

- Some cases have high *leverage*, the potential to greatly affect the fit.
- These cases are outliers in the space of predictors.
- Often the residuals for these cases are not large because
 - the response is in line with the other values, or
 - the high leverage has caused the fitted model to be pulled toward the observed response.

- ① The leverage exerted by the i 'th case is h_{ii} , the i 'th diagonal element of the hat matrix.
- ② Properties:
 - $0 \leq h_{ii} \leq 1$
 - if there is an intercept term in a regression model $h_{ii} \geq \frac{1}{n}$
 - if there are r observations with the same $\mathbf{x}$, the leverage for those observations is $\leq 1/r$. (groups of potentially influential cases are masked)
 - a general guideline is to flag cases where $h_{ii} > 2p/n$, where p is the number of columns of $\mathbf{X}$, equal to $k + 1$ in a multiple regression with k predictors and an intercept.
- ③ To get leverage values in R, use the command `hat(model.matrix(output))`, where *output* is the output from a call to *lm*.

- The fitted value at case i is

$$\hat{y}_i = (\mathbf{H}\mathbf{y})_i = \sum_{j=1}^n h_{ij}y_j = h_{ii}y_i + \sum_{j \neq i}^n h_{ij}y_j$$

a linear combination of all the responses.

- Ideally all cases contribute, with those at and closest to $\mathbf{x}_i$ dominating.
- In influential cases h_{ii} approaches 1, and h_{ij} approaches 0, for $j \neq i$.
- One can inspect the $h_{ii} = \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i$, called *leverage values*, to identify those which are large.
- In R you use the command `hat(model.matrix(output))` to get the leverage values, where `output` is the output from `lm`.

- Often it is difficult to find a case with high leverage by examining each predictor separately or in pairs using bivariate plots
 - the case may not be extreme in any particular predictor, but still be far from the centroid of the predictors.
 - Recall that $Var(\hat{y}_i) = h_{ii}\sigma^2$ and $Var(e_i) = (1 - h_{ii})\sigma^2$, so cases with high leverage have large estimation variance and small residual variance.
 - In simple linear regression

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{j=1}^n (x_j - \bar{x})^2}$$

so the minimum is $1/n$ at $\bar{x}$ and the maximum occurs when x is furthest from $\bar{x}$.

- More generally, h_{ii} measures the distance of the predictors from their centroid.
- The sum of the h_{ii} is $tr(\mathbf{H}) = k + 1 = p$, so their average is $\bar{h} = (k + 1)/n = p/n$.

How to identify hidden extrapolation

- Our book points out the danger of hidden extrapolation when predicting (Section 3.8).
- They note that any $\mathbf{x}_0$ with $\mathbf{x}_0^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_0 > h_{max}$, where h_{max} is the largest value in the dataset, will imply extrapolation beyond the cases in the dataset.

$$0 \leq h_{ii} \leq 1$$

- Because $\mathbf{H} = \mathbf{H}\mathbf{H}$ and $\mathbf{H} = \mathbf{H}^T$

$$h_{ii} = \sum_{j=1}^n h_{ij} h_{ji} = h_{ii}^2 + \sum_{j \neq i}^n h_{ij}^2 \quad (1)$$

so

$$h_{ii}(1 - h_{ii}) \geq 0$$

and

$$0 \leq h_{ii} \leq 1.$$

- Some statistical packages flag cases where $h_{ii} > 2(k+1)/n = 2p/n$.

When an intercept β_0 is included in a multiple regression model $h_{ii} \geq \frac{1}{n}$

- In the notes about adding variables to a regression we partitioned the $\mathbf{X}$ matrix into $\mathbf{X}_1$ and $\mathbf{X}_2$, and saw that $\mathbf{H} = \mathbf{H}_1 + \mathbf{H}_{2.1}$.
- Let $\mathbf{X}_1$ be the vector of 1's, so that $\mathbf{H}_1 = \mathbf{J}/n$ and

$$\mathbf{H}_{2.1} = \tilde{\mathbf{X}}(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T$$

where $\tilde{\mathbf{X}} = (\mathbf{I} - \mathbf{J}/n)\mathbf{X}$ contains the deviations of the predictors from their means.

- The i th diagonal entry of $\mathbf{H}$ is

$$h_{ii} = \frac{1}{n} + [\tilde{\mathbf{X}}(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T]_{ii}.$$

- The second term is positive so

$$h_{ii} \geq 1/n.$$

Maximum leverage with replicate $\mathbf{x}$

- The second term is of the form

$$\sum_j \sum_k (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k) \tilde{C}_{jk}$$

where $\tilde{C}_{jk}$ is the jk th entry of $(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1}$, and so measures the distance of the predictors in the i th case from the centroid $\bar{\mathbf{x}} = (\bar{x}_1, \dots, \bar{x}_k)^T$ in the k dimensional space of predictors.

