## **Classification Problem**

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## Introduction

We used the Breast Cancer dataset to solve the classification problem. The analysis consists of 4 parts:

- 1: logistic regression;
- 2: decision tree;
- 3: random forest;
- 4: SVM

These 4 methods were applied to the Breast Cancer dataset to compare their differences and gain a better understanding of each approach.

### Logistic Regression

First, we'll load the data and check if there are any missing values in the dataset. After that, we'll transform the data into the proper format. Then, we'll split the dataset into a training set and a test set, with a ratio of 70% for training and 30% for testing.

```
library("mlbench")
data("BreastCancer")
head(BreastCancer)
```

	Id	Cl.thickness	Cell.size	Cell.shape	Marg.adhesion	Epith.c.size
1	1000025	5	1	1	1	2
2	1002945	5	4	4	5	7
3	1015425	3	1	1	1	2
4	1016277	6	8	8	1	3
5	1017023	4	1	1	3	2

```
6 1017122
                       8
                                 10
                                              10
                                                               8
                                                                             7
  Bare.nuclei Bl.cromatin Normal.nucleoli Mitoses
                                                            Class
             1
                           3
                                             1
                                                           benign
1
                                                      1
2
            10
                           3
                                             2
                                                      1
                                                           benign
             2
3
                           3
                                            1
                                                      1
                                                           benign
4
             4
                           3
                                             7
                                                           benign
5
             1
                           3
                                            1
                                                           benign
6
            10
                           9
                                             7
                                                      1 malignant
```

#### names(BreastCancer)

- [1] "Id" "Cl.thickness" "Cell.size" "Cell.shape" [5] "Marg.adhesion" "Epith.c.size" "Bare.nuclei" "Bl.cromatin"
- [9] "Normal.nucleoli" "Mitoses" "Class"

#### str(BreastCancer)

```
699 obs. of 11 variables:
'data.frame':
                 : chr "1000025" "1002945" "1015425" "1016277" ...
$ Id
$ Cl.thickness : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<...: 5 5 3 6 4 8 1 2 2 4 ...
                  : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 1 1 2 ...
$ Cell.size
                 : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 2 1 1 ...
$ Cell.shape
$ Marg.adhesion : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 5 1 1 3 8 1 1 1 1 ...
                 : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<...: 2 7 2 3 2 7 2 2 2 2 ...
$ Epith.c.size
$ Bare.nuclei
                 : Factor w/ 10 levels "1", "2", "3", "4", ...: 1 10 2 4 1 10 10 1 1 1 ...
$ Bl.cromatin
                 : Factor w/ 10 levels "1", "2", "3", "4", ...: 3 3 3 3 3 9 3 3 1 2 ...
$ Normal.nucleoli: Factor w/ 10 levels "1","2","3","4",..: 1 2 1 7 1 7 1 1 1 1 ...
                 : Factor w/ 9 levels "1","2","3","4",..: 1 1 1 1 1 1 1 5 1 ...
$ Mitoses
                  : Factor w/ 2 levels "benign", "malignant": 1 1 1 1 1 2 1 1 1 1 ...
$ Class
```

# df <- BreastCancer[-1] df</pre>

	Cl.thickness	Cell.size	Cell.shape	Marg.adhesion	Epith.c.size	Bare.nuclei
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2	5	4	4	5	7	10
3	3	1	1	1	2	2
4	6	8	8	1	3	4
5	4	1	1	3	2	1
6	8	10	10	8	7	10

7	1	1	1	1	2	10
8	2	1	2	1	2	1
9	2	1	1	1	2	1
10	4	2	1	1	2	1
11	1	1	1	1	1	1
12	2	1	1	1	2	1
13	5	3	3	3	2	3
14	1	1	1	1	2	3
15	8	7	5	10	7	9
16	7	4	6	4	6	1
17	4	1	1	1	2	1
18	4	1	1	1	2	1
19	10	7	7	6	4	10
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22	10	5	5	3	6	7
23	3	1	1	1	2	1
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26	5	2	3	4	2	7
27	3	2	1	1	1	1
28	5	1	1	1	2	1
29	2	1	1	1	2	1
30	1	1	3	1	2	1
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32	2	1	1	1	2	1
33	10	7	7	3	8	5
34	2	1	1	2	2	1
35	3	1	2	1	2	1
36	2	1	1	1	2	1
37	10	10	10	8	6	1
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39	5	4	4	9	2	10
40	2	5	3	3	6	7
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46	1	1	1	1	2	1
47	3	7	7	4	4	9
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421	3	2	2	3	2	3
422	10	10	10	7	10	10
423	4	3	3	1	2	1
424	5	1	3	1	2	1
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427	5	3	6	1	2	1
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350	7	6	1	malignant
351	1	1	1	benign
352	3	1	1	benign
353	4	6	1	benign
354	4	9	4	malignant
355	2	1	1	benign
356	2	2	1	benign
357	3	3	3	malignant
358	7	3	8	malignant
359	4	10	3	malignant
360	3	5	3	malignant
361	8	10	10	malignant
362	5	1	4	malignant
363	2	1	1	benign
364	2	1	1	benign
365	3	1	1	benign
366	2	1	1	benign
367	7	10	7	malignant
368	8	10	3	malignant
369	1	1	1	benign
370	2	1	1	benign
371	2	1	1	benign
372	1	1	1	benign
373	2	1	1	benign
374	2	1	1	benign
375	2	1	1	benign
376	1	1	1	benign
377	2	1	1	benign
378	2	1	1	benign
379	2	2	1	benign
380	3	1	1	benign
381	1	1	1	benign
				9

