Compsci 571 HW2

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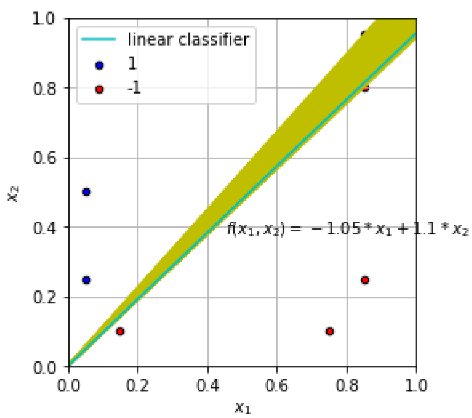
1 Classifier for Basketball Courts

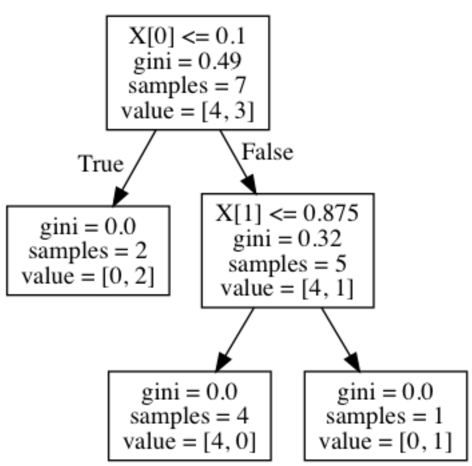
(a) When running Perceptron algorithm on the dataset, it takes 7 iterations (updates) to converge. The decision boundary is $f(x_1, x_2) = -1.05 * x_1 + 1.1 * x_2$. Because after it converges, all training points are correctly classified, the error rate is 0.

Assume another linear classifier that goes through origin and achieves the same training error rate (0) as the perceptron classifier is $f(x_1, x_2) = w_1 * x_1 + w_2 * x_2$. Set $f(x_1, x_2) = 0$, we get the slope of the boundary is $-\frac{w_1}{w_2}$. From the plot of training data, we know that the boundary should go above point $[0.85, 0.80]$, and go below point $[0.85, 0.95]$. So $\frac{0.80}{0.85} < -\frac{w_1}{w_2} < \frac{0.95}{0.85}$. If we set $w_2 = 1$, we get $-1.12 < w_1 < -0.94$.

The plot of observed data, the perceptron decision boundary (the light blue line), and all other linear boundaries that achieve the same training error (the yellow area) is:



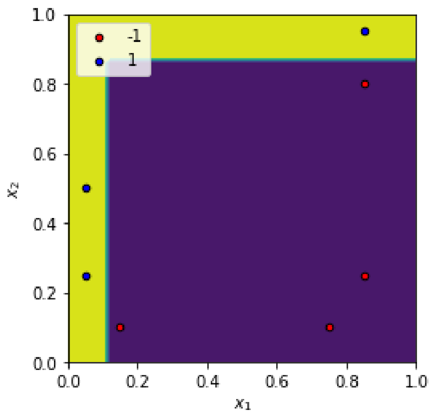
(b) The fully-grown decision tree using Gini index as splitting criterion on the observed data is:



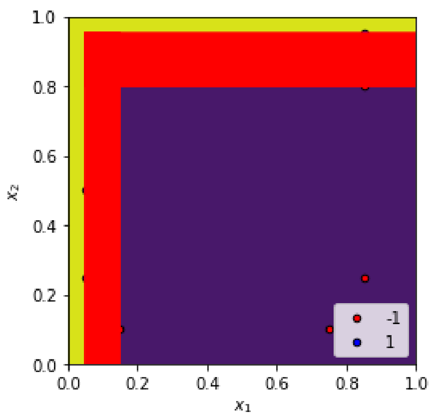
Because all training points are correctly classified by this tree, its training error is 0.

Assume another decision tree with same training error (0) splits on the same feature order but different splitting threshold (v_1 for x_1 and v_2 for x_2). Then the threshold of the first split on x_1 should be able to separate points $[0.05, 0.25], [0.05, 0.5]$ (+1) with $[0.15, 0.1]$ (-1). So v_1 should be $\in (0.05, 0.15)$. The threshold of the second split on x_2 should be able to separate points $[0.85, 0.8]$ (-1) with $[0.85, 0.95]$ (+1). So v_2 should be $\in (0.8, 0.95)$.

