Compsci 571 HW2

Yilin Gao (yg95)

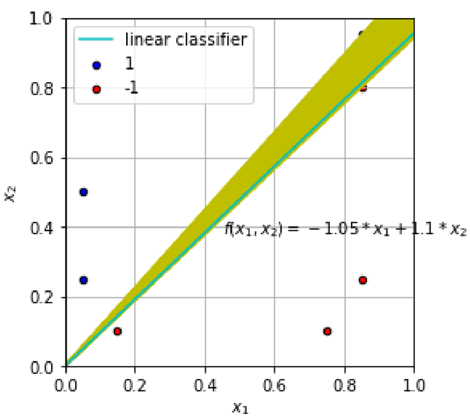
February 4, 2018

1 Classifier for Basketball Courts

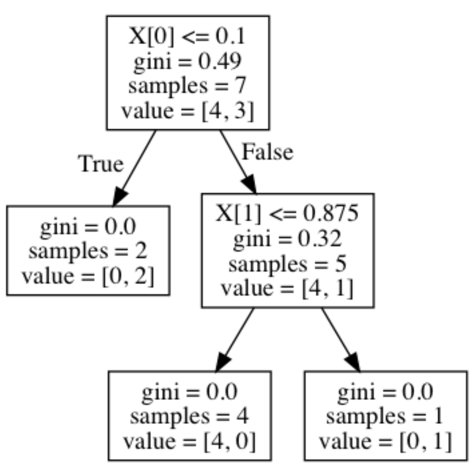
(a) When running Perceptron algorithm on the dataset, it takes 7 iterations (updates) to converge. The decision boundary is $f(x_1, x_2) = -1.05 * x_1 + 1.1 * x_2$. Because after it converges, all training points are correctly classified, the error rate is 0.

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 $w_2 = 1.1$ as the perceptron boundary, we get $-1.229 < w_1 < -1.035$.

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:



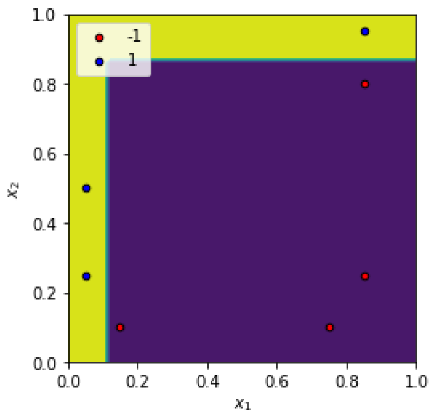
(b) The fully-grown decision tree using Gini index as splitting criterion on the observed data is:



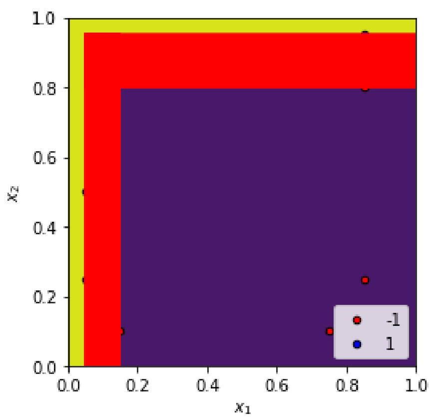
Because all training points are correctly classified by this tree, its training error is 0.

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 $R^{true}(f)$.

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

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

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

$$= \mathbf{P}(y = 1) * \mathbf{P}(f(\mathbf{x}) \leq 0 | y = 1) + \mathbf{P}(y = -1) * \mathbf{P}(f(\mathbf{x}) \geq 0 | y = -1) \tag{4}$$

$$= (1 - \frac{\pi}{4}) * \mathbf{P}(w_1 * x_1 + w_2 * x_2 \leq 0 | 0 \leq x_1 \leq 1, \sqrt{x_1} \leq x_2 \leq 1) + \frac{\pi}{4} * \mathbf{P}(w_1 * x_1 + w_2 * x_2 \geq 0 | 0 \leq x_1 \leq 1, 0 \leq x_2 \leq \sqrt{x_1}) \tag{5}$$

$$= (1 - \frac{\pi}{4}) * \mathbf{P}(x_2 \leq -\frac{w_1}{w_2} x_1 | 0 \leq x_1 \leq 1, \sqrt{x_1} \leq x_2 \leq 1) + \frac{\pi}{4} * \mathbf{P}(x_2 \geq -\frac{w_1}{w_2} x_1 | 0 \leq x_1 \leq 1, 0 \leq x_2 \leq \sqrt{x_1}) \tag{6}$$

Step (2) is from the property of expectation on indicator function. Step (4) is from the rule of conditional probability. In step (5), $\mathbf{P}(y=1)=\frac{\pi}{4}$ and $\mathbf{P}(y=-1)=1-\frac{\pi}{4}$ because of the uniform distribution of (x_1, x_2).

