Compsci 571 HW2

Yilin Gao (yg95)

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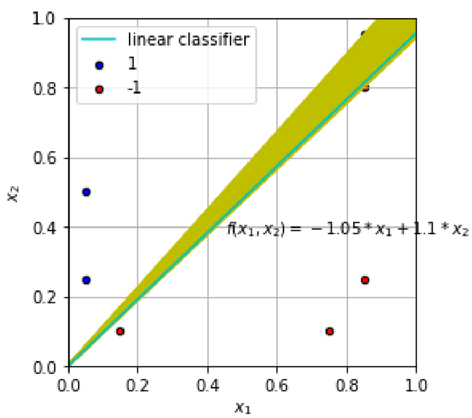
1 Classifier for Basketball Courts

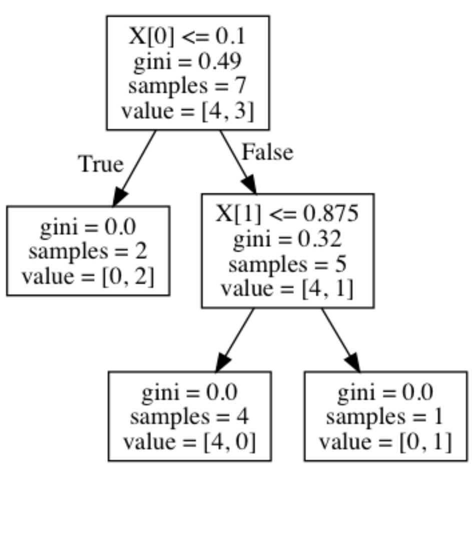
(a) When running Perceptron algorithm on the dataset, it takes 7 iterations (updates) to converge. The decision boundary is $f(x_1, x_2) = -1.05 * x_1 + 1.1 * x_2$. Because after it converges, all training points are correctly classified, the error rate is 0.

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 $w_2 = 1.1$ 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:



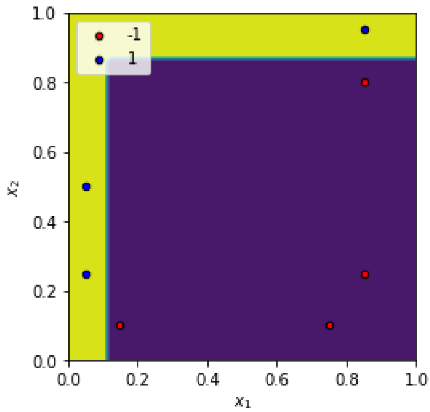
(b) The fully-grown decision tree using Gini index as splitting criterion on the observed data is:



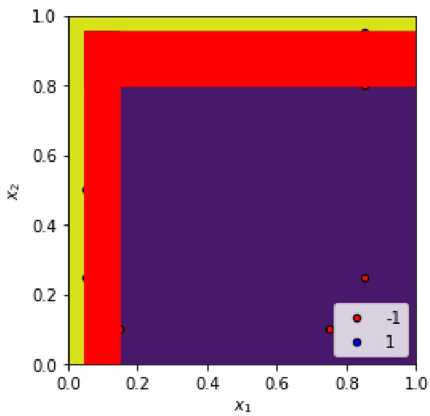
Because all training points are correctly classified by this tree, its training error is 0.

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 $R^{true}(f)$.

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

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

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

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

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

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

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:

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

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

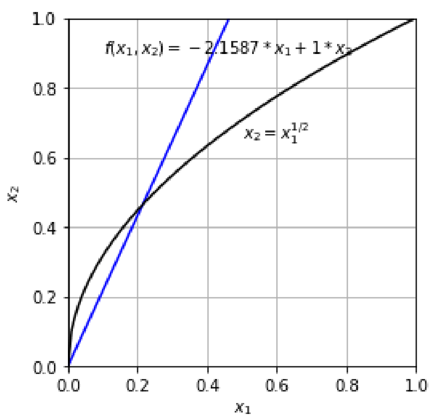
If $p\in[0,1]$, $T=\frac{\pi}{4}*(\frac{\pi}{4}-\frac{1}{2}*1*p)$, and local optimized $p'=1$ minimizes $T'=\frac{\pi}{4}[\frac{\pi}{4}-\frac{1}{2}]$.

