

Fundamentals of Predictive Analytics with JMP[®]

Third Edition

Ron Klimberg

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Fundamentals of Predictive Analytics with JMP®, Third Edition

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About This Book

What Does This Book Cover?

This book focuses on the business statistics intelligence component of business analytics. It covers processes to perform a statistical study that might include data mining or predictive analytics techniques. Some real-world business examples of using these techniques are as follows:

- target marketing
- customer relation management
- market basket analysis
- cross-selling
- forecasting
- market segmentation
- customer retention
- improved underwriting
- quality control
- competitive analysis
- fraud detection and management
- churn analysis

Specific applications can be found at <u>https://www.jmp.com/en_my/customer-stories/customer-listing/featured.html</u>. The bottom line, as reported by the KDNuggets poll (2008), is this: The median return on investment for data mining projects is in the 125–150% range. (See <u>http://www.kdnuggets.com/polls/2008/roi-data-mining.htm</u>.)

This book is *not* an introductory statistics book, although it does introduce basic data analysis, data visualization, and analysis of multivariate data. For the most part, your introductory statistics course has not completely prepared you to move on to real-world statistical analysis. The primary objective of this book is, therefore, to provide a bridge from your introductory statistics course to practical statistical analysis. This book is also not a highly technical book that dives deeply into the theory or algorithms, but it will provide insight into the "black box" of the methods covered. Analytics techniques covered by this book include the following:

- regression
- ANOVA
- logistic regression
- principal component analysis

- LASSO and Elastic Net
- cluster analysis
- decision trees
- k-nearest neighbors
- neural networks
- bootstrap forests and boosted trees
- text mining
- time series forecasting
- association rules

Is This Book for You?

This book is designed for the student who wants to prepare for his or her professional career and who recognizes the need to understand both the concepts and the mechanics of predominant analytic modeling tools for solving real-world business problems. This book is designed also for the practitioner who wants to obtain a hands-on understanding of business analytics to make better decisions from data and models, and to apply these concepts and tools to business analytics projects.

This book is for you if you want to explore the use of analytics for making better business decisions and have been either intimidated by books that focus on the technical details, or discouraged by books that focus on the high-level importance of using data without including the how-to of the methods and analysis.

Although not required, your completion of a basic course in statistics will prove helpful. Experience with the book's software, JMP Pro 17, is not required.

What's New in This Edition?

This third edition includes one new chapter on time series forecasting. All the old chapters from the second edition are updated to JMP 17. In addition, about 60% more end-of-chapter exercises are provided.

What Should You Know about the Examples?

This book includes tutorials for you to follow to gain hands-on experience with JMP.

Software Used to Develop the Book's Content

JMP Pro 17 is the software used throughout this book.

Example Code and Data

You can access the example code and data for this book by linking to its author page at http://support.sas.com/klimberg. Some resources, such as instructor resources and add-ins used in the book, can be found on the JMP User Community file exchange at https://community.jmp.com.

Where Are the Exercise Solutions?

We strongly believe that for you to obtain maximum benefit from this book you need to complete the examples in each chapter. At the end of each chapter are suggested exercises so that you can practice what has been discussed in the chapter. Professors and instructors can obtain the exercise solutions by requesting them through the author's SAS Press webpage at http://support.sas.com/klimberg.

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Learn more about the author by visiting his author page, where you can download free book excerpts, access example code and data, read the latest reviews, get updates, and more: http://support.sas.com/klimberg.

Chapter 13: Bootstrap Forests and Boosted Trees

Introduction

Decision trees, discussed in Chapter 10, are easy to comprehend, easy to explain, can handle qualitative variables without the need for dummy variables, and (as long as the tree isn't too large) are easily interpreted. Despite all these advantages, trees suffer from one grievous problem: they are unstable.

In this context, unstable means that a small change in the input can cause a large change in the output. For example, if one variable is changed even a little, and if the variable is important, then it can cause a split high up in the tree to change and, in so doing, cause changes all the way down the tree. Trees can be very sensitive not just to changes in variables, but also to the inclusion or exclusion of variables.

Fortunately, there is a remedy for this unfortunate state of affairs. As shown in Figure 13.1, this chapter discusses two techniques, bootstrap forests and boosted trees, which overcome this instability and many times result in better models.



Figure 13.1: A Framework for Multivariate Analysis

Bootstrap Forests

The first step in constructing a remedy involves a statistical method known as "the bootstrap." The idea behind the bootstrap is to take a single sample and turn it into several "bootstrap samples," each of which has the same number of observations as the original sample. In particular, a bootstrap sample is produced by random sampling with replacement from the original sample. These several bootstrap samples are then used to build trees. The results for each observation for each tree are averaged to obtain a prediction or classification for each observation. This averaging process implies that the result will not be unstable. Thus, the bootstrap remedies the great deficiency of trees.

