STAT 462

Applied Regression Analysis

Lesson 11: Model Building

Overview of this Lesson

For all of the regression analyses that we have performed so far in this course, it has been obvious which of the major predictors we should include in our regression model. Unfortunately, this is typically not the case. More often than not, a researcher has a large set of candidate predictor variables from which to try to identify the most appropriate predictors to include in the regression model.

Of course, the larger the number of candidate predictor variables, the larger the number of possible regression models. For example, if a researcher has (only) 10 candidate predictor variables, there are $2^{10} = 1024$ possible regression models from which to choose. Clearly, some assistance would be needed in evaluating all of the possible regression models. That's where two variable selection methods — **stepwise regression** and **best subsets regression** — come in handy.

In this lesson, we'll learn about the above two variable selection methods. Our goal throughout will be to choose a small subset of predictors from the larger set of candidate predictors so that the resulting regression model is **simple** yet **useful**. That is, as always, our resulting regression model should:

- provide a good summary of the trend in the response,
- provide good predictions of the response, and
- provide good estimates of the slope coefficients.

Note. The data sets herein are not really all that large. For the sake of illustration, they necessarily have to be small, so that the largeness of the data set does not obscure the pedagogical point being made.

Key Learning Goals for this Lesson:
▪ Understand the impact of the four different kinds of models with respect to their "correctness" — correctly specified, underspecified, overspecified, and correct but with extraneous predictors. ▪ As a way of ensuring that you understand the general idea behind stepwise regression, be able to conduct stepwise regression "by hand." ▪ Know the limitations of stepwise regression. ▪ Know the general idea behind best subsets regression. ▪ Know how to choose an optimal model based on the R^2 value, the adjusted R^2 value, MSE and the C_p criterion. ▪ Know the limitations of best subsets regression. ▪ Know the general principles behind good model building strategies.

11.1 - What if the Regression Equation Contains "Wrong" Predictors? › (/stat462/node/195)

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11.1 - What if the Regression Equation Contains "Wrong" Predictors?

Before we can go off and learn about the two variable selection methods, we first need to understand the consequences of a regression equation containing the "wrong" or "inappropriate" variables. Let's do that now!

There are four possible outcomes when formulating a regression model for a set of data:

- The regression model is "**correctly specified**."
- The regression model is "**underspecified**."
- The regression model contains one or more "**extraneous variables**."
- The regression model is "**overspecified**."

Let's consider the consequence of each of these outcomes on the regression model. Before we do, we need to take a brief aside to learn what it means for an estimate to have the good characteristic of being unbiased.

Unbiased estimates

An estimate is **unbiased** if the average of the values of the estimates determined from all possible random samples equals the parameter you're trying to estimate. That is, if you take a random sample from a population and calculate the mean of the sample, then take another random sample and calculate its mean, and take another random sample and calculate its mean, and so on — the average of the means from all of the samples that you have taken should equal the true population mean. If that happens, the sample mean is considered an unbiased estimate of the population mean μ.

An estimated regression coefficient b_i is an unbiased estimate of the population slope β_i if the mean of all of the possible estimates b_i equals β_i. And, the predicted response $\hat{y}_i$ is an unbiased estimate of μ_Y if the mean of all of the possible predicted responses $\hat{y}_i$ equals μ_Y.

So far, this has probably sounded pretty technical. Here's an easy way to think about it. If you hop on a scale every morning, you can't expect that the scale will be perfectly accurate every day —some days it might run a little high, and some days a little low. That you can probably live with. You certainly don't want the scale, however, to *consistently* report that you weigh five pounds more than you actually do — your scale would be biased upward. Nor do you want it to *consistently* report that you weigh five pounds less than you actually do — errr..., scratch that, maybe you do — in this case, your scale would be biased downward. What you do want is for the scale to be correct on average — in this case, your scale would be unbiased. And, that's what we want!

The four possible outcomes

Now, back to the business on hand. **A regression model is correctly specified (outcome 1)** if the regression equation contains all of the relevant predictors, including any necessary transformations and interaction terms. That is, there are no missing, redundant or extraneous predictors in the model. Of course, this is the best possible outcome and the one we hope to achieve!

The good thing is that a correctly specified regression model yields unbiased regression coefficients and unbiased predictions of the response. And, the mean squared error (*MSE*) — which appears in some form in every hypothesis test we conduct or confidence interval we calculate — is an unbiased estimate of the error variance σ^2.

A regression model is underspecified (outcome 2) if the regression equation is missing one or more important predictor variables. This situation is perhaps the worst-case scenario, because an underspecified model yields biased regression coefficients and biased predictions of the response. That is, in using the model, we would consistently underestimate or overestimate the population slopes and the population means. To make already bad matters even worse, the mean square error *MSE* tends to overestimate σ^2, thereby yielding wider confidence intervals than it should.

Let's take a look at an example of a model that is likely underspecified. It involves an analysis of the height and weight of martians. The data set (martian.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/martian.txt)) — which was obviously contrived just for the sake of this example — contains the weights (in *g*), heights (in *cm*), and amount of daily water consumption (0, 10 or 20 *cups per day*) of 12 martians.

If we regress y = *weight* on the predictors x_1 = *height* and x_2 = *water*, we obtain the following estimated regression equation:

```
Regression Equation

weight = -1.220 + 0.28344 height + 0.11121 water
```

and the following estimate of the error variance σ^2:

```
MSE = 0.017
```

If we regress y = *weight* on only the one predictor x_1 = *height*, we obtain the following estimated regression equation:

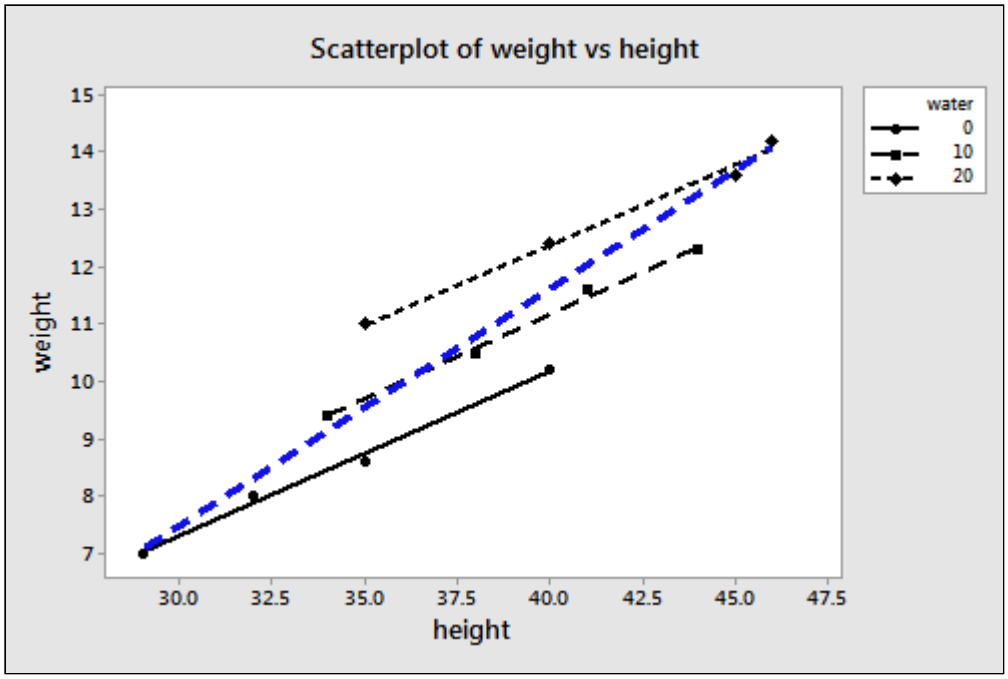
```
Regression Equation

weight = -4.14 + 0.3889 height
```

and the following estimate of the error variance σ^2:

```
MSE = 0.653
```

Plotting the two estimated regression equations, we obtain:



The three black lines represent the estimated regression equation when the amount of water consumption is taken into account — the first line for 0 cups per day, the second line for 10 cups per day, and the third line for 20 cups per day. The blue dashed line represents the estimated regression equation when we leave the amount of water consumed out of the regression model.

The second model — in which water is left out of the model — is likely an underspecified model. Now, what is the effect of leaving water consumption out of the regression model?

- The slope of the line (0.3889) obtained when height is the only predictor variable is much *steeper* than the slopes of the three parallel lines (0.28344) obtained by including the effect of water consumption, as well as height, on martian weight. That is, the slope likely *overestimates* the actual slope.
- The intercept of the line (-4.14) obtained when height is the only predictor variable is *smaller* than the intercepts of the three parallel lines (-1.220, -1.220 + 0.11121(10) = -0.108, and -1.220 + 0.11121(20) = 1.004) obtained by including the effect of water consumption, as well as height, on martian weight. That is, the intercept likely *underestimates* the actual intercepts.
- The estimate of the error variance σ^2 (MSE = 0.653) obtained when height is the only predictor variable is *about 38 times larger* than the estimate obtained (MSE = 0.017) by including the effect of water consumption, as well as height, on martian weight. That is, MSE likely *overestimates* the actual error variance σ^2.

This contrived example is nice in that it allows us to visualize how an underspecified model can yield biased estimates of important regression parameters. Unfortunately, in reality, we don't know the correct model. After all, if we did we wouldn't have a need to conduct the regression analysis! Because we don't know the correct form of the regression model, we have no way of knowing the exact nature of the biases.

Another possible outcome is that **the regression model contains one or more extraneous variables (outcome 3)**. That is, the regression equation contains extraneous variables that are neither related to the response nor to any of the other predictors. It is as if we went overboard and included extra predictors in the model that we didn't need!

The good news is that such a model does yield unbiased regression coefficients, unbiased predictions of the response, and an unbiased MSE. The bad news is that — because we have more parameters in our model — MSE has fewer degrees of freedom associated with it. When this happens, our confidence intervals tend to be wider and our hypothesis tests tend to have lower power. It's not the worst thing that can happen, but it's not too great either.

By including extraneous variables, we've also made our model more complicated and hard to understand than necessary.

If the regression model is overspecified (outcome 4), then the regression equation contains one or more redundant predictor variables. That is, part of the model is correct, but we have gone overboard by adding predictors that are redundant. Redundant predictors lead to problems such as inflated standard errors for the regression coefficients. (Such problems are also associated with multicollinearity, which we covered in Lesson 10).

Regression models that are overspecified yield unbiased regression coefficients, unbiased predictions of the response, and an unbiased MSE. Such a regression model can be used, with caution, for prediction of the response, but should not be used to ascribe the effect of a predictor on the response. Also, as with including extraneous variables, we've also made our model more complicated and hard to understand than necessary.

A goal and a strategy

Okay, so now we know the consequences of having the "wrong" variables in our regression model. The challenge, of course, is that we can never really be sure which variables are "wrong" and which variables are "right." All we can do is use the statistical methods at our fingertips and our knowledge of the situation to help build our regression model.

Here's my recommended approach to building a good and useful model:

1. **Know your goal, know your research question.** Knowing how you plan to use your regression model can assist greatly in the model building stage. Do you have a few particular predictors of interest? If so, you should make sure your final model includes them. Are you just interested in predicting the response? If so, then multicollinearity should worry you less. Are you interested in the effects that specific predictors have on the response? If so, multicollinearity should be a serious concern. Are you just interested in summary description? What is it that you are trying to accomplish?
2. **Identify all of the possible candidate predictors.** This may sound easier than it actually is to accomplish. Don't worry about interactions or the appropriate functional form — such as x^2 and $\log x$ — just yet. Just make sure you identify all the possible important predictors. If you don't consider them, there is no chance for them to appear in your final model.
3. **Use variable selection procedures to find the middle ground between an underspecified model and a model with extraneous or redundant variables.** Two possible variable selection procedures are *stepwise regression* and *best subsets regression*. We'll learn about both methods here in this lesson.
4. **Fine-tune the model to get a correctly specified model.** If necessary, change the functional form of the predictors and/or add interactions. Check the behavior of the residuals. If the residuals suggest problems with the model, try a different functional form of the predictors or remove some of the interaction terms. Iterate back and forth between formulating different regression models and checking the behavior of the residuals until you are satisfied with the model

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11.2 - Stepwise Regression

In this section, we learn about the stepwise regression procedure. While we will soon learn the finer details, the general idea behind the stepwise regression procedure is that we build our regression model from a set of candidate predictor variables by entering and removing predictors — in a stepwise manner — into our model until there is no justifiable reason to enter or remove any more.

Our hope is, of course, that we end up with a reasonable and useful regression model. There is one sure way of ending up with a model that is certain to be underspecified — and that's if the set of candidate predictor variables doesn't include *all* of the variables that actually predict the response. This leads us to a fundamental rule of the stepwise regression procedure — the list of candidate predictor variables must include *all* of the variables that actually predict the response. Otherwise, we are sure to end up with a regression model that is underspecified and therefore misleading.

An example

Let's learn how the stepwise regression procedure works by considering a data set that concerns the hardening of cement. Sounds interesting, eh? In particular, the researchers were interested in learning how the composition of the cement affected the heat evolved during the hardening of the cement. Therefore, they measured and recorded the following data (cement.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/cement.txt)) on 13 batches of cement:

- Response y: heat evolved in calories during hardening of cement on a per gram basis
- Predictor x_1: % of tricalcium aluminate
- Predictor x_2: % of tricalcium silicate
- Predictor x_3: % of tetracalcium alumino ferrite
- Predictor x_4: % of dicalcium silicate

Now, if you study the scatter plot matrix of the data:

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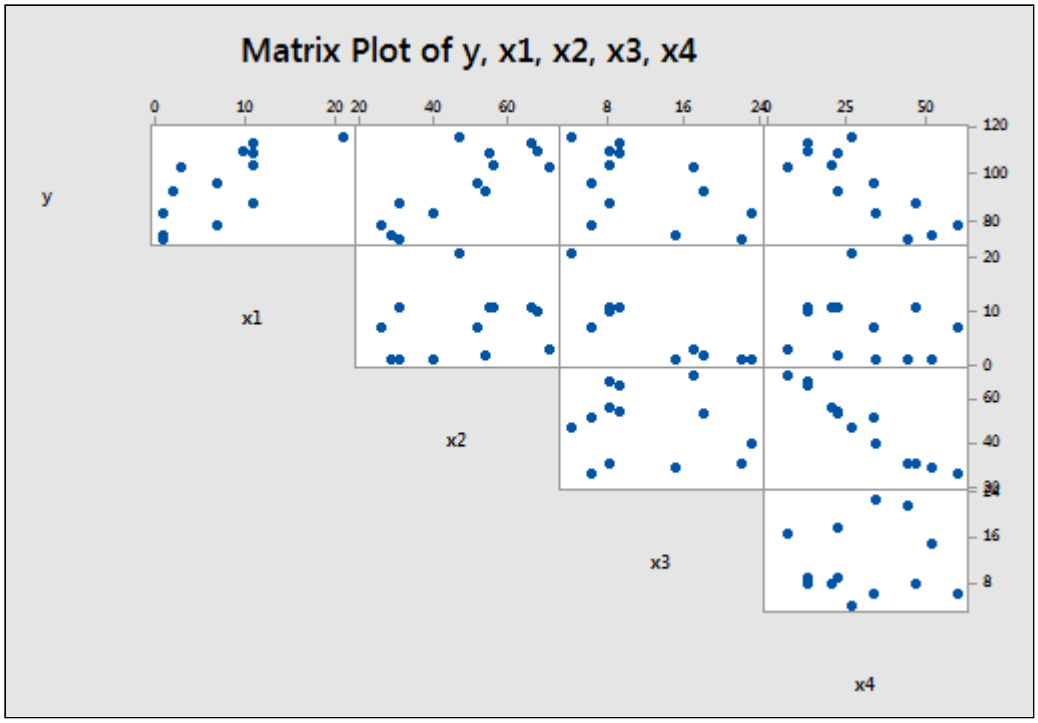

you can get a hunch of which predictors are good candidates for being the first to enter the stepwise model. It looks as if the strongest relationship exists between either y and x_2 or between y and x_4 — and therefore, perhaps either x_2 or x_4 should enter the stepwise model first. Did you notice what else is going on in this data set though? A strong correlation also exists between the predictors x_2 and x_4! How does this correlation among the predictor variables play out in the stepwise procedure? Let's see what happens when we use the stepwise regression method to find a model that is appropriate for these data.

