

Interpreting Residuals

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January 26, 2021

Biol 520C: Statistical modelling for biological data

1. Housekeeping
2. Model Residuals
3. Diagnosing Residuals

Housekeeping

- Practical 03 is up on canvas, and due next Tuesday.

Model Residuals



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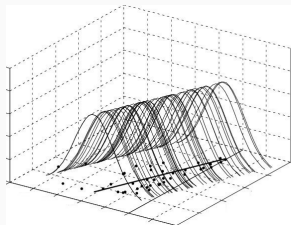
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The difference between the predicted and observed value is called the residual:

$$\text{Residual} = \text{Observed} - \text{Predicted}$$

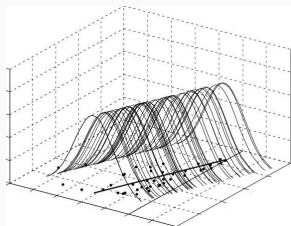


By definition, if these models are behaving properly they should result in some amount of residual spread around values predicted by a model's deterministic component.



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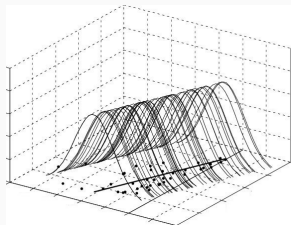
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Today we'll cover how to interpret a model's residuals to help you both understand and improve a regression model.



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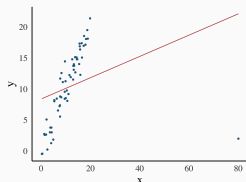
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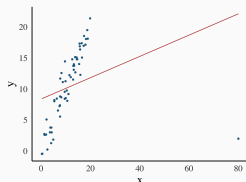
Rule of thumb: If your data are normally distributed, 95% of your data should be ± 2 SDs from the mean. If you have something greater than that, then you're probably looking at an outlier.



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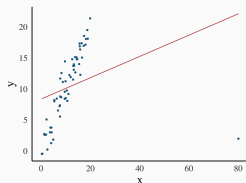


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The basic idea behind studentised residuals is to drop observations one at a time and refit the regression model on the remaining $n-1$ observations. Then, we compare the observed y_i values to their expected values based on the models with the i^{th} observation removed. This produces deleted residuals. Standardising these residuals produces studentised residuals.

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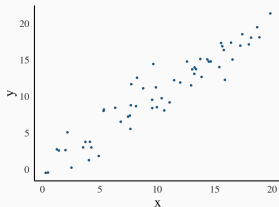
If data point i is ‘influential’ it pulls the regression line towards itself, and the observation would be close to the predicted response. But, if you removed the outlier, then the regression line would bounce back to the bulk of the data, resulting in a large studentised residual.



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linear <- function(x){  
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  eps <- rnorm(n = length(x), sd = sig)  
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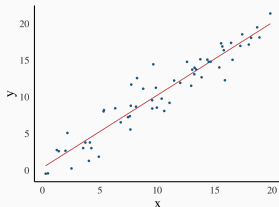
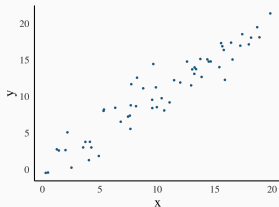
Residuals:

	Min	1Q	Median	3Q	Max
	-3.7911	-1.1243	-0.1473	0.9906	4.5536

Coefficients:

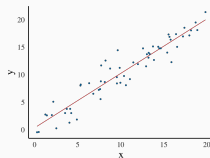
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	0.35535	0.49162	0.723	0.473
x	0.98904	0.04255	23.244	<2e-16 ***

Residual standard error: 1.763 on 58 degrees of freedom
Multiple R-squared: 0.9031, Adjusted R-squared: 0.9014
F-statistic: 540.3 on 1 and 58 DF, p-value: < 2.2e-16



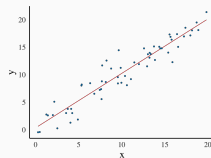


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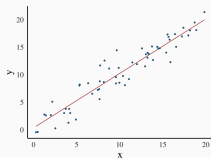
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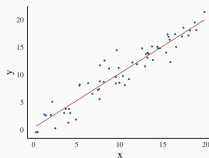


