

Exercises, STK4040, week 45

November 5, 2007

Exercise 1: MSE

Let f be a regression trained (estimated) on a data set \mathbf{X} and \mathbf{y} , and let $\hat{y} = f(\mathbf{x})$ be the predicted response value for a given new observation \mathbf{x} . Show that

$$\text{MSE}(\hat{y}) = \text{Bias}^2(\hat{y}) + \text{Var}(\hat{y} - Y), \quad (1)$$

where Y is (the unknown) response value corresponding to \mathbf{x} . (We treat \mathbf{X} and \mathbf{x} as given.) Note that this is true for regressions in general; we have not assumed anything about the shape of f (for instance that it should be a linear regression).

Exercise 2: leverage

Assume the model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad (2)$$

where \mathbf{X} is known and $\boldsymbol{\varepsilon} \sim N_n(0, \sigma^2\mathbf{I})$.

Given a data set \mathbf{X} and \mathbf{y} . Let $e_i = y_i - \hat{y}_i$ be the residuals from a linear regression of \mathbf{y} onto \mathbf{X} . Let h_i be the diagonal entries of the ‘hat matrix’ $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$. h_i is called the ‘leverage’ of \mathbf{x}_i , and is a measure of how much \mathbf{x}_i potentially can affect the regression. Note that $h_i = \mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i$.

a)

Let $\mathbf{X}_{(i)}$ and $\mathbf{y}_{(i)}$ be \mathbf{X} and \mathbf{y} with the i th observation removed, and let $\mathbf{b}_{(i)}$ be the estimate of $\boldsymbol{\beta}$ using $\mathbf{X}_{(i)}$ and $\mathbf{y}_{(i)}$. Show that

$$e_{(i)} = y_i - \mathbf{x}_i^T \mathbf{b}_{(i)} = e_i / (1 - h_i). \quad (3)$$

(In other words: one can calculate the residuals from a full cross-validation (A.K.A. leave one out cross-validation) of a linear regression without having to refit the regression for each observation.)

Tip: to save a bit of calculation, you can use the fact that

$$(\mathbf{X}_{(i)}^T \mathbf{X}_{(i)})^{-1} = (\mathbf{X}^T \mathbf{X})^{-1} + \frac{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1}}{1 - h_i}. \quad (4)$$

(Extra exercise: Use the fact that $\mathbf{X}_{(i)}^T \mathbf{X}_{(i)} = \mathbf{X}^T \mathbf{X} - \mathbf{x}_i \mathbf{x}_i^T$ to show (4).)

b)

Assume that $\mathbf{X} = (\mathbf{1} \ \mathbf{X}_1)$ in (2). Let \mathbf{X}_c and \mathbf{y}_c be \mathbf{X}_1 and \mathbf{y} centered, and let $\mathbf{y}_c = \mathbf{X}_c \boldsymbol{\beta}_c + \boldsymbol{\varepsilon}$ be the corresponding centered model. Call the leverages for this model g_i , and show that

$$h_i = g_i + 1/n, \quad (5)$$

where n is the number of observations, and h_i are the leverages for the observations in model (2). (Tip: Note that if we write the observations in model (2) as $(\mathbf{1} \ \mathbf{x}_i)$, then the corresponding observations in the centered model can be written as $\mathbf{x}_i - \bar{\mathbf{x}}$, where $\bar{\mathbf{x}}$ is the column means of \mathbf{X}_1 .)