- When two cases i and k have the same predictors, ($\mathbf{x}_i = \mathbf{x}_k$), (or equivalently, when there are two y values at the same $\mathbf{x}$)

$$h_{ik} = \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_k = h_{ii}$$

- From equation (1)

$$h_{ii} = 2h_{ii}^2 + \sum_{j \neq i, k}^n h_{ij}^2$$

so

$$h_{ii}(1 - 2h_{ii}) \geq 0$$

and

$$0 \leq h_{ii} \leq 1/2.$$

- So, the maximum leverage value is halved when there are two cases with the same values for the predictors.
- More generally, if r cases have the same predictors, (or equivalently, when there are r replicate values of y at $\mathbf{x}$), the maximum possible leverage value for these cases is $1/r$.
- Groups of potentially influential cases are *masked*, and cannot be detected by examining the h_{ii} .

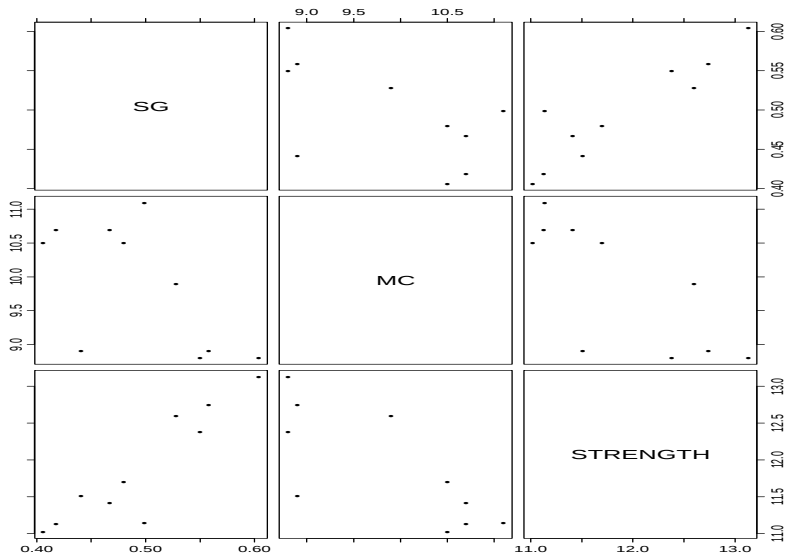
Example: strength of wood beams

Example: Data on the strength of wood beams was given by Hoaglin and Welsch (*The American Statistician*, 1978, vol 32, pp 17-22). The response is *Strength* and the predictors are *Specific Gravity* and *Moisture Content*. The data are

Beam Number	Specific Gravity	Moisture Content	Strength
1	.499	11.1	11.14
2	.558	8.9	12.74
3	.604	8.8	13.13
4	.441	8.9	11.51
5	.550	8.8	12.38
6	.528	9.9	12.60
7	.418	10.7	11.13
8	.480	10.5	11.70
9	.406	10.5	11.02
10	.467	10.7	11.41

- The correlation matrix of the data is

	SG	MC	STRENGTH
SG	1.0000000	-0.6077351	0.9131352
MC	-0.6077351	1.0000001	-0.7592328
STRENGTH	0.9131352	-0.7592328	1.0000000



- There is a positive association between *Strength* and *SG* and a negative association with *MC*.
- There is also a negative association between *Strength* and *MC*, with one value (in the lower left corner) quite different from the others.
- The linear model

$$\textit{Strength} = \beta_0 + \beta_1 \textit{SG} + \beta_2 \textit{MC} + \epsilon$$

gives output as follows.

```
> summary(woodlm.out)
```

```
Call: lm(formula = wood.Str ~ wood.SG + wood.MC)
```

```
Residuals:
```

Min	1Q	Median	3Q	Max
-0.4442	-0.1278	0.05365	0.1052	0.4499

```
Coefficients:
```

	Value	Std. Error	t value	Pr(> t)
(Intercept)	10.3015	1.8965	5.4319	0.0010
wood.SG	8.4947	1.7850	4.7589	0.0021
wood.MC	-0.2663	0.1237	-2.1522	0.0684

```
Residual standard error: 0.2754 on 7 degrees of freedom
```

```
Multiple R-Squared: 0.9
```

```
F-statistic: 31.5 on 2 and 7 degrees of freedom, the p-value
```

- The leverage values for the linear model in the two predictors are.