This chapter does not dwell on the intricacies of the bootstrap method. (If interested, see "The Bootstrap," an article written by Shalizi (2010) in *American Scientist*. Suffice it to say that bootstrap methods are very powerful and, in general, do no worse than traditional methods that analyze only the original sample, and very often (as in the present case) can do much better.

It seems obvious now that you should take your original sample, turn it into several bootstrap samples, and construct a tree for each bootstrap sample. You could then combine the results of these several trees. In the case of classification, you could grow each tree so that it classified each observation—knowing that each tree would not classify each observation the same way.

Bootstrap forests, also called *random forests* in the literature, are a very powerful method, probably the most powerful method, presented in this book. On any particular problem, some other method might perform better. In general, however, bootstrap forests will perform better than other methods. Beware, though, of this great power. On some data sets, bootstrap forests can fit the data perfectly or almost perfectly. However, such a model will not predict perfectly or almost perfectly on new data. This is the phenomenon of "overfitting" the data, which is discussed in detail in Chapter 14. For now, the important point is that there is no reason to try to fit the data as well as possible. Just try to fit it well enough. You might use other algorithms as benchmarks, and then see whether bootstrap forests can do better.

Understand Bagged Trees

Suppose you grew 101 bootstrap trees. Then you would have 101 classifications ("votes") for the first observation. If 63 of the votes were "yes" and 44 were "no," then you would classify the first observation as a "yes." Similarly, you could obtain classifications for all the other observations. This method is called "bagged trees," where "bag" is shorthand for "bootstrap aggregation"— bootstrap the many trees and then aggregate the individual answers from all the trees. A similar approach can obtain predictions for each observation in the case of regression trees. This method uses the same data to build the tree and to compute the classification error.

An alternative method of obtaining predictions from bootstrapped trees is the use of "in-bag" and "out-of-bag" observations. Some observations, say two-thirds, are used to build the tree (these are the "in-bag" observations) and then the remaining one-third out-of-bag observations are dropped down the tree to see how they are classified. The predictions are compared to the truth for the out-of-bag observations, and the error rate is calculated on the out-of-bag observations. The reasons for using out-of-bag observations will be discussed more fully in Chapter 14. Suffice it to say that using the same observations to build the tree and then also to compute the error rate results in an overly optimistic error rate that can be misleading.

There is a problem with bagged trees, and it is that they are all quite similar, so their structures are highly correlated. We could get better answers if the trees were not so correlated, if each of the trees was more of an independent solution to the classification problem at hand. The way to achieve this was discovered by Breiman (2001). Breiman's insight was to not use all the independent variables for making each split. Instead, for each split, a subset of the independent variables is used.

To see the advantage of this insight, consider a node that needs to be split. Suppose variable X1 would split this node into two child nodes. Each of the two child nodes contains about the same number of observations, and each of the observations is only moderately homogeneous. Perhaps variable X2 would split this into two child nodes. One of these child nodes is small but relatively pure; the other child node is much larger and moderately homogenous. If X1 and X2 have to compete against each other in this spot, and if X1 wins, then you would never uncover the small, homogeneous node. On the other hand, if X1 is excluded and X2 is included so that X2 does not have to compete against X1, then the small, homogeneous pocket will be uncovered. A large number of trees is created in this manner, producing a forest of bootstrap trees. Then, after each tree has classified all the observations, voting is conducted to obtain a classification for each observation. A similar approach is used for regression trees.

Perform a Bootstrap Forest

To demonstrate bootstrap forests, use the Titanic data set, TitanicPassengers.jmp, the variables of which are described below in Table 13.1. It has 1,309 observations.

You want to predict who will survive:

- 1. Open the TitanicPassengers.jmp data set.
- In the course of due diligence, you will engage in exploratory data analysis before beginning any modeling. This exploratory data analysis will reveal that **Body** correlates perfectly with not surviving (Survived), as selecting Analyze ► Tabulate (or Fit Y by X), for these two variables will show. Also, Lifeboat correlates very highly with surviving (Survived), because very few of the people who got into a lifeboat failed to survive. So, use only the variables marked with an asterisk in Table 13.1.
- 3. Select Analyze > Predictive Modeling > Partition.

Variable	Description
Passenger Class *	1 = first, 2 = second, 3 = third
Survived *	No, Yes
Name	Passenger name
Sex *	Male, female
Age *	Age in years
Siblings and Spouses *	Number of Siblings and Spouses aboard
Parents and Children *	Number of Parents and Children aboard
Ticket #	Ticket number
Fare *	Fare in British pounds
Cabin	Cabin number (known only for a few passengers)
Port *	Q = Queenstown, C = Cherbourg, S = Southampton
Lifeboat	16 lifeboats 1–16 and four inflatables A–D
Body	Body identification number for deceased
Home/Destination	Home or destination of traveler

Table 13.1: Variables in the TitanicPassengers.jmp Data Set

- 4. Select **Survived** as **Y**, **response**. The other variables with asterisks in Table 13.1 are **X**, **Factor**.
- 5. For **Method**, choose **Bootstrap Forest**. **Validation Portion** is zero by default. **Validation** will be discussed in Chapter 14. For now, leave this at zero.
- 6. Click **OK**.

or

- 3. Select Analyze > Predictive Modeling > Bootstrap Forest.
- 4. Select **Survived** as **Y**, **response**. The other variables with asterisks in Table 13.1 are **X**, **Factor**.
- 5. Validation Portion is zero by default. Leave this at zero.
- 6. Click **OK**.