382	7	8	4	${\tt malignant}$
383	3	2	1	benign
384	1	1	1	benign
385	1	1	1	benign
386	1	2	3	benign
387	7	1	1	${\tt malignant}$
388	3	1	1	benign
389	2	2	1	benign
390	2	2	1	benign
391	2	1	1	benign
392	7	9	1	malignant
393	2	1	1	benign
394	1	1	1	benign
395	2	1	1	benign
396	2	1	1	benign
397	3	1	1	benign
398	1	1	1	benign
399	2	2	1	benign
400	1	1	1	benign
401	9	3	8	malignant
402	1	1	1	benign
403	2	1	1	benign
404	1	1	1	benign
405	1	2	1	benign
406	2	1	1	benign
407	2	1	1	benign
408	2	1	1	benign
409	3	1	1	benign
410	2	1	1	benign
411	2	1	1	benign
412	2	1	1	benign
413	8	5	1	malignant
414	3	1	1	benign
415	6	6	1	malignant
416	3	5	1	benign
417	7	2	1	malignant
418	2	1	1	benign
419	3	2	2	benign
420	1	1	1	benign
421	3	1	1	benign
422	8	2	1	malignant
423	3	3	1	benign
424	2	1	1	benign
	_	•	_	0

	_	_		
425	1	1	1	benign
426	10	10	1	malignant
427	1	1	1	benign
428	5	10	1	malignant
429	2	1	1	benign
430	2	1	1	benign
431	2	2	1	benign
432	3	2	1	benign
433	2	2	1	benign
434	1	1	1	benign
435	4	2	1	benign
436	5	1	1	malignant
437	2	8	1	${\tt malignant}$
438	1	1	1	benign
439	1	1	1	benign
440	1	1	1	benign
441	10	1	1	${\tt malignant}$
442	1	1	1	benign
443	1	1	1	benign
444	1	1	1	benign
445	2	1	1	benign
446	1	1	1	benign
447	1	1	1	benign
448	1	1	1	benign
449	1	1	1	benign
450	8	10	1	malignant
451	2	1	1	benign
452	1	1	1	benign
453	1	1	1	benign
454	10	7	1	malignant
455	1	1	1	benign
456	1	1	2	malignant
457	8	6	1	malignant
458	10	10	1	malignant
459	1	1	1	benign
460	1	1	1	benign
461	1	1	1	benign
462	1	1	1	benign
463	1	1	1	benign
464	1	2	1	benign
465	1	1	1	benign
466	7	10	3	malignant
467	9	7	1	malignant
				5

468	7	6	2	${\tt malignant}$
469	1	1	1	benign
470	2	1	1	benign
471	2	1	1	benign
472	1	1	1	benign
473	1	1	1	benign
474	1	1	1	benign
475	1	1	1	benign
476	1	1	1	benign
477	1	1	1	benign
478	1	1	1	benign
479	1	1	1	benign
480	7	5	1	malignant
481	1	1	1	benign
482	1	1	1	benign
483	10	10	10	malignant
484	9	10	1	malignant
485	1	1	1	benign
486	1	1	1	benign
487	2	1	1	benign
488	8	1	5	malignant
489	3	4	1	malignant
490	4	1	1	malignant
491	1	1	1	benign
492	7	1	1	malignant
493	2	1	1	benign
494	6	5	2	malignant
495	2	1	1	benign
496	2	1	1	benign
497	1	1	1	benign
498	1	1	1	benign
499	2	1	1	benign
500	2	1	1	benign
501	3	1	1	benign
502	2	1	1	benign
503	2	1	1	benign
504	3	1	1	benign
505	1	1	1	benign
506	1	1	1	benign
507	4	8	7	malignant
508	1	1	1	benign
509	1	1	1	benign
510	1	1	1	benign

511	1	1	1	benign
512	2	1	1	benign
513	1	1	1	benign
514	2	1	1	benign
515	8	10	2	malignant
516	9	10	1	malignant
517	1	1	1	benign
518	2	1	1	benign
519	1	1	1	benign
520	9	1	1	malignant
521	1	1	1	benign
522	1	1	1	benign
523	7	3	1	malignant
524	5	3	1	malignant
525	2	1	1	benign
526	1	1	1	benign
527	1	1	1	benign
528	3	1	1	benign
529	1	1	1	benign
530	2	1	1	benign
531	6	9	1	malignant
532	2	1	1	benign
533	3	1	1	benign
534	2	1	1	benign
535	2	1	1	benign
536	3	1	1	benign
537	3	1	1	benign
538	3	1	1	benign
539	2	1	1	benign
540	2	1	1	benign
541	2	1	1	benign
542	1	1	1	benign
543	1	1	1	benign
544	2	1	1	benign
545	2	1	1	benign
546	2	1	1	benign
547	7	10	1	malignant
548	1	1	1	benign
549	1	1	1	benign
550	7	8	2	malignant
551	2	1	1	benign
552	3	1	1	benign
553	4	2	1	benign
				_

554	2	1	2	benign
555	1	1	1	benign
556	4	8	1	benign
557	2	1	1	benign
558	1	1	1	benign
559	2	1	1	benign
560	2	1	1	benign
561	3	1	1	benign
562	3	1	1	benign
563	3	1	1	benign
564	2	1	1	benign
565	3	2	1	benign
566	10	10	1	malignant
567	3	1	1	benign
568	2	1	1	benign
569	2	5	2	malignant
570	10	3	1	malignant
571	8	2	1	malignant
572	9	10	2	malignant
573	2	1	1	benign
574	2	1	1	benign
575	7	7	1	malignant
576	3	1	1	benign
577	2	1	1	benign
578	2	1	1	benign
579	2	1	1	benign
580	3	1	1	benign
581	2	1	1	benign
582	7	5	1	malignant
583	6	10	1	malignant
584	1	1	1	benign
585	1	1	1	benign
586	1	1	1	benign
587	10	10	1	malignant
588	2	2	1	benign
589	4	1	1	malignant
590	1	1	1	benign
591	10	1	1	malignant
592	7	6	1	malignant
593	4	1	1	malignant
594	1	1	1	benign
595	7	1	1	malignant
596	2	1	1	benign
	_	-	_	- 3011