Assign $p=-\frac{w_1}{w_2}$, $p \in [0,\infty)$, equation (6) becomes:

$$= (1-\frac{\pi}{4}) * \mathbf{P}(x_2 \leq px_1 | 0 \leq x_1 \leq 1, \sqrt{x_1} \leq x_2 \leq 1) + \frac{\pi}{4} * \mathbf{P}(x_2 \geq px_1 | 0 \leq x_1 \leq 1, 0 \leq x_2 \leq \sqrt{x_1}) \quad (7)$$

So we need to find the optimized p that minimizes $R^{true}(f)$, or equivalently equation (7).

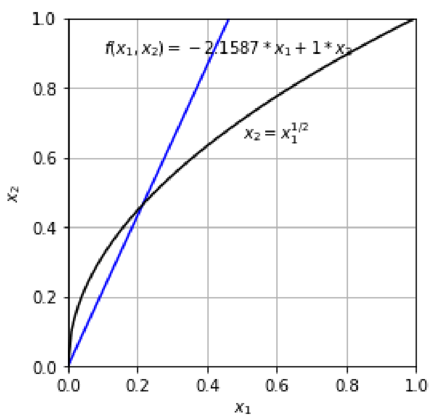
If $p \in [0,1]$, $T=\frac{\pi}{4}*(\frac{\pi}{4}-\frac{1}{2}*1*p)$, and local optimized $p'=1$ minimizes $T'=\frac{\pi}{4}[\frac{\pi}{4}-\frac{1}{2}]$.

If $p \in (1,\infty)$, based on geometry in the 2D space and integration, I get $T=\frac{1}{6}p^{-3}+(\frac{1}{2}-\frac{\pi}{8})p^{-1}+(1-\frac{\pi}{4})$. So local optimized $p''=(1-\frac{\pi}{4})^{-2}$, and $T''=\frac{1}{6}(1-\frac{\pi}{4})^6-\frac{1}{2}(1-\frac{\pi}{4})^3+(1-\frac{\pi}{4})$.

So the global optimized $p^*=p''=(1-\frac{\pi}{4})^{-2} \approx \mathbf{2.158655221735395}$, the optimal linear classifier that passes through the origin is $\mathbf{f(x_1,x_2)=-2.1587*x_1+1*x_2=0}$, and the corresponding minimal $R^{true}(f)=\frac{1}{6}(1-\frac{\pi}{4})^6-\frac{1}{2}(1-\frac{\pi}{4})^3+(1-\frac{\pi}{4}) \approx \mathbf{0.18146363796206844}$.

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) 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.

$$T = R^{true}(f) = \mathbf{P}(y=1) * \mathbf{P}(f(\mathbf{x}) \leq 0 | y=1) + \mathbf{P}(y=-1) * \mathbf{P}(f(\mathbf{x}) \geq 0 | y=-1) \quad (8)$$

$$= (1-\frac{\pi}{4}) * \mathbf{P}(f(\mathbf{x}) \leq 0 | y=1) + \frac{\pi}{4} * \mathbf{P}(f(\mathbf{x}) \geq 0 | y=-1) \quad (9)$$

Step (8) comes from the same steps as in (c).

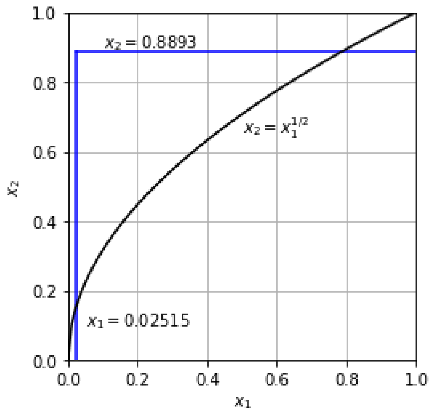
If $0 \leq n \leq \sqrt{m}$, $T=\frac{\pi}{4}[1-\frac{4}{\pi}(1-m)n] \geq \frac{\pi}{4}[1-\frac{4}{\pi}(1-m)\sqrt{m}]$. So the local optimized $m'=\frac{1}{3}$, local optimized $n'=\sqrt{m'}=\sqrt{\frac{1}{3}}$, and local minimal $T'=\frac{\pi}{4}-\frac{2}{3}\sqrt{\frac{1}{3}} \approx 0.4004979839376978$.