Note. The number of predictors in this data set is not large. The stepwise procedure is typically used on much larger data sets, for which it is not feasible to attempt to fit all of the possible regression models. For the sake of illustration, the data set here is necessarily small, so that the largeness of the data set does not obscure the pedagogical point being made.

The procedure

Again, before we learn the finer details, let me again provide a broad overview of the steps involved. First, we start with no predictors in our "**stepwise model**." Then, at each step along the way we either enter or remove a predictor based on the partial F-tests — that is, the t-tests for the slope parameters — that are obtained. We stop when no more predictors can be justifiably entered or removed from our stepwise model, thereby leading us to a "**final model**."

Now, let's make this process a bit more concrete. Here goes:

Starting the procedure. The first thing we need to do is set a significance level for deciding when to enter a predictor into the stepwise model. We'll call this the **Alpha-to-Enter** significance level and will denote it as α_E. Of course, we also need to set a significance level for deciding when to remove a predictor from the stepwise model. We'll call this the **Alpha-to-Remove** significance level and will denote it as α_R. That is, first:

- Specify an Alpha-to-Enter significance level. This will typically be greater than the usual 0.05 level so that it is not too difficult to enter predictors into the model. Many software packages set this significance level by

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- Specify an Alpha-to-Remove significance level. This will typically be greater than the usual 0.05 level so that it is not too easy to remove predictors from the model. Again, many software packages set this significance level by default to $\alpha_R = 0.15$.

Step #1. Once we've specified the starting significance levels, then we:

1. Fit each of the one-predictor models — that is, regress y on x_1, regress y on x_2, ..., and regress y on x_k.
2. Of those predictors whose t-test P-value is less than $\alpha_E = 0.15$, the first predictor put in the stepwise model is the predictor that has the smallest t-test P-value.
3. If no predictor has a t-test P-value less than $\alpha_E = 0.15$, stop.

Step #2. Then:

1. Suppose x_1 had the smallest t-test P-value below $\alpha_E = 0.15$ and therefore was deemed the "best" single predictor arising from the the first step.
2. Now, fit each of the two-predictor models that include x_1 as a predictor — that is, regress y on $x_1$and x_2, regress y on $x_1$and x_3, ..., and regress y on x_1 and x_k.
3. Of those predictors whose t-test P-value is less than $\alpha_E = 0.15$, the second predictor put in the stepwise model is the predictor that has the smallest t-test P-value.
4. If no predictor has a t-test P-value less than $\alpha_E = 0.15$, stop. The model with the one predictor obtained from the first step is your final model.
5. But, suppose instead that x_2 was deemed the "best" second predictor and it is therefore entered into the stepwise model.
6. Now, since x_1 was the first predictor in the model, step back and see if entering x_2 into the stepwise model somehow affected the significance of the x_1 predictor. That is, check the t-test P-value for testing $\beta_1 = 0$. If the t-test P-value for $\beta_1 = 0$ has become not significant — that is, the P-value is greater than $\alpha_R = 0.15$ — remove x_1 from the stepwise model.

Step #3. Then:

1. Suppose both x_1 and x_2 made it into the two-predictor stepwise model and remained there.
2. Now, fit each of the three-predictor models that include x_1 and x_2 as predictors — that is, regress y on x_1, x_2, and x_3, regress y on x_1, x_2, and x_4, ..., and regress y on x_1, x_2, and x_k.
3. Of those predictors whose t-test P-value is less than $\alpha_E = 0.15$, the third predictor put in the stepwise model is the predictor that has the smallest t-test P-value.
4. If no predictor has a t-test P-value less than $\alpha_E = 0.15$, stop. The model containing the two predictors obtained from the second step is your final model.
5. But, suppose instead that x_3 was deemed the "best" third predictor and it is therefore entered into the stepwise model.
6. Now, since x_1 and x_2 were the first predictors in the model, step back and see if entering x_3 into the stepwise model somehow affected the significance of the x_1 and x_2 predictors. That is, check the t-test P-values for testing $\beta_1 = 0$ and $\beta_2 = 0$. If the t-test P-value for either $\beta_1 = 0$ or $\beta_2 = 0$ has become not significant — that is, the P-value is greater than $\alpha_R = 0.15$ — remove the predictor from the stepwise model.

Stopping the procedure. Continue the steps as described above until adding an additional predictor does not yield a

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Whew! Let's return to our cement data example so we can try out the stepwise procedure as described above.

The example again

To start our stepwise regression procedure, let's set our Alpha-to-Enter significance level at $\alpha_E = 0.15$, and let's set our Alpha-to-Remove significance level at $\alpha_R = 0.15$. Now, regressing y on x_1, regressing y on x_2, regressing y on x_3, and regressing y on x_4, we obtain:

Predictor	Coef	SE Coef	T	P
Constant	81.479	4.927	16.54	0.000
x1	1.8687	0.5264	**3.55**	**0.005**

Predictor	Coef	SE Coef	T	P
Constant	57.424	8.491	6.76	0.000
x2	0.7891	0.1684	**4.69**	**0.001**

Predictor	Coef	SE Coef	T	P
Constant	110.203	7.948	13.87	0.000
x3	-1.2558	0.5984	**-2.10**	**0.060**

Predictor	Coef	SE Coef	T	P
Constant	117.568	5.262	22.34	0.000
x4	-0.7382	0.1546	**-4.77**	**0.001**

Each of the predictors is a candidate to be entered into the stepwise model because each t-test P-value is less than $\alpha_E = 0.15$. The predictors x_2 and x_4 tie for having the smallest t-test P-value — it is 0.001 in each case. But note the tie is an artifact of rounding to three decimal places. The t-statistic for x_4 is *larger in absolute value* than the t-statistic for x_2—4.77 versus 4.69—and therefore the P-value for x_4 must be smaller. As a result of the first step, we enter x_4 into our stepwise model.

Now, following step #2, we fit each of the two-predictor models that include x_4 as a predictor — that is, we regress y on x_4 and x_1, regress y on x_4 and x_2, and regress y on x_4 and x_3, obtaining:

Predictor	Coef	SE Coef	T	P
Constant	103.097	2.124	48.54	0.000
x4	-0.61395	0.04864	-12.62	0.000
x1	1.4400	0.1384	**10.40**	**0.000**

Predictor	Coef	SE Coef	T	P
Constant	94.16	56.63	1.66	0.127
x4	-0.4569	0.6960	-0.66	0.526
x2	0.3109	0.7486	**0.42**	**0.687**

Predictor	Coef	SE Coef	T	P
Constant	131.282	3.275	40.09	0.000
x4	-0.72460	0.07233	-10.02	0.000
	999	0.1890	**-6.35**	**0.000**

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The predictor x_2 is not eligible for entry into the stepwise model because its *t*-test *P*-value (0.687) is greater than $\alpha_E = 0.15$. The predictors x_1 and x_3 are candidates because each *t*-test *P*-value is less than $\alpha_E = 0.15$. The predictors x_1 and x_3 tie for having the smallest *t*-test *P*-value—it is < 0.001 in each case. But, again the tie is an artifact of rounding to three decimal places. The *t*-statistic for x_1 is *larger in absolute value* than the *t*-statistic for x_3—10.40 versus 6.35—and therefore the *P*-value for x_1 must be smaller. As a result of the second step, we enter x_1 into our stepwise model.

Now, since x_4 was the first predictor in the model, we must step back and see if entering x_1 into the stepwise model affected the significance of the x_4 predictor. It did not—the *t*-test *P*-value for testing $\beta_1 = 0$ is less than 0.001, and thus smaller than $\alpha_R = 0.15$. Therefore, we proceed to the third step with both x_1 and x_4 as predictors in our stepwise model.

Now, following step #3, we fit each of the three-predictor models that include $x1$ and x_4 as predictors — that is, we regress y on x_4, x_1, and x_2; and we regress y on x_4, x_1, and x_3, obtaining:

Predictor	Coef	SE Coef	T	P
Constant	71.65	14.14	5.07	0.001
x4	-0.2365	0.1733	-1.37	0.205
x1	1.4519	0.1170	12.41	0.000
x2	0.4161	0.1856	**2.24**	**0.052**

Predictor	Coef	SE Coef	T	P
Constant	111.684	4.562	24.48	0.000
x4	-0.64280	0.04454	-14.43	0.000
x1	1.0519	0.2237	4.70	0.001
x3	-0.4100	0.1992	**-2.06**	**0.070**

Both of the remaining predictors—x_2 and x_3—are candidates to be entered into the stepwise model because each *t*-test *P*-value is less than $\alpha_E = 0.15$. The predictor x_2 has the smallest *t*-test *P*-value (0.052). Therefore, as a result of the third step, we enter x_2 into our stepwise model.

Now, since x_1 and x_4 were the first predictors in the model, we must step back and see if entering x_2 into the stepwise model affected the significance of the x_1 and x_4 predictors. Indeed, it did—the *t*-test *P*-value for testing $\beta_4 = 0$ is 0.205, which is greater than $\alpha_R = 0.15$. Therefore, we remove the predictor x_4 from the stepwise model, leaving us with the predictors x_1 and x_2 in our stepwise model:

Predictor	Coef	SE Coef	T	P
Constant	52.577	2.286	23.00	0.000
x1	1.4683	0.1213	12.10	0.000
x2	0.66225	0.04585	14.44	0.000

Now, we proceed fitting each of the three-predictor models that include x_1 and x_2 as predictors — that is, we regress y on x_1, x_2, and x_3; and we regress y on x_1, x_2, and x_4, obtaining:

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Predictor	Coef	SE Coef	T	P
Constant	71.65	14.14	5.07	0.001
x1	1.4519	0.1170	12.41	0.000
x2	0.4161	0.1856	2.24	0.052
x4	-0.2365	0.1733	**-1.37**	**0.205**

Predictor	Coef	SE Coef	T	P
Constant	48.194	3.913	12.32	0.000
x1	1.6959	0.2046	8.29	0.000
x2	0.65691	0.04423	14.85	0.000
x3	0.2500	0.1847	**1.35**	**0.209**

Neither of the remaining predictors—x_3 and x_4—are eligible for entry into our stepwise model, because each t-test P-value—0.209 and 0.205, respectively—is greater than $\alpha_E = 0.15$. That is, we stop our stepwise regression procedure. Our final regression model, based on the stepwise procedure contains only the predictors x_1 and x_2:

Predictor	Coef	SE Coef	T	P
Constant	52.577	2.286	23.00	0.000
x1	1.4683	0.1213	12.10	0.000
x2	0.66225	0.04585	14.44	0.000

Whew! That took a lot of work! The good news is that most statistical software provides a stepwise regression procedure that does all of the dirty work for us.

Here's what stepwise regression output looks like for our cement data example:

Regression Analysis: y versus x1, x2, x3, x4

Stepwise Selection of Terms

Candidate terms: x1, x2, x3, x4

	-----Step 1----		-----Step 2-----		-----Step 3----		-----Step 4----	
	Coef	P	Coef	P	Coef	P	Coef	P
Constant	117.57		103.10		71.6		52.58	
x4	-0.738	0.001	-0.6140	0.000	-0.237	0.205		
x1			1.440	0.000	1.452	0.000	1.468	0.000
x2					0.416	0.052	0.6623	0.000
S		8.96390		2.73427		2.30874		2.40634
R-sq		67.45%		97.25%		98.23%		97.87%
R-sq(adj)		64.50%		96.70%		97.64%		97.44%
R-sq(pred)		56.03%		95.54%		96.86%		96.54%
Mallows' Cp		138.73		5.50		3.02		2.68

α to enter = 0.15, α to remove = 0.15

The output tells us that :

- a stepwise regression procedure was conducted on the response y and four predictors x_1, x_2, x_3, and x_4
- the Alpha-to-Enter significance level was set at $\alpha_E = 0.15$ and the Alpha-to-Remove significance level was set

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The remaining portion of the output contains the results of the various steps of the stepwise regression procedure. One thing to keep in mind is that this output numbers the steps a little differently than described above. This output considers a step any addition or removal of a predictor from the stepwise model, whereas our steps—step #3, for example—considers the addition of one predictor and the removal of another as one step.

The results of each step are reported in a column labeled by the step number. It took four steps before the procedure was stopped. Here's what the output tells us:

- Just as our work above showed, as a result of the **first step**, the predictor x_4 is entered into the stepwise model. The output tells us that the estimated intercept ("Constant") $b_0 = 117.57$ and the estimated slope $b_4 = -0.738$. The P-value for testing $\beta_4 = 0$ is 0.001. The estimate S, which equals the square root of MSE, is 8.96. The R^2-value is 67.45% and the adjusted R^2-value is 64.50%. Mallows' Cp-statistic, which we learn about in the next section, is 138.73. The output also includes a predicted R^2-value, which we'll come back to in Section 10.5.
- As a result of the **second step**, the predictor x_1 is entered into the stepwise model already containing the predictor x_4. The output tells us that the estimated intercept $b_0 = 103.10$, the estimated slope $b_4 = -0.614$, and the estimated slope $b_1 = 1.44$. The P-value for testing $\beta_4 = 0$ is < 0.001. The P-value for testing $\beta_1 = 0$ is < 0.001. The estimate S is 2.73. The R^2-value is 97.25% and the adjusted R^2-value is 96.70%. Mallows' Cp-statistic is 5.5.
- As a result of the **third step**, the predictor x_2 is entered into the stepwise model already containing the predictors x_1 and x_4. The output tells us that the estimated intercept $b_0 = 71.6$, the estimated slope $b_4 = -0.237$, the estimated slope $b_1 = 1.452$, and the estimated slope $b_2 = 0.416$. The P-value for testing $\beta_4 = 0$ is 0.205. The P-value for testing $\beta_1 = 0$ is < 0.001. The P-value for testing $\beta_2 = 0$ is 0.052. The estimate S is 2.31. The R^2-value is 98.23% and the adjusted R^2-value is 97.64%. Mallows' Cp-statistic is 3.02.
- As a result of the **fourth and final step**, the predictor x_4 is removed from the stepwise model containing the predictors x_1, x_2, and x_4, leaving us with the final model containing only the predictors x_1 and x_2. The output tells us that the estimated intercept $b_0 = 52.58$, the estimated slope $b_1 = 1.468$, and the estimated slope $b_2 = 0.6623$. The P-value for testing $\beta_1 = 0$ is < 0.001. The P-value for testing $\beta_2 = 0$ is < 0.001. The estimate S is 2.41. The R^2-value is 97.87% and the adjusted R^2-value is 97.44%. Mallows' Cp-statistic is 2.68.

Does the stepwise regression procedure lead us to the "best" model? No, not at all! Nothing occurs in the stepwise regression procedure to guarantee that we have found the optimal model. Case in point! Suppose we defined the best model to be the model with the largest adjusted R^2-value. Then, here, we would prefer the model containing the three predictors x_1, x_2, and x_4, because its adjusted R^2-value is 97.64%, which is higher than the adjusted R^2-value of 97.44% for the final stepwise model containing just the two predictors x_1 and x_2.

Again, nothing occurs in the stepwise regression procedure to guarantee that we have found the optimal model. This, and other cautions of the stepwise regression procedure, are delineated in the next section.

Cautions!

Here are some things to keep in mind concerning the stepwise regression procedure:

- The final model is not guaranteed to be optimal in any specified sense.
- The procedure yields a single final model, although there are often several equally good models.
- The procedure does not take into account a researcher's knowledge about the predictors. It may be necessary to force the procedure to include important predictors.

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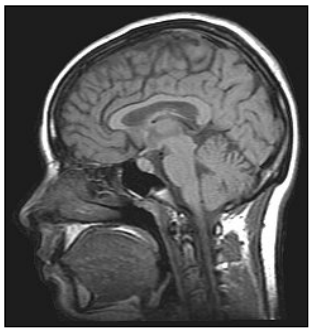
- One should not over-interpret the order in which predictors are entered into the model.
- One should not jump to the conclusion that all the important predictor variables for predicting y have been identified, or that all the unimportant predictor variables have been eliminated. It is, of course, possible that we may have committed a Type I or Type II error along the way.
- Many t-tests for testing $\beta_k = 0$ are conducted in a stepwise regression procedure. The probability is therefore high that we included some unimportant predictors or excluded some important predictors.

