Applied Regression Modeling: A Business Approach Chapter 3: Multiple Linear Regression Sections 3.1–3.3.2

by Iain Pardoe

Multiple linear regression

- Y is a quantitative *response* variable (a.k.a. dependent, outcome, or output variable).
- $(X_1, X_2, \dots)$ are quantitative *predictor* variables (a.k.a. independent/input variables, or covariates).
- Important to identify variables and define them carefully, e.g.:
  - Y is final exam score, out of 100;
  - X_1 is time spent partying during last week of term, in hours;
  - X_2 is average time spent studying during term, in hours per week.
- How much do we expect Y to change by when we change the values of X_1 and/or X_2?
- What do we expect the value of Y to be when $X_1 = 7.5$ and $X_2 = 1.3$?

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Multiple linear regression model

- Suppose exam score is (on average) 70 minus 1.6 times party hours plus 2.0 times study hours.
  - $\mathrm{E}(Y\,|\,(X_{1i}, X_{2i})) = 70 - 1.6X_{1i} + 2.0X_{2i}$, where $\mathrm{E}(Y\,|\,(X_{1i}, X_{2i}))$ means "the expected value of Y given that $X_1 = X_{1i}$ and $X_2 = X_{2i}$".
- Individual scores can deviate from this expected value by an amount e_i (called a "random error").
  - $Y_i\,|\,(X_{1i}, X_{2i})$ $= 70 - 1.6X_{1i} + 2.0X_{2i} + e_i \quad (i = 1, \dots, n)$ $=$ deterministic part $+$ random error.
- Error, e_i, represents variation in Y due to factors other than X_1 and X_2 which we haven't measured, e.g., quantitative skills, exam-taking ability.
- Example: $\mathrm{E}(Y) = 70 - 1.6(7.5) + 2.0(1.3) = 60.6$. If $Y = 65$, then $e = 65 - 60.6 = 4.4$.

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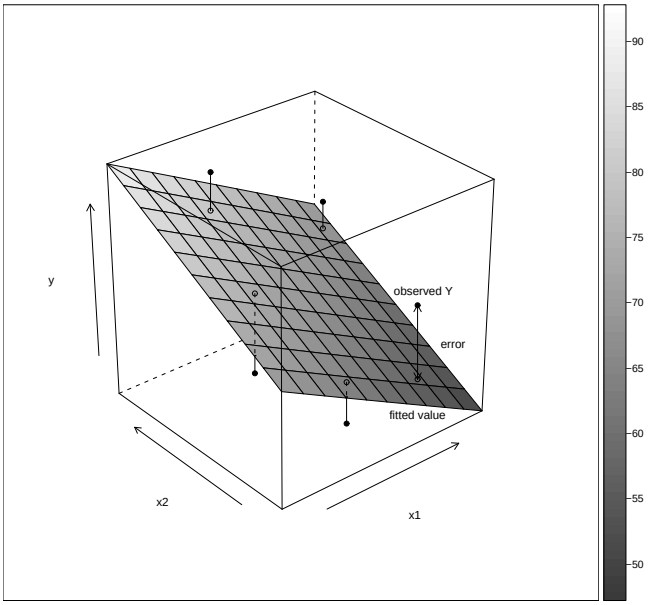
3D-scatterplot of (Y, X_1, X_2)

$Y =$ exam score, $X_1 =$ party time, $X_2 =$ study time



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Multiple linear regression equation

- Population: $\mathrm{E}(Y \,|\, (X_1, X_2, \ldots)) = b_0 + b_1 X_1 + b_2 X_2 + \cdots$.
- Interpretation:
  - b_0: expected Y-value when $X_1 = X_2 = \ldots = 0$;
  - b_1: "slope in the X_1-direction" (i.e., when $X_2, X_3, \ldots$ are held constant);
  - b_2: "slope in the X_2-direction" (i.e., when $X_1, X_3, \ldots$ are held constant).
- Sample: $\hat{Y} = \hat{b}_0 + \hat{b}_1 X_1 + \hat{b}_2 X_2 + \cdots$.
  - How can we estimate $\hat{b}_0, \hat{b}_1, \hat{b}_2, \cdots$?