Understand the Options in the Dialog Box

Some of the options presented in the Bootstrap Forest dialog box, shown in Figure 13.2, are as follows:

- Number of trees in the forest is self-explanatory. There is no theoretical guidance on what this number should be. But empirical evidence suggests that there is no benefit to having a very large forest. 100 is the default. Try also 300 and 500. Setting the number of trees to be in the thousands probably will not be helpful.
- Number of terms sampled per split is the number of variables to use at each split. The default value is 6. If the original number of predictors is *p*, use V*p* rounded down for

classification, and for regression use p/3 rounded down (Hastie et al. 2009, p. 592). These are only rough recommendations. After trying \sqrt{p} , try $2\sqrt{p}$ and $\sqrt{p}/2$, as well as other values, if necessary.

- **Bootstrap sample rate** is the proportion of the data set to resample with replacement. Just leave this at the default 1 so that the bootstrap samples have the same number of observations as the original data set.
 - Minimum Splits Per Tree and Maximum Splits Per Tree are self-explanatory.
 - Minimum Size Split is the minimum number of observations in a node that is a candidate for splitting. For classification problems, the minimum node size should be one. For regression problems, the minimum node size should be five as recommended by Hastie et al. (2009, page 592).
 - Do not check the box Multiple Fits over number of terms. The associated Max Number of Terms is only used when the box is checked. The interested reader is referred to the user guide for additional details.

For now, change the Number of Terms Sampled per Split to 1 and just click OK.

The output of the Bootstrap Forest should look like Figure 13.3.

👺 Bootstrap Forest		×
Bootstrap Forest Specification		
Number of Rows: 1309 Number of Terms: 7 Forest Number of Trees in the Forest Number of Terms Sampled per Split: Bootstrap Sample Rate Minimum Splits per Tree: Maximum Splits per Tree Minimum Size Split:	100 6 1 10 2000 5	Multiple Fits
		OK Cancel

Figure 13.2: The Bootstrap Forest Dialog Box

Figure 13.3: Bootstrap Forest Output for the TitanicPassengers.jmp Data Set

	orect	for Surv	ived		
Bootstrap Fo	orest				
Specification	IS				
larget			Survived	Training Rows:	
				Validation Rows:	
Number of Trees	in the	Forest:	100	Test Rows:	
Number of Term	s Samp	led per Sp	lit: 1	Number of Terms:	
				Bootstrap Samples:	
				Minimum Splits per Tree:	
				Minimum Size Split:	
Overall Statis	stics				
Measure		Training	Definition		
Entropy RSquar	e	0.1789	1-Loglike(mod	lel)/Loglike(0)	
Generalized RSc	quare	0.2878	(1-(L(0)/L(mod	del))^(2/n))/(1-L(0)^(2/n))	
Mean -Log p		0.5461	∑ -Log(p[j])/n		
RASE		0.4247	√∑(y[j]-ρ[j])²/r	n	
Mean Abs Dev		0.4022	Σlv[i]-o[i]l/n		
Micelassificatio			Z 0 01 P 01P 11		
Wisclassificatio	n Rate	0.2231	∑(p[j]≠pMax)/	'n	
N	n Rate	0.2231 1309	∑ (ρ[j]≠ρMax)/ n	'n	
N Confusion	n Rate Matri	0.2231 1309 X	∑(p[j]≠pMax)/ n	'n	
N Confusion Tra	n Rate Matri aining	0.2231 1309 X	∑ (ρ[j]≠ρMax)/ n	'n	
N Confusion Tra	n Rate Matri aining Predic	0.2231 1309 x	∑(ρ[j]≠ρMax)/ n	'n	
N Confusion Tra Actual	n Rate Matri aining Predic Cou	0.2231 1309 X :ted nt	∑ (ρ[j]≠ρMax)/ n	'n	
Confusion Tra Actual Survived	n Rate Matri aining Predic Cour No	0.2231 1309 X :ted nt Yes	∑ (ρ[j]≠ρMax)/ n	'n	
A Confusion A Confusion Tra Actual Survived No	n Rate Matri aining Predic Cour No 775	0.2231 1309 x :ted nt Yes 34	∑ (ρ[j]≠ρMax)/ n	'n	
Actual Survived No Yes	n Rate Matri aining Predic Cou No 775 258	0.2231 1309 X ted nt Yes 34 242	Σ(ρ[j]≠ρMax)/ n	'n	
Confusion Tra Actual Survived No Yes	n Rate Matri aining Predic Cour No 775 258 Pred	0.2231 1309 x ted nt Yes 34 242 icted	Σ(ρ[]]≠ρMax)/ n	'n	
Confusion Tra Actual Survived No Yes Actual	n Rate Matri aining Predic Cou No 775 258 Pred Ra	0.2231 1309 X :ted nt Yes 34 242 icted ite	Σ(ρ[]]≠ρMax)/ n	'n	
Actual Survived Survived Survived Survived	n Rate Matri aining Predic Cou No 775 258 Pred Ra No	0.2231 1309 X :ted nt Yes 34 242 icted nte Yes	Σ(ρ[]]≠ρMax)/ n	'n	
N Confusion Tra Actual Survived No Yes Actual Survived No No	n Rate Matri aining Predic Cou No 775 258 Pred Ra No 0.958	0.2231 1309 X :ted nt Yes 34 242 iicted nte Yes 0.042	Σ(ρ[]≠ρMax)/ n	'n	