It's for all of these reasons that one should be careful not to overuse or overstate the results of any stepwise regression procedure.

More examples

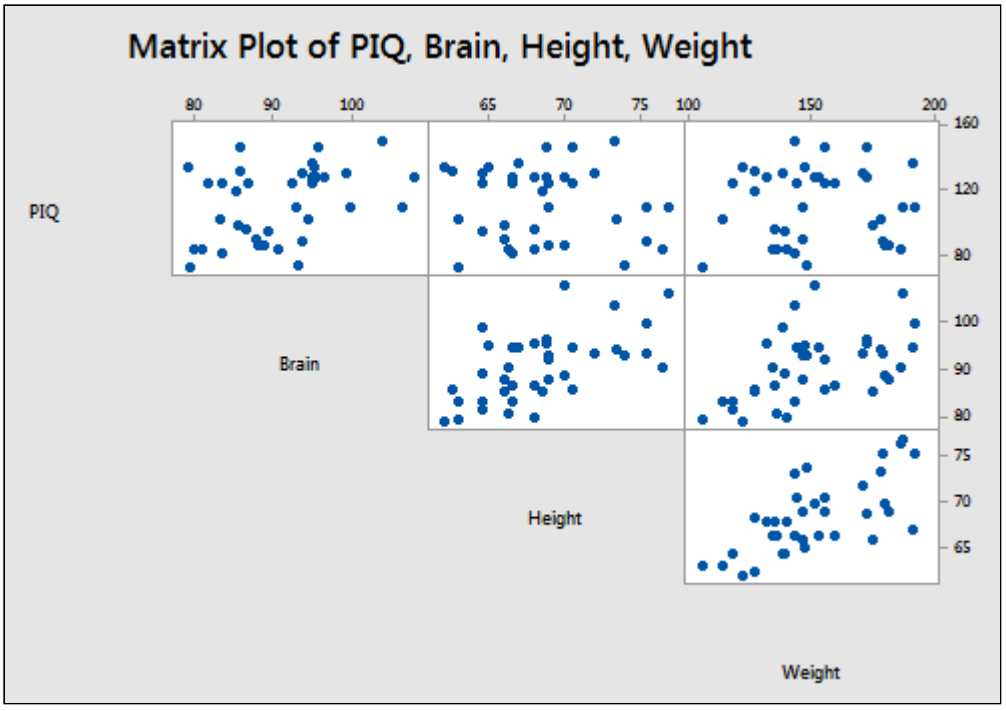
Let's close up our discussion of stepwise regression by taking a quick look at two more examples.



Example #1. Are a person's brain size and body size predictive of his or her intelligence? Interested in this question, some researchers (Willerman, et al, 1991) collected the following data (iqsize.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/iqsize.txt)) on a sample of $n = 38$ college students:

- Response (y): Performance IQ scores (**PIQ**) from the revised Wechsler Adult Intelligence Scale. This variable served as the investigator's measure of the individual's intelligence.
- Potential predictor (x_1): **Brain** size based on the count obtained from MRI scans (given as count/10,000).
- Potential predictor (x_2): **Height** in inches.
- Potential predictor (x_3): **Weight** in pounds.

A matrix plot of the resulting data looks like:



Loading [MathJax]/extensions/MathZoom.js rform the stepwise regression procedure, we obtain:

Regression Analysis: PIQ versus Brain, Height, Weight

Stepwise Selection of Terms

Candidate terms: Brain, Height, Weight

	Step 1		Step 2	
	Coef	P	Coef	P
Constant	4.7		111.3	
Brain	1.177	0.019	2.061	0.001
Height			-2.730	0.009
S	21.2115		19.5096	
R-sq	14.27%		29.49%	
R-sq(adj)	11.89%		25.46%	
R-sq(pred)	4.60%		17.63%	
Mallows' Cp	7.34		2.00	

α to enter = 0.15, α to remove = 0.15

The output tells us:

- The first predictor entered into the stepwise model is **Brain**. The output tells us that the estimated intercept is 4.7 and the estimated slope for **Brain** is 1.177. The *P*-value for testing $\beta_{\text{Brain}} = 0$ is 0.019. The estimate *S* is 21.2, the R^2-value is 14.27%, the adjusted R^2-value is 11.89%, and Mallows' *Cp*-statistic is 7.34.
- The second and final predictor entered into the stepwise model is **Height**. The output tells us that the estimated intercept is 111.3, the estimated slope for **Brain** is 2.061, and the estimated slope for **Height** is -2.730. The *P*-value for testing $\beta_{\text{Brain}} = 0$ is 0.001. The *P*-value for testing $\beta_{\text{Height}} = 0$ is 0.009. The estimate *S* is 19.5, the R^2-value is 29.49%, the adjusted R^2-value is 25.46%, and Mallows' *Cp*-statistic is 2.00.
- At no step is a predictor removed from the stepwise model.
- When $\alpha_E = \alpha_R = 0.15$, the final stepwise regression model contains the predictors **Brain** and **Height**.

Example #2. Some researchers observed the following data (bloodpress.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/bloodpress.txt)) on 20 individuals with high blood pressure:

- blood pressure ($y = BP$, in mm Hg)
- age ($x_1 = Age$, in years)
- weight ($x_2 = Weight$, in kg)
- body surface area ($x_3 = BSA$, in sq m)
- duration of hypertension ($x_4 = Dur$, in years)
- basal pulse ($x_5 = Pulse$, in beats per minute)
- stress index ($x_6 = Stress$)

The researchers were interested in determining if a relationship exists between blood pressure and age, weight, body surface area, duration, pulse rate and/or stress level.

The matrix plot of *BP*, *Age*, *Weight*, and *BSA* looks like:

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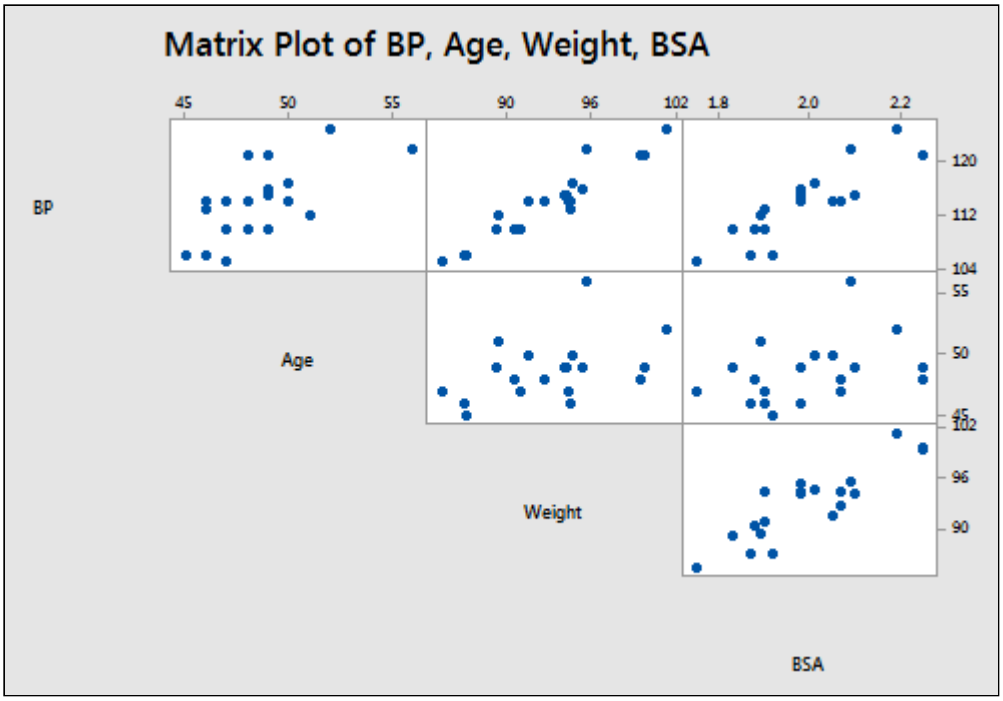
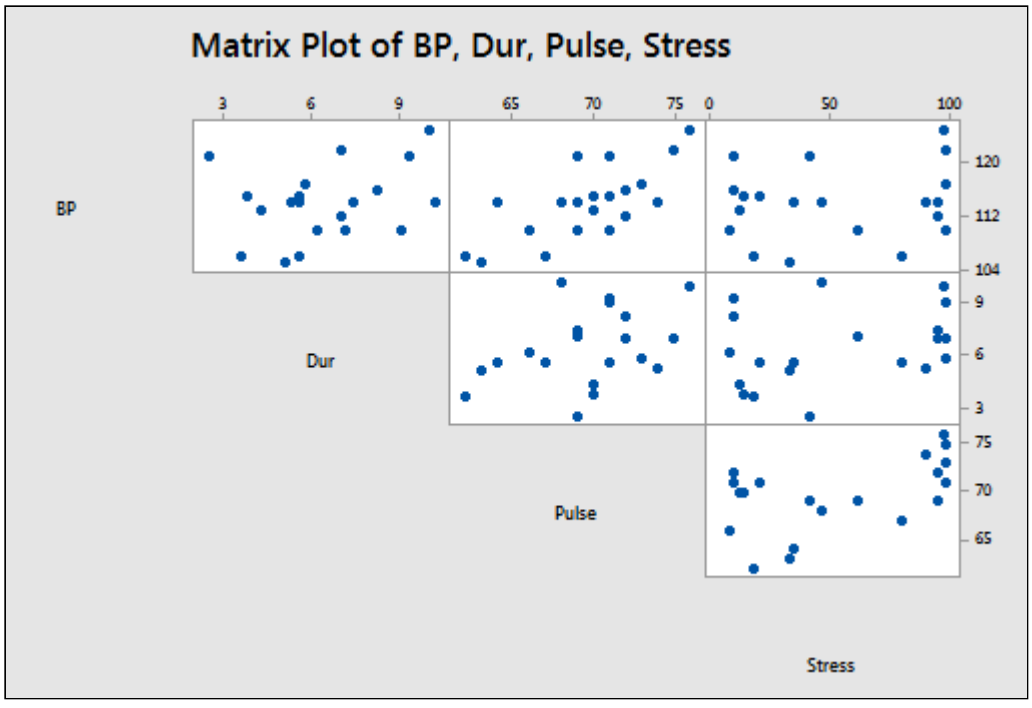


and the matrix plot of *BP*, *Dur*, *Pulse*, and *Stress* looks like:



Using statistical software to perform the stepwise regression procedure, we obtain:

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Regression Analysis: BP versus Age, Weight, BSA, Dur, Pulse, Stress

```
Stepwise Selection of Terms

Candidate terms: Age, Weight, BSA, Dur, Pulse, Stress

             -----Step 1----    -----Step 2-----    -----Step 3-----
               Coef        P      Coef         P      Coef         P
Constant       2.21             -16.58             -13.67
Weight       1.2009    0.000    1.0330     0.000    0.9058     0.000
Age                             0.7083     0.000    0.7016     0.000
BSA                                                  4.63     0.008

S                   1.74050           0.532692           0.437046
R-sq                 90.26%             99.14%             99.45%
R-sq(adj)            89.72%             99.04%             99.35%
R-sq(pred)           88.53%             98.89%             99.22%
Mallows' Cp          312.81              15.09               6.43

α to enter = 0.15, α to remove = 0.15
```

When $\alpha_E = \alpha_R = 0.15$, the final stepwise regression model contains the predictors **Weight**, **Age**, **and BSA**.

‹ 11.1 - What if the Regression Equation Contains "Wrong" Predictors? (/stat462/node/195) | up (/stat462/node/89) | 11.3 - Best Subsets Regression, Adjusted R-Sq, Mallows Cp › (/stat462/node/197)

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STAT 462

Applied Regression Analysis

11.3 - Best Subsets Regression, Adjusted R-Sq, Mallows Cp

In this section, we learn about the **best subsets regression** procedure (or the **all possible subsets regression** procedure). While we will soon learn the finer details, the general idea behind best subsets regression is that we select the subset of predictors that do the best at meeting some well-defined objective criterion, such as having the largest R^2 value or the smallest *MSE*.

Again, our hope is that we end up with a reasonable and useful regression model. There is one sure way of ending up with a model that is certain to be underspecified—and that's if the set of candidate predictor variables doesn't include *all* of the variables that actually predict the response. Therefore, just as is the case for the stepwise regression procedure, a fundamental rule of the best subsets regression procedure is that the list of candidate predictor variables must include *all* of the variables that actually predict the response. Otherwise, we are sure to end up with a regression model that is underspecified and therefore misleading.

The procedure

A regression analysis utilizing the best subsets regression procedure involves the following steps:

Step #1. First, identify *all* of the possible regression models derived from all of the possible combinations of the candidate predictors. Unfortunately, this can be a huge number of possible models.

For the sake of example, suppose we have k=**3** candidate predictors—x_1, x_2, and x_3—for our final regression model. Then, there are 2^3=**8** possible regression models we can consider:

- the one (1) model with no predictors
- the three (3) models with only one predictor each — the model with x_1 alone; the model with x_2 alone; and the model with x_3 alone
- the three (3) models with two predictors each — the model with x_1 and x_2; the model with x_1 and x_3; and the model with x_2 and x_3
- and the one (1) model with all three predictors — that is, the model with x_1, x_2 and x_3

That's 1 + 3 + 3 + 1 = 8 possible models to consider. It can be shown that when there are four candidate predictors—x_1, x_2, x_3 and x_4—there are 16 possible regression models to consider. In general, if there are k possible candidate predictors, then there are 2^k possible regression models containing the predictors. For example, 10 predictors yield 2^{10} = 1024 possible regression models.

That's a heck of a lot of models to consider! The good news is that statistical software does all of the dirty work for us.

Step #2. From the possible models identified in the first step, determine the one-predictor models that do the "best" at meeting some well-defined criteria, the two-predictor models that do the "best," the three-predictor models that do the "best," and so on. For example, suppose we have three candidate predictors—x_1, x_2, and x_3—for our final regression model. Of the three possible models with one predictor, identify the one or two that does "best." Of the three possible two-predictor models, identify the one or two that does "best." By doing this, it cuts down considerably the number of possible regression models to consider!

But, have you noticed that we have not yet even defined what we mean by "best"? What do you think "best" means? Of course, you'll probably define it differently than me or than your neighbor. Therein lies the rub—we might not be able to agree on what's best! In thinking about what "best" means, you might have thought of any of the following:

- the model with the largest R^2
- the model with the largest adjusted R^2
- the model with the smallest *MSE* (or *S* = square root of *MSE*)

There are other criteria you probably didn't think of, but we could consider, too, for example, Mallows' C_p-statistic, the *PRESS* statistic, and Predicted R^2 (which is calculated from the PRESS statistic). We'll learn about Mallows' C_p-statistic in this section and about the *PRESS* statistic and Predicted R^2 in Section 11.5.

To make matters even worse—the different criteria quantify different aspects of the regression model, and therefore often yield different choices for the best set of predictors. That's okay—as long as we don't misuse best subsets regression by claiming that it yields the best model. Rather, we should use best subsets regression as a screening tool—that is, as a way to reduce the large number of possible regression models to just a handful of models that we can evaluate further before arriving at one final model.

Step #3. Further evaluate and refine the handful of models identified in the last step. This might entail performing residual analyses, transforming the predictors and/or response, adding interaction terms, and so on. Do this until you are satisfied that you have found a model that meets the model conditions, does a good job of summarizing the trend in the data, and most importantly allows you to answer your research question.

