rings (for all other errors). Make sure that the functions parms.error and parms.aggregateError are invoked for these calculations. The format of the table is as follows:

	$\partial I / \partial x$	$\partial I/\partial y$
Numerical		
Training		
Out-of-Bag		
Testing		

10. How do the values in the Training and Out-of-Bag rows in the previous table tell you whether your regressor generalizes well or overfits? Briefly explain the conclusion you draw from these values.

11. Compare the Out-of-Bag and Testing rows in the table above. How can you explain the results of this comparison?

12. Explain how you can use the field phi.used of a random forest to verify that each tree is trained on about 63 percent of all training samples. Show the result of doing so on any one of your forests (it does not matter which one you use).