If $\sqrt{m} \leq n \leq 1$, according to geometry in 2D space and integration, $T=\frac{1}{3}n^3+(\frac{\pi}{4}-1)mn-\frac{\pi}{4}n+\frac{2}{3}m^{\frac{3}{2}}+\frac{\pi}{6}$. So the local optimized $m''=\frac{(4-\pi)^2}{4^2+4(4-\pi)+\pi^2} \approx 0.025146138400079843$, local optimized $n''=(1-\frac{\pi}{4})m''+\frac{\pi}{4} \approx 0.8892663104388737$, and the local minimal $T'' \approx 0.0574391669843608$.

So the global optimized $m^*=\frac{(4-\pi)^2}{4^2+4(4-\pi)+\pi^2} \approx \mathbf{0.025146138400079843}$, the global optimized $n^*=(1-\frac{\pi}{4})m''+\frac{\pi}{4} \approx \mathbf{0.8892663104388737}$, and the global minimal $R^{true}(f) \approx \mathbf{0.0574391669843608}$.

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 $f(x_1, x_2^*) = w_1 x_1 + w_2^* x_2^*$.

$$T = R^{true}(f) = \mathbf{P}(y=1) * \mathbf{P}(f(\mathbf{x}^*) \le 0|y=1) + \mathbf{P}(y=-1) * \mathbf{P}(f(\mathbf{x}^*) \ge 0|y=-1) \tag{10}$$
$$= \frac{1}{2}\mathbf{P}(x_2^* \le -\frac{w_1}{w_2^*}x_1|0 \le x_1 \le 1, x_2^* \ge x_1) + \frac{1}{2}\mathbf{P}(x_2^* \ge -\frac{w_1}{w_2^*}x_1|0 \le x_1 \le 1, x_2^* \le x_1) \tag{11}$$

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), suppose the optimal depth 2 decision tree splits on $x_1 = m$ and $x_2^* = n$, $R^{real}(f)$ goes as following:

$$T = R^{true}(f) = \mathbf{P}(y=1) * \mathbf{P}(f(\mathbf{x}^*) \le 0|y=1) + \mathbf{P}(y=-1) * \mathbf{P}(f(\mathbf{x}^*) \ge 0|y=-1) \tag{12}$$
$$= \frac{1}{2} * \mathbf{P}(f(\mathbf{x}^*) \le 0|y=1) + \frac{1}{2} * \mathbf{P}(f(\mathbf{x}^*) \ge 0|y=-1) \tag{13}$$

If $0 \le n \le m \le 1$, $\mathbf{P}(f(\mathbf{x}^*) \le 0|y=1) = 0$, $T = \frac{1}{2}[\frac{1}{2} - n(1-m)] \ge \frac{1}{2}[1 - m(1-m)]$. So the local optimal $m' = \frac{1}{2}$, the local optimal $n' = \frac{1}{2}$, and the corresponding local minimal $T' = \frac{1}{8}$.

If $0 \le m < n \le 1$, $\mathbf{P}(f(\mathbf{x}^*) \le 0|y=1) = \frac{1}{2}(n-m)^2$, $\mathbf{P}(f(\mathbf{x}^*) \ge 0|y=-1) = \frac{1}{2}m^2 + \frac{1}{2}(1-n)^2$, $T = \frac{1}{4}[(n-m)^2 + m^2 + (1-n)^2]$. The local optimized $m' = \frac{1}{3}$, $n' = \frac{2}{3}$, and the corresponding $T' = \frac{5}{24}$.

So the global minimal true risk generated by a depth 2 decision tree under this transformation is $\frac{1}{8}$. The decision tree **cannot** achieve the same minimal true error (0) as the linear classifier in part (e).

(g) For paint, assume the part inside paint ($0.5 \le x_1 \le 1$ and $0 \le x_2 \le 0.25$) 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 $R^{true}(f)$.

$$T = R^{true}(f) = \mathbf{P}(y=1) * \mathbf{P}(f(\mathbf{x}) \le 0|y=1) + \mathbf{P}(y=-1) * \mathbf{P}(f(\mathbf{x}) \ge 0|y=-1) \tag{14}$$
$$= \frac{7}{8} * \mathbf{P}(x_2 \le -\frac{w_1}{w_2}x_1|y=1) + \frac{1}{8} * \mathbf{P}(x_2 \ge -\frac{w_1}{w_2}x_1|y=-1) \tag{15}$$

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

$$= \frac{7}{8} * \mathbf{P}(x_2 \le px_1|y=1) + \frac{1}{8} * \mathbf{P}(x_2 \ge px_1|y=-1) \tag{16}$$

If $p \ge \frac{1}{2}$, $\mathbf{P}(x_2 \ge px_1|y=-1) = 0$, $T = \frac{7}{8} * \mathbf{P}(x_2 \le px_1|y=1)$.