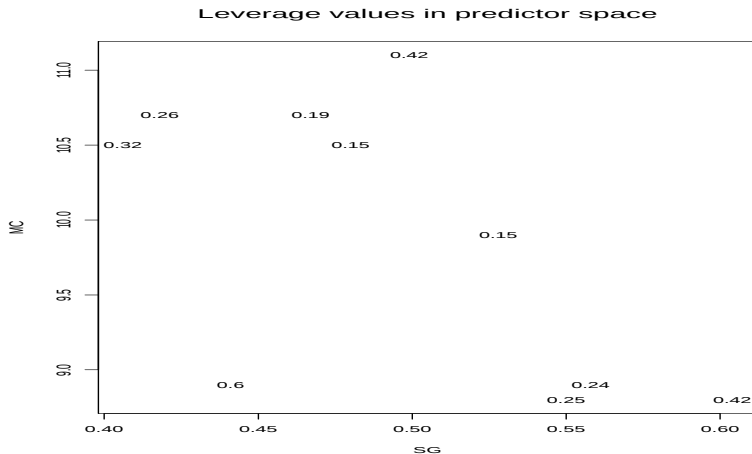
```
> hat(model.matrix(woodlm.out))
```

```
[1] 0.4178935 0.2418666 0.4172806 0.6043904 0.2521824 0.14
```

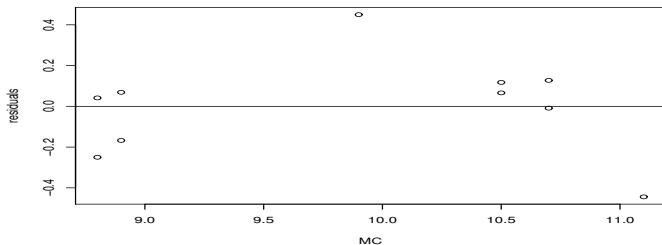
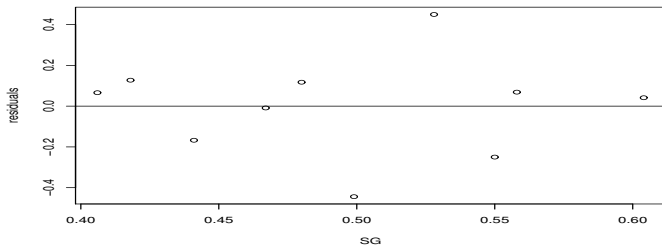
```
[7] 0.2616385 0.1540321 0.3155106 0.1873364
```

- Case 4 has the largest leverage, this is the case with low *SG* and *MC*.
- Note that the leverage values sum to 3, and that $2\bar{h} = 2(3)/10 = .6$ so that case 4 would be flagged as high leverage by some packages.

- The leverage values are plotted in the SG , MC space below.
- One can see how the values increase as you move toward the extremes of the data.



- The residuals from this model are shown below.



- This is only a small data set, but one possible extension to the model is to add a quadratic term in MC.

```
>wood.MC2 = wood.MC^2  
>woodlm2.out=lm(wood.Str~wood.SG + wood.MC + wood.MC2)  
>summary(woodlm2.out)
```

Call:

```
lm(formula = wood.Str ~ wood.SG + wood.MC + wood.MC2)
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-42.59511	8.49356	-5.015	0.002416	**
wood.SG	9.68175	0.72851	13.290	1.12e-05	***
wood.MC	10.42822	1.71125	6.094	0.000889	***
wood.MC2	-0.54221	0.08672	-6.252	0.000776	***

Residual standard error: 0.1085 on 6 degrees of freedom

Multiple R-Squared: 0.9867,

Adjusted R-squared: 0.98

F-statistic: 148.3 on 3 and 6 DF, p-value: 5.13e-06

- The fit has been improved (s has been reduced from .2754 to .1085, R^2 has increased from .9 to .99) and the MC^2 term is highly significant.
- The leverage values change with the model - $\mathbf{X}$ has one more column.

```
> hat(model.matrix(woodlm2.out))  
[1] 0.7657191 0.2418690 0.4241376 0.6469168  
0.2836093 0.6163116 0.2662545  
[8] 0.2304277 0.3371019 0.1876526
```

- The first case now has the largest leverage value.
- With an extra predictor, however, $2\bar{h} = .8$, so none of these values meet the threshold.