The plot of observed data, and the calculated decision boundary is:



The plot of observed data, the calculated decision boundary, and all other decision boundaries that achieve the same training area (the red area) is:



(c) Suppose the real optimal linear classifier that passes through the origin is $f(x_1, x_2) = w_1 * x_1 + w_2 * x_2$, such that it is able to minimize $R^{true}(f)$.

$$T = R^{true}(f) = \mathbb{E}_{(\mathbf{x},y)\sim D} l(f(\mathbf{x}), y) = \mathbb{E}_{(\mathbf{x},y)\sim D} \mathbf{1}_{[sign(f(\mathbf{x}))\neq y]} \tag{1}$$

$$= \mathbf{P}(sign(f(\mathbf{x})) \neq y) \tag{2}$$

$$= \mathbf{P}(y = 1, f(\mathbf{x}) \leq 0) + \mathbf{P}(y = -1, f(\mathbf{x}) \geq 0) \tag{3}$$

$$= \mathbf{P}(w_1x_1 + w_2x_2 \leq 0, 0 \leq x_1 \leq 1, \sqrt{x_1} \leq x_2 \leq 1) + \mathbf{P}(w_1x_1 + w_2x_2 \geq 0, 0 \leq x_1 \leq 1, 0 \leq x_2 \leq \sqrt{x_1}) \tag{4}$$

$$= \mathbf{P}(x_2 \leq -\frac{w_1}{w_2}x_1, 0 \leq x_1 \leq 1, \sqrt{x_1} \leq x_2 \leq 1) + \mathbf{P}(x_2 \geq -\frac{w_1}{w_2}x_1, 0 \leq x_1 \leq 1, 0 \leq x_2 \leq \sqrt{x_1}) \tag{5}$$

Step (2) is from the property of expectation on indicator function.

Assign $k = -\frac{w_1}{w_2}$, $k \in [0, \infty)$, equation (5) becomes:

$$= \mathbf{P}(x_2 \leq kx_1, 0 \leq x_1 \leq 1, \sqrt{x_1} \leq x_2 \leq 1) + \mathbf{P}(x_2 \geq kx_1, 0 \leq x_1 \leq 1, 0 \leq x_2 \leq \sqrt{x_1}) \tag{6}$$

So we need to find the optimized k that minimizes $R^{true}(f)$, or equivalently equation (6).

Because (x_1, x_2) follow a uniform distribution, the 2 probability values in equation (6) are just areas formed by the border lines. We could use integration to compute them. (Here I use Python packages to compute the optimized values, see code for details.)

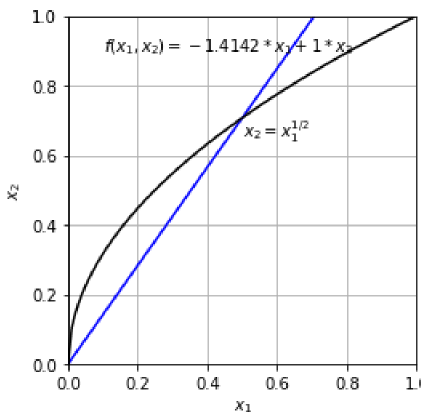
If $k \in [0, 1]$, local optimized $k' = 1$ minimizes $T' = \frac{\pi}{4} - \frac{1}{2}$.

If $k \in (1, \infty)$, local optimized $k'' = 1.4142$, and $T'' = 0.09763107$.

So the global optimized $k^* = k'' = 1.4142$, the optimal linear classifier that passes through the origin is $\mathbf{f(x_1, x_2) = -1.4142 * x_1 + 1 * x_2 = 0}$, and the corresponding minimal $R^{true}(f) = 0.09763107$.

This solution **is not** among the solutions that achieved the same loss (0) in part (a).