Select Options and Relaunch

Your results will be slightly different because this algorithm uses a random number generator to select the bootstrap samples. The sample size is 1,309. The lower left value in the first column of the Confusion Matrix, 258, and the top right value in the right-most column, 34, are the classification errors (discussed further in Chapter 14). Added together, 258 + 34 = 292, they compose the numerator of the reported misclassification rate in Figure 13.3: 292/1309 = 22.31%. Now complete the following steps:

- 1. Click the **Bootstrap Forest for Survived** red triangle and select **Redo** ► **Relaunch Analysis**.
- 2. The Partition dialog box appears. Click **OK**.
- 3. Now you are back in the Bootstrap Forest dialog box, as in Figure 13.2. Click **OK**. This time, double **the Number of Terms Sampled Per Split** to **2**.
- 4. Click **OK**.

The Bootstrap Forest output should look similar to Figure 13.4.

Specification	ns			
arget				Survived Training Rows:
				Validation Rows:
Number of Tree	s in the	Forest	:	100 Test Rows:
Number of Tern	ns Samp	led pe	r Spli	t: 2 Number of Terms:
				Bootstrap Samples:
				Minimum Splits per Tree:
				Minimum Size Split:
Overall Stati	stics			
Measure		Train	ning	Definition
Entropy RSqua	re	0.3	645	1-Loglike(model)/Loglike(0)
Generalized RS	quare	0.5	223	(1-(L(0)/L(model))^(2/n))/(1-L(0)^(2/n))
Mean -Log p		0.4	226	Σ -Log(p[j])/n
RASE		0.3	606	√∑(y[j]-p[j])²/n
Mean Abs Dev		0.3	030	Σ [y[j]-p[j]]/n
Misclassificatio	on Rate	0.1	597	∑ (p[j]≠pMax)/n
N		18	309	n
Confusion	Matri	ix		
Tr	aining			
	Predie	cted		
Actual	Cou	nt		
Survived	No	Yes		
No	761	48		
Yes	Yes 161 339			
	Predicted			
	Actual Ra			
Actual	N			
Actual Survived	No	Ye	s	
Actual Survived No	No 0.941	Ye : 0.059	s 9	

Figure 13.4: Bootstrap Forest Output with the Number of Terms Sampled per Split to 2

Examine the Improved Results

Notice the dramatic improvement. The error rate is now 15.97%. You could run the model again, this time increasing the **Number of Terms Sampled Per Split** to **3** and increasing the **Number of Trees** to **500**. These changes will again produce another dramatic improvement. Notice also that, although there are many missing values in the data set, Bootstrap Forest uses the full 1309 observations. Many other algorithms (for example, logistic regression) have to drop observations that have missing values.

An additional advantage of random forests is that, just like basic decision trees in Chapter 10 produced column contributions to show the important variables, random forests produce a similar ranking of variables. To get this list, click the **Bootstrap Forest for Survived** and select **Column Contributions**. This ranking can be especially useful in providing guidance for variable selection when later building logistic regressions or neural network models.

Perform a Bootstrap Forest for Regression Trees

Now briefly consider random forests for regression trees. Use the data set MassHousing.jmp in which the target variable is median value:

- 1. Select Analyze ► Predictive Modeling ► Partition.
- 2. Select mvalue for Y, Response and all the other variables as X, Factor.
- 3. For method, select **Bootstrap Forest**.
- 4. Click **OK**.
- 5. In the Bootstrap Forest dialog box, leave everything at default and click **OK**.

The Bootstrap Forest output should look similar to Figure 13.5.

Under **Overall Statistics**, see the In-Bag and Out-of-Bag RMSE. Notice that the Out-of-Bag RMSE is much larger than the In-Bag RMSE. This is to be expected because the algorithm is fitting on the In-Bag data. It then applies the estimated model to data that were not used to fit the model to obtain the Out-of-Bag RMSE. You will learn much more about this topic in Chapter 14. What's important for your purposes is that you obtained RSquare = 0.946 and RMSE = 1.863 for the full data set (remember that your results will be different because of the random number generator). These values compare quite favorably with the results from a linear regression: RSquare = 0.7406 and RMSE = 4.745. You can see that bootstrap forest regression can offer a substantial improvement over traditional linear regression. Additionally, bootstrap forest regression addresses nonlinearity better than ordinary least squares.