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Estimating the model

- Model: $\mathrm{E}(Y) = b_0 + b_1 X_1 + b_2 X_2 + \cdots + b_k X_k$.
- Estimate: $\hat{Y} = \hat{b}_0 + \hat{b}_1 X_1 + \hat{b}_2 X_2 + \cdots + \hat{b}_k X_k$.
- Obtain $\hat{b}_0, \hat{b}_1, \hat{b}_2, \cdots, \hat{b}_k$ by finding best fit "hyperplane" (using least squares).
- Mathematically, minimize sum of squared errors:

$$\begin{aligned} \text{SSE} &= \sum_{i=1}^{n} \hat{e}_i^2 \\ &= \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 \\ &= \sum_{i=1}^{n} (Y_i - \hat{b}_0 - \hat{b}_1 X_{1i} - \hat{b}_2 X_{2i} - \cdots - \hat{b}_k X_{ki})^2. \end{aligned}$$

- Can use calculus (partial derivatives), but we'll use computer software to find $\hat{b}_0, \hat{b}_1, \hat{b}_2, \cdots, \hat{b}_k$.

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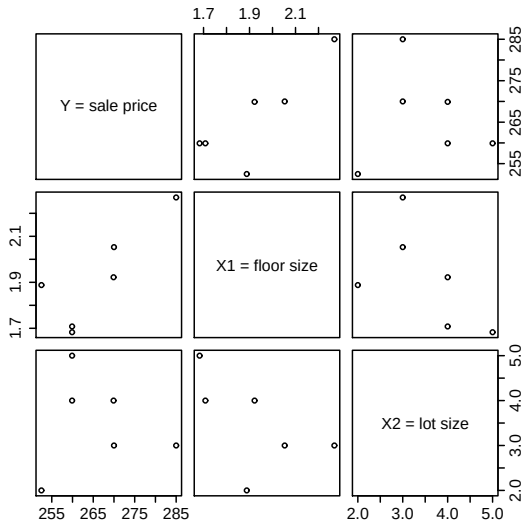
HOMES3 data

Y	252.5	259.9	259.9	269.9	270.0	285.0
X_1	1.888	1.683	1.708	1.922	2.053	2.269
X_2	2	5	4	4	3	3



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Scatterplot matrix

- A matrix of scatterplots showing all bivariate relationships in a multivariate dataset (e.g., previous slide).
- However, patterns *cannot* tell us whether a multiple linear regression model can provide a useful mathematical approximation to these bivariate relationships.
- Primarily useful for identifying any strange patterns or odd-looking values that might warrant further investigation *before* we start modeling.
- Home price–floor size example:
  no odd values to worry about.

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Multiple linear regression model

- Propose this multiple linear regression model:

$$\begin{aligned} Y &= \mathrm{E}(Y) + e \\ &= b_0 + b_1 X_1 + b_2 X_2 + e. \end{aligned}$$

- Random errors, e, represent variation in Y due to factors other than X_1 and X_2 that we haven't measured, e.g., numbers of bedrooms/bathrooms, property age, garage size, or nearby schools.
- Use least squares to estimate the deterministic part of the model, $\mathrm{E}(Y)$, as $\hat{Y} = \hat{b}_0 + \hat{b}_1 X_1 + \hat{b}_2 X_2$.
  - i.e., use statistical software to find the values of b_0, b_1, and b_2 that minimize $\mathrm{SSE} = \sum_{i=1}^{n} (Y_i - \hat{b}_0 - \hat{b}_1 X_{1i} - \hat{b}_2 X_{2i})^2$.

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Computer output

Parameters [a]

Model		Estimate	Std. Error	t-stat	Pr(>|t|)
1	(Intercept)	122.357	14.786	8.275	0.004
	X1	61.976	6.113	10.139	0.002
	X2	7.091	1.281	5.535	0.012

[a] Response variable: Y.

- Fitted model: $\hat{Y} = 122.36 + 61.98X_1 + 7.09X_2$.
- Expect $Y = \hat{b}_0$ when $X_1 = X_2 = 0$, but *only* if this makes sense and we have data close to $X_1 = X_2 = 0$
- Expect Y to change by $\hat{b}_1$ when X increases by one and other predictor X-variables stay constant, i.e., expect sale price to increase $\$6200$ when floor size increases 100 sq. feet and lot size stays constant.
- Expect Y to change by $\hat{b}_2$ when X increases by one and other predictor X-variables stay constant, i.e., expect sale price to increase $\$7090$ when lot size increases one category and floor size stays constant.

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3.3 Model evaluation

Evaluating fit numerically

Three methods:

- How close are the actual observed Y-values to the model-based fitted values, $\hat{Y}$?
  - Calculate *regression standard error*, s (3.3.1).
- How much of the variability in Y have we been able to explain with our model?
  - Calculate *coefficient of determination*, R^2 (3.3.2).
- How strong is the evidence of our modeled relationship between Y and $(X_1, X_2, \ldots)$?
  - Estimate/test *regression parameters*, $b_1, b_2, \ldots$
  - Globally (3.3.3), in subsets (3.3.4), individually (3.3.5).