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 $m\le x_1\le 1$ and $0\le x_2\le n$, $f(\mathbf{x})=1$ otherwise.

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

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

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

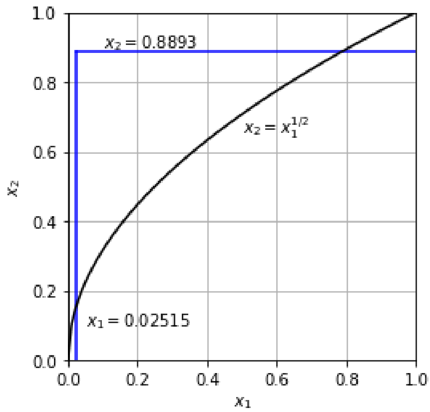
If $0\le n\le\sqrt{m}$, $T=\frac{\pi}{4}[1-\frac{4}{\pi}(1-m)n]\ge\frac{\pi}{4}[1-\frac{4}{\pi}(1-m)\sqrt{m}]$. So the local optimized $m'=\frac{1}{3}$, local optimized $n'=\sqrt{m'}=\sqrt{\frac{1}{3}}$, and local minimal $T'=\frac{\pi}{4}-\frac{2}{3}\sqrt{\frac{1}{3}}\approx 0.4004979839376978$.

If $\sqrt{m}\le n\le 1$, 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 $f(x_1, x_2^*) = w_1 x_1 + w_2^* x_2^*$.

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

$$= \frac{1}{2}\mathbf{P}(x_2^* \leq -\frac{w_1}{w_2^*}x_1 | 0 \leq x_1 \leq 1, x_2^* \geq x_1) + \frac{1}{2}\mathbf{P}(x_2^* \geq -\frac{w_1}{w_2^*}x_1 | 0 \leq x_1 \leq 1, x_2^* \leq x_1) \tag{11}$$

And it is easy to find out that the optimal value of $-\frac{\mathbf{w_1}}{\mathbf{w_2^*}} = \mathbf{1}$, 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:

$$T = R^{true}(f) = \mathbf{P}(y=1) * \mathbf{P}(f(\mathbf{x}^*) \leq 0 | y=1) + \mathbf{P}(y=-1) * \mathbf{P}(f(\mathbf{x}^*) \geq 0 | y=-1) \tag{12}$$

$$= \frac{1}{2} * \mathbf{P}(f(\mathbf{x}^*) \leq 0 | y=1) + \frac{1}{2} * \mathbf{P}(f(\mathbf{x}^*) \geq 0 | y=-1) \tag{13}$$

If $0 \leq n \leq m \leq 1$, $\mathbf{P}(f(\mathbf{x}^*) \leq 0 | y=1) = 0$, $T = \frac{1}{2}[\frac{1}{2} - n(1-m)] \geq \frac{1}{2}[1 - m(1-m)]$. 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 $0 \leq m < n \leq 1$, $\mathbf{P}(f(\mathbf{x}^*) \leq 0 | y=1) = \frac{1}{2}(n-m)^2$, $\mathbf{P}(f(\mathbf{x}^*) \geq 0 | y=-1) = \frac{1}{2}m^2 + \frac{1}{2}(1-n)^2$, $T = \frac{1}{4}[(n-m)^2 + m^2 + (1-n)^2]$. 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 ($0.5 \leq x_1 \leq 1$ 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 $R^{true}(f)$.