Specificat	ions				
Target	Target		mvalue	Training Rows:	50
				Validation Rows:	
Number of T	rees in the Fo	rest:	100	Test Rows:	
Number of T	erms Sample	d per Split:	10	Number of Terms:	1
				Bootstrap Samples:	50
				Minimum Splits per Tree:	1
				Minimum Size Split:	
Overall St	atistics				
Individual					
Trees	RASE				
In Bag	1.862558				
Out of Bag	4.777244				
RSquare	RASE	Ν			
0.946	2.1411069	506			

Figure 13.5: Bootstrap Forest Output for the MassHousing.jmp Data Set

Boosted Trees

Boosting is a general approach to combining a sequence of models in which each successive model changes slightly in response to the errors from the preceding model.

Understand Boosting

Boosting starts with estimating a model and obtaining residuals. The observations with the biggest residuals (where the model did the worst job) are given additional weight, and then the model is re-estimated on this transformed data set. In the case of classification, the misclassified observations are given more weight. After several models have been constructed, the estimates from these models are averaged to produce a prediction or classification for each observation. As was the case with bootstrap forests, this averaging implies that the predictions or classifications from the boosted tree model will not be unstable. When boosting, there is often no need to build elaborate models; simple models often suffice. In the case of trees, there is no need to grow the tree completely out; a tree with just a few splits often will do the trick. Indeed, simply fitting "stumps" (trees with only a single split and two leaves) at each stage often produces good results.

A boosted tree builds a large tree by fitting a sequence of smaller trees. At each stage, a smaller tree is grown on the scaled residuals from the prior stage, and the magnitude of the scaling is governed by a tuning parameter called the learning rate. The essence of boosting is that, on the current tree, it gives more weight to the observations that were misclassified on the prior tree.

Perform Boosting

Use Boosted Trees on the data set TitanicPassengers.jmp:

- 1. Select Analyze ► Predictive Modeling ► Partition.
- 2. For Method, select Boosted Tree.
- 3. Use the same variables as you did with Bootstrap Forests. Select **Survived** as **Y**, **response**. The other variables with asterisks in Table 13.1 are **X**, **Factor**.
- 4. Click **OK**.

or

- 1. Select Analyze > Predictive Modeling > Boosted Tree.
- 2. Select Survived as Y, response. The other variables with asterisks in Table 13.1 are X, Factor.
- 3. Click **OK**.

The Boosted Tree dialog box will appear, as shown in Figure 13.6.

Boosted Tree Gradient-Boosted Trees Specification	×
BoostingNumber of Layers:Splits per Tree:9Learning Rate:0.106Overfit Penalty:0.0001Minimum Size Split:5	Multiple Fits
Stochastic Boosting Row Sampling Rate 1.0000 Column Sampling Rate 1.0000	Reproducibility Suppress Multithreading Random Seed 0

Figure 13.6: The Boosted Tree Dialog Box

Understand the Options in the Dialog Box

The options are as follows:

- **Number of Layers** is the number of stages in the final tree. It is the number of trees to grow.
- **Splits Per Tree** is the number of splits for each stage (tree). If the number of splits is one, then "stumps" are being used.
- Learning Rate is a number between zero and one. A number close to one means faster learning, but at the risk of overfitting. Set this number close to one when the Number of Layers (trees) is small.
- **Overfit Penalty** helps protect against fitting probabilities equal to zero. It applies only to categorical targets.
- **Minimum Split Size** is the smallest number of observations to be in a node before it can be split.
- Multiple Fits over splits and learning rate will have JMP build a separate boosted tree for all combinations of splits and learning rate that the user chooses. Leave this box unchecked.

Select Options and Relaunch

For now, leave everything at default and click **OK**. The Bootstrap Tree output is shown in Figure 13.7. It shows a misclassification rate of 11.5%.

Figure 13.7: Boosted Tree Output for the TitanicPassengers.jmp Data Set

Boost	ed Tree	for	Surv	ivec	I					
Specifi	cations									
Target Survi			ived	N	Number of training rows: 130					
Number	of Layers:		198	N	umber of validation rows:	0				
Splits per	Tree:		9							
Learning	Rate:	0	.106							
Overfit P	enalty:	0.0	001							
Overal	Statist	ics								
Measur	e		Trai	ning	Definition					
Entropy	RSquare		0.5	5664	1-Loglike(model)/Loglike(0)				
General	ized RSqu	are	0.7	7195	(1-(L(0)/L(model))^(2/n))/((1-L(0)^(2				
Mean -l	.og p		0.2	2884	∑ -Log(p[j])/n					
RASE			0.2	2970	√∑(y[j]-p[j])²/n					
Mean Abs Dev			0.1	1994	Σ [y[j]-p[j]]/n					
Misclassification Rate		0.1	.1146 ∑(ρ[j]≠ρMax)/n							
N			1	309	n					
⊿ Conf	usion N	/latri	ix							
	Trai	ning								
	ctual I	Predic	ted							
	vived	No	Voc							
No	viveu	775	34							
Yes		116	384							
A	ctual	Ra	licted ate							
Su	vived	No	Ye	es						
No		0.958	0.04	2						
Yes		0.232	0.76	8						

Using the guidance given about the options, set the Learning rate high, to 0.9.