597	2	1	1	benign
598	3	1	1	benign
599	2	1	1	benign
600	1	1	1	benign
601	2	1	1	benign
602	2	1	1	benign
603	2	1	1	benign
604	8	10	1	malignant
605	8	1	2	malignant
606	7	8	3	malignant
607	1	1	1	benign
608	1	1	1	benign
609	10	1	1	malignant
610	1	1	1	benign
611	7	1	2	malignant
612	8	5	1	malignant
613	10	10	10	malignant
614	2	1	1	benign
615	2	1	1	benign
616	2	1	1	benign
617	2	1	1	benign
618	1	1	1	benign
619	2	1	1	benign
620	2	1	1	benign
621	2	1	1	benign
622	6	1	1	benign
623	2	1	1	benign
624	1	1	1	benign
625	2	1	1	benign
626	1	1	1	benign
627	7	7	3	malignant
628	1	1	1	benign
629	1	1	1	benign
630	1	1	1	benign
631	1	1	1	benign
632	2	1	1	benign
633	1	1	1	benign
634	5	10	1	malignant
635	1	1	1	benign
636	1	1	1	benign
637	10	10	3	malignant
638	2	1	1	benign
639	1	1	1	benign
009	1	1	1	penign

0.40	_			
640	1	1	1	benign
641	1	1	1	benign
642	2	1	1	benign
643	2	1	1	benign
644	1	1	1	benign
645	1	1	1	benign
646	2	1	1	benign
647	1	1	1	benign
648	1	1	1	benign
649	10	10	10	malignant
650	2	1	1	benign
651	1	1	1	benign
652	2	1	1	benign
653	2	2	1	benign
654	2	1	1	benign
655	3	1	1	benign
656	2	1	1	benign
657	2	1	1	benign
658	3	6	1	benign
659	7	2	3	malignant
660	1	1	1	benign
661	2	1	1	benign
662	3	1	1	benign
663	2	1	1	benign
664	2	1	1	benign
665	2	1	1	benign
666	1	1	1	benign
667	1	1	2	benign
668	3	1	1	benign
669	7	10	3	malignant
670	7	10	1	malignant
671	7	4	1	malignant
672	3	1	1	benign
673	3	1	1	benign
674	1	1	1	benign
675	2	1	1	benign
676	1	1	1	benign
677	2	1	1	benign
678	1	1	1	benign
679	1	1	1	benign
680	1	1	1	benign
681	10	10	7	malignant
682	5	6		malignant
	-	-	_	3

```
683
               3
                                  2
                                           1
                                                 benign
684
               1
                                  1
                                           1
                                                 benign
685
               1
                                  1
                                           1
                                                 benign
686
               1
                                  1
                                           1
                                                 benign
687
               1
                                  1
                                           1
                                                 benign
688
               2
                                  3
                                           1
                                                 benign
689
               1
                                  1
                                           1
                                                 benign
690
               1
                                  1
                                           8
                                                 benign
691
               1
                                  1
                                           1
                                                 benign
692
               4
                                  4
                                           1 malignant
693
               1
                                  1
                                           1
                                                 benign
694
               2
                                  1
                                           2
                                                 benign
695
                                  1
               1
                                           1
                                                 benign
696
               1
                                  1
                                                 benign
697
               8
                                 10
                                           2 malignant
698
              10
                                  6
                                           1 malignant
699
              10
                                           1 malignant
```

```
sum(is.na(df))
```

#### [1] 16

#### colSums(is.na(df))

```
Cl.thickness Cell.size Cell.shape Marg.adhesion Epith.c.size
0 0 0 0 0 0 0

Bare.nuclei Bl.cromatin Normal.nucleoli Mitoses Class
16 0 0 0 0
```

```
df <- na.omit(df)
df$Cl.thickness <- as.numeric(df$Cl.thickness)
df$Cell.size <- as.numeric(df$Cell.size)
df$Cell.shape <- as.numeric(df$Cell.shape)
df$Marg.adhesion <- as.numeric(df$Marg.adhesion)
df$Epith.c.size <- as.numeric(df$Epith.c.size)
df$Bare.nuclei <- as.numeric(df$Bare.nuclei)
df$Bl.cromatin <- as.numeric(df$Bl.cromatin)
df$Normal.nucleoli <- as.numeric(df$Normal.nucleoli)
df$Mitoses <- as.numeric(df$Mitoses)</pre>
```

```
index <- sample(nrow(df), 0.7*nrow(df))
train <- df[index,]
test <- df[-index,]</pre>
```

Then, we use the nine variables to perform logistic regression for classification, where the class is the dependent variable. We use the summary function to examine the details of the fit result. Next, we use the test data for prediction and set type = 'response' to see the probability of the malignant class.