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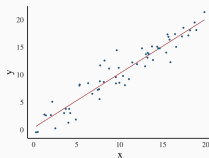
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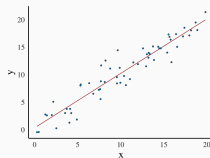
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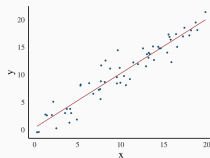
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head(Residuals)

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Alternatively, you can use the `residuals()` function, ultimately, the result is the same

```
Residuals2 <- residuals(MODEL)

head(Residuals2)

      1      2      3      4      5      6
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SS_res <- sum(Residuals^2)

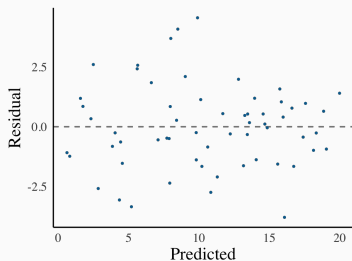
SS_tot <- sum((Observed - mean(Observed))^2)

Rsquare <- 1 - (SS_res/SS_tot)

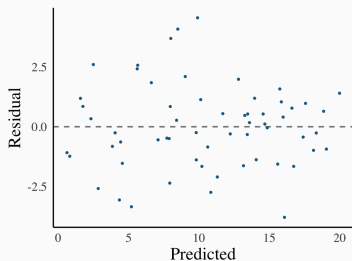
Rsquare
[1] 0.9030564
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The most useful way to examine the residuals is by plotting the predicted values of on the x-axis, and the residuals on the y-axis.

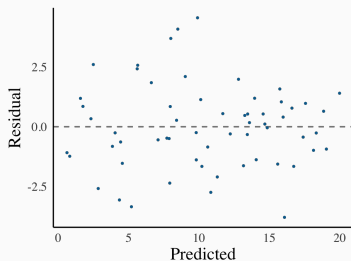


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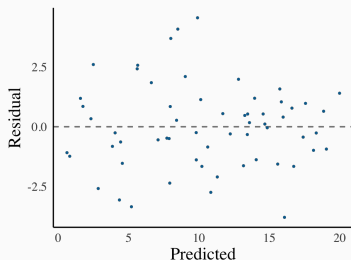
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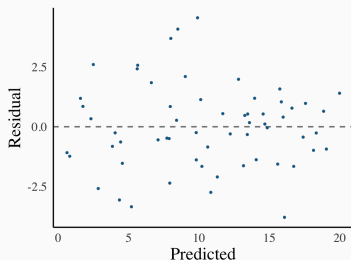
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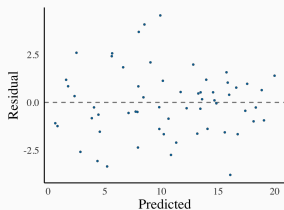


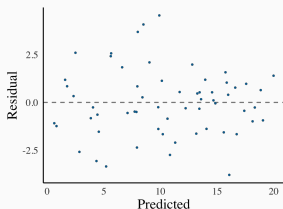
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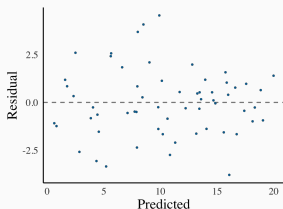


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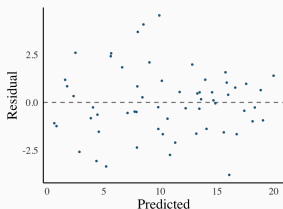


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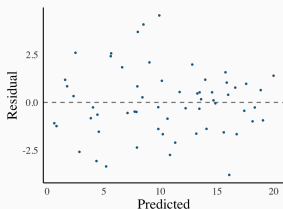
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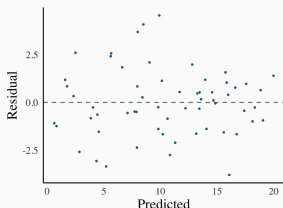
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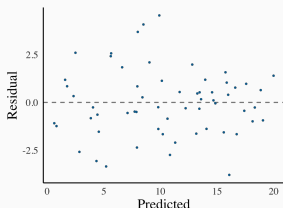
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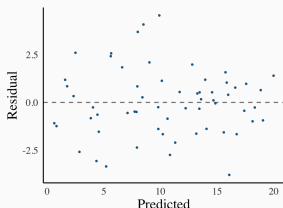
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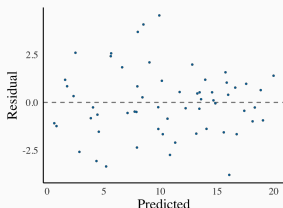
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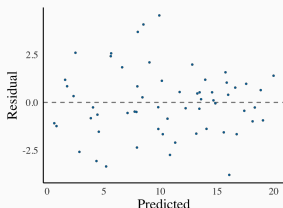
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This is what you hope to see if a model is performing well. The predictions aren't far from the observations, and there are no remaining patterns that aren't being explained by the model. If the residuals aren't evenly distributed vertically, or they have an outlier, or they have clear patterns, then the model has room for improvement.

Diagnosing Residuals



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Let's take a look at what happens to the residuals when there are known issues in the data.



Problem: What if the normal range of your data was ~ 0 to 20, but one of your datapoints had an x value of 80?

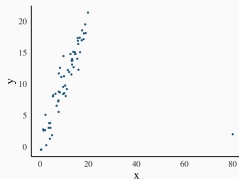
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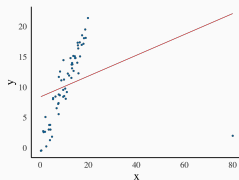
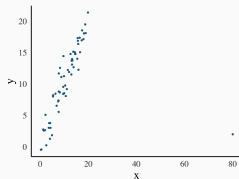
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Call:
lm(formula = y ~ x)
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```
Residuals:
    Min       1Q   Median       3Q      Max
-20.110  -3.024   1.158   3.905   9.580
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```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  8.39362    1.03457   8.113 3.52e-11 ***
x             0.17146    0.06731   2.547  0.0135 *
---

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Residual standard error: 5.428 on 59 degrees of freedom
Multiple R-squared:  0.09907, Adjusted R-squared:  0.0838
F-statistic: 6.488 on 1 and 59 DF,  p-value: 0.01349
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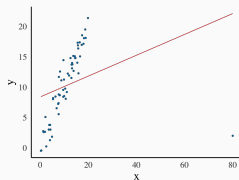
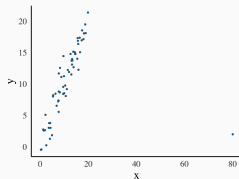
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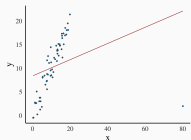
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Remember, our intercept was 0 and our slope was 1. What about the R^2

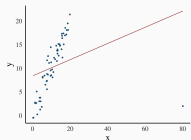


Implications: Because the outlier is so far from the bulk of the data, it has a disproportionate effect on the model and pulls the fit towards itself

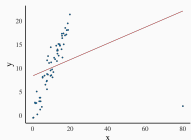


Implications: Because the outlier is so far from the bulk of the data, it has a disproportionate effect on the model and pulls the fit towards itself

How to solve the issue:



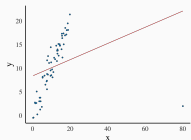
Implications: Because the outlier is so far from the bulk of the data, it has a disproportionate effect on the model and pulls the fit towards itself



How to solve the issue:

- It's possible that this is a measurement or data entry error. If this is the case, remove the outlier as it is providing misinformation.

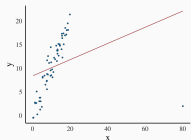
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How to solve the issue:

- It's possible that this is a measurement or data entry error. If this is the case, remove the outlier as it is providing misinformation.
- It's possible that what appear to be just a couple outliers are in fact the result of a non-linear relationship between x and y . Consider transforming or adding a variable.

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How to solve the issue:

- It's possible that this is a measurement or data entry error. If this is the case, remove the outlier as it is providing misinformation.
- It's possible that what appear to be just a couple outliers are in fact the result of a non-linear relationship between x and y . Consider transforming or adding a variable.
- If the data is not an entry/measurement error, you should assess the impact of the outlier. E.g., note the coefficients of your current model, then filter out that datapoint from the regression. If the model doesn't change much, there's not much to worry about. If there's a big change, examine the models and decide which one feels better to you given your knowledge of the system. It's okay to discard outliers in a defensible way.

Correction: Filtering outliers



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$$\text{Standardised Residual}_i = \frac{\text{Residual}_i}{\text{Standard Deviation of Residuals}}$$

$$\text{Standardised Residual}_i = \frac{\text{Residual}_i}{\text{Standard Deviation of Residuals}}$$