- 1. Click the **Boosted Tree for Survived** red triangle and select **Redo**. Choose **Relaunch Analysis**. The Partition dialog box appears. Click **OK**.
- 2. The Boosted Tree dialog box appears. Change the Learning rate to 0.9.
- 3. Click **OK**.

Examine the Improved Results

The Bootstrap Tree output will look like Figure 13.8, which has an error rate of 4.7%.

This is a substantial improvement over the default model and better than the Bootstrap Forest models. You could run the model again and this time change the **Number of Layers** to 250. Because this is bigger than the default, you could have chosen 200 or 400. Change the **Learning Rate** to 0.4. Because this is somewhere between 0.9 and 0.1, you could have chosen 0.3 or 0.6. Change the number of **Splits Per Tree** to **5** (again, there is nothing magic about this number).

	teu mee	101	Juiv	IVCC	•	
⊿ Speci	fications					
Target	Target Surv			N	lumber of training rows:	1309
Numbe	r of Layers:		198	N	lumber of validation rows:	0
Splits p	er Tree:		9			
Learnin	ig Rate:		0.9			
Overfit	Penalty:	0.0	001			
⊿ Overa	all Statist	ics				
Meas	ure		Trai	ning	Definition	
Entrop	by RSquare		0.	7974	1-Loglike(model)/Loglike(0))
Gener	alized RSqu	are	0.8888		(1-(L(0)/L(model))^(2/n))/	(1-L(0)^(
Mean	Mean -Log p		0.1347		∑ -Log(p[j])/n	
RASE	RASE		0.	1970	√ ∑(y[j]-p[j])²/n	
Mean	Abs Dev		0.0	0953	∑ y[j]-p[j] /n	
Miscla	ssification	Rate	0.0	0466	∑(p[j]≠pMax)/n	
N			1	1309	n	
⊿ Cor	fusion N	latri	ix			
	Trair	ning				
	Predicted					
	Actual	Cou	nt			
S	urvived	No	Yes			
N	o	789	20			
V	es	41				
1						
		Pred	licted			
	Actual	Pred Ra	licted ate			
s	Actual urvived	Pred Ra No	licted ate Ye	es		
S	Actual urvived	Pred Ra No 0.975	licted ate Ye 0.02	es 25		

Figure 13.8: Boosted Tree Output with a Learning Rate of 0.9

Boosted Trees is a very powerful method that also works for regression trees as you will see immediately below.

Perform a Boosted Tree for Regression Trees

Again, use the data set MassHousing.jmp.

- 1. Select Analyze ► Predictive Modeling ► Partition.
- 2. For Method, select Boosted Tree.
- 3. Select **mvalue** for the dependent variable, and all the other variables for independent variables.
- 4. Click **OK**.
- 5. Leave everything at default and click **OK**.

You should get the Boosted Tree output shown in Figure 13.9.

Specificat	ions			
Target	mvalu	e	Number of training rows:	506
Number of L	ayers: 171		Number of validation rows:	0
Splits per Tre	e:	5		
Learning Rat	e: 0.0	79		
Overall St	atistics			
RSquare	RASE	N		
0.973	1.4969641	506		

Figure 13.9: Boosted Tree Output for the MassHousing.jmp Data Set

Boosting is better than the Bootstrap Forest in Figure 13.5 (look at RSquare and RMSE), to say nothing of the linear regression.

Next, relaunch the analysis and change the **Learning rate** to 0.9. This is a substantial improvement with a perfect fit with an RSquare of 1.0. This is not really surprising, because both Bootstrap Forests and Boosted Trees are so powerful and flexible that they often can fit a data set perfectly.

Use Validation and Training Samples

When using such powerful methods, you should not succumb to the temptation to the make the RSquared as high as possible because such models rarely predict well on new data. To gain some insight into this problem, you will consider one more example in this chapter in which you will use a manually selected holdout sample.

You will divide the data into two samples, a "training" sample that consists of, for example, 75% of the data, and a "validation" sample that consists of the remaining 25%. You will then rerun your three boosted tree models on the TitanicPassengers.jmp data set on the training sample. JMP will automatically use the estimated models to make predictions on the validation sample.