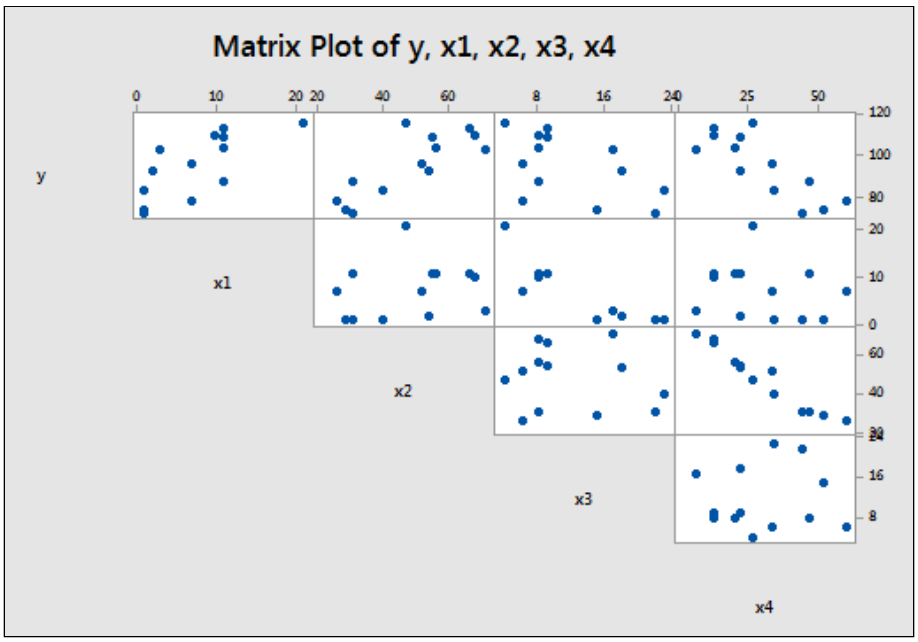
An example

For the remainder of this section, we discuss how the criteria identified above can help us reduce the large number of possible regression models to just a handful of models suitable for further evaluation.

For the sake of example, we will use the cement data to illustrate use of the criteria. Therefore, let's quickly review—the researchers measured and recorded the following data (cement.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/cement.txt)) on 13 batches of cement:

- Response *y*: heat evolved in calories during hardening of cement on a per gram basis
- Predictor x_1: % of tricalcium aluminate
- Predictor x_2: % of tricalcium silicate
- Predictor x_3: % of tetracalcium alumino ferrite
- Predictor x_4: % of dicalcium silicate

And, the matrix plot of the data looks like:



The R^2-values

As you may recall, the R^2-value, which is defined as:

$$R^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO}$$

can only increase as more variables are added. Therefore, it makes no sense to define the "best" model as the model with the largest R^2-value. After all, if we did, the model with the largest number of predictors would always win.

All is not lost, however. We can instead use the R^2-values to find the point where adding more predictors is not worthwhile, because it yields a *very small increase in the R^2-value*. In other words, we look at the size of the increase in R^2, not just its magnitude alone. Because this is such a "wishy-washy" criteria, it is used most often in combination with the other criteria.

Let's see how this criterion works on the cement data example.

Best Subsets Regression: y versus x1, x2, x3, x4

Response is y

Vars	R-Sq	R-Sq (adj)	R-Sq (pred)	Mallows Cp	S	x1	x2	x3	x4
1	67.5	64.5	56.0	138.7	8.9639				X
1	66.6	63.6	55.7	142.5	9.0771		X		
2	97.9	97.4	96.5	2.7	2.4063	X	X		
2	97.2	96.7	95.5	5.5	2.7343	X			X
3	98.2	97.6	96.9	3.0	2.3087	X	X		X
3	98.2	97.6	96.7	3.0	2.3121	X	X	X	
4	98.2	97.4	95.9	5.0	2.4460	X	X	X	X

Each row in the table represents information about one of the possible regression models. The first column—labeled **Vars**—tells us how many predictors are in the model. The last four columns—labeled downward **x1**, **x2**, **x3**, and **x4**—tell us which predictors are in the model. If an "X" is present in the column, then that predictor is in the model. Otherwise, it is not. For example, the first row in the table contains information about the model in which x_4 is the only predictor, whereas the fourth row contains information about the model in which x_1 and x_4 are the two predictors in the model. The other five columns—labeled **R-sq, R-sq(adj), R-sq(pred), Cp and S**—pertain to the criteria that we use in deciding which models are "best."

As you can see, this output reports only the two best models for each number of predictors based on the size of the R^2-value—that is, the output reports the two one-predictor models with the largest R^2-values, followed by the two two-predictor models with the largest R^2-values, and so on.

So, using the R^2-value criterion, which model (or models) should we consider for further evaluation? Hmmm—going from the "best" one-predictor model to the "best" two-predictor model, the R^2-value jumps from 67.5 to 97.9. That is a jump worth making! That is, with such a substantial increase in the R^2-value, one could probably not justify—with a straight face at least—using the one-predictor model over the two-predictor model. Now, should we instead consider the "best" three-predictor model? Probably not! The increase in the R^2-value is very small—from 97.9 to 98.2—and therefore, we probably can't justify using the larger three-predictor model over the simpler, smaller two-predictor model. Get it? Based on the R^2-value criterion, the "best" model is the model with the two predictors x_1 and x_2.

The adjusted R^2-value and *MSE*

The adjusted R^2-value, which is defined as:

$$R^2_a = 1 - \left(\frac{n-1}{n-k-1}\right)\left(\frac{SSE}{SSTO}\right) = 1 - \left(\frac{n-1}{SSTO}\right) MSE = \frac{\frac{SSTO}{n-1} - \frac{SSE}{n-k-1}}{\frac{SSTO}{n-1}}$$

makes us pay a penalty for adding more predictors to the model. Therefore, we can just use the adjusted R^2-value outright. That is, according to the adjusted R^2-value criterion, the best regression model is the one with the *largest adjusted R^2-value.*

Now, you might have noticed that the adjusted R^2-value is a function of the mean square error (*MSE*). And, you may—or may not—recall that *MSE* is defined as:

$$MSE = \frac{SSE}{n-k-1} = \frac{\sum(y_i - \hat{y}_i)^2}{n-k-1}$$

That is, *MSE* quantifies how far away our predicted responses are from our observed responses. Naturally, we want this distance to be small. Therefore, according to the *MSE* criterion, the best regression model is the one with the *smallest MSE.*

But, aha—the two criteria are equivalent! If you look at the formula again for the adjusted R^2-value:

$$R^2_a = 1 - \left(\frac{n-1}{SSTO}\right) MSE$$

you can see that the adjusted R^2-value increases only if *MSE* decreases. That is, the adjusted R^2-value and *MSE* criteria always yield the same "best" models.

Back to the cement data example! One thing to note is that *S* is the square root of *MSE*. Therefore, finding the model with the smallest *MSE* is equivalent to finding the model with the smallest *S*:

Best Subsets Regression: y versus x1, x2, x3, x4

Response is y

		R-Sq	R-Sq	Mallows		x	x	x	x
Vars	R-Sq	(adj)	(pred)	Cp	S	1	2	3	4
1	67.5	64.5	56.0	138.7	8.9639				X
1	66.6	63.6	55.7	142.5	9.0771		X		
2	97.9	97.4	96.5	2.7	2.4063	X	X		
2	97.2	96.7	95.5	5.5	2.7343	X			X
3	98.2	97.6	96.9	3.0	2.3087	X	X		X
3	98.2	97.6	96.7	3.0	2.3121	X	X	X	
4	98.2	97.4	95.9	5.0	2.4460	X	X	X	X

The model with the largest adjusted R^2-value (97.6) and the smallest *S* (2.3087) is the model with the three predictors x_1, x_2, and x_4.

See?! Different criteria can indeed lead us to different "best" models. Based on the R^2-value criterion, the "best" model is the model with the two predictors x_1 and x_2. But, based on the adjusted R^2-value and the smallest *MSE* criteria, the "best" model is the model with the three predictors x_1, x_2, and x_4.

Mallows' C_p-statistic

Recall that an underspecified model is a model in which important predictors are missing. And, an underspecified model yields biased regression coefficients and biased predictions of the response. Well, in short, Mallows' C_p-statistic estimates the size of the bias that is introduced into the predicted responses by having an underspecified model.

Now, we could just jump right in and be told how to use Mallows' C_p-statistic as a way of choosing a "best" model. But, then it wouldn't make any sense to you—and therefore it wouldn't stick to your craw. So, we'll start by justifying the use of the Mallows' C_p-statistic. The problem is it's kind of complicated. So, be patient, don't be frightened by the scary looking formulas, and before you know it, we'll get to the moral of the story. Oh, and by the way, in case you're wondering—it's called Mallows' C_p-statistic, because a guy named Mallows thought of it!

Here goes! At issue in any regression model are two things, namely:

- The **bias** in the predicted responses.
- The **variation** in the predicted responses.

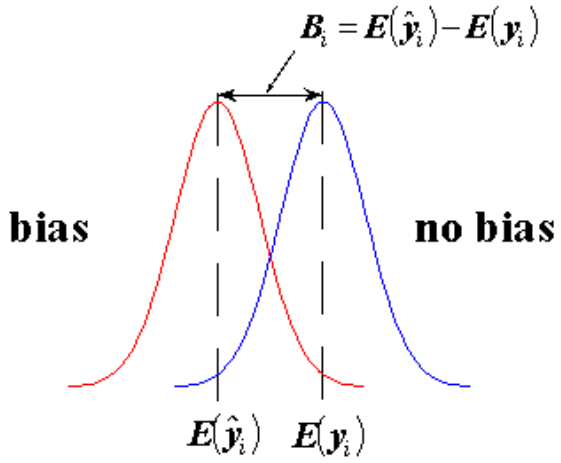
Bias in predicted responses

Recall that, in fitting a regression model to data, we attempt to estimate the average—or expected value—of the observed responses $E(y_i)$ at any given predictor value x. That is, $E(y_i)$ is the population regression function. Because the average of the observed responses depends on the value of x, we might also denote this population average or population regression function as $\mu_{Y|x}$.

Now, if there is no bias in the predicted responses, then the average of the observed responses $E(y_i)$ and the average of the predicted responses $E(\hat{y}_i)$ both equal the thing we are trying to estimate, namely the average of the responses in the population $\mu_{Y|x}$. On the other hand, if there is bias in the predicted responses, then $E(y_i) = \mu_{Y|x}$ and $E(\hat{y}_i)$ do not equal each other. The difference between $E(y_i)$ and $E(\hat{y}_i)$ is the bias B_i in the predicted response. That is, the bias:

$$B_i = E(\hat{y}_i) - E(y_i)$$

We can picture this bias as follows:



The quantity $E(y_i)$ is the value of the population regression line at a given x. Recall that we assume that the error terms ε_i are normally distributed. That's why there is a normal curve—in blue—drawn around the population regression line $E(y_i)$. You can think of the quantity $E(\hat{y}_i)$ as being the predicted regression line—well, technically, it's the average of all of the predicted regression lines you could obtain based on your formulated regression model. Again, since we always assume the error terms ε_i are normally distributed, we've drawn a normal curve—in red—around the average predicted regression line $E(\hat{y}_i)$. The difference between the population regression line $E(y_i)$ and the average predicted regression line $E(\hat{y}_i)$ is the bias $B_i = E(\hat{y}_i) - E(y_i)$.

Earlier in this lesson, we saw an example in which bias was likely introduced into the predicted responses because of an underspecifed model. The data concerned the heights and weights of martians. The data set (martian.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/martian.txt)) contains the weights (in *g*), heights (in *cm*), and amount of daily water consumption (0, 10 or 20 *cups per day*) of 12 martians.

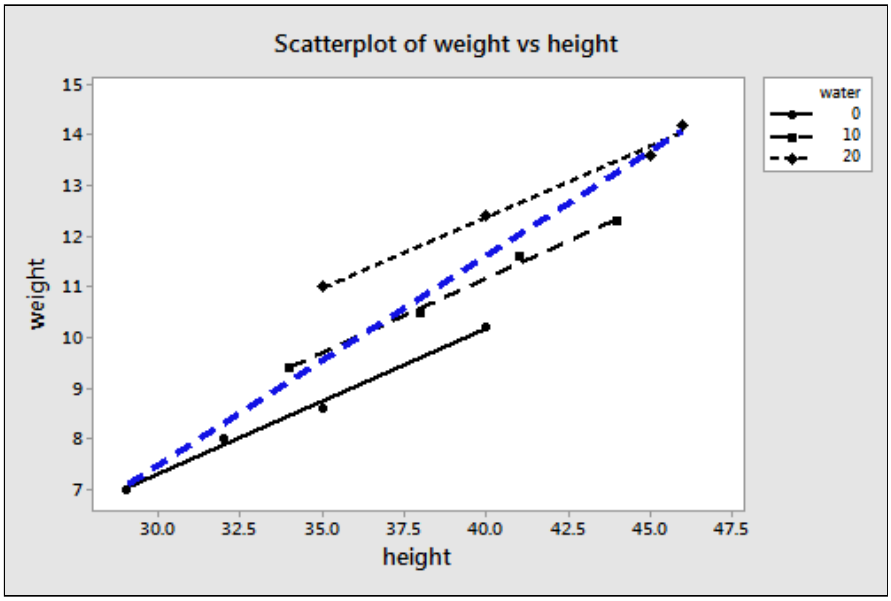
If we regress y = *weight* on the predictors x_1 = *height* and x_2 = *water*, we obtain the following estimated regression equation:

```
Regression Equation

weight = -1.220 + 0.28344 height + 0.11121 water
```

But, if we regress y = *weight* on only the one predictor x_1 = *height*, we obtain the following estimated regression equation:

```
Regression Equation

weight = -4.14 + 0.3889 height
```

A plot of the data containing the two estimated regression equations looks like:



The three **black** lines represent the estimated regression equation when the amount of water consumption is taken into account — the first line for 0 cups per day, the second line for 10 cups per day, and the third line for 20 cups per day. The dashed **blue** line represents the estimated regression equation when we leave the amount of water consumed out of the regression model.

As you can see, if we use the blue line to predict the weight of a randomly selected martian, we would consistently overestimate the weight of martians who drink 0 cups of water a day, and we would consistently understimate the weight of martians who drink 20 cups of water a day. That is, our predicted responses would be biased.

Variation in predicted responses

When a bias exists in the predicted responses, the variance in the predicted responses for a data point *i* is due to two things:

- the ever-present random sampling variation, that is $(\sigma^2_{\hat{y}_i})$
- the variance associated with the bias, that is (B_i^2)

Now, if our regression model is biased, it doesn't make sense to consider the bias at just one data point *i*. We need to consider the bias that exists for all *n* data points. Looking at the plot of the two estimated regression equations for the martian data, we see that the predictions for the underspecified model are more biased for certain data points than for others. And, we can't just consider the variation in the predicted responses at one data point *i*. We need to consider the *total* variation in the predicted responses.

To quantify the total variation in the predicted responses, we just sum the two variance components—$(\sigma^2_{\hat{y}_i})$ and (B_i^2)—over all *n* data points to obtain a **(standardized) measure of the total variation in the predicted responses Γ_p** (that's the greek letter "gamma"):

$$\Gamma_p = \frac{1}{\sigma^2}\left\{\sum_{i=1}^{n}\sigma^2_{\hat{y}_i} + \sum_{i=1}^{n}\left[E(\hat{y}_i) - E(y_i)\right]^2\right\}$$

I warned you about not being overwhelmed by scary looking formulas! The first term in the brackets quantifies the random sampling variation summed over all *n* data points, while the second term in the brackets quantifies the amount of bias (squared) summed over all *n* data points. Because the size of the bias depends on the measurement units used, we divide by σ^2 to get a standardized unitless measure.

Now, we don't have the tools to prove it, but it can be shown that if there is no bias in the predicted responses—that is, if the bias = 0 —then Γ_p achieves its smallest possible value, namely *k+1*, the number of parameters:

$$\Gamma_p = \frac{1}{\sigma^2}\left\{\sum_{i=1}^{n}\sigma^2_{\hat{y}_i} + 0\right\} = k+1$$

Now, because it quantifies the amount of bias and variance in the predicted responses, Γ_p seems to be a good measure of an underspecified model:

$$\Gamma_p = \frac{1}{\sigma^2}\left\{\sum_{i=1}^{n}\sigma^2_{\hat{y}_i} + \sum_{i=1}^{n}\left[E(\hat{y}_i) - E(y_i)\right]^2\right\}$$

The best model is simply the model with the *smallest value of* Γ_p. We even know that the theoretical minimum of Γ_p is the number of parameters *k+1*.

Well, it's not quite that simple—we still have a problem. Did you notice all of those greek parameters—σ^2, $(\sigma^2_{\hat{y}_i})$, and Γ_p? As you know, greek parameters are generally used to denote unknown population quantities. That is, we don't or can't know the value of Γ_p—we must estimate it. That's where Mallows' C_p-statistic comes into play!