$$T = R^{true}(f) = \mathbf{P}(y=1) * \mathbf{P}(f(\mathbf{x}) \leq 0 | y=1) + \mathbf{P}(y=-1) * \mathbf{P}(f(\mathbf{x}) \geq 0 | y=-1) \tag{14}$$

$$= \frac{7}{8} * \mathbf{P}(x_2 \leq -\frac{w_1}{w_2}x_1 | y=1) + \frac{1}{8} * \mathbf{P}(x_2 \geq -\frac{w_1}{w_2}x_1 | y=-1) \tag{15}$$

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

$$= \frac{7}{8} * \mathbf{P}(x_2 \leq p x_1 | y=1) + \frac{1}{8} * \mathbf{P}(x_2 \geq p x_1 | y=-1) \tag{16}$$

If $p \geq \frac{1}{2}$, $\mathbf{P}(x_2 \geq p x_1 | y=-1) = 0$, $T = \frac{7}{8} * \mathbf{P}(x_2 \leq p x_1 | y=1)$.

(i) If $1 \geq p \geq \frac{1}{2}$, $T = \frac{7}{8}[\frac{p}{2} - \frac{1}{8}]$, 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 $\frac{1}{2} > p \geq 0$,

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

(ii) If $\frac{1}{4} > p \geq 0$, $\mathbf{P}(x_2 \geq px_1|y = -1) = \frac{1}{4}[\frac{1}{2} - \frac{3p}{2}]$, $\mathbf{P}(x_2 \leq px_1|y = 1) = \frac{p}{8}$, $T = \frac{4p}{64} + \frac{1}{64}$. 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 $m \leq x_1 \leq 1$ and $0 \leq x_2 \leq n$, $f(\mathbf{x}) = 1$ otherwise.

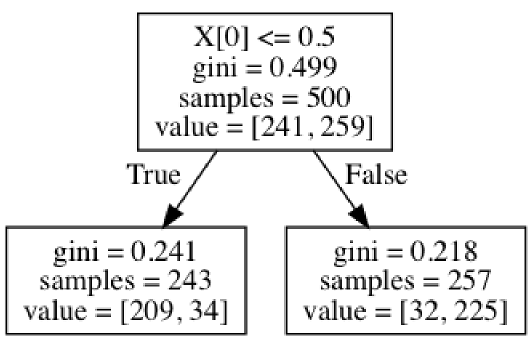
$$T = R^{true}(f) = \mathbf{P}(y = 1) * \mathbf{P}(f(\mathbf{x}) \leq 0|y = 1) + \mathbf{P}(y = -1) * \mathbf{P}(f(\mathbf{x}) \geq 0|y = -1) \tag{17}$$

$$= \frac{7}{8} * \mathbf{P}(f(\mathbf{x}) \leq 0|y = 1) + \frac{1}{8} * \mathbf{P}(f(\mathbf{x}) \geq 0|y = -1) \geq 0 \tag{18}$$

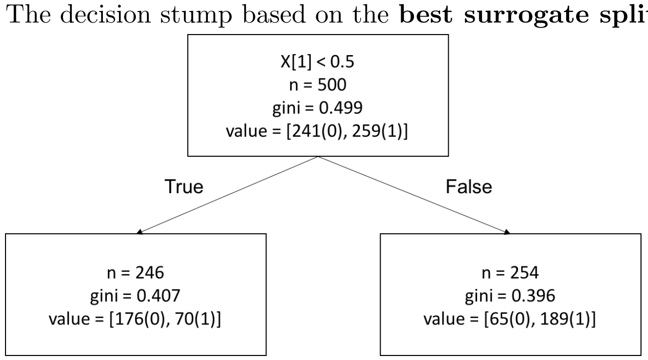
It's easy to find out that when $\mathbf{m = \frac{1}{2}}$ and $\mathbf{n = \frac{1}{4}}$, both $\mathbf{P}(f(\mathbf{x}) \leq 0|y = 1)$ and $\mathbf{P}(f(\mathbf{x}) \geq 0|y = -1)$ are equal to 0, and T achieves its minimal value $\mathbf{0}$.