The plot of the decision boundary (blue line) on the basketball court is:



(d)

$$T = R^{true}(f) = \mathbf{P}(f(\mathbf{x}) \leq 0, y = 1) + \mathbf{P}(f(\mathbf{x}) \geq 0, y = -1) \tag{7}$$

For tree 1 which starts splitting on X_1, there are 4 different conditions regarding s_1, s_2, s_3:

If $0 \leq s_2 < \sqrt{s_1}$ and $\sqrt{s_1} < s_3 \leq 1$, $\min_{s_1,s_2,s_3} T = \int_0^{s_2^2}(s_2 - \sqrt{x})dx + \int_{s_2^2}^{s_1}(\sqrt{x} - s_2)dx + \int_{s_1}^{s_3^2}(s_3 - \sqrt{x})dx + \int_{s_3^2}^{1}(\sqrt{x} - s_3)dx$

If $0 \leq s_2 < \sqrt{s_1}$ and $0 \leq s_3 \leq \sqrt{s_1}$, $\min_{s_1,s_2,s_3} T = \int_0^{s_2^2}(s_2 - \sqrt{x})dx + \int_{s_2^2}^{s_1}(\sqrt{x} - s_2)dx + \int_{s_1}^{1}(\sqrt{x} - s_3)dx = \min_{s_1,s_2,s_3=\sqrt{s_1}}(\int_0^{s_2^2}(s_2 - \sqrt{x})dx + \int_{s_2^2}^{s_1}(\sqrt{x} - s_2)dx + \int_{s_1}^{1}(\sqrt{x} - \sqrt{s_1}dx)$

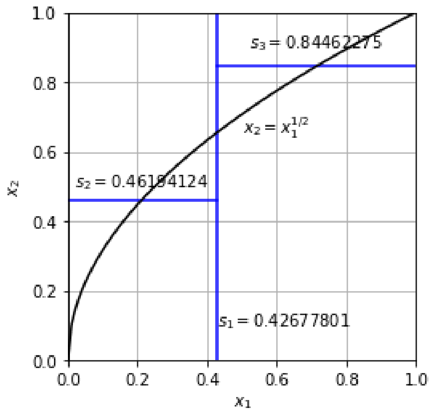
If $\sqrt{s_1} \leq s_2 \leq 1$ and $\sqrt{s_1} < s_3 \leq 1$, $\min_{s_1,s_2,s_3} T = \int_0^{s_1}(s_2 - \sqrt{x})dx + \int_{s_1}^{s_3^2}(s_3 - \sqrt{x})dx + \int_{s_3^2}^{1}(\sqrt{x} - s_3)dx = \min_{s_1,s_2=\sqrt{s_1},s_3}(\int_0^{s_1}(\sqrt{s_1} - \sqrt{x})dx + \int_{s_1}^{s_3^2}(s_3 - \sqrt{x})dx + \int_{s_3^2}^{1}(\sqrt{x} - s_3)dx)$

If $\sqrt{s_1} \leq s_2 \leq 1$ and $0 \leq s_3 \leq \sqrt{s_1}$, $\min_{s_1,s_2,s_3} T = \int_0^{s_1}(s_2 - \sqrt{x})dx + \int_{s_1}^{1}(\sqrt{x} - s_3)dx = \min_{s_1,s_2=\sqrt{s_1},s_3=\sqrt{s_1}}(\int_0^{s_1}(\sqrt{s_1} - \sqrt{x})dx + \int_{s_1}^{1}(\sqrt{x} - \sqrt{s_1})dx)$

The global optimized solutions are $\mathbf{s_1 = 0.42677801, s_2 = 0.46194124, s_3 = 0.84462275}$ which gives minimal $R^{true}(f) = \mathbf{0.1035845342551841}$. (See code for calculation details.)

The real optimized tree decision boundary **is not** among those achieved in part (b).

The plot of the decision boundary (blue line) on the basketball court is:



For the tree which starts splitting from X_2, there are also 4 different conditions regarding s_1, s_2, s_3:

If $0 \le s_2 < s_1^2$ and $s_1^2 < s_3 \le 1$, $\min_{s_1,s_2,s_3} T = \int_0^{s_2} \sqrt{x}dx + \int_{s_2}^{s_1^2}(s_1 - \sqrt{x})dx + \int_{s_1^2}^{s_3}(\sqrt{x} - s_1)dx + \int_{s_3}^{1}(1 - \sqrt{x})dx$