C_p as an estimate of Γ_p

If we know the population variance σ^2, we can estimate Γ_p:

$$C_p = k + 1 + \frac{(MSE_k - \sigma^2)(n-k-1)}{\sigma^2}$$

where MSE_k is the mean squared error from fitting the model containing the subset of *k* predictors.

But we don't know σ^2. So, we estimate it using MSE_{all}, the mean squared error obtained from fitting the model containing *all* of the candidate predictors. That is:

$$C_p = k + 1 + \frac{(MSE_k - MSE_{all})(n-k-1)}{MSE_{all}} = k + 1 + \frac{(n-k-1)MSE_k}{MSE_{all}} - (n-k-1) = \frac{SSE_k}{MSE_{all}} + 2(k+1) - n.$$

A couple of things to note though. Estimating σ^2 using MSE_{all}:

- assumes that there are no biases in the full model with all of the predictors, an assumption that may or may not be valid, but can't be tested without additional information (at the very least you have to have all of the important predictors involved)
- guarantees that $C_p = k+1$ for the full model because in that case $MSE_k = MSE_{all}$.

Using the C_p criterion to identify "best" models

Finally—we're getting to the moral of the story! Just a few final facts about Mallows' C_p-statistic will get us on our way. Recalling that *k* denotes the number of predictor terms in the model:

- Subset models with small C_p values have a small estimated total (standardized) variation in predicted responses.
- When the C_p value is ...
  - ... near *k+1*, the bias is small (next to none)
  - ... much greater than *k+1*, the bias is substantial
  - ... below *k+1*, it is due to sampling error; interpret as no bias
- For the largest model containing all of the candidate predictors, $C_p = k+1$ (always). Therefore, **you shouldn't use C_p to evaluate the full model** (the model containing all of the candiate predictors).

That all said, here's a reasonable strategy for using C_p to identify "best" models:

- Identify subsets of predictors for which the C_p value is **near *k+1*** (if possible).
- The full model always yields $C_p = k+1$, so don't select the full model based on C_p.
- If all models, except the full model, yield a large C_p not near *k+1*, it suggests some important predictor(s) are missing from the analysis. In this case, we are well-advised to identify the predictors that are missing!

- If a number of models have C_p near $k+1$, choose the model with the smallest C_p value, thereby insuring that the combination of the bias and the variance is at a minimum.
- When more than one model has a small value of C_p value near k+*1*, in general, choose the simpler model or the model that meets your research needs.

The cement data example

Ahhh—an example! Let's see what model the C_p criterion leads us to for the cement data:

Best Subsets Regression: y versus x1, x2, x3, x4

Response is y

Vars	R-Sq	R-Sq (adj)	R-Sq (pred)	Mallows Cp	S	x1	x2	x3	x4
1	67.5	64.5	56.0	138.7	8.9639				X
1	66.6	63.6	55.7	142.5	9.0771		X		
2	97.9	97.4	96.5	2.7	2.4063	X	X		
2	97.2	96.7	95.5	5.5	2.7343	X			X
3	98.2	97.6	96.9	3.0	2.3087	X	X		X
3	98.2	97.6	96.7	3.0	2.3121	X	X	X	
4	98.2	97.4	95.9	5.0	2.4460	X	X	X	X

The first thing you might want to do here is "pencil in" a column to the left of the **Vars** column. Recall that the Vars column tells us the number of predictor terms (k) that are in the model. But, we need to compare C_p to the number of parameters ($k+1$). There is always one more parameter—the intercept parameter—than predictor terms. So, you might want to add—at least mentally—a column containing the number of parameters—here, 2, 2, 3, 3, 4, 4, and 5.

Here, the model in the third row (containing predictors x_1 and x_2), the model in the fifth row (containing predictors x_1, x_2 and x_4), and the model in the sixth row (containing predictors x_1, x_2 and x_3) are all unbiased models, because their C_p values equal (or are below) the number of parameters $k+1$. For example:

- the model containing the predictors x_1 and x_2 contains 3 parameters and its C_p value is 2.7. Since C_p is less than k+1=3, it suggests the model is unbiased;
- the model containing the predictors x_1, x_2 and x_4 contains 4 parameters and its C_p value is 3.0. Since C_p is less than k+1=4, it suggests the model is unbiased;
- the model containing the predictors x_1, x_2 and x_3 contains 4 parameters and its C_p value is 3.0. Since C_p is less than k+1=4, it suggests the model is unbiased.

So, in this case, based on the C_p criterion, the researcher has three legitimate models from which to choose with respect to bias. Of these three, the model containing the predictors x_1 and x_2 has the smallest C_p value, but the C_p values for the other two models are similar and so there is little to separate these models based on this criterion.

Incidentally, you might also want to conclude that the last model—the model containing all four predictors—is a legitimate contender because C_p = 5.0 equals $k+1$ = 5. However, don't forget that the model with all of the predictor terms is *assumed* to be unbiased. Therefore, you should not use the C_p criterion as a way of evaluating the full model with all of the candidate predictor terms.

Incidentally, how did the statistical software detemine that the C_p value for the third model is 2.7, while for the fourth model the C_p value is 5.5? We can verify these calculated C_p values!

First, consider the third model containing the predictors x_1 and x_2 for which k=2. The following output obtained by first regressing y on the predictors x_1, x_2, x_3 and x_4 and then by regressing y on the predictors x_1 and x_2 :

```
The regression equation is
y = 62.4 + 1.55 x1 + 0.510 x2 + 0.102 x3 - 0.144 x4

Source          DF       SS        MS         F       P
Regression       4  2667.90    666.97    111.48   0.000
Residual Error   8    47.86      5.98
Total           12  2715.76
```

```
The regression equation is y = 52.6 + 1.47 x1 + 0.662 x2

Source          DF       SS        MS         F       P
Regression       2  2657.9    1328.9    229.50   0.000
Residual Error  10    57.9       5.8
Total           12  2715.8
```

tells us that, here, $SSE_k = 57.9$ and $MSE_{all} = 5.98$. Therefore, just as the output claims:

$$C_p = \frac{SSE_k}{MSE_{all}} + 2(k+1) - n = \frac{57.9}{5.98} + 2(2+1) - 13 = 2.7.$$

Next, consider the fourth model containing the predictors x_1 and x_4 for which k =2. The following output obtained by first regressing y on the predictors x_1, x_2, x_3 and x_4 and then by regressing y on the predictors x_1 and x_4:

```
The regression equation is
y = 62.4 + 1.55 x1 + 0.510 x2 + 0.102 x3 - 0.144 x4

Source          DF       SS        MS         F       P
Regression       4  2667.90    666.97    111.48   0.000
Residual Error   8    47.86      5.98
Total           12  2715.76
```

```
The regression equation is y = 103 + 1.44 x1 - 0.614 x4

Source          DF       SS        MS         F       P
Regression       2  2641.0    1320.5    176.63   0.000
Residual Error  10    74.8       7.5
Total           12  2715.8
```

tells us that, here, $SSE_k = 74.8$ and $MSE_{all} = 5.98$. Therefore, just as the output claims:

$$C_p = \frac{SSE_k}{MSE_{all}} + 2(k+1) - n = \frac{74.8}{5.98} + 2(2+1) - 13 = 5.5.$$

‹ 11.2 - Stepwise Regression (/stat462/node/196) up (/stat462/node/89) 11.4 - Some Automated Variable Selection Examples › (/stat462/node/198)

STAT 462

Applied Regression Analysis

11.4 - Some Automated Variable Selection Examples

Let's take a look at a few more examples to see how the best subsets and stepwise regression procedures assist us in identifying a final regression model.

Example #1

Let's return one more time to the cement data example (cement.txt

(https://onlinecourses.science.psu.edu/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/cement.txt)). Recall that the stepwise regression procedure:

Regression Analysis: y versus x1, x2, x3, x4

Stepwise Selection of Terms

Candidate terms: x1, x2, x3, x4

	-----Step 1----		-----Step 2-----		-----Step 3----		-----Step 4----	
	Coef	P	Coef	P	Coef	P	Coef	P
Constant	117.57		103.10		71.6		52.58	
x4	-0.738	0.001	-0.6140	0.000	-0.237	0.205		
x1			1.440	0.000	1.452	0.000	1.468	0.000
x2					0.416	0.052	0.6623	0.000
S		8.96390		2.73427		2.30874		2.40634
R-sq		67.45%		97.25%		98.23%		97.87%
R-sq(adj)		64.50%		96.70%		97.64%		97.44%
R-sq(pred)		56.03%		95.54%		96.86%		96.54%
Mallows' Cp		138.73		5.50		3.02		2.68

α to enter = 0.15, α to remove = 0.15

yielded the final stepwise model with y as the response and x_1 and x_2 as predictors.

The best subsets regression procedure:

Best Subsets Regression: y versus x1, x2, x3, x4

Response is y

Vars	R-Sq	R-Sq (adj)	R-Sq (pred)	Mallows Cp	S	x 1	x 2	x 3	x 4
1	67.5	64.5	56.0	138.7	8.9639				X
1	66.6	63.6	55.7	142.5	9.0771		X		
2	97.9	97.4	96.5	2.7	2.4063	X	X		
2	97.2	96.7	95.5	5.5	2.7343	X			X
3	98.2	97.6	96.9	3.0	2.3087	X	X		X
3	98.2	97.6	96.7	3.0	2.3121	X	X	X	
4	98.2	97.4	95.9	5.0	2.4460	X	X	X	X

yields various models depending on the different criteria:

- Based on the R^2-value criterion, the "best" model is the model with the two predictors x_1 and x_2.
- Based on the adjusted R^2-value and *MSE* criteria, the "best" model is the model with the three predictors is the model with the three predictors x_1, x_2, and x_4.
- Based on the C_p criterion, there are three possible "best" models — the model containing x_1 and x_2; the model containing x_1, x_2 and x_3; and the model containing x_1, x_2 and x_4.

So, which model should we "go with"? That's where the final step — the refining step — comes into play. In the refining step, we evaluate each of the models identified by the best subsets and stepwise procedures to see if there is a reason to select one of the models over the other. This step may also involve adding interaction or quadratic terms, as well as transforming the response and/or predictors. And, certainly, when selecting a final model, don't forget why you are performing the research to begin with — the reason may make the choice of the model obvious.

Well, let's evaluate the three remaining candidate models. We don't have to go very far with the model containing the predictors x_1, x_2 and x_4:

Regression Analysis: y versus x1, x2, x4

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	3	2667.79	889.263	166.83	0.000
x1	1	820.91	820.907	154.01	0.000
x2	1	26.79	26.789	5.03	0.052
x4	1	9.93	9.932	1.86	0.205
Error	9	47.97	5.330		
Total	12	2715.76			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
2.30874	98.23%	97.64%	96.86%

Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	71.6	14.1	5.07	0.001	
x1	1.452	0.117	12.41	0.000	1.07
x2	0.416	0.186	2.24	0.052	18.78
x4	-0.237	0.173	-1.37	0.205	18.94

Regression Equation

$y = 71.6 + 1.452\ x1 + 0.416\ x2 - 0.237\ x4$

The variance inflation factors of 18.78 and 18.94 for x_2 and x_4 indicate that the model exhibits substantial multicollinearity. You may recall that the predictors x_2 and x_4 are strongly negatively correlated—indeed, $r = -0.973$.

While not perfect, the variance inflation factors for the model containing the predictors x_1, x_2 and x_3:

Regression Analysis: y versus x1, x2, x3

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	3	2667.65	889.22	166.34	0.000
x1	1	367.33	367.33	68.72	0.000
x2	1	1178.96	1178.96	220.55	0.000
x3	1	9.79	9.79	1.83	0.209
Error	9	48.11	5.35		
Total	12	2715.76			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
2.31206	98.23%	97.64%	96.69%

Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	48.19	3.91	12.32	0.000	
x1	1.696	0.205	8.29	0.000	3.25
x2	0.6569	0.0442	14.85	0.000	1.06
x3	0.250	0.185	1.35	0.209	3.14

Regression Equation

$$y = 48.19 + 1.696\ x1 + 0.6569\ x2 + 0.250\ x3$$

are much better (smaller) than the previous variance inflation factors. But, unless there is a good scientific reason to go with this larger model, it probably makes more sense to go with the smaller, simpler model containing just the two predictors x_1 and x_2:

Regression Analysis: y versus x1, x2

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	2	2657.86	1328.93	229.50	0.000
x1	1	848.43	848.43	146.52	0.000
x2	1	1207.78	1207.78	208.58	0.000
Error	10	57.90	5.79		
Total	12	2715.76			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
2.40634	97.87%	97.44%	96.54%

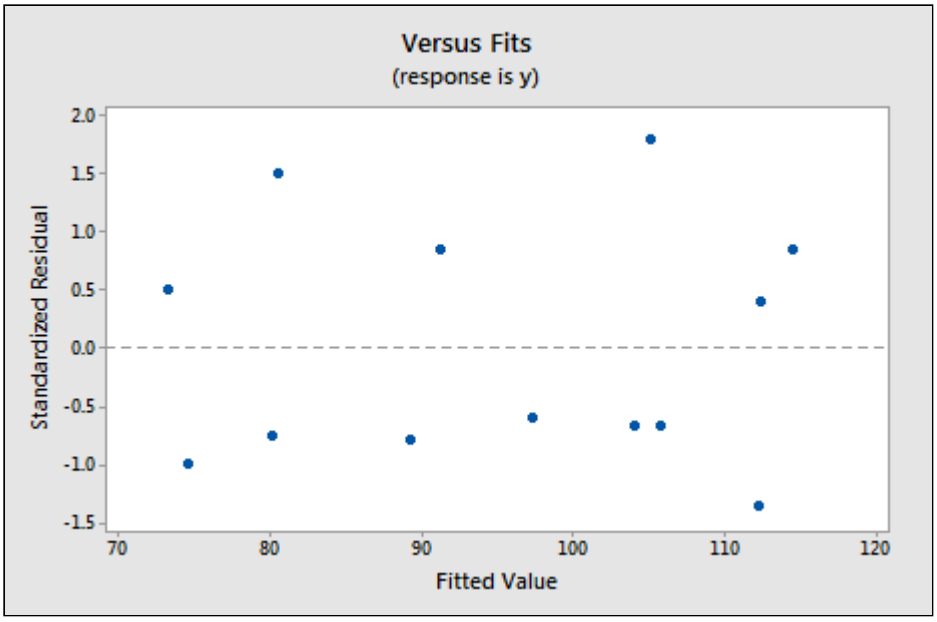
Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	52.58	2.29	23.00	0.000	
x1	1.468	0.121	12.10	0.000	1.06
x2	0.6623	0.0459	14.44	0.000	1.06

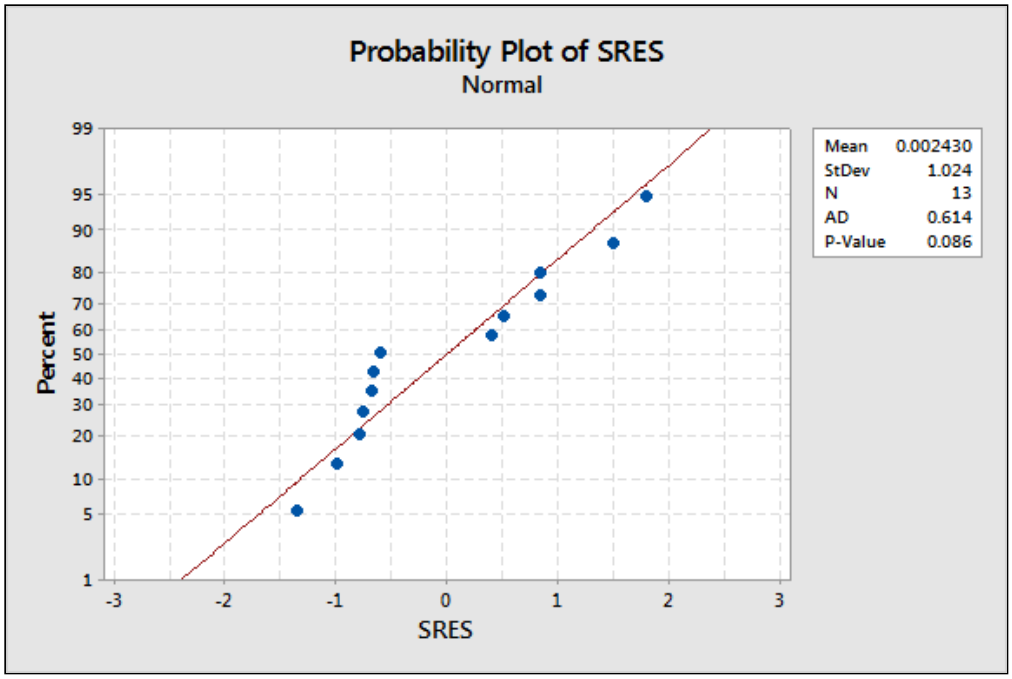
Regression Equation

$$y = 52.58 + 1.468\ x1 + 0.6623\ x2$$

For this model, the variance inflation factors are quite satisfactory (both 1.06), the adjusted R^2-value (97.44%) is large, and the residual analysis yields no concerns. That is, the residuals versus fits plot:

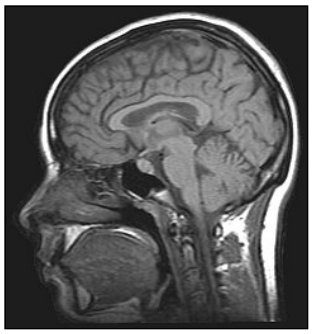


suggests that the relationship is indeed linear and that the variances of the error terms are constant. Furthermore, the normal probability plot:



suggests that the error terms may not be normally distributed, but the Anderson-Darling normality test p-value is not significant at a 0.05 significance level. The regression model with y as the response and x_1 and x_2 as the predictors has been evaluated fully and appears to be ready to answer the researcher's questions.