Create a Dummy Variable

To effect this division into training and validation samples, you will need a dummy variable that randomly splits the data into a 75% / 25% split:

- 1. Open TitanicPassengers.jmp.
- 2. Select Analyze ► Predictive Modeling ► Make Validation Column. Click OK.
- 3. The Make Validation Column report dialog box will appear, as shown in Figure 13.10.
- 4. Click Go.

to cho option	omly partitions the cose a model by co nal test set to inde	rows of omparing pendentl	the data table in the predictive y evaluate perfo	nto a training s performance o prmance after	set to estimate the of several candidat the model is chos	e model, a validation se te models, and an en.
⊿ Spe	ecify rates or r	elative	rates			
			Adjusted Rates	Row Counts		
	Training Set	0.75	0.75019	982		
	Validation Set	0.25	0.24981	327		
	Test Set	0	0	0		
	Excluded Rows			0		
	Total Rows			1309		
⊿ Op	tions					
	New Column Na	ime	Validation			
	Validation Colur	nn Type	Fixed	~		
	Random Seed					
	Go					

Figure 13.10: The Make Validation Column Report Dialog Box

You will see that a new column called **Validation** has been added to the data table. You specified that the training set is to be 0.75 of the total rows, but this is really just a suggestion. The validation set will contain about 0.25 of the total rows.

Perform a Boosting at Default Settings

Run a Boosted Tree at default as before:

- 1. Select Analyze ► Predictive Modeling ► Partition.
- 2. As you did before, select **Survived** as **Y**, **response**. The other variables with asterisks in Table 13.1 are **X**, **Factor**.
- 3. Select the Validation column and then click Validation.
- 4. For Method, select **Boosted Tree**.
- 5. Click OK.
- 6. Click **OK** again for the options window. You are initially estimating this model with the defaults.

Examine Results and Relaunch

The results are presented in Figure 13.11. There are 982 observations in the training sample and 327 in the validation sample. Because 0.75 is just a suggestion and because the random number generator is used, your results will not agree exactly with the output in Figure 13.11. The error rate in the training sample is 15.1%, and the error rate in the validation sample is 21.4.

This strongly suggests that the model estimated on the training data predicts at least as well, if not better, on brand new data. The important point is that the model does not overfit the data (which can be detected when the performance on the training data is significantly better than the performance on new data). Now relaunch:

Figure 13.11: Boosted Tree Results for the TitanicPassengers.jmp Data Set with a Training and Validation Set

 Boosted Tree 	ee for	Surv	ivec	ł						
Specificatio	ns									
Target	get Survive			Number of t	training	rows:	982			
Validation Colu	mn: Vali	idation		Number of	/alidati	on rows	s: 327			
Number of Laye	ers:	40								
Splits per Tree:		9								
Learning Rate:		0.106								
Overfit Penalty:	(0.0001								
Overall Stat	istics									
Measure		Trair	ning	Validation	Defin	ition				
Entropy RSqua	are	0.4	764	0.2812	1-Log	1-Loglike(model)/Loglike(0)				
Generalized RS	quare	0.6	377	0.4252	(1-(L(0)/L(model))^(2/n))/(1-L(0)^(2					
Mean -Log p		0.3474		0.4812	2 ∑-Log(p[j])/n					
RASE		0.3294		0.3919 √∑(y[j]-p[j])²/n						
Mean Abs Dev		0.2365		0.2836	Σ ly[j]	-p[j] /n				
Misclassification Rate		0.1507		0.2141	∑ (ρ[j]	≠pMax)/n			
N			982	327	n					
	n Matr	ix								
Т	raining			Vali	dation					
	Predi	cted			Predic	ted				
Actual	Cou	int		Actual	Cou	nt				
Survived	No	Yes		Survived	No	Yes				
No	572	38		No	184	15				
Yes	110	262		Yes	55	73				
	Prec	Predicted			Pred	icted				
Actual	R	Rate		Actual	Ra	ate				
Survived	No	Ye	s	Survived	No	Yes				
No	0.938	0.06	2	No	0.925	0.075				
Yes	0.296	0.70	4	Yes	0.430	0.570				
Cumulative	Valida	ation								

- 1. Click the Boosted Tree for Survived red triangle and select Redo and Relaunch Analysis.
- 2. Click **OK** to get the Boosted Trees dialog box for the options and change the learning rate to **0.9**.
- 3. Click **OK**.

Compare Results to Choose the Least Misleading Model

You should get results similar to Figure 13.12, where the training error rate is 11.7% and the validation error rate is 22.0%.

Now you see that the model does a better job of "predicting" on the sample data than on brand new data. This makes you think that perhaps you should prefer the default model because it does not mislead you into thinking you have more accuracy than you really do.