(i) If $1 \ge p \ge \frac{1}{2}$, $T = \frac{7}{8}[\frac{p}{2} - \frac{1}{8}]$, and local optimized $p' = \frac{1}{2}$ generates local minimal $p' = \frac{7}{64}$.
(ii) If $p > 1$, $T = \frac{7}{8}[\frac{7}{8} - \frac{1}{2p}]$, and local optimized $p' = 1$ generates local minimal $p' = \frac{21}{64}$.

If $\frac{1}{2} > p \ge 0$,

(i) If $\frac{1}{2} > p \ge \frac{1}{4}$, $\mathbf{P}(x_2 \ge px_1 | y = -1) = \frac{1}{8}(\frac{1}{4p} + p - 1)$, $\mathbf{P}(x_2 \le px_1 | y = 1) = \frac{5p}{8} - \frac{1}{4} + \frac{1}{32p}$. $T = \frac{9p}{16} + \frac{1}{32p} - \frac{15}{64}$. So the local optimized $p' = \frac{1}{4}$ generates local minimal $T' = \frac{2}{64}$.
(ii) If $\frac{1}{4} > p \ge 0$, $\mathbf{P}(x_2 \ge px_1 | y = -1) = \frac{1}{4}[\frac{1}{2} - \frac{3p}{2}]$, $\mathbf{P}(x_2 \le px_1 | y = 1) = \frac{p}{8}$, $T = \frac{4p}{64} + \frac{1}{64}$. So the local optimal $p' = 0$ generates local minimal $T' = \frac{1}{64}$.

So in conclusion, the global optimized $-\frac{w_1}{w_2} = p = \mathbf{0}$, the optimal linear classifier that passes through the origin is $\mathbf{f(x_1, x_2) = x_2 = 0}$, and the corresponding minimal true error rate $R^{true}(f) = \mathbf{\frac{1}{64}}$.

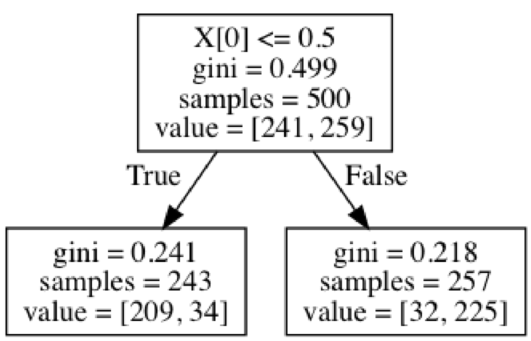
(h) The optimal depth 2 decision tree will split on $x_1 = m$ and $x_2 = n$. And $f(\mathbf{x}) = -1$ if $m \le x_1 \le 1$ and $0 \le x_2 \le n$, $f(\mathbf{x}) = 1$ otherwise.

$$T = R^{true}(f) = \mathbf{P}(y = 1) * \mathbf{P}(f(\mathbf{x}) \le 0 | y = 1) + \mathbf{P}(y = -1) * \mathbf{P}(f(\mathbf{x}) \ge 0 | y = -1) \tag{17}$$
$$= \frac{7}{8} * \mathbf{P}(f(\mathbf{x}) \le 0 | y = 1) + \frac{1}{8} * \mathbf{P}(f(\mathbf{x}) \ge 0 | y = -1) \ge 0 \tag{18}$$

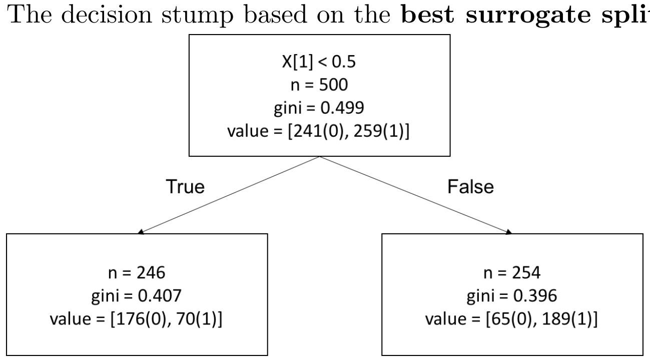
It's easy to find out that when $\mathbf{m} = \mathbf{\frac{1}{2}}$ and $\mathbf{n} = \mathbf{\frac{1}{4}}$, both $\mathbf{P}(f(\mathbf{x}) \le 0 | y = 1)$ and $\mathbf{P}(f(\mathbf{x}) \ge 0 | y = -1)$ are equal to 0, and T achieves its minimal value $\mathbf{0}$.