Next, we set a threshold for the probability: if the probability is greater than 0.5, we label it as 'malignant', and if it is less than 0.5, we label it as 'benign'. Then, we convert these 'benign' and 'malignant' labels into factors for further classification, as we will use the table function.

```
fit <- glm(Class ~ ., data = train, family = binomial())
summary(fit)</pre>
```

```
Call:
glm(formula = Class ~ ., family = binomial(), data = train)
Coefficients:
                Estimate Std. Error z value Pr(>|z|)
(Intercept)
                -9.69151
                            1.29558 -7.480 7.41e-14 ***
Cl.thickness
                 0.48040
                            0.15234
                                      3.154 0.00161 **
Cell.size
                            0.29262
                 0.05705
                                      0.195
                                            0.84541
Cell.shape
                 0.13100
                            0.31630
                                      0.414 0.67874
                                             0.00372 **
Marg.adhesion
                 0.40724
                            0.14038
                                      2.901
Epith.c.size
                -0.03252
                            0.18088
                                    -0.180 0.85731
Bare.nuclei
                 0.44746
                            0.11178
                                      4.003 6.26e-05 ***
Bl.cromatin
                 0.48273
                            0.19220
                                      2.512 0.01202 *
Normal.nucleoli 0.23560
                            0.12904
                                      1.826 0.06788 .
                 0.66368
                            0.28592
                                      2.321 0.02028 *
Mitoses
               0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Signif. codes:
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 629.040
                            on 477
                                    degrees of freedom
Residual deviance: 80.061
                            on 468 degrees of freedom
AIC: 100.06
```

```
prob <- predict(fit,test,type="response")
prediction <- factor(prob>0.5, levels=c(FALSE,TRUE), labels = c("benign","malignant"))
prediction
```

3	5	6	8	9	16	17	21
benign	benign	malignant	benign	benign	benign	benign	malignant
25	27	28	30	33	38	39	46
benign	benign	benign	benign	malignant	benign	malignant	benign
49	50	57	58	59	64	71	74
benign	malignant	malignant	malignant	malignant	benign	benign	malignant
75	82	83	84	87	92	93	94
malignant	benign	benign	benign	${\tt malignant}$	benign	benign	benign
95	98	111	112	113	114	119	126
benign	benign	benign	${\tt malignant}$	${\tt malignant}$	${\tt malignant}$	benign	benign
130	131	132	134	135	136	139	142
benign	benign						
143	152	155	157	163	173	178	179
${\tt malignant}$	${\tt malignant}$	benign	benign	benign	benign	${\tt malignant}$	benign
182	186	191	193	196	199	203	206
benign	benign	${\tt malignant}$	benign	benign	benign	benign	malignant
210	215	228	231	232	239	240	244
benign	${\tt malignant}$	${\tt malignant}$	_	_	_	_	benign
245	246	253	254	255	261	272	274
benign	benign	${\tt malignant}$	${\tt malignant}$	${\tt malignant}$	•	benign	benign
275	277	284	287	288	291	297	299
benign	benign	malignant	malignant	benign	_	malignant	benign
301	304	311	312	313	314	317	319
malignant	benign	benign	benign	malignant	benign	malignant	•
326	329	332	335	339	341	343	344
•	malignant	_	malignant	_	_	benign	benign
346	351	354	368	369	373	381	383
benign	· ·	malignant	•	benign	· ·	benign	benign
395	405	407	408	413	416	417	425
benign	benign	benign	_	${\tt malignant}$	_	malignant	benign
426	429	430	431	434	437	448	450
malignant	benign	benign	· ·	_	${\tt malignant}$	_	malignant
452	453	463	466	467	469	470	479
benign	benign	•	malignant	•	•	•	benign
480	481	488	498	502	505	509	511

malignant	benign	malignant	benign	benign	benign	benign	benign
519	520	522	524	529	532	536	539
benign	malignant	benign	malignant	benign	benign	benign	benign
540	546	548	551	554	557	560	564
benign	benign	benign	benign	benign	benign	benign	benign
566	570	573	574	575	578	579	580
malignant	${\tt malignant}$	benign	benign	malignant	benign	benign	benign
583	596	598	600	601	603	605	606
${\tt malignant}$	benign	benign	benign	benign	benign	${\tt malignant}$	${\tt malignant}$
608	609	611	613	628	629	632	638
benign	${\tt malignant}$	malignant	malignant	benign	benign	benign	benign
640	641	646	648	655	656	658	660
benign	benign	benign	benign	benign	benign	benign	benign
665	667	668	670	672	676	678	679
benign	benign	benign	malignant	benign	benign	benign	benign
680	681	684	686	694			
benign	${\tt malignant}$	benign	benign	benign			
Levels: benign malignant							

Finally, we generate a table comparing the actual classification with the predicted classification, which allows us to view the final results. Based on this table, we calculate four key metrics to evaluate the model's performance: Accuracy, Precision, Recall, and F1 Score. From these metrics, we observe that the result is generally acceptable and high.

```
perf1 <- table(test$Class, prediction, dnn=c("Actual", "Predicted"))
perf1</pre>
```

```
Actual benign malignant benign 140 2 malignant 3 60
```

```
TN1 <- perf1[1, 1] # True Negatives
TP1 <- perf1[2, 2] # True Positives

FP1 <- perf1[1, 2] # False Positives
FN1 <- perf1[2, 1] # False Negatives

# (Accuracy)
accuracy1 <- (TP1 + TN1) / sum(perf1)</pre>
```

```
# (Precision)
precision1 <- TP1 / (TP1 + FP1)

# (Recall)
recall1 <- TP1 / (TP1 + FN1)

spcificity1 <- TN1/(TN1 + FP1)

list(
   Accuracy1 = accuracy1,
   Precision1 = precision1,
   Recall1 = recall1,
   Spcificity1 = spcificity1
)</pre>
```