Figure 13.12: Boosted Tree Results with Learning Rate of 0.9

Spe	cification	S								
Targe	et	Sun	vived		Number of t	raining	rows		982	
Valid	ation Colum	nn: Vali	dation		Number of	/alidati	on rov	VS:	327	
Num	ber of Layer	S:	22							
Splits	per Tree:		9							
Learn	ning Rate:		0.9							
Over	fit Penalty:	(0.0001							
Ove	rall Statis	stics								
Me	asure		Trainir	ng	Validation	Defin	ition			
Entr	opy RSquar	e	0.60	22	-0.157	1-Log	like(m	odel)/L	oglike((D)
Gen	eralized RSc	uare	0.74	B9	-0.317	(1-(L(0)/L(n	nodel))^	(2/n))/	(1-L(0)^(2/
Mean -Log p			0.26	40	0.7744	/44 ∑ -Log(ρ[j])/n				
RASE		0.28	74	0.4119	√∑(y[j]-p(j]))²/n			
Mean Abs Dev 0.1		0.17	69	0.2569	Σ [y[j]	-p[j]//	n			
Mis	classificatio	n Rate	0.11	71	0.2202	∑ (ρ[j]	≠ρMa	ix)/n		
N			98	82	327	n				
⊿ Co	onfusion	Matri	ix							
	Tra	aining			Vali	dation				
		Predic	redicted			Predicted				
	Actual	Cou	nt		Actual	Cou	nt			
	Survived	No	Yes		Survived	No	Yes			
	No	588	22		No	182	17			
	Yes	93	279		Yes	55	73			
[Pred	licted			Pred	icted			
	Actual	Ra	ate		Actual	Ra	te			
	Survived	No	Yes		Survived	No	Ye	s		
	No	0.964	0.036		No	0.915	0.08	5		
	Ves	0.250	0.750		Yes	0.430	0.57	0		

See if this pattern persists for the third model. Observe that the Number of Layers has decreased to 22, even though you specified it to be 198. This adjustment is automatically performed by JMP. As you did before, change the Learning Rate to 0.4. You should get similar results as shown in Figure 13.13, where the training error rate is 13.2% and the validation error rate is 21.4%. JMP again has changed the Number of Layers from the default 198 to 24.

It seems that no matter how you tweak the model to achieve better "in-sample" performance (that is, performance on the training sample), you always get about a 20% error rate on the brand-new data. So, which of the three models should you choose? The one that misleads you the least? The default model because its training sample performance is close to its validation sample performance? This idea of using "in-sample" and "out-of-sample" predictions to select the best model will be fully explored in the next chapter.

Bo	osted Tre	e for	Surv	iveo	1							
⊿ Spe	cification	s										
Targ	et	Survived			Number of t	raining	rows:	98	2			
Valio	lation Colum	nn: Vali	Validation		Number of v	alidati	on row	s: 32	7			
Num	ber of Layer	S:	24									
Split	s per Tree:		9									
Lear	ning Rate:		0.4									
Over	fit Penalty:	C	.0001									
⊿ Ove	erall Statis	stics										
Me	asure		Trai	nina	Validation	Defin	ition					
Ent	ropy RSquar	e	0.5	5407	0.1132	0.1132 1-Loglike(model)/Loglike(0)						
Ger	Generalized RSquare		0.6	5969	0.1906	(1-(L(0)/L(m	odel))^(2/	/n))/(1-L(0)^(2/n))			
Me	Mean -Log p		0.3	3047	0.5936	0.5936 ∑ -Log(p[j])/n						
RAS	RASE		0.3105		0.4122							
Me	Mean Abs Dev		0.2082		0.2785	Σ ly[j]·	-p[j]/n	1				
Mis	Misclassification Rate		0.1324		0.2141 ∑(p[j]≠pMax)/n			()/n				
N				982	327	n						
⊿C	onfusion	Matri	x									
	Tra	aining			Vali	dation						
		Predic	edicted			Predicted						
	Actual	Cou	nt		Actual	Cour	Count					
	Survived	No	Yes		Survived	No	Yes					
	No	577	33		No	177	22					
	Yes	97	275		Yes	48	80					
		Pred	Predicted			Pred	icted					
	Actual	Ra	Rate		Actual	Ra	te					
	Survived	No	Ye	es	Survived	No	Yes	;				
	No	0.946	0.05	4	No	0.889	0.111					
	Yes	0.261	0.73	9	Yes	0.375	0.625					
Cur	nulative	/alida	tion									

Figure 13.13: Boosted Tree Results with Learning Rate of 0.4

Predictions are created in the following way for both bootstrap forests and boosted trees. Suppose 38 trees are grown. The data for the new case is dropped down each tree (just as predictions were made for a single Decision Tree), and each tree makes a prediction. Then a "vote" is taken of all the trees, with a majority determining the winner. If, of the 38 trees, 20 predict "No" and the remaining 18 predict "Yes," then that observation is predicted to not survive.

Exercises

- 1. Without using a Validation column, run a logistic regression on the Titanic data and compare to the results in this chapter.
- 2. Can you improve on the results in Figure 13.3?
- 3. How high can you get the RSquare in the MassHousing example?
- 4. Without using a validation column, apply logistic regression, bootstrap forests, and boosted tree to the Churn data set.
- 5. Use a validation sample on boosted regression trees with MassHousing. How high can you get the RSquared on the validation sample? Compare this to your answer for Question 3.
- 6. Use a validation sample, and apply logistic regression, bootstrap forests, and boosted trees to the Churn data set. Compare this answer to your answer for Question 4.