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Regression standard error, s

Model Summary

Model	Multiple R	R Squared	Adjusted R Squared	Regression Std. Error
1	0.986 [a]	0.972	0.953	2.4753

[a] Predictors: (Intercept), X1, X2.

- Regression standard error, s, estimates the std. dev. of the multiple linear regression random errors:

$$s = \sqrt{\frac{\text{SSE}}{n-k-1}}.$$

- Unit of measurement for s is the same as unit of measurement for Y.
- Approximately 95% of the observed Y-values lie within plus or minus $2s$ of their fitted $\hat{Y}$-values.
- $2s = 4.95$, so expect to predict an unobserved sale price from particular floor and lot size values to within approx. $\pm\$4950$ (at a 95% confidence level).

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Calculating R^2

- Without model, estimate Y with sample mean m_Y.
- With model, estimate Y using fitted $\hat{Y}$-value.
- How much do we reduce our error when we do this?
- Total error without model: $\text{TSS} = \sum_{i=1}^{n}(Y_i - m_Y)^2$, variation in Y about m_Y.
- Remaining error with model: $\text{SSE} = \sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$, unexplained variation.
- Proportional reduction in error: $R^2 = \frac{\text{TSS}-\text{SSE}}{\text{TSS}}$.
- Home price–floor size example: $R^2 = 0.972$.
- 97.2% of the variation in sale price (about its mean) can be explained by a multiple linear regression relationship between sale price and (floor size, lot size).

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Interpreting R^2

Model Summary

Model	Multiple R	R Squared	Adjusted R Squared	Regression Std. Error
1	0.986^{a}	0.972	0.953	2.4753

[a] Predictors: (Intercept), X1, X2.

- R^2 measures the proportion of variation in Y (about its mean) that can be explained by a multiple linear regression relationship between Y and $(X_1, X_2, \ldots)$.
- If TSS = SSE then $R^2 = 0$: using $(X_1, X_2, \ldots)$ to predict Y hasn't helped and we may as well use m_Y to predict Y regardless of the $(X_1, X_2, \ldots)$ values.
- If SSE $= 0$ then $R^2 = 1$: using $(X_1, X_2, \ldots)$ allows us to predict Y perfectly (with no random errors).
- Such extremes rarely occur and usually R^2 lies between zero and one, with higher values of R^2 corresponding to better fitting models.

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Disadvantage of R^2 for model building

- Model building: what is the best way to model the relationship between Y and $(X_1, X_2, \ldots, X_k)$?
  - e.g., should we use all k predictors, or just a subset?
- Consider a sequence of *nested* models, with each model in the sequence adding predictors to the previous model.
- Which model would R^2 say is the "best" model? The final model with k predictors.
- Geometrical argument: start with a regression line on a 2D-scatterplot, then add a second predictor to make the line a plane in a 3D-scatterplot.
- In other words, R^2 always increases (or stays the same) as you add predictors to a model.

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Adjusted R^2

- R^2 has a clear interpretation since it represents the proportion of variation in Y (about its mean) explained by a multiple linear regression relationship between Y and $(X_1, X_2, \ldots)$.
- *But*, R^2 is not appropriate for finding a model that captures the major, important population relationships without overfitting every slight twist and turn in the sample relationships.
- We need an alternate criterion, which penalizes models that contain too many unimportant predictor variables:

$$\text{adjusted } R^2 = 1 - \left(\frac{n-1}{n-k-1}\right)\left(1-R^2\right).$$

- In practice, we can obtain the value for adjusted R^2 directly from statistical software.

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Using adjusted R^2

Model Summary

Model	Multiple R	R Squared	Adjusted R Squared	Regression Std. Error
1	0.826 [a]	0.682	0.603	7.1775
[a] Predictors: (Intercept), X1.				
2	0.986 [a]	0.972	0.953	2.4753
[a] Predictors: (Intercept), X1, X2.				

- Since adjusted R^2 is 0.603 for the single-predictor model, but 0.953 for the two-predictor model, the two-predictor model is better than the single-predictor model (according to this criterion).
- In other words, there is no indication that adding $X_2 =$ lot size to the model causes overfitting.
- What happens to R^2 and s?