\$Accuracy1 [1] 0.9756098 \$Precision1 [1] 0.9677419 \$Recall1 [1] 0.952381 \$Spcificity1 [1] 0.9859155

## **Decision Tree**

Next, we move on to the Decision Tree method. We set the parameters to use information gain instead of the Gini index. By using the print and summary functions, we can examine the details of the decision tree.

```
library("rpart")
dtree <- rpart(Class ~ .,data= train, method="class",parms=list(split="information"))
print(dtree)</pre>
```

n = 478

```
node), split, n, loss, yval, (yprob)
      * denotes terminal node
 1) root 478 176 benign (0.63179916 0.36820084)
   2) Cell.size< 2.5 279
                           8 benign (0.97132616 0.02867384) *
   3) Cell.size>=2.5 199 31 malignant (0.15577889 0.84422111)
     6) Cell.size< 4.5 69 28 malignant (0.40579710 0.59420290)
      12) Bare.nuclei < 2.5 25
                                3 benign (0.88000000 0.12000000) *
                                6 malignant (0.13636364 0.86363636) *
      13) Bare.nuclei>=2.5 44
     7) Cell.size>=4.5 130
                             3 malignant (0.02307692 0.97692308) *
summary(dtree)
Call:
rpart(formula = Class ~ ., data = train, method = "class", parms = list(split = "information
 n = 478
          CP nsplit rel error
                                 xerror
                                              xstd
1 0.77840909
                  0 1.0000000 1.0000000 0.05991467
                  1 0.2215909 0.2556818 0.03627635
2 0.05397727
3 0.01000000
                  3 0.1136364 0.1250000 0.02602958
Variable importance
      Cell.size
                                   Epith.c.size
                     Cell.shape
                                                     Bare.nuclei
                                                                     Bl.cromatin
             22
                                                                              15
                             18
                                             16
                                                              15
Normal.nucleoli
                  Marg.adhesion
             14
Node number 1: 478 observations,
                                    complexity param=0.7784091
  predicted class=benign
                             expected loss=0.3682008 P(node) =1
    class counts:
                    302
                          176
   probabilities: 0.632 0.368
  left son=2 (279 obs) right son=3 (199 obs)
  Primary splits:
      Cell.size
                   < 2.5 to the left,
                                       improve=192.1333, (0 missing)
      Cell.shape
                   < 2.5 to the left,
                                       improve=188.4330, (0 missing)
      Bare.nuclei < 2.5 to the left,
                                       improve=168.9610, (0 missing)
                                       improve=163.3498, (0 missing)
      Bl.cromatin < 3.5 to the left,
      Epith.c.size < 2.5 to the left,
                                       improve=157.6645, (0 missing)
  Surrogate splits:
      Cell.shape
                      < 2.5 to the left, agree=0.918, adj=0.804, (0 split)
```

```
agree=0.897, adj=0.754, (0 split)
      Epith.c.size
                     < 2.5 to the left,
      Bl.cromatin
                     < 3.5 to the left,
                                          agree=0.868, adj=0.683, (0 split)
                     < 2.5 to the left,
                                          agree=0.860, adj=0.663, (0 split)
      Bare.nuclei
      Normal.nucleoli < 2.5 to the left,
                                          agree=0.860, adj=0.663, (0 split)
Node number 2: 279 observations
 predicted class=benign
                             expected loss=0.02867384 P(node) =0.583682
    class counts:
                    271
   probabilities: 0.971 0.029
                                    complexity param=0.05397727
Node number 3: 199 observations,
 predicted class=malignant expected loss=0.1557789 P(node) =0.416318
    class counts:
                     31
                          168
   probabilities: 0.156 0.844
  left son=6 (69 obs) right son=7 (130 obs)
 Primary splits:
      Cell.size
                    < 4.5 to the left,
                                        improve=25.22106, (0 missing)
      Bare.nuclei
                    < 2.5 to the left,
                                        improve=24.73323, (0 missing)
                    < 2.5 to the left,
                                        improve=21.68253, (0 missing)
      Cell.shape
      Marg.adhesion < 5.5 to the left,
                                        improve=19.06313, (0 missing)
                    < 3.5 to the left,
      Bl.cromatin
                                        improve=18.80490, (0 missing)
  Surrogate splits:
     Cell.shape
                     < 4.5 to the left,
                                          agree=0.794, adj=0.406, (0 split)
                                          agree=0.759, adj=0.304, (0 split)
     Epith.c.size
                     < 3.5 to the left,
                     < 2.5 to the left,
                                          agree=0.749, adj=0.275, (0 split)
      Marg.adhesion
      Bl.cromatin
                      < 3.5 to the left,
                                          agree=0.749, adj=0.275, (0 split)
                                          agree=0.724, adj=0.203, (0 split)
      Normal.nucleoli < 3.5 to the left,
Node number 6: 69 observations,
                                   complexity param=0.05397727
 predicted class=malignant expected loss=0.4057971 P(node) =0.1443515
                     28
    class counts:
   probabilities: 0.406 0.594
  left son=12 (25 obs) right son=13 (44 obs)
 Primary splits:
     Bare.nuclei
                      < 2.5 to the left,
                                          improve=19.896530, (0 missing)
      Cell.shape
                      < 2.5 to the left,
                                          improve= 9.967081, (0 missing)
      Cl.thickness
                     < 9 to the left,
                                          improve= 8.481164, (0 missing)
      Normal.nucleoli < 2.5 to the left,
                                          improve= 7.230538, (0 missing)
                                          improve= 7.094551, (0 missing)
      Marg.adhesion
                     < 5.5 to the left,
 Surrogate splits:
     Cell.shape
                     < 2.5 to the left,
                                          agree=0.812, adj=0.48, (0 split)
                                          agree=0.739, adj=0.28, (0 split)
      Bl.cromatin
                     < 1.5 to the left,
     Marg.adhesion
                     < 1.5 to the left,
                                          agree=0.710, adj=0.20, (0 split)
```

```
Cl.thickness < 2.5 to the left, agree=0.681, adj=0.12, (0 split) Normal.nucleoli < 2.5 to the left, agree=0.681, adj=0.12, (0 split)
```