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) and threshold 0.5 (actually this value doesn't really matter) as the best surrogate split.

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

X_1	0.2706
X_2	NA
X_3	NA
X_4	NA
X_5	NA

Variable importance measures from equation (3) are:

X_1	0.2706
X_2	0.1058
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 least-squares error of predictions on the test data from the decision stump based on the best split is 0.1.

The mean least-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) (i) The table for best split variable for each K is:

K	variable	time as best split variable (out of 1000)
1	X_1	223
	X_2	185
	X_3	196
	X_4	210
	X_5	186
2	X_1	368
	X_2	290
	X_3	134
	X_4	128
	X_5	80
3	X_1	488
	X_2	293
	X_3	96
	X_4	79
	X_5	44
4	X_1	578
	X_2	289
	X_3	58
	X_4	54
	X_5	21

5	X_1	672
	X_2	256
	X_3	27
	X_4	31
	X_5	14

The table for best split surrogate split variable for each K is:

K	variable	time as best surrogate split variable (out of 1000)
1	X_1	0
	X_2	0
	X_3	0
	X_4	0
	X_5	0
2	X_1	38
	X_2	108
	X_3	269
	X_4	273
	X_5	312
3	X_1	104
	X_2	261
	X_3	206
	X_4	176
	X_5	253
4	X_1	195
	X_2	333
	X_3	180
	X_4	116
	X_5	176
5	X_1	242
	X_2	412
	X_3	124
	X_4	53
	X_5	169

According to best split variable, 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 best surrogate split variable, 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	0.317459	
	X_2	0.185158	
	X_3	0.086647	
	X_4	0.100492	
	X_5	0.091785	

2	X_1	0.316218	
	X_2	0.184409	
	X_3	0.087232	
	X_4	0.100509	
	X_5	0.091449	
3	X_1	0.316162	
	X_2	0.185297	
	X_3	0.087645	
	X_4	0.100699	
	X_5	0.091544	
4	X_1	0.316481	
	X_2	0.185115	
	X_3	0.087517	
	X_4	0.100573	
	X_5	0.091798	
5	X_1	0.315904	
	X_2	0.184598	
	X_3	0.087999	
	X_4	0.101263	
	X_5	0.091400	

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

K	method 1	method 2
1		
2		
3		
4		
5		

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

q	variable	variable importance (5)	variable importance (6)
0.4	X_1	0.406475	
	X_2	0.342298	
	X_3	0.287157	
	X_4	0.299625	
	X_5	0.290382	
0.5	X_1	0.383594	
	X_2	0.302990	
	X_3	0.237279	
	X_4	0.249938	
	X_5	0.240827	
0.6	X_1	0.361578	
	X_2	0.263266	
	X_3	0.187936	
	X_4	0.200152	
	X_5	0.191461	
0.7	X_1	0.339114	
	X_2	0.224404	
	X_3	0.136833	
	X_4	0.150833	
	X_5	0.141829	

0.8	X_1	0.316477	
	X_2	0.184955	
	X_3	0.087182	
	X_4	0.100499	
	X_5	0.092076	

From the results,

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

q	variable	std (5)	std (6)
0.4	X_1	0.01137653	
	X_2	0.00949841	
	X_3	0.00916807	
	X_4	0.00306012	
	X_5	0.00746454	
0.5	X_1	0.01164611	
	X_2	0.00982521	
	X_3	0.00777255	
	X_4	0.00330059	
	X_5	0.00602257	
0.6	X_1	0.01104073	
	X_2	0.00930425	
	X_3	0.0057956	
	X_4	0.00211394	
	X_5	0.00434062	
0.7	X_1	0.01024229	
	X_2	0.00865117	
	X_3	0.00500432	
	X_4	0.00177119	
	X_5	0.00424676	
0.8	X_1	0.00910605	
	X_2	0.00715279	
	X_3	0.00380045	
	X_4	0.00121756	
	X_5	0.00330985	