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SHIPDEPT data

Y (labor hours)	X_1 (weight shipped)	X_2 (truck proportion)	X_3 (average weight)	X_4 (week)
100	5.1	90	20	1
85	3.8	99	22	2
...	...	...	...	...
85	4.8	58	25	20

- $Y =$ weekly labor hours
- $X_1 =$ total weight shipped in thousands of pounds
- $X_2 =$ proportion shipped by truck
- $X_3 =$ average shipment weight in pounds
- $X_4 =$ week
- Compare two models:
  - $\mathrm{E}(Y) = b_0 + b_1X_1 + b_3X_3$;
  - $\mathrm{E}(Y) = b_0 + b_1X_1 + b_2X_2 + b_3X_3 + b_4X_4$.

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Adjusted R^2 for SHIPDEPT data

Model Summary

Model	Multiple R	R Squared	Adjusted R Squared	Regression Std. Error
1	0.899 [a]	0.808	0.786	8.815
[a] Predictors: (Intercept), X1, X3.				
2	0.905 [a]	0.820	0.771	9.103
[a] Predictors: (Intercept), X1, X2, X3, X4.				

- Since adjusted R^2 is 0.786 for the two-predictor model, but 0.771 for the four-predictor model, the two-predictor model is better than the four-predictor model (according to this criterion).
- In other words, there is a suggestion that adding $X_2 =$ truck proportion and $X_4 =$ week to the model causes overfitting.
- What happens to R^2 and s?

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Multiple correlation

Model Summary

Model	Multiple R	R Squared	Adjusted R Squared	Regression Std. Error
1	0.986 [a]	0.972	0.953	2.4753
[a] Predictors: (Intercept), X1, X2.				

- The multiple correlation coefficient, multiple R, measures the strength and direction of linear association between the observed Y-values and the fitted $\hat{Y}$-values from the model.
- Multiple linear regression: multiple $R = +\sqrt{R^2}$.
  - e.g., $0.986 = \sqrt{0.972}$ for the home price–floor size example above.
- Beware: intuition about correlation can be seriously misleading when it comes to multiple linear regression (see next two slides).

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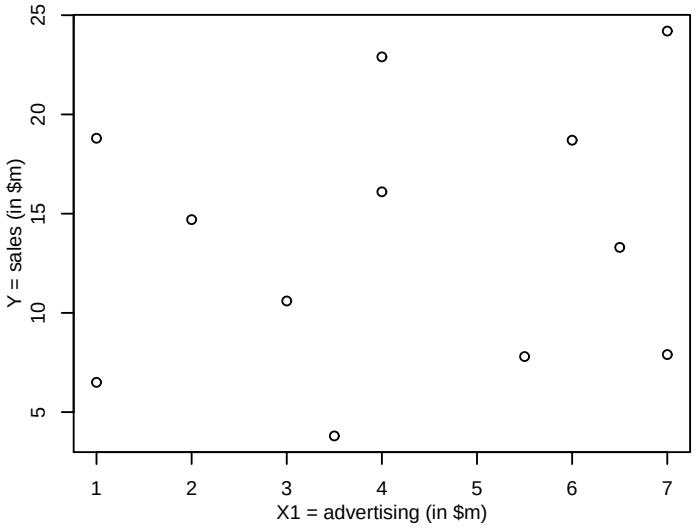
Low correlation between Y and X_1

X_1 can still be a useful predictor of Y in a MLR model.



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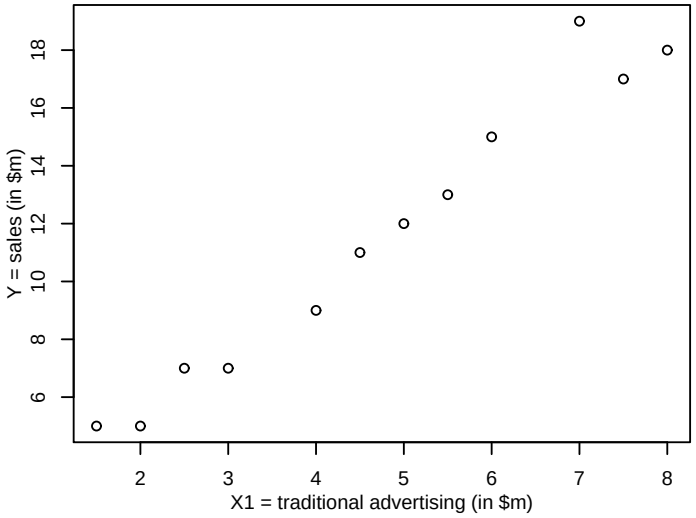
High correlation between Y and X_1

X_1 may be a poor predictor of Y in a MLR model.



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