Node number 7: 130 observations

predicted class=malignant expected loss=0.02307692 P(node) =0.2719665

class counts: 3 127 probabilities: 0.023 0.977

Node number 12: 25 observations

predicted class=benign expected loss=0.12 P(node) =0.05230126

class counts: 22 3 probabilities: 0.880 0.120

Node number 13: 44 observations

predicted class=malignant expected loss=0.1363636 P(node) =0.09205021

class counts: 6 38 probabilities: 0.136 0.864

In order to simplify the model, improve calculation efficiency, and enhance stability, we use the prune function to help optimize the decision tree.

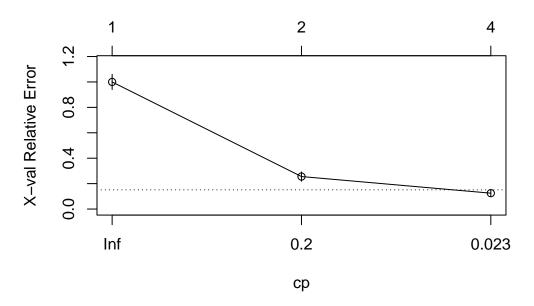
By examining the complexity parameter table, we can determine the optimal pruning point for the decision tree, which shows different values of cp, the number of branches in the tree (nsplit), the relative error (rel error), the cross-validation error (xerror), and its standard deviation (xstd).

The general approach is to choose the value of **CP** that minimizes the **cross-validation error** (**xerror**).

In that case, we will choose the 0.01 for the CP value. After pruning the decision tree, we can use fancyRpartPlot function to visualize the decision tree and its structure clearly.

plotcp(dtree)

## size of tree



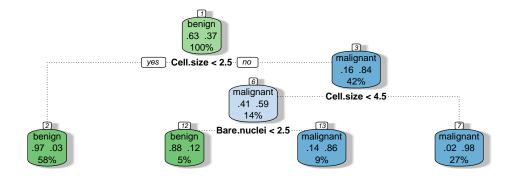
## dtree\$cptable

```
dtree.pruned <- prune(dtree,cp=0.01)
library(rattle)</pre>
```

Loading required package: tibble

Loading required package: bitops

Rattle: A free graphical interface for data science with R. Version 5.5.1 Copyright (c) 2006-2021 Togaware Pty Ltd. Type 'rattle()' to shake, rattle, and roll your data.



#### Classification Tree

After pruning the decision tree, we can use the test data to make predictions. Similar to logistic regression, we can use the table() function to compare the actual classifications with the predicted classifications.

```
dtree.pred <- predict(dtree.pruned,test,type="class")
perf2 <- table(test$Class,dtree.pred,dnn=c("Actual","Predicted"))
perf2</pre>
```

#### Predicted

Actual benign malignant benign 138 4 malignant 6 57

```
TN2 <- perf2[1, 1] # True Negatives
FP2 <- perf2[1, 2] # False Positives
FN2 <- perf2[2, 1] # False Negatives
TP2 <- perf2[2, 2] # True Positives
# (Accuracy)
accuracy2 <- (TP2 + TN2) / sum(perf2)</pre>
```

```
# (Precision)
precision2 <- TP2 / (TP2 + FP2)

# (Recall)
recall2 <- TP2 / (TP2 + FN2)

spcificity2 <- TN2/(TN2 + FP2)

list(
   Accuracy2 = accuracy2,
   Precision2 = precision2,
   Recall2 = recall2,
   Spcificity2 = spcificity2
)</pre>
```

\$Accuracy2
[1] 0.9512195

\$Precision2
[1] 0.9344262

\$Recall2
[1] 0.9047619

\$Spcificity2
[1] 0.971831

#### RandomForestModel

#### RandomForest

Now, let's move on to the random forest method. We use the randomForest function to build the model and the importance function to evaluate and rank the variables based on their importance.

```
library(randomForest)
```

```
randomForest 4.7-1.2
```

Type rfNews() to see new features/changes/bug fixes.

```
Attaching package: 'randomForest'
The following object is masked from 'package:rattle':
    importance
set.seed(1234)
fit.forest <- randomForest(Class ~ ., data=train,importance= TRUE)</pre>
fit.forest
Call:
 randomForest(formula = Class ~ ., data = train, importance = TRUE)
              Type of random forest: classification
                    Number of trees: 500
No. of variables tried at each split: 3
        OOB estimate of error rate: 2.93%
Confusion matrix:
         benign malignant class.error
benign
            293
                    9 0.02980132
malignant
           5
                      171 0.02840909
```

<pre>var_importance &lt;- fit.forest\$importance</pre>	
<pre>print(var_importance)</pre>	

	benign	${\tt malignant}$	MeanDecreaseAccuracy	MeanDecreaseGini
Cl.thickness	0.042688778	0.026907087	0.036757666	9.794852
Cell.size	0.090035717	0.087705808	0.088954598	58.635963
Cell.shape	0.021820598	0.073103200	0.040661838	49.754466
Marg.adhesion	0.011159602	0.032511581	0.018912111	8.373530
Epith.c.size	0.019658049	0.005981130	0.014562683	16.814313
Bare.nuclei	0.074536451	0.069801310	0.072818091	36.621347
Bl.cromatin	0.018291504	0.038034280	0.025639056	25.179804
Normal.nucleoli	0.022615855	0.017624908	0.020754772	14.177153
Mitoses	0.005865146	0.003703546	0.004991195	2.015803