If $s_1^2 \le s_2 \le 1$ and $s_1^2 < s_3 \le 1$, $\min_{s_1,s_2=s_1^2,s_3} T = \int_0^{s_1^2} \sqrt{x}dx + \int_{s_1^2}^{s_3}(\sqrt{x} - s_1)dx + \int_{s_3}^{1}(1 - \sqrt{x})dx$

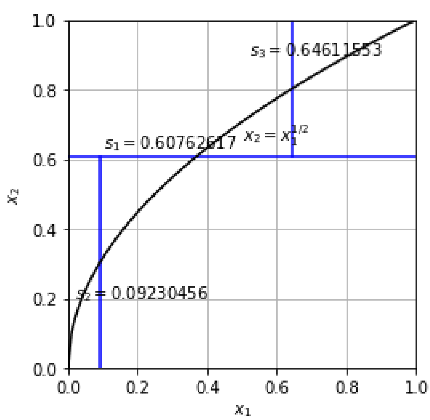
If $0 \le s_2 < s_1^2$ and $0 \le s_3 \le s_1^2$, $\min_{s_1,s_2,s_3=s_1^2} T = \int_0^{s_2} \sqrt{x}dx + \int_{s_2}^{s_1^2}(s_1 - \sqrt{x})dx + \int_{s_1^2}^{1}(1 - \sqrt{x})dx$

If $s_1^2 \le s_2 \le 1$ and $0 \le s_3 \le s_1^2$, $\min_{s_1,s_2=s_1^2,s_3=s_1^2} T = \int_0^{s_1^2} \sqrt{x}dx + \int_{s_1^2}^{1}(1 - \sqrt{x})dx$

The global optimized solutions are $\mathbf{s_1 = 0.60762617, s_2 = 0.09230456, s_3 = 0.64611553}$ which gives minimal $R^{true}(f) = \mathbf{0.11796176307566364}$. (See code for calculation details.)

The real optimized tree decision boundary **is not** among those achieved in part (b).

The plot of the decision boundary (blue line) on the basketball court is:



(e) Transform x_2 into $\mathbf{x_2^* = x_2^2}$. So now $x_1 \in [0,1]$, $x_2^* \in [0,1]$, and the true boundary for the 3-point line is $x_2^* = x_1$.

Suppose the real optimal linear classifier that passes through the origin is $f(x_1, x_2^*) = w_1 x_1 + w_2^* x_2^*$.

$$T = R^{true}(f) = \mathbf{P}(f(\mathbf{x}^*) \le 0, y = 1) + \mathbf{P}(f(\mathbf{x}^*) \ge 0, y = -1) \tag{8}$$

$$= \mathbf{P}(x_2^* \le -\frac{w_1}{w_2^*}x_1, 0 \le x_1 \le 1, x_2^* \ge x_1) + \mathbf{P}(x_2^* \ge -\frac{w_1}{w_2^*}x_1, 0 \le x_1 \le 1, x_2^* \le x_1) \tag{9}$$

And it is easy to find out that the optimal value of $-\mathbf{\frac{w_1}{w_2^*} = 1}$, the optimal linear classifier that passes through the origin is $\mathbf{f(x_1, x_2^*) = -x_1 + x_2^* = 0}$, and the corresponding minimal true error is $\mathbf{0}$.

(f) With the same transformation of x_2 as in part (e), a decision tree **cannot** achieve the same minimal true error (0) as the linear classifier in part (e). This is because the splitting boundary of decision tree can never be a line going through the origin.

(g) For paint, assume the part inside paint ($0.5 \leq x_1 \leq 1$ and $0 \leq x_2 \leq 0.25$) has label $y = -1$ and the part outside paint has $y = 1$.

Same as in part (c), suppose the real optimal linear classifier that passes through the origin is $f(x_1, x_2) = w_1 x_1 + w_2 x_2$, such that it is able to minimize $R^{true}(f)$.

$$T = R^{true}(f) = \mathbf{P}(f(\mathbf{x}) \leq 0, y = 1) + \mathbf{P}(f(\mathbf{x}) \geq 0, y = -1) \tag{10}$$

$$= \mathbf{P}(x_2 \leq -\frac{w_1}{w_2} x_1, y = 1) + \mathbf{P}(x_2 \geq -\frac{w_1}{w_2} x_1, y = -1) \tag{11}$$