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

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

K	variable	time as best split variable (out of 1000)
1	X_1	200
	X_2	205
	X_3	196
	X_4	209
	X_5	190
2	X_1	333
	X_2	278
	X_3	157
	X_4	156
	X_5	76
3	X_1	509
	X_2	283
	X_3	79
	X_4	93
	X_5	36
4	X_1	588
	X_2	280
	X_3	56
	X_4	53
	X_5	23

5	X_1	668
	X_2	237
	X_3	46
	X_4	29
	X_5	20

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	29
	X_2	115
	X_3	275
	X_4	263
	X_5	318
3	X_1	109
	X_2	254
	X_3	237
	X_4	167
	X_5	233
4	X_1	177
	X_2	345
	X_3	173
	X_4	107
	X_5	198
5	X_1	258
	X_2	398
	X_3	127
	X_4	68
	X_5	149

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	0.315591	0.365900
	X_2	0.184543	0.230439
	X_3	0.087096	-0.017959
	X_4	0.100569	0.009761
	X_5	0.091519	-0.026316

2	X_1	0.315598	0.364745
	X_2	0.184487	0.227410
	X_3	0.086678	-0.010318
	X_4	0.100980	-0.007949
	X_5	0.091208	-0.022895
3	X_1	0.316503	0.367819
	X_2	0.184912	0.228975
	X_3	0.086697	-0.010125
	X_4	0.101133	-0.008817
	X_5	0.091880	-0.038887
4	X_1	0.316615	0.364218
	X_2	0.185013	0.233357
	X_3	0.088056	-0.013214
	X_4	0.100946	-0.001885
	X_5	0.091464	-0.031304
5	X_1	0.316620	0.363772
	X_2	0.185098	0.228608
	X_3	0.087510	-0.013913
	X_4	0.100940	-0.014481
	X_5	0.090950	-0.037

(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	0.407452	0.367130
	X_2	0.341932	0.229640
	X_3	0.286466	-0.015229
	X_4	0.300333	0.001737
	X_5	0.290861	-0.012727
0.5	X_1	0.383744	0.367407
	X_2	0.301408	0.233945
	X_3	0.236769	-0.012283
	X_4	0.250323	0.003333
	X_5	0.241498	-0.016509
0.6	X_1	0.361694	0.367335
	X_2	0.263844	0.226786
	X_3	0.187090	-0.017031
	X_4	0.200351	0.002857
	X_5	0.191520	-0.020842
0.7	X_1	0.339353	0.365197
	X_2	0.224097	0.224492
	X_3	0.137176	-0.020660
	X_4	0.150509	0.003743
	X_5	0.141717	-0.016368

0.8	X_1	0.315598	0.364745
	X_2	0.184488	0.227410
	X_3	0.086678	-0.010318
	X_4	0.100980	-0.007947
	X_5	0.091208	-0.022893

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	0.01112367	0.03103856
	X_2	0.00870762	0.03255196
	X_3	0.00952271	0.03317124
	X_4	0.00323389	0.04077185
	X_5	0.00681136	0.0327284
0.5	X_1	0.01124836	0.03793574
	X_2	0.00902561	0.03685835
	X_3	0.00797128	0.03568958
	X_4	0.0028276	0.04255715
	X_5	0.00608335	0.04003311
0.6	X_1	0.01055884	0.04240423
	X_2	0.00876408	0.04514072
	X_3	0.00609878	0.04217448
	X_4	0.00215396	0.0493615
	X_5	0.00455622	0.03715297
0.7	X_1	0.01003214	0.04752654
	X_2	0.00857417	0.04998027
	X_3	0.00480541	0.04686512
	X_4	0.00181428	0.05767446
	X_5	0.00400655	0.04974323
0.8	X_1	0.00833034	0.06041158
	X_2	0.00750252	0.0628672
	X_3	0.00366868	0.06426875
	X_4	0.00133906	0.06270319
	X_5	0.00315306	0.05855308