Use the test data

```
forest.pred <- predict(fit.forest,test)
perf3 <- table(test$Class,forest.pred,dnn=c("Actual","Predicted"))
perf3</pre>
```

#### Predicted

Actual benign malignant benign 140 2 malignant 3 60

```
TN3 <- perf3[1, 1] # True Negatives
FP3 <- perf3[1, 2] # False Positives
FN3 <- perf3[2, 1] # False Negatives
TP3 <- perf3[2, 2] # True Positives

accuracy3 <- (TP3 + TN3) / sum(perf3)

precision3 <- TP3 / (TP3 + FP3)

recall3 <- TP3 / (TP3 + FN3)
spcificity3 <- TN3/(TN3 + FP3)

list(
    Accuracy3 = accuracy3,
    Precision3 = precision3,
    Recall3 = recall3,
    Spcificity3 = spcificity3
)</pre>
```

### \$Accuracy3

[1] 0.9756098

#### \$Precision3

[1] 0.9677419

#### \$Recall3

[1] 0.952381

#### \$Spcificity3

[1] 0.9859155

#### Black-box characteristic

These classification models are really important in real-world applications, as they can have a significant impact on people's decisions. For example, if someone applies for a bank loan and gets rejected, we would want to know the reason. If the decision is based on a logistic regression model or a decision tree model, we can easily understand the exact reason from the coefficients of the logistic regression model or the decision tree plot. However, if the decision is based on a random forest model, how can we get the answer? In random forest, multiple decision trees are used, and the paths of each tree are determined by various factors. As a result, we don't have a clear understanding of the decision path. To address this, there are methods we can use to interpret black box characteristics. One way is by applying explainable artificial intelligence (XAI) techniques to make these decisions more transparent and understandable.

For example, if we randomly generate data for Amy and use the model to calculate her probability of being malignant, and the result shows that her probability of being malignant is nearly 67%, which is greater than 50%, we want to understand how this result is influenced by the nine variables. Specifically, we want to know the contribution of each variable to the final decision. To do this, we use the explainer and plot to clearly visualize how each variable contributes to the model's output.

From the two charts below, we can observe that the results are consistent. The most important factor is the CL thickness, as its contribution is the highest among all the variables

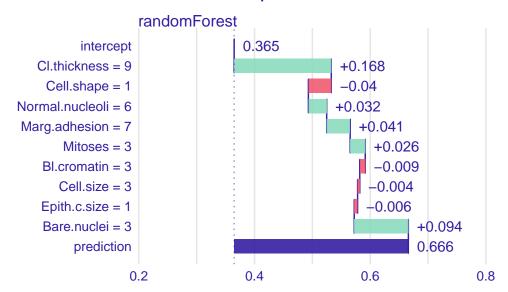
```
library("DALEX")
```

Welcome to DALEX (version: 2.4.3). Find examples and detailed introduction at: http://ema.drwhy.ai/

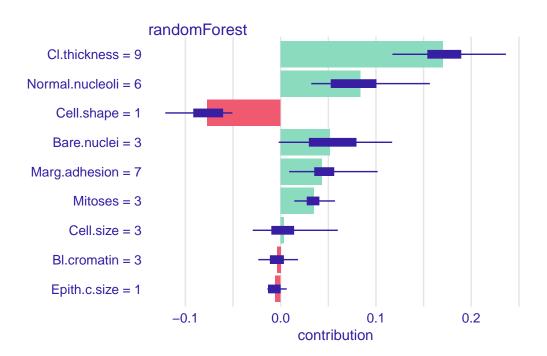
```
Amy <- data.frame(
   Cl.thickness = 9,
   Cell.size = 3,
   Cell.shape = 1,
   Marg.adhesion = 7,
   Epith.c.size = 1,
   Bare.nuclei = 3,
   Bl.cromatin = 3,
   Normal.nucleoli = 6,
   Mitoses = 3
)</pre>
```

```
benign malignant
1 0.334
            0.666
attr(,"class")
[1] "matrix" "array" "votes"
explainer_fr_malignant <- explain(fit.forest, data=train, y=train$Class == "malignant",
                     predcit_function = function(m,x) predict(m,x,type = "prob")[,2])
Preparation of a new explainer is initiated
  -> model label
                     : randomForest ( default )
  -> data
                     : 478 rows 10 cols
  -> target variable : 478 values
  -> predict function : yhat.randomForest will be used ( default )
  -> predicted values : No value for predict function target column. ( default )
                     : package randomForest , ver. 4.7.1.2 , task classification ( defau
  -> model_info
 -> model_info
                     : Model info detected classification task but 'y' is a logical . Con
  \rightarrow predicted values : numerical, min = 0 , mean = 0.3647782 , max = 1
  -> residual function : difference between y and yhat ( default )
                      : numerical, min = -0.364, mean = 0.003422594, max = 0.416
  -> residuals
  A new explainer has been created!
rf_pparts1 <- predict_parts(explainer_fr_malignant,new_observation = Amy,type="break_down")
plot(rf_pparts1 )
```

# Break Down profile



rf\_pparts2 <- predict\_parts(explainer\_fr\_malignant,new\_observation = Amy,type="shap")
plot(rf\_pparts2 )</pre>