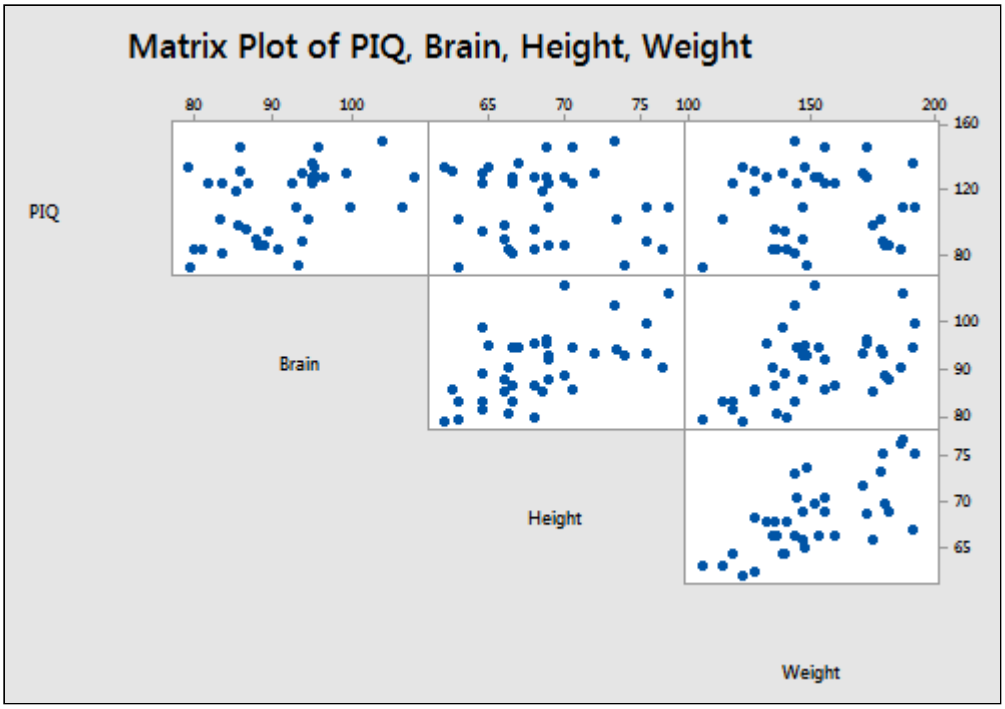
Example #2



Let's return to the brain size and body size study, in which the researchers were interested in determinig whether or not a person's brain size and body size are predictive of his or her intelligence? The researchers (Willerman, *et al*, 1991) collected the following data (iqsize.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/iqsize.txt)) on a sample of $n = 38$ college students:

- Response (y): Performance IQ scores (**PIQ**) from the revised Wechsler Adult Intelligence Scale. This variable served as the investigator's measure of the individual's intelligence.
- Potential predictor (x_1): **Brain** size based on the count obtained from MRI scans (given as count/10,000).
- Potential predictor (x_2): **Height** in inches.
- Potential predictor (x_3): **Weight** in pounds.

A matrix plot of the resulting data looks like:



The stepwise regression procedure:

Regression Analysis: PIQ versus Brain, Height, Weight

```
Stepwise Selection of Terms

Candidate terms: Brain, Height, Weight

             ----Step 1----    -----Step 2----
              Coef        P      Coef        P
Constant       4.7              111.3
Brain        1.177    0.019     2.061    0.001
Height                        -2.730    0.009

S                  21.2115           19.5096
R-sq                14.27%            29.49%
R-sq(adj)           11.89%            25.46%
R-sq(pred)           4.60%            17.63%
Mallows' Cp           7.34              2.00

α to enter = 0.15, α to remove = 0.15
```

yielded the final stepwise model with *PIQ* as the response and *Brain* and *Height* as predictors. In this case, the best subsets regression procedure:

Best Subsets Regression: PIQ versus Brain, Height, Weight

Response is PIQ

Vars	R-Sq	R-Sq (adj)	R-Sq (pred)	Mallows Cp	S	Brain	Height	Weight
1	14.3	11.9	4.6	7.3	21.212	X		
1	0.9	0.0	0.0	13.8	22.810		X	
2	29.5	25.5	17.6	2.0	19.510	X	X	
2	19.3	14.6	5.9	6.9	20.878	X		X
3	29.5	23.3	12.8	4.0	19.794	X	X	X

yields the same model regardless of criterion used:

- Based on the R^2-value criterion, the "best" model is the model with the two predictors *Brain* and *Height*.
- Based on the adjusted R^2-value and *MSE* criteria, the "best" model is the model with the two predictors *Brain* and *Height*.
- Based on the C_p criterion, the "best" model is the model with the two predictors *Brain* and *Height*.

Well, at least in this case, we have only one model to evaluate further:

Regression Analysis: PIQ versus Brain, Height

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	2	5573	2786.4	7.32	0.002
Brain	1	5409	5408.8	14.21	0.001
Height	1	2876	2875.6	7.56	0.009
Error	35	13322	380.6		
Total	37	18895			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
19.5096	29.49%	25.46%	17.63%

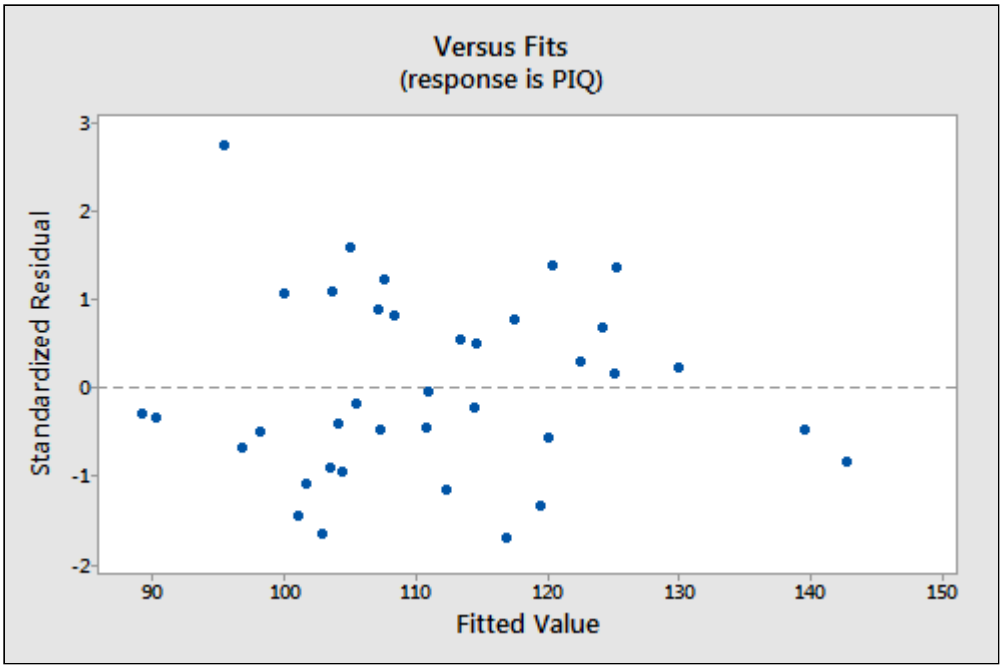
Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	111.3	55.9	1.99	0.054	
Brain	2.061	0.547	3.77	0.001	1.53
Height	-2.730	0.993	-2.75	0.009	1.53

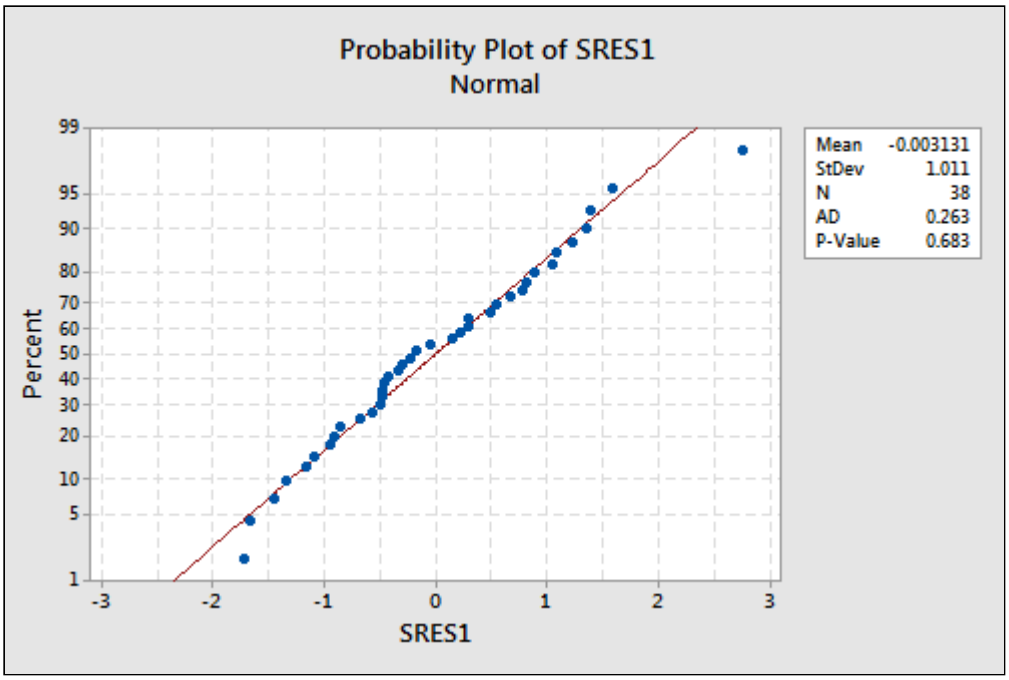
Regression Equation

PIQ = 111.3 + 2.061 Brain - 2.730 Height

For this model, the variance inflation factors are quite satisfactory (both 1.53), the adjusted R^2-value (25.46%) is not great but can't get any better with these data, and the residual analysis yields no concerns. That is, the residuals versus fits plot:



suggests that the relationship is indeed linear and that the variances of the error terms are constant. The researcher might want to investigate the one outlier, however. The normal probability plot:



suggests that the error terms are normally distributed. The regression model with *PIQ* as the response and *Brain* and *Height* as the predictors has been evaluated fully and appears to be ready to answer the researchers' questions.

Example #3

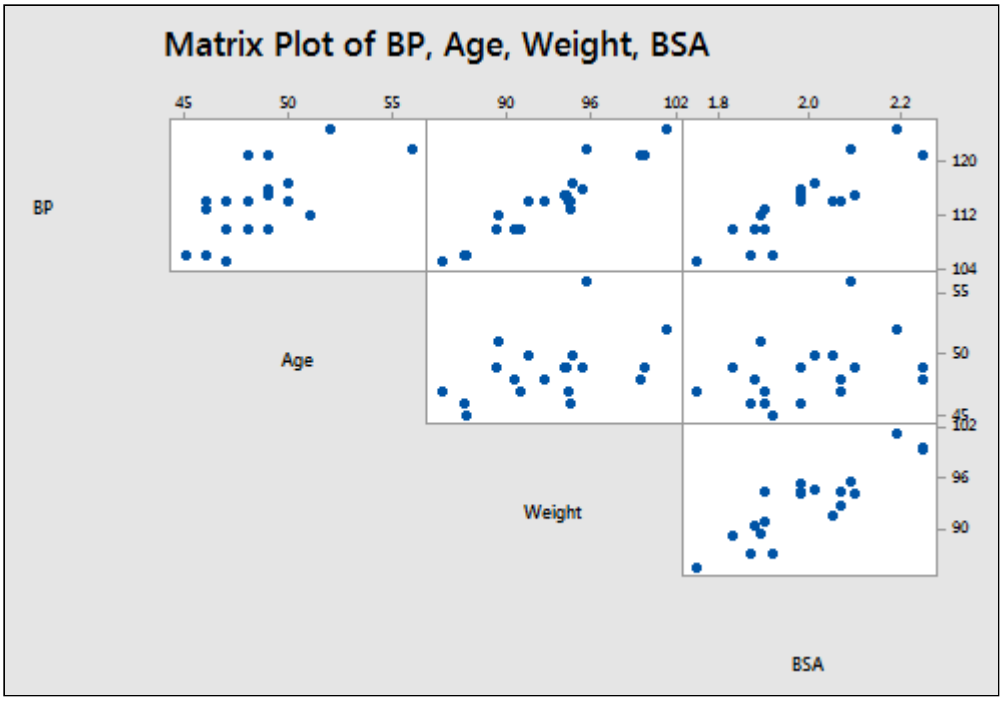
Let's return to the blood pressure study in which we observed the following data (bloodpress.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/bloodpress.txt)) on 20 individuals with hypertension:

- blood pressure ($y = BP$, in mm Hg)
- age ($x_1 = Age$, in years)

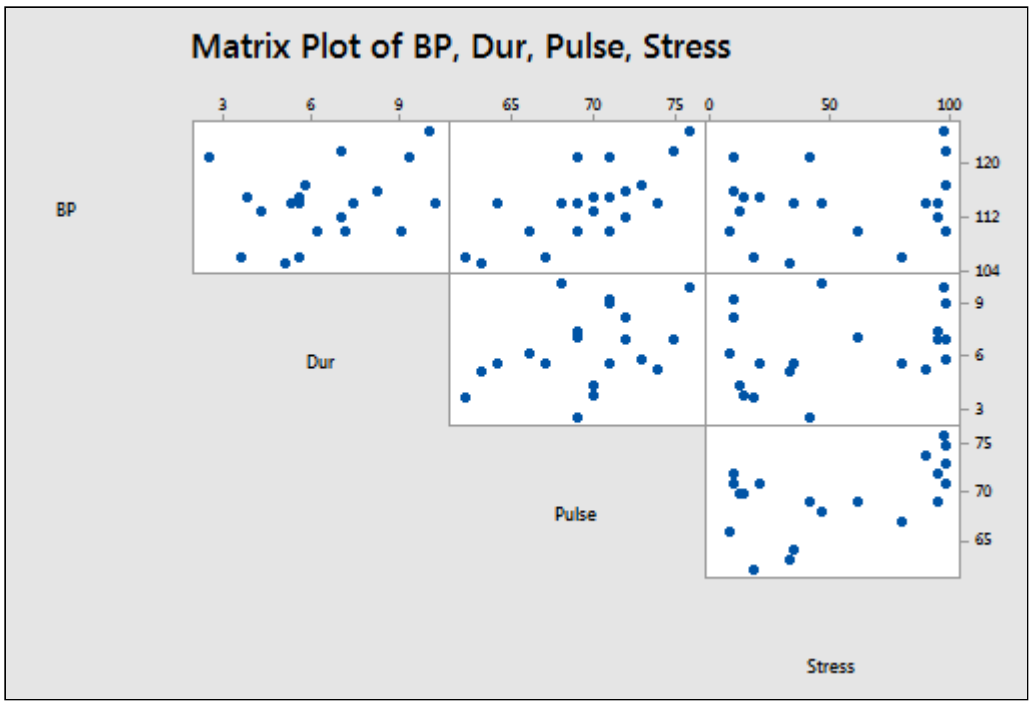
- weight (x_2 = *Weight*, in kg)
- body surface area (x_3 = *BSA*, in sq m)
- duration of hypertension (x_4 = *Dur*, in years)
- basal pulse (x_5 = *Pulse*, in beats per minute)
- stress index (x_6 = *Stress*)

The researchers were interested in determining if a relationship exists between blood pressure and age, weight, body surface area, duration, pulse rate and/or stress level.