```
Observed <- y
```

```
Predicted <- MODEL$coefficients[1] + MODEL$coefficients[2]*x
```

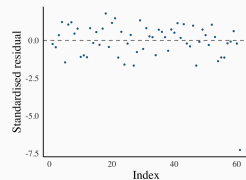
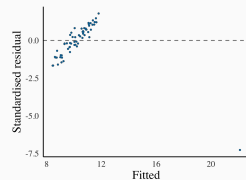
```
Residuals <- Observed - Predicted
```

$$\text{Standardised Residual}_i = \frac{\text{Residual}_i}{\text{Standard Deviation of Residuals}}$$

```
Observed <- y  
  
Predicted <- MODEL$coefficients[1] + MODEL$coefficients[2]*x  
  
Residuals <- Observed - Predicted  
  
Residuals <- Residuals/sd(Residuals)
```

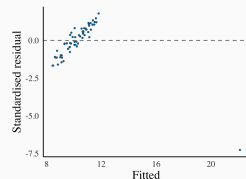

$$\text{Standardised Residual}_i = \frac{\text{Residual}_i}{\text{Standard Deviation of Residuals}}$$

```
Observed <- y  
Predicted <- MODEL$coefficients[1] + MODEL$coefficients[2]*x  
Residuals <- Observed - Predicted  
Residuals <- Residuals/sd(Residuals)  
head(Residuals)  
  
[1] -0.2371666 -0.4519790  0.3482399  1.2166389 -1.4501977  
     1.0522036
```



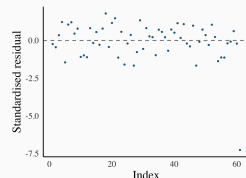
$$\text{Standardised Residual}_i = \frac{\text{Residual}_i}{\text{Standard Deviation of Residuals}}$$

```
Observed <- y  
Predicted <- MODEL$coefficients[1] + MODEL$coefficients[2]*x  
Residuals <- Observed - Predicted  
Residuals <- Residuals/sd(Residuals)  
head(Residuals)  
  
[1] -0.2371666 -0.4519790  0.3482399  1.2166389 -1.4501977  
     1.0522036
```



Alternatively, you can use `rstandard()`

```
Residuals2 <- rstandard(MODEL)  
head(Residuals2)  
  
      1      2      3      4      5      6  
-0.2378209 -0.4524664  0.3481916  1.2208638 -1.4561621  1.0556393
```



Correction: Filtering outliers cont.



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```
R_Student <- vector()  
for(i in 1:length(x)){
```



```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]
```



```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)
```

```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)

  Predicted <- coef(SUB_MODEL)[1] + coef(SUB_MODEL)[2]*x[i]
```

```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)

  Predicted <- coef(SUB_MODEL)[1] + coef(SUB_MODEL)[2]*x[i]

  Observed <- y[i]

  RESIDUAL <- Observed - Predicted
```



```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)

  Predicted <- coef(SUB_MODEL)[1] + coef(SUB_MODEL)[2]*x[i]

  Observed <- y[i]

  RESIDUAL <- Observed - Predicted

  R_Student[i] <- RESIDUAL/sd(residuals(SUB_MODEL))
}
```

```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)

  Predicted <- coef(SUB_MODEL)[1] + coef(SUB_MODEL)[2]*x[i]

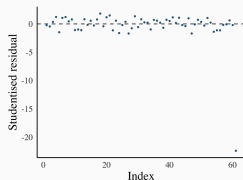
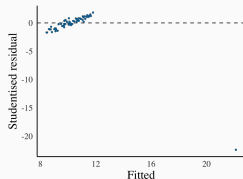
  Observed <- y[i]

  RESIDUAL <- Observed - Predicted

  R_Student[i] <- RESIDUAL/sd(residuals(SUB_MODEL))
}

head(R_Student)

[1] -0.2406048 -0.4575714  0.3514427  1.2513493 -1.5017222
     1.0782553
```



```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)

  Predicted <- coef(SUB_MODEL)[1] + coef(SUB_MODEL)[2]*x[i]

  Observed <- y[i]