## Support vector machines

#### **SVM**

The results from the Support Vector Machine (SVM) model demonstrate strong performance, as evidenced by the four performance metrics.

```
library(e1071)
set.seed(1234)
fit.svm <- svm(Class ~ ., data=train)</pre>
fit.svm
Call:
svm(formula = Class ~ ., data = train)
Parameters:
   SVM-Type: C-classification
 SVM-Kernel: radial
       cost: 1
Number of Support Vectors: 84
svm.pred <- predict(fit.svm,test)</pre>
svm.perf <- table(test$Class,svm.pred,dnn=c("Actual","Predicted"))</pre>
svm.perf
           Predicted
           benign malignant
Actual
               138
  benign
                           62
  malignant
                1
TN <- svm.perf[1, 1] # True Negatives
FP <- svm.perf[1, 2] # False Positives</pre>
FN <- svm.perf[2, 1] # False Negatives
TP <- svm.perf[2, 2] # True Positives
accuracy <- (TP + TN) / sum(svm.perf)</pre>
precision <- TP / (TP + FP)</pre>
recall <- TP / (TP + FN)
```

```
spcificity <- TN/(TN + FP)

list(
   Accuracy = accuracy,
   Precision = precision,
   Recall = recall,
   Spcificity =spcificity
)</pre>
```

```
$Accuracy
[1] 0.9756098

$Precision
[1] 0.9393939

$Recall
[1] 0.984127

$Spcificity
[1] 0.971831
```

#### **Parameters**

There are two key hyperparameters in Support Vector Machines (SVM): gamma and cost. By adjusting these parameters, we can enhance the model's performance. From the code results below, the optimal parameter values are found to be gamma = 0.01 and cost = 1. After updating the default parameters with these values and re-running the model, we observe that the results improve marginally, with one additional benign instance being accurately predicted. While the overall performance remains largely unchanged, it's important to note that tuning parameters in SVM typically leads to improvements in model performance.

```
#SVM
set.seed(1234)
tuned <- tune.svm(Class~.,data=train,gamma=10^(-6:1),cost=10^(-10:10))
tuned</pre>
```

```
Parameter tuning of 'svm':
- sampling method: 10-fold cross validation
```

```
- best parameters:
   gamma cost
   0.01   1
- best performance: 0.03355496

fit.svm1 <- svm(Class~., data=train,gamma=0.01,cost=1)
svm.pred1 <- predict(fit.svm1,na.omit(test))
svm.perf1 <- table(na.omit(test)$Class,svm.pred1,dnn=c("Actual","Predicted"))
svm.perf1</pre>
```

```
Predicted

Actual benign malignant benign 139 3 malignant 1 62
```

## **Summary**

Among the four models—Logistic Regression, Decision Tree, Random Forest, and Support Vector Machine—the results from all models are generally acceptable, with good performance across the board. However, in practice, the decision to choose the best model depends on the specific context. In this case, while the Support Vector Machine (SVM) appears to offer slightly better performance, the differences among the models are minimal.

From a cancer diagnosis perspective, recall is a critical metric, as it reflects the model's ability to accurately identify malignant cases. Therefore, this metric should be prioritized when selecting the most suitable model. Among the four models, the Support Vector Machine (SVM) demonstrates the highest recall rate, making it the preferred choice for this task.

Logistic regression is a simple and interpretable model that provides probabilities, making it easy to understand and useful for decision-making. It works well with linear data but struggles with nonlinear relationships, limiting its performance in more complex scenarios. Decision trees, on the other hand, can handle nonlinear data and provide a clear, interpretable structure through a tree diagram. They are capable of capturing more complex patterns than logistic regression. Random forests, an ensemble of multiple decision trees, improve upon decision trees by reducing overfitting and improving accuracy. They excel at handling missing data and complex nonlinear relationships, making them more robust and accurate than individual decision trees, but at the cost of interpretability. The Support Vector Machine (SVM) is a widely used and popular method, known for its versatility across various applications. It is particularly useful in scenarios where the number of variables exceeds the number of observations, a

common challenge in the pharmaceutical industry. Like Random Forest, SVM's classification principle can be difficult to interpret, as it functions as a black-box model. Additionally, when dealing with large datasets, SVM may not perform as well as Random Forest. However, once a successful model is developed, it is highly effective for classifying new observations.

```
list(
  Accuracy1 = accuracy1,
  Precision1 = precision1,
  Recall1 = recall1,
  spcificity1 = spcificity1
)
$Accuracy1
[1] 0.9756098
$Precision1
[1] 0.9677419
$Recall1
[1] 0.952381
$spcificity1
[1] 0.9859155
list(
  Accuracy2 = accuracy2,
  Precision2 = precision2,
  Recall2 = recall2,
  Spcificity2 = spcificity2
$Accuracy2
[1] 0.9512195
$Precision2
[1] 0.9344262
$Recall2
[1] 0.9047619
$Spcificity2
[1] 0.971831
```

```
list(
  Accuracy3 = accuracy3,
 Precision3 = precision3,
 Recall3 = recall3,
  Spcificity3 = spcificity3
$Accuracy3
[1] 0.9756098
$Precision3
[1] 0.9677419
$Recall3
[1] 0.952381
$Spcificity3
[1] 0.9859155
list(
 Accuracy4 = accuracy,
  Precision4 = precision,
 Recall4 = recall,
  Spcificity4 = spcificity
$Accuracy4
[1] 0.9756098
$Precision4
[1] 0.9393939
$Recall4
[1] 0.984127
$Spcificity4
[1] 0.971831
```