The matrix plot of *BP*, *Age*, *Weight*, and *BSA* looks like:



and the matrix plot of *BP*, *Dur*, *Pulse*, and *Stress* looks like:



The stepwise regression procedure:

Regression Analysis: BP versus Age, Weight, BSA, Dur, Pulse, Stress

```
Stepwise Selection of Terms

Candidate terms: Age, Weight, BSA, Dur, Pulse, Stress

             -----Step 1----    -----Step 2-----    -----Step 3-----
               Coef        P      Coef         P      Coef         P
Constant       2.21             -16.58             -13.67
Weight       1.2009    0.000    1.0330     0.000    0.9058     0.000
Age                             0.7083     0.000    0.7016     0.000
BSA                                                  4.63     0.008

S                    1.74050           0.532692           0.437046
R-sq                  90.26%             99.14%             99.45%
R-sq(adj)             89.72%             99.04%             99.35%
R-sq(pred)            88.53%             98.89%             99.22%
Mallows' Cp           312.81              15.09               6.43

α to enter = 0.15, α to remove = 0.15
```

yielded the final stepwise model with *PIQ* as the response and *Age*, *Weight*, and *BSA* (body surface area) as predictors. The best subsets regression procedure:

Best Subsets Regression: BP versus Age, Weight, BSA, Dur, Pulse, Stress

```
Response is BP

                                                  W       S
                                                  e     P t
                                                  i     u r
                                              A g B D l e
             R-Sq    R-Sq  Mallows             g h S u s s
Vars  R-Sq  (adj)  (pred)      Cp        S      e t A r e s
   1  90.3   89.7    88.5   312.8   1.7405      X
   1  75.0   73.6    69.5   829.1   2.7903        X
   2  99.1   99.0    98.9    15.1  0.53269    X X
   2  92.0   91.0    89.3   256.6   1.6246      X       X
   3  99.5   99.4    99.2     6.4  0.43705    X X X
   3  99.2   99.1    98.8    14.1  0.52012    X X     X
   4  99.5   99.4    99.2     6.4  0.42591    X X X X
   4  99.5   99.4    99.1     7.1  0.43500    X X X     X
   5  99.6   99.4    99.1     7.0  0.42142    X X X   X X
   5  99.5   99.4    99.2     7.7  0.43078    X X X X X
   6  99.6   99.4    99.1     7.0  0.40723    X X X X X  X
```

yields various models depending on the different criteria:

- Based on the R^2-value criterion, the "best" model is the model with the two predictors *Age* and *Weight*.
- Based on the adjusted R^2-value and *MSE* criteria, the "best" model is the model with all six of the predictors — *Age*, *Weight*, *BSA*, *Duration*, *Pulse*, and *Stress* — in the model. However, one could easily argue that any number of sub-models are also satisfactory based on these criteria — such as the model containing *Age*, *Weight*, *BSA*, and *Duration*.
- Based on the C_p criterion, a couple of models stand out — namely the model containing *Age*, *Weight*, and *BSA*; and the model containing *Age*, *Weight*, *BSA*, and *Duration*.

Incidentally, did you notice how large some of the C_p values are for some of the models? Those are the models that you should be concerned about exhibiting substantial bias. Don't worry too much about C_p values that are only slightly larger than p.

Here's a case in which I might argue for thinking practically over thinking statistically. There appears to be nothing substantially wrong with the two-predictor model containing *Age* and *Weight*:

Regression Analysis: BP versus Age, Weight

Analysis of Variance

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Regression	2	555.176	277.588	978.25	0.000
Age	1	49.704	49.704	175.16	0.000
Weight	1	311.910	311.910	1099.20	0.000
Error	17	4.824	0.284		
Lack-of-Fit	16	4.324	0.270	0.54	0.807
Pure Error	1	0.500	0.500		
Total	19	560.000			

Model Summary

S	R-sq	R-sq(adj)	R-sq(pred)
0.532692	99.14%	99.04%	98.89%

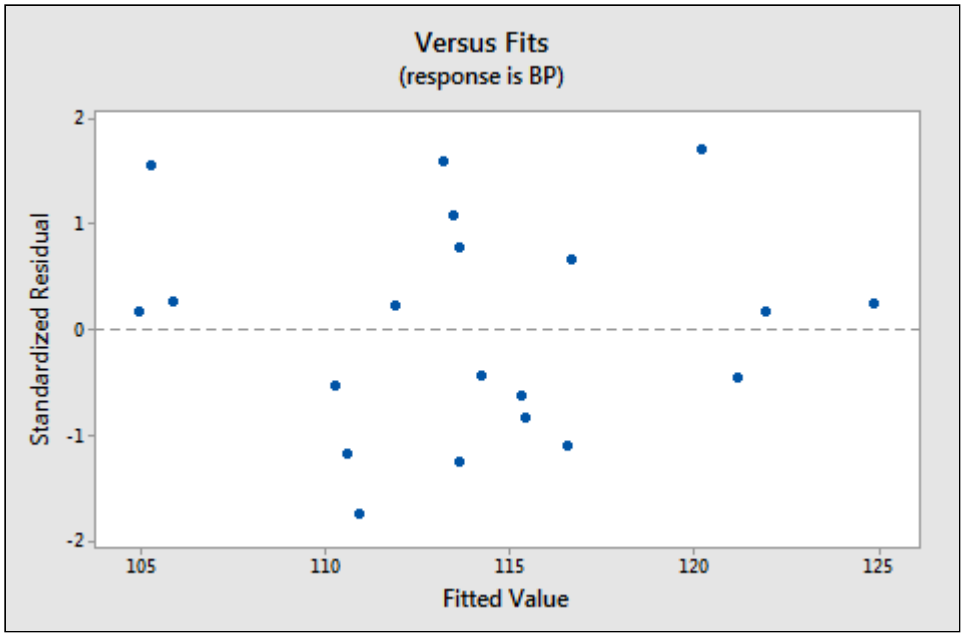
Coefficients

Term	Coef	SE Coef	T-Value	P-Value	VIF
Constant	-16.58	3.01	-5.51	0.000	
Age	0.7083	0.0535	13.23	0.000	1.20
Weight	1.0330	0.0312	33.15	0.000	1.20

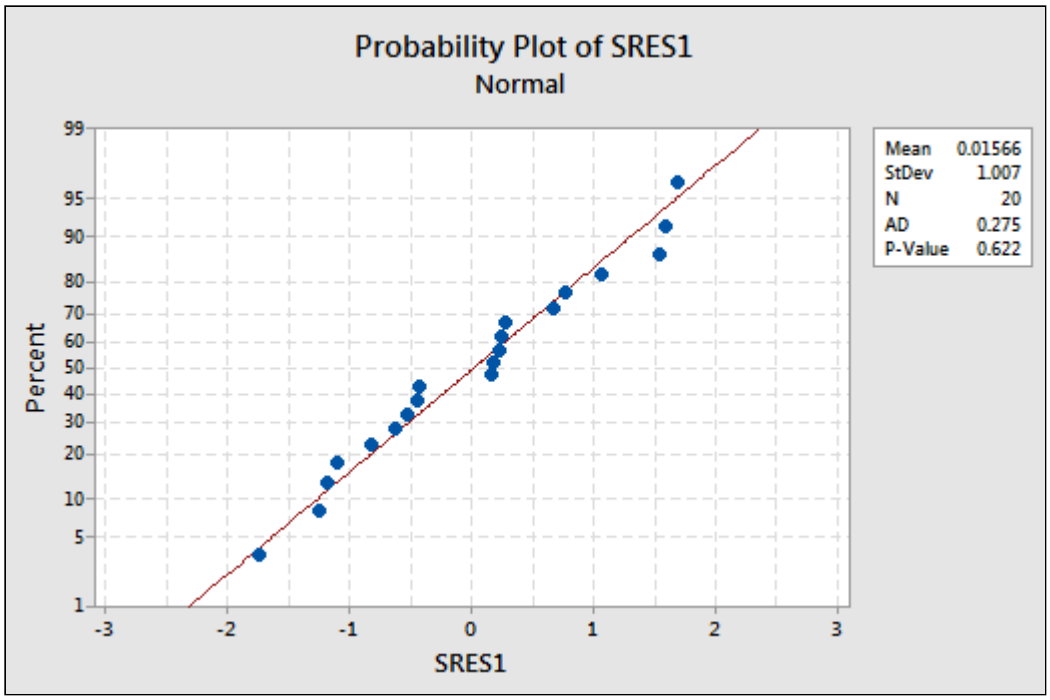
Regression Equation

BP = -16.58 + 0.7083 Age + 1.0330 Weight

For this model, the variance inflation factors are quite satisfactory (both 1.20), the adjusted R^2-value (99.04%) can't get much better, and the residual analysis yields no concerns. That is, the residuals versus fits plot:



is just right, suggesting that the relationship is indeed linear and that the variances of the error terms are constant. The normal probability plot:



suggests that the error terms are normally distributed.

Now, why might I prefer this model over the other legitimate contenders? It all comes down to simplicity! What's your age? What's your weight? Perhaps more than 90% of you know the answer to those two simple questions. But, now what is your body surface area? And, how long have you had hypertension? Answers to these last two questions are almost certainly less immediate for most (all?) people. Now, the researchers might have good arguments for why we should instead use the larger, more complex models. If that's the case, fine. But, if not, it is almost always best to go with the simpler model. And, certainly the model containing only *Age* and *Weight* is simpler than the other viable models.

‹ 11.3 - Best Subsets Regression, Adjusted R-Sq, Mallows Cp (/stat462/node/197) up (/stat462/node/89) 11.5 - Information Criteria and PRESS › (/stat462/node/199)

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11.5 - Information Criteria and PRESS

To compare regression models, some statistical software may also give values of statistics referred to as **information criterion** statistics. For regression models, these statistics combine information about the SSE, number of parameters in the model, and the sample size. A low value, compared to values for other possible models, is good. Some data analysts feel that these statistics give a more realistic comparison of models than the C_p statistic because C_p tends to make models seem more different than they actually are.

Three information criteria that we present are called **Akaike's Information Criterion** (**AIC**), the **Bayesian Information Criterion** (**BIC**) (which is sometimes called **Schwartz's Bayesian Criterion** (**SBC**)), and **Amemiya's Prediction Criterion** (**APC**). The respective formulas are as follows:

$$AIC_k = n\ln(SSE) - n\ln(n) + 2(k+1)$$

$$BIC_k = n\ln(SSE) - n\ln(n) + (k+1)\ln(n)$$

$$APC_k = \frac{(n+k+1)}{n(n-k-1)}SSE$$

In the formulas, n = sample size and k = number of predictor terms (so k+1 = number of regression parameters in the model being evaluated, including the intercept). Notice that the only difference between AIC and BIC is the multiplier of *(k+1)*, the number of parameters. Each of the information criteria is used in a similar way—in comparing two models, the model with the *lower* value is preferred.

The BIC places a higher penalty on the number of parameters in the model so will tend to reward more parsimonious (smaller) models. This stems from one criticism of AIC in that it tends to favor models that overfit.

The **prediction sum of squares** (or **PRESS**) is a model validation method used to assess a model's predictive ability that can also be used to compare regression models. For a data set of size n, PRESS is calculated by omitting each observation individually and then the remaining $n - 1$ observations are used to calculate a regression equation which is used to predict the value of the omitted response value (which, recall, we denote by $\hat{y}_{i(i)}$). We then calculate the i^{th} PRESS residual as the difference $y_i - \hat{y}_{i(i)}$. Then, the formula for PRESS is given by

$$\text{PRESS} = \sum_{i=1}^{n}(y_i - \hat{y}_{i(i)})^2.$$

In general, the *smaller* the PRESS value, the better the model's predictive ability.

PRESS can also be used to calculate the **predicted** R^2 (denoted by R^2_{pred}) which is generally more intuitive to interpret than PRESS itself. It is defined as

$$R^2_{pred} = 1 - \frac{\text{PRESS}}{\text{SSTO}}$$

and is a helpful way to validate the predictive ability of your model without selecting another sample or splitting the data into training and validation sets in order to assess the predictive ability (see Section 11.7). Together, PRESS and R^2_{pred} can help prevent overfitting because both are calculated using observations not included in the model estimation. Overfitting refers to models that appear to provide a good fit for the data set at hand, but fail to provide valid predictions for new observations.

You may notice that R^2 and R^2_{pred} are similar in form. While they will not be equal to each other, it is possible to have R^2 quite high relative to R^2_{pred}, which implies that the fitted model is overfitting the sample data. However, unlike R^2, R^2_{pred} ranges from values below 0 to 1. $R^2_{pred} < 0$ occurs when the underlying PRESS gets inflated beyond the level of the SSTO. In such a case, we can simply truncate R^2_{pred} at 0.

Finally, if the PRESS value appears to be large due to a few outliers, then a variation on PRESS (using the absolute value as a measure of distance) may also be calculated:

$$\text{PRESS}^* = \sum_{i=1}^{n} |y_i - \hat{y}_{i(i)}|,$$

which also leads to

$$R^{2*}_{pred} = 1 - \frac{\text{PRESS}^*}{\text{SSTO}}.$$

‹ 11.4 - Some Automated Variable Selection Examples (/stat462/node/198) | up (/stat462/node/89) | 11.6 - Further Automated Variable Selection Examples › (/stat462/node/203)

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11.6 - Further Automated Variable Selection Examples

Example: Peruvian Blood Pressure Data

First we will illustrate the "Best Subsets" procedure and a "by hand" calculation of the information criteria from earlier. Recall from Lesson 5 that this dataset consists of variables possibly relating to blood pressures of $n = 39$ Peruvians who have moved from rural high altitude areas to urban lower altitude areas (peru.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/peru.txt)). The variables in this dataset (where we have omitted the calf skinfold variable from the first time we used this example) are:

Y = systolic blood pressure
X_1 = age
X_2 = years in urban area
$X_3 = X_2 / X_1$ = fraction of life in urban area
X_4 = weight (kg)
X_5 = height (mm)
X_6 = chin skinfold
X_7 = forearm skinfold
X_8 = resting pulse rate

The results from the best subsets procedure are presented below.

Best Subsets Regression: Systol versus Age, Years, ...

Response is Systol

Vars	R-Sq	R-Sq (adj)	R-Sq (pred)	Mallows Cp	S	Age	Years	fraclife	Weight	Height	Chin	Forearm	Pulse
1	27.2	25.2	20.7	30.5	11.338			X					
1	7.6	5.1	0.0	48.1	12.770		X						
2	47.3	44.4	37.6	14.4	9.7772		X	X					
2	42.1	38.9	30.3	19.1	10.251	X		X					
3	50.3	46.1	38.6	13.7	9.6273		X	X		X			
3	49.0	44.7	34.2	14.8	9.7509	X	X	X					
4	59.7	55.0	44.8	7.2	8.7946	X	X	X	X				
4	52.5	46.9	31.0	13.7	9.5502	X	X	X		X			
5	63.9	58.4	45.6	5.5	8.4571	X	X	X	X		X		
5	63.1	57.6	44.2	6.1	8.5417	X	X	X	X			X	
6	64.9	58.3	43.3	6.6	8.4663	X	X	X	X		X	X	
6	64.3	57.6	44.0	7.1	8.5337	X	X	X	X	X	X		
7	66.1	58.4	42.6	7.5	8.4556	X	X	X	X	X	X	X	
7	65.5	57.7	41.3	8.0	8.5220	X	X	X	X		X	X	X
8	66.6	57.7	39.9	9.0	8.5228	X	X	X	X	X	X	X	X

To interpret the results, we start by noting that the lowest C_p value (= 5.5) occurs for the five-variable model that includes the variables **Age**, **Years**, **fraclife**, **Weight**, and **Chin**. The "**X**"s to the right side of the display tell us which variables are in the model (look up to the column heading to see the variable name). The value of R^2 for this model is 63.9% and the value of R^2_{adj} is 58.4%. If we look at the best six-variable model, we see only minimal changes in these values, and the value of $S = \sqrt{MSE}$ increases. A five-variable model most likely will be sufficient. We should then use multiple regression to explore the five-variable model just identified. Note that two of these *x*-variables relate to how long the person has lived at the urban lower altitude.