Assign $k = -\frac{w_1}{w_2}$, $k \in [0, \infty)$,

$$= \mathbf{P}(x_2 \leq k x_1, y = 1) + \mathbf{P}(x_2 \geq k x_1, y = -1) \tag{12}$$

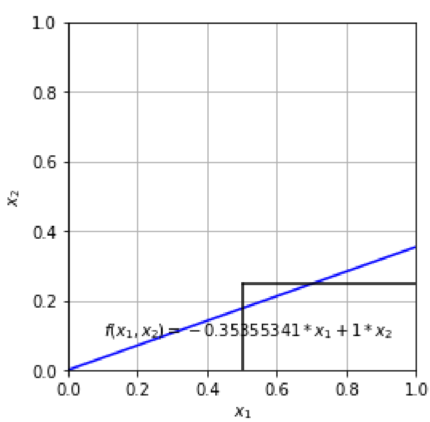
If $k \in [\frac{1}{2}, \infty)$, local optimized $k' = \frac{1}{2}$ minimizes $T' = \frac{1}{8}$.

If $k \in (\frac{1}{4}, \frac{1}{2})$, $min_k T = \int_0^{\frac{1}{2}} kx dx + \int_{\frac{1}{2}}^{\frac{1}{4k}} (\frac{1}{4} - kx) dx$. And the local optimized $k'' = 0.35355341$ minimizes $T'' = 0.0517766952966372$.

If $k \in [0, \frac{1}{4}]$, $min_k T = \int_0^{\frac{1}{2}} kx dx + \int_{\frac{1}{2}}^{1} (\frac{1}{4} - kx) dx = 0.0625$ when $k = \frac{1}{4}$.

So in conclusion, the global optimized $-\frac{w_1}{w_2} = k = \mathbf{0.35355341}$, the optimal linear classifier that passes through the origin is $\mathbf{f(x_1, x_2) = -0.35355341 x_1 + x_2 = 0}$, and the corresponding minimal true error rate $R^{true}(f) = \mathbf{0.0517766952966372}$.

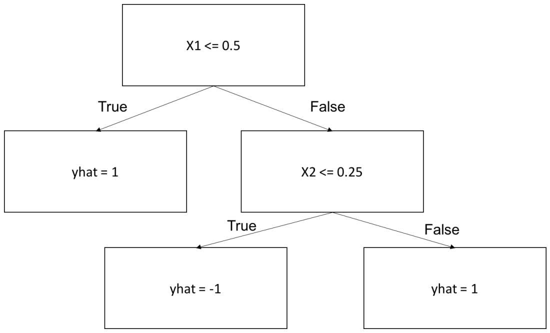
The plot of the decision boundary on the basketball court is:



(h) The optimal depth 2 decision tree will split on $x_1 = m$ and $x_2 = n$. And $f(\mathbf{x}) = -1$ if $m \leq x_1 \leq 1$ and $0 \leq x_2 \leq n$, $f(\mathbf{x}) = 1$ otherwise.

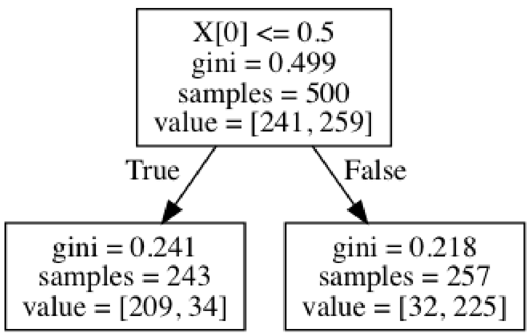
$$T = R^{true}(f) = \mathbf{P}(f(\mathbf{x}) \leq 0, y = 1) + \mathbf{P}(f(\mathbf{x}) \geq 0, y = -1) \tag{13}$$

It's easy to find out that when $\mathbf{m} = \mathbf{\frac{1}{2}}$ and $\mathbf{n} = \mathbf{\frac{1}{4}}$, both $\mathbf{P}(f(\mathbf{x}) \leq 0, y = 1)$ and $\mathbf{P}(f(\mathbf{x}) \geq 0, y = -1)$ are equal to 0, and T achieves its minimal value $\mathbf{0}$. The depth 2 decision tree looks like:

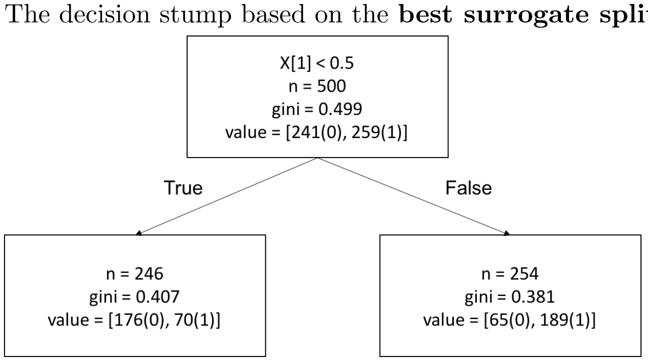


2 Variable Importance for Trees and Random Forests

(a) (i) The decision stump based on the **best split** (for each node, split on the variable with largest reduction in Gini Index) is:



At root it splits on independent variable X_1 (shown as $X[0]$ in picture) on the threshold $s_1 = 0.5$. The decision stump based on the **best surrogate split** is:



This tree is generated by choosing the best surrogate split on the root (by comparing the predictive similarity measure on variables X_2, X_3, X_4 and X_5). At root it chooses X_2 (shown as $X[1]$ in picture) as the best surrogate split, with threshold 0.5 (actually this value doesn't really matter).

(ii) Variable importance measures from equation (2) are:

X_1	0.2703
X_2	NA
X_3	NA
X_4	NA
X_5	NA

Variable importance measures from equation (3) are:

X_1	0.2703
X_2	0.1056
X_3	NA
X_4	NA
X_5	NA

(See code for calculation process)

If we only refer to the variable importance measures from equation (2), we can only say variable X_1 is the known most important variable among the five, but not sure if any other variables has similar importance as it.

With the variable importance measures from equation (3), we could see comparing variable X_1 and its most close substitute/surrogate X_2, X_1 is still more important than X_2. So we could suggest with more confidence that X_1 is more important than others.

(iii) The mean squares error of predictions on the test data from the decision stump based on the best split is 0.1.

The mean squares error of predictions on the test data from the decision stump based on the best surrogate split is 0.27.

(see code for calculation process)

(b) For all following random forests in (b) and (c), I set the Python numpy random seed to 111.

(i) The table for best split variable and best surrogate variable for each K is:

(Note that when $K = 1$ there are only 999 trees in the forest, because there is one potential tree generating negative reduction in Gini index, and this tree is dropped. And whether this happens or not depends on the bootstrap training sample selected for each tree.)

K	variable	time as best split variable	time as best surrogate variable
1	X_1	215	0
	X_2	203	0
	X_3	186	0
	X_4	192	0
	X_5	203	0
2	X_1	399	0
	X_2	312	106
	X_3	119	291
	X_4	116	268
	X_5	54	335
3	X_1	585	0
	X_2	321	291
	X_3	48	288
	X_4	39	146
	X_5	7	275
4	X_1	788	0
	X_2	212	582
	X_3	0	168
	X_4	0	22
	X_5	0	228
5	X_1	1000	0
	X_2	0	1000
	X_3	0	0
	X_4	0	0
	X_5	0	0

First of all, we need to make clear the implication of different values of K. When K is smaller (like 1), variables are given more equal opportunities to become the best split variable. When K is larger (like 5), the competition between variables to become the best split gets more fierce, and important variables are more likely to win out as the best split.

So according to the frequency of best split variables, X_1 is selected as the best split variable more as K increases. So this suggests variable X_1 is more important than others.

And according to the frequency of best surrogate split variables, X_2 is selected more as K increases. So this suggests while X_1 is important, the importance of X_2 could have been masked by that of X_1. So we also need to consider the importance of X_2.

