3.2: Variable Selection

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1 Why Variable Selection

- Up until now, we have focused on trying to make predictions/inference using all the potential explanatory variables we have available to us.
- We now wish to consider several candidate models, ultimately making a judgment as to which model is "best."
 - Selection is more than an art than it is a science: no "right" decisions, several wrong decisions, several "reasonables."
 - This is an iterative process, that makes it difficult to know when we are "done" (see Figure 1 on last page).
- One element of the model building process involves **selecting a subset** of potential explanatory variables for use in the final model.
 - Follows the Ockham's razor principle: entia non sunt multiplicanda praeter necessitatem

(Groups) Why might we prefer simpler models to complex ones? *Should* we prefer simpler models to more complex ones?

(Groups) Why is variable selection not something we would normally want to use in an experimental setting?

2 Methods of Variable Selection

How to pick the "best" subset of variables?

- Whenever possible, remove variables based on **context**, which comes with **expertise**.
- Automatic Methods:
 - All possible regressions: Consider all possible combinations of predictor variables, select the "best" model according to some measurement criteria.
 - **Stepwise methods:** Take a structured approach that takes a (semi) intelligent search through a subset of all possible models.
 - Penalized regression: more in Module 4.

2.1 All Possible Regressions

Consider all subsets of predictor variables X_1, \ldots, X_{p-1} .

- Number of subsets of size $\binom{p-1=P-1}{p-1=\frac{(P-1)!}{(p-1)!(P-p)!}}$.
- Number of subsets of all possible sizes: $\binom{\sum_{p=1}^{P}P-1}{p-1=2^{P-1}}$.

2.1.1 Measures of "goodness"

• R-square - but which model will always have the highest R^2 ?

$$R_p^2 = 1 - \frac{SS_{Error,p}}{SS_{Total}}$$

• Adjusted R-square - balances against # of predictors

$$R_{a,p}^2 = 1 - \frac{n-1}{n-p} \cdot \frac{SS_{Error,p}}{SS_{Total}}$$

As p increases, $R_{a,p}^2$ first increases, then decreases

• Mallow's C_p - for a certain subset of p-1 predictors:

$$C_p = \frac{SS_{Error} \text{ from model with } p - 1 \text{ predictors}}{MSE \text{ from model with } P - 1 \text{ predictors}} + 2p - n$$

When a subset of p-1 predictors gives unbiased \hat{Y} 's, $E[C_p] \approx p$. – so look for model with smallest p such that $C_p \approx p$, i.e., want $C_p \approx \#$ predictors +1.

Akaike's information criteria & Schwarz's Bayesian criterion
 both penalize larger numbers of predictors (want small):

$$AIC_p = n \log SS_{Error,p} - n \log n + 2p$$

$$SBC_p = n \log SS_{Error,p} - n \log n + p \log n$$

• Prediction sum of squares – based on leave-one-out philosophy $(\hat{Y}_{i(i)})$

$$PRESS_p = \sum_{i=1}^{n} \left(Y_i - \hat{Y}_{i(i)} \right)^2$$

- look for models with small $PRESS_n$

2.2 Stepwise Selection

Stepwise methods:

- automatically select a model based on some criterion (convenient)
- less satisfactory, do not "guarantee" the "right" model
- best used as "confirmatory" approaches
- three main: backward (okay), forward (worst), stepwise (hybrid)

Backward Elimination – basic algorithm

- 1. Fit model with all P-1 predictors
 - (a) Compare each predictor's individual P-value to some threshold (slstay; default in SAS is 0.10)
 - (b) If any predictor's P-value > slstay, drop predictor with largest P-value
- 2. Repeat with P-2 predictors
- 3. Continue until all predictors remaining have P-values below slstay

Forward Selection – basic algorithm

- 1. Find predictor with highest correlation with response
 - (a) Regress response on this predictor
 - (b) Leave predictor in model if P-value is below some threshold (slentry; default in SAS is 0.50)
- 2. Given the previously entered predictor, find the predictor with the highest partial correlation with response
 - (a) Add this predictor to the model
 - (b) Leave in model if P-value is below slentry
- 3. Continue until no more predictors warrant inclusion (P-value of "next" predictor above threshold)

Big problem here: best 2-variable model does not necessarily contain best 1-variable model (first step(s) can throw everything off)

Stepwise Selection – basic algorithm:

- 1. Take a "forward" step: add "best" predictor with P-value below slentry (default 0.15)
- 2. Take a "backward" step: evaluate all predictors in model and drop the variable with the highest P-value above slstay (default 0.15)
- 3. Iterate "forward" and "backward" steps until model stays the same

Note: in all these automatic stepwise procedures (backward, forward, stepwise), the slentry and slstay thresholds are deceptive. After the first step (really a hypothesis test), they are <u>not</u> significance levels (α), but "conditional" significance levels, which are harder to interpret.

(Individual) Clearly, it would be better to compare all possible models, rather than a subset (in stepwise methods). Why do stepwise methods even exist?

2.3 Remember this...

- In order to have reliable results, we need n >> P (often 6*10 times larger).
- Each described technique measures how well your models fit the data you already have, which might not translate to new data (in production).

We get a sense of how our models perform on new data by:

- Splitting our data into "training" and "test" sets.
- Fit each model using only the training data, then use the model to predict on the test data.
- Calculate the mean square prediction error:

$$MSPR = \frac{\sum_{i=1}^{n^*} \left(Y_i - \hat{Y}_i\right)^2}{n^*}$$



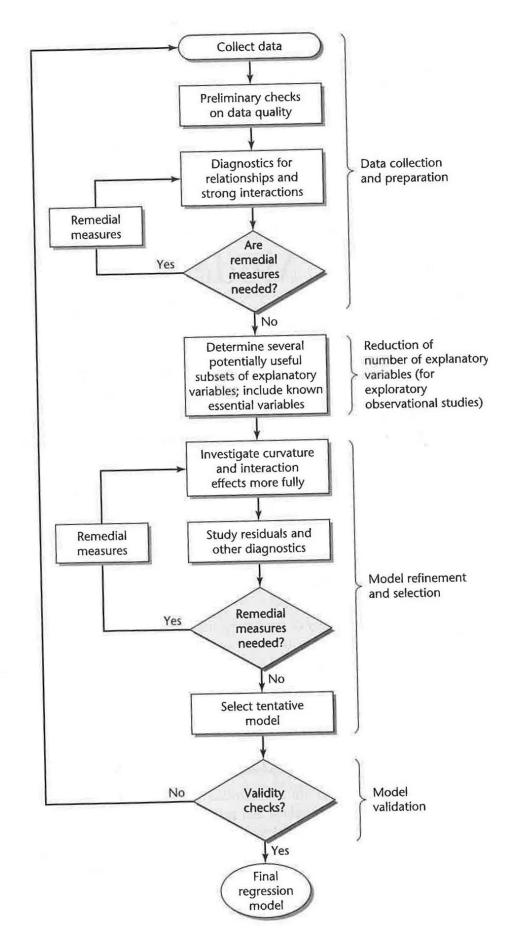


Figure 1: General model for multiple regression model selection (taken from Kutner et. al. (2004)).