



Model Building

Part 3: Prediction Models

STAT 705: Regression and Analysis of Variance

Prediction vs. Estimation

- Linear models can be used for estimation or prediction
- Equations for the models can be the same, but our method of assessing a 'good' model is different
- For estimation models
 - Assess 'goodness' via AIC, SBC, Adjusted R^2 , etc.
 - These measure how well the model fits the sample data
- For prediction models
 - Need a measure for how well the model will predict new observations
 - One option: PRESS (PREdicted Sum of Squares)

Deleted Residuals

- For each observation
 - Temporarily delete the observation
 - Fit the model using the remaining $n - 1$ observations
 - Use the fitted model to predict the response for this observation
 - » Notation: Put the subscript in parenthesis, $\hat{Y}_{(i)}$
 - The *deleted residual* is the difference between the observed and predicted values
$$r_{(i)} = Y_i - \hat{Y}_{(i)}$$
- Repeat this for every observation

PRESS Statistic

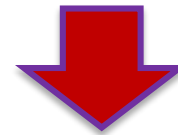
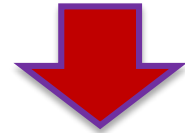
- PREdiction Sum of Squares
 - Sum of the squared deleted residuals
 - $$\text{PRESS} = \sum_{i=1}^n \left(Y_i - \hat{Y}_{(i)} \right)^2$$
- Software uses a shortcut for the calculations
 - No need to fit n separate regression models
- Small PRESS values are desirable
 - Small prediction errors

SAS Implementation

Use the 'press' option on the model statement

```
proc reg data=senic outest=pressinfo;
  WithNurses:    model InfRisk = Stay CulRatio XRay Nurses
                  Services MedSch Reg1 Reg2 Reg3 / press;
  WithoutNurses: model InfRisk = Stay CulRatio XRay
                  Services MedSch Reg1 Reg2 Reg3 / press;

  output press=press;
run;
proc print data=pressinfo; run;
```



Obs	_MODEL_	_TYPE_	_DEPVAR_	_RMSE_	_PRESS_	Intercept	Stay	CulRatio	XRay
1	WithNurses	PARMS	InfRisk	0.90912	104.997	-0.14941	0.26708	0.051606	0.011606
2	WithoutNurses	PARMS	InfRisk	0.91120	104.444	-0.32966	0.27469	0.052336	0.011326

Obs	Nurses	Services	MedSch	Reg1	Reg2	Reg3	InfRisk
1	.001304167	0.017633	-0.61838	-1.07183	-0.74377	-0.77185	-1
2	.	0.025459	-0.50274	-1.10697	-0.76674	-0.75937	-1

Interpreting PRESS

- For the model that predicts Infection Risk (in the SENIC dataset)
 - PRESS = 104.997 when 'Nurses' is used as a predictor
 - PRESS = 104.444 when 'Nurses' is not used
- Smaller PRESS \Rightarrow better predictive ability
- In this case, excluding a predictor *improves* the predictive ability (but not by much)

***ADDING MORE PREDICTORS IS SOMETIMES
DETRIMENTAL TO THE MODEL***

Model Validation

- There is no assurance that a model that is a good fit to the existing data will also be successful for future predictions
- There could be
 - influential factors that were unknown during model building
 - a different correlation structure among the predictors
- The key idea: Test the model in the environment in which it is going to perform
- This is especially important for observational studies
- PRESS is one method for assessing the predictive ability of the model
 - PRESS is sometimes called ‘leave one out’ cross validation, LOOCV

K-fold Cross Validation

- Similar to PRESS, but operates on groups of observations instead of individual observations
- Split the observations into K groups
- For each group
 - Temporarily remove this group from the data
 - Fit the model using the observations in the other groups
 - Predict the response value of the observations that were removed
 - Calculate the residuals
- Do this for all the groups
- Calculate the sum of the squared residuals

Data Splitting

- Another way to assess predictive ability of the model
- Requires a lot of data
 - At least 30 observations; more for complex models
- Split observations into two groups
 - Training set (about $2/3$ of all observations)
 - » Use these observations to estimate the regression equation
 - Prediction set (about $1/3$ of all observations)
 - » Apply the estimated regression equation to these observations
 - » Predict the value for the response
 - » Calculate the residuals

Mean Square for Prediction

- Analogous to MSE, but specifically designed to assess the predictive ability

$$MSPR = \frac{1}{n^*} \sum_{k=1}^{n^*} (Y_k - \hat{Y}_k)^2$$

- Y_k is the observed response for the k^{th} observation in the prediction set, $k = 1, 2, \dots, n^*$
- \hat{Y}_k is the predicted response for the k^{th} observation in the prediction set
 - Use the regression equation estimated with the training set.
- MSPR is a measure of the error, so smaller is better

What You Should Know

- How to assess model adequacy
 - Models for Estimation vs. Models for Prediction
- Understand why we need different methods of assessing the adequacy of prediction models
- For the PRESS statistic
 - Describe how it is calculated
 - Use SAS to calculate it
 - Interpret the results
- How is the MSPR different from the sum of squared residuals in K-fold cross validation?