(ii) The variable importance according to equations (5) and (6) for each K is:

K	variable	variable importance (5)	variable importance (6)
1	X_1	0.269419	0.370326
	X_2	0.105597	0.228473
	X_3	0.000926	-0.024192
	X_4	0.000908	0.009479
	X_5	0.000405	-0.033300
2	X_1	0.270229	0.364712
	X_2	0.106150	0.225641
	X_3	0.001206	-0.019158
	X_4	0.001266	-0.018274
	X_5	0.000684	-0.040000
3	X_1	0.270640	0.363863
	X_2	0.105558	0.227726
	X_3	0.001323	-0.021665
	X_4	0.001396	-0.023588
	X_5	0.001013	-0.034284
4	X_1	0.270346	0.364391
	X_2	0.105903	0.230000
	X_3	NaN	NaN
	X_4	NaN	NaN
	X_5	NaN	NaN
5	X_1	0.270640	0.36388
	X_2	NaN	NaN
	X_3	NaN	NaN
	X_4	NaN	NaN
	X_5	NaN	NaN

As these are all average variable importance over all trees, importance of each variable under different values of K shouldn't show significant difference, which is consistent with the empirical results. And if some variables are never selected as the best split variable, they won't have either variable importance (5) or (6).

Both variable importance (5) and (6) for all the $K = \{1, 2, 3, 4, 5\}$ suggest variable X_1 is the most important one, and X_2 is the second important one. And the importance of X_1 and X_2 are much higher that that of other variables.

As K increase, the problem of masking is exaggerated. When $K = 5$, only variable X_1 is selected as the best split, thus only its importance can be computed. We can never know the importance of other variables.

But when K is small, each variable is given more opportunities to be selected as the best split. And when a variable is selected as the best split, it is able to demonstrate its importance. So the results of $K = 1$ could lessen the impact of masking.

(iii) The mean squares loss on the test data using the random forest with 2 methods:

K	method 1	method 2
1	0.17	0.358240
2	0.15	0.262910
3	0.1	0.189990
4	0.1	0.136040
5	0.1	0.100000

Method 1 is the correct one to compute the prediction error on random forest. Because for a random forest, its estimation/prediction is computed as the majority vote of all trees (for classification) or the average prediction of all trees (for regression). So to compute prediction error, we should get the predicted label in the previous way, and then compare it with the true label to compute mean squares loss.

(c) (i) The variable importance according to equations (5) and (6) for each q is:

q	variable	variable importance (5)	variable importance (6)
	X_1	0.269617	0.366979
	X_2	0.105768	0.234229
0.4	X_3	0.003900	-0.007961
	X_4	0.004054	-0.000769
	X_5	0.002572	-0.015064
	X_1	0.269642	0.365378
	X_2	0.105405	0.227849
0.5	X_3	0.002632	-0.005097
	X_4	0.002545	-0.008703
	X_5	0.001845	-0.015529
	X_1	0.273054	0.363852
	X_2	0.104674	0.229203
065	X_3	0.001848	-0.013398
	X_4	0.001544	0.000625
	X_5	0.001848	-0.025526
	X_1	0.269012	0.363795
	X_2	0.105991	0.226984
0.7	X_3	0.001697	-0.004348
	X_4	0.001333	-0.006955
	X_5	0.000993	-0.021554
	X_1	0.270229	0.364712
	X_2	0.106150	0.225641
0.8	X_3	0.001206	-0.019158
	X_4	0.001266	-0.018274
	X_5	0.000684	-0.040000

From the results, both equations (5) and (6) suggest variable X_1 is the most important one, and X_2 is the second important one. And the importance of X_1 and X_2 is much higher that that of other variables.

(ii) The standard deviation of variable importance according to equations (5) and (6) for each q is:

q	variable	std (5)	std (6)
	X_1	0.027299	0.031448
	X_2	0.022169	0.034970
0.4	X_3	0.003543	0.033055
	X_4	0.003339	0.038799

	X_5	0.002730	0.033652
0.5	X_1	0.021400	0.037146
	X_2	0.017976	0.039988
	X_3	0.002717	0.037081
	X_4	0.002402	0.036587
	X_5	0.001781	0.036883
0.6	X_1	0.017279	0.041339
	X_2	0.015590	0.044078
	X_3	0.001722	0.048822
	X_4	0.001376	0.048858
	X_5	0.002246	0.042717
0.7	X_1	0.014476	0.046987
	X_2	0.012524	0.047612
	X_3	0.001305	0.045928
	X_4	0.001538	0.050301
	X_5	0.000838	0.049596
0.8	X_1	0.010818	0.056496
	X_2	0.009347	0.061802
	X_3	0.000963	0.058462
	X_4	0.000908	0.065893
	X_5	0.000813	0.064061