Next, we turn our attention to calculating AIC and BIC. Here are the multiple regression results for the best five-variable model (which has $C_p = 5.5$) and the best four-variable model (which has $C_p = 7.2$).

Best 5-variable model results:

```
Analysis of Variance

Source      DF  Adj SS   Adj MS  F-Value  P-Value
Regression   5  4171.2   834.24    11.66    0.000
  Age        1   782.6   782.65    10.94    0.002
  Years      1   751.2   751.19    10.50    0.003
  fraclife   1  1180.1  1180.14    16.50    0.000
  Weight     1   970.3   970.26    13.57    0.001
  Chin       1   269.5   269.48     3.77    0.061
Error       33  2360.2    71.52
Total       38  6531.4


Model Summary

      S    R-sq  R-sq(adj)  R-sq(pred)
8.45707  63.86%     58.39%      45.59%


Coefficients

Term        Coef  SE Coef  T-Value  P-Value    VIF
Constant   109.4     21.5     5.09    0.000
Age       -1.012    0.306    -3.31    0.002   2.94
Years      2.407    0.743     3.24    0.003  29.85
fraclife  -110.8     27.3    -4.06    0.000  20.89
Weight     1.098    0.298     3.68    0.001   2.38
Chin      -1.192    0.614    -1.94    0.061   1.48


Regression Equation

Systol = 109.4 - 1.012 Age + 2.407 Years - 110.8 fraclife + 1.098 Weight - 1.192 Chin
```

Best 4-variable model results

```
Analysis of Variance

Source      DF  Adj SS   Adj MS  F-Value  P-Value
Regression   4  3901.7   975.43    12.61    0.000
  Age        1   698.1   698.07     9.03    0.005
  Years      1   711.2   711.20     9.20    0.005
  fraclife   1  1125.5  1125.55    14.55    0.001
  Weight     1   706.5   706.54     9.14    0.005
Error       34  2629.7    77.34
Total       38  6531.4


Model Summary

      S    R-sq  R-sq(adj)  R-sq(pred)
8.79456  59.74%     55.00%      44.84%


Coefficients

Term        Coef  SE Coef  T-Value  P-Value    VIF
Constant   116.8     22.0     5.32    0.000
Age       -0.951    0.316    -3.00    0.005   2.91
Years      2.339    0.771     3.03    0.005  29.79
fraclife  -108.1     28.3    -3.81    0.001  20.83
Weight     0.832    0.275     3.02    0.005   1.88


Regression Equation

Systol = 116.8 - 0.951 Age + 2.339 Years - 108.1 fraclife + 0.832 Weight
```

AIC Comparison: The five-variable model still has a slight edge (a lower AIC is better).

- For the five-variable model:

$$\text{AIC}_k = 39 \ln(2360.23) - 39 \ln(39) + 2(6) = 172.015.$$

- For the four-variable model:

$$\text{AIC}_k = 39 \ln(2629.71) - 39 \ln(39) + 2(5) = 174.232.$$

BIC Comparison: The values are nearly the same; the five-variable model has a slightly lower value (a lower BIC is better).

- For the five-variable model:

$$\text{BIC}_k = 39 \ln(2360.23) - 39 \ln(39) + \ln(39) \times 6 = 181.997.$$

- For the four-variable model:

$$\text{BIC}_k = 39 \ln(2629.71) - 39 \ln(39) + \ln(39) \times 5 = 182.549.$$

Our decision is that the five-variable model has better values than the four-variable models, so it seems to be the winner. Interestingly, the **Chin** variable is not quite at the 0.05 level for significance in the five-variable model so we could consider dropping it as a predictor. But, the cost will be an increase in MSE and 4.2% drop in R^2. Given the closeness of the **Chin**-value (0.061) to the 0.05 significance level and the relatively small sample size (39), we probably should keep the **Chin** variable in the model for prediction purposes. When we have a p-value that is only

slightly higher than our significance level (by slightly higher, we mean usually no more than 0.05 above the significance level we are using), we usually say a variable is **marginally significant**. It is usually a good idea to keep such variables in the model, but one way or the other, you should state why you decided to keep or drop the variable.

Example: Measurements of College Students

Next we will illustrate stepwise procedures. Recall from Lesson 5 that this dataset consists of $n = 55$ college students with measurements for the following seven variables (Physical.txt (/stat462/sites/onlinecourses.science.psu.edu.stat462/files/data/Physical.txt)):

Y = height (in)
X_1 = left forearm length (cm)
X_2 = left foot length (cm)
X_3 = left palm width
X_4 = head circumference (cm)
X_5 = nose length (cm)
X_6 = gender, coded as 0 for male and 1 for female

Here is the output for a stepwise procedure.

```
Stepwise Selection of Terms

Candidate terms: LeftArm, LeftFoot, LeftHand, HeadCirc, nose, Gender

             ----Step 1----     ----Step 2----
              Coef         P     Coef         P
Constant     31.22              21.86
LeftFoot     1.449     0.000    1.023     0.000
LeftArm                         0.796     0.000

S                   2.55994           2.14916
R-sq                 67.07%            77.23%
R-sq(adj)            66.45%            76.35%
R-sq(pred)           64.49%            73.65%
Mallows' Cp           20.69              0.57

α to enter = 0.15, α to remove = 0.15
```

All six x-variables were candidates for the final model. The procedure took two forward steps and then stopped. The variables in the model at that point are left foot length and left forearm length. The left foot length variable was selected first (in Step 1), and then left forearm length was added to the model. The procedure stopped because no other variables could enter at a significant level. Notice that the significance level used for entering variables was 0.15. Thus, after Step 2 there were no more x-variables for which the p-value would be less than 0.15.

It is also possible to work backwards from a model with all the predictors included and only consider steps in which the least significant predictor is removed. Output for this *backward elimination* procedure is given below.

```
Backward Elimination of Terms

Candidate terms: LeftArm, LeftFoot, LeftHand, HeadCirc, nose, Gender

             -----Step 1----    ----Step 2----    ----Step 3----    ----Step 4----
               Coef        P     Coef        P     Coef        P     Coef        P
Constant       21.1             19.7             16.60             21.25
LeftArm       0.762    0.000    0.751    0.000    0.760    0.000    0.766    0.000
LeftFoot      0.912    0.000    0.915    0.000    0.961    0.000    1.003    0.000
LeftHand      0.191    0.510    0.198    0.490    0.248    0.332    0.225    0.370
HeadCirc      0.076    0.639    0.081    0.611    0.100    0.505
nose         -0.230    0.654
Gender        -0.55    0.632    -0.43    0.696

S                   2.20115          2.18317          2.16464          2.15296
R-sq                 77.95%           77.86%           77.79%           77.59%
R-sq(adj)            75.19%           75.60%           76.01%           76.27%
R-sq(pred)           70.58%           71.34%           72.20%           73.27%
Mallows' Cp            7.00             5.20             3.36             1.79

             ----Step 5----
               Coef        P
Constant      21.86
LeftArm       0.796    0.000
LeftFoot      1.023    0.000
LeftHand
HeadCirc
nose
Gender

S                   2.14916
R-sq                 77.23%
R-sq(adj)            76.35%
R-sq(pred)           73.65%
Mallows' Cp            0.57

α to remove = 0.1
```

The procedure took five steps (counting Step 1 as the estimation of a model with all variables included). At each subsequent step, the weakest variable is eliminated until all variables in the model are significant (at the default 0.10 level). At a particular step, you can see which variable was eliminated by the new blank spot in the display (compared to the previous step). For instance, from Step 1 to Step 2, the nose length variable was dropped (it had the highest *p*-value.) Then, from Step 2 to Step 3, the gender variable was dropped, and so on.

The stopping point for the backward elimination procedure gave the same model as the stepwise procedure did, with left forearm length and left foot length as the only two *x*-variables in the model. It will not always necessarily be the case that the two methods used here will arrive at the same model.

Finally, it is also possible to work forwards from a base model with no predictors included and only consider steps in which the most significant predictor is added. We leave it as exercise to see how this *forward selection* procedure works for this dataset (you can probably guess given the results of the Stepwise procedure above).

‹ 11.5 - Information Criteria and PRESS (/stat462/node/199) up (/stat462/node/89) 11.7 - Cross-validation › (/stat462/node/200)

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11.7 - Cross-validation

How do we know that an estimated regression model is generalizable beyond the sample data used to fit it? Ideally, we can obtain new independent data with which to validate our model. For example, we could refit the model to the new dataset to see if the various characteristics of the model (e.g., estimates regression coefficients) are consistent with the model fit to the original dataset. Alternatively, we could use the regression equation of the model fit to the original dataset to make predictions of the response variable for the new dataset. Then we can calculate the prediction errors (differences between the actual response values and the predictions) and summarize the predictive ability of the model by the **mean squared prediction error (MSPE)**. This gives an indication of how well the model will predict in the future. Sometimes the MSPE is rescaled to provide a cross-validation R^2.

However, most of the time we cannot obtain new independent data to validate our model. An alternative is to partition the sample data into a **training (or model-building) set**, which we can use to develop the model, and a **validation (or prediction) set**, which is used to evaluate the predictive ability of the model. This is called **cross-validation**. Again, we can compare the model fit to the training set to the model refit to the validation set to assess consistency. Or we can calculate the MSPE for the validation set to assess the predictive ability of the model.

Another way to employ cross-validation is to use the validation set to help determine the final selected model. Suppose we have found a handful of "good" models that each provide a satisfactory fit to the training data and satisfy the model (LINE) conditions. We can calculate the MSPE for each model on the validation set. Our final selected model is the one with the smallest MSPE.

The simplest approach to cross-validation is to partition the sample observations randomly with 50% of the sample in each set. This assumes there is sufficient data to have 6-10 observations per potential predictor variable in the training set; if not, then the partition can be set to, say, 60%/40% or 70%/30%, to satisfy this constraint.

If the dataset is too small to satisfy this constraint even by adjusting the partition allocation then ***K*-fold cross-validation** can be used. This partitions the sample dataset into K parts which are (roughly) equal in size. For each part, we use the remaining $K - 1$ parts to estimate the model of interest (i.e., the training sample) and test the predictability of the model with the remaining part (i.e., the validation sample). We then calculate the sum of squared prediction errors, and combine the K estimates of prediction error to produce a K-fold cross-validation estimate.

When $K = 2$, this is a simple extension of the 50%/50% partition method described above. The advantage of this method is that it is usually preferable to residual diagnostic methods and takes not much longer to compute. However, its evaluation can have high variance since evaluation may depend on which data points end up in the training sample and which end up in the test sample.

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When $K = n$, this is called **leave-one-out cross-validation**. That means that n separate data sets are trained on all of the data (except one point) and then prediction is made for that one point. The evaluation of this method is very good, but often computationally expensive. Note that the K-fold cross-validation estimate of prediction error is identical to the PRESS statistic.

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Applied Regression Analysis

11.8 - One Model Building Strategy

We've talked before about the "art" of model building. Unsurprisingly, there are many approaches to model building, but here is one strategy—consisting of seven steps—that is commonly used when building a regression model.

The first step

Decide on the type of model that is needed in order to achieve the goals of the study. In general, there are five reasons one might want to build a regression model. They are:

- For **predictive** reasons — that is, the model will be used to predict the response variable from a chosen set of predictors.
- For **theoretical** reasons — that is, the researcher wants to estimate a model based on a known theoretical relationship between the response and predictors.
- For **control** purposes — that is, the model will be used to control a response variable by manipulating the values of the predictor variables.
- For **inferential** reasons — that is, the model will be used to explore the strength of the relationships between the response and the predictors.
- For **data summary** reasons — that is, the model will be used merely as a way to summarize a large set of data by a single equation.

The second step

Decide which predictor variables and response variable on which to collect the data. Collect the data.

The third step

Explore the data. That is:

- On a univariate basis, check for outliers, gross data errors, and missing values.
- Study bivariate relationships to reveal other outliers, to suggest possible transformations, and to identify possible multicollinearities.

I can't possibly over-emphasize the importance of this step. There's not a data analyst out there who hasn't made the mistake of skipping this step and later regretting it when a data point was found in error, thereby nullifying hours of work.

The fourth step

Randomly divide the data into a training set and a validation set:

- The **training set**, with at least 15-20 error degrees of freedom, is used to estimate the model.
- The **validation set** is used for cross-validation of the fitted model.

The fifth step

Using the training set, identify several candidate models:

- Use best subsets regression.
- Use stepwise regression, which of course only yields one model unless different alpha-to-remove and alpha-to-enter values are specified.

The sixth step

Select and evaluate a few "good" models:

- Select the models based on the criteria we learned, as well as the number and nature of the predictors.
- Evaluate the selected models for violation of the model conditions.
- If none of the models provide a satisfactory fit, try something else, such as collecting more data, identifying different predictors, or formulating a different type of model.

The seventh and final step

Select the final model:

- Compare the competing models by cross-validating them against the validation data.
- The model with a smaller mean square prediction error (or larger cross-validation R^2) is a better predictive model.
- Consider residual plots, outliers, parsimony, relevance, and ease of measurement of predictors.

And, most of all, don't forget that there is not necessarily only **one** good model for a given set of data. There might be a few equally satisfactory models.

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Applied Regression Analysis

11.9 - Another Model Building Strategy

Here is another strategy that outlines some basic steps for building a regression model.

1. After establishing a research hypothesis, proceed to design an appropriate experiment or experiments. Identify variables of interest, what variable(s) will be the response, and what levels of the predictor variables you wish to cover in the study. If costs allow for it, then a pilot study may be helpful (or necessary).

2. Collect the data and make sure to "clean" it for any bugs (e.g., entry errors). If data from many variables are recorded, then variable selection and screening should be performed.

3. Consider the regression model to be used for studying the relationship and assess the adequacy of such a model. Oftentimes, a linear regression model will be implemented. But as these notes show, there are numerous regression models and regression strategies for dealing with different data structures. How you assess the adequacy of the fitted model will be dependent on the type of regression model that is being used as well as the corresponding assumptions. For linear regression, the following need to be checked:

   (a) Check for normality of the residuals. This is often done through a variety of visual displays, but formal statistical testing can also be performed.

   (b) Check for constant variance of the residuals. Again, visual displays and formal testing can both be performed.

   (c) Check the linearity condition using residual plots.

   (d) After time-ordering your data (if appropriate), assess the independence of the observations. Independence is best assessed by looking at a time-ordered plot of the residuals, but other time series techniques exist for assessing the assumption of independence (see Lesson 10). Regardless, checking the assumptions of your model as well as the model's overall adequacy is usually accomplished through residual diagnostic procedures.

4. Look for any outlying or influential data points that may be affecting the overall fit of your current model (see Lesson 9). Care should be taken with how you handle these points as they could actually be legitimate in how they were measured. While the option does exist for excluding such problematic points, this should only be done after careful consideration about if such points are recorded in error or are truly not representative of the data you collected. If any corrective actions are taken in this step, then return to Step 3.

5. Assess multicollinearity, i.e., linear relationships amongst your predictor variables (see Lesson 10). Multicollinearity issues can provide incorrect estimates as well as other issues. If you proceed to omit variables y be causing multicollinearity, then return to Step 3.

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6. Use the measures discussed in this Lesson to assess the predictability and overall goodness-of-fit of your model. If these measures turn out to be unsatisfactory, then modifications to the model may be in order (e.g., a different functional form or down-weighting certain observations). If you must take such actions, then return to Step 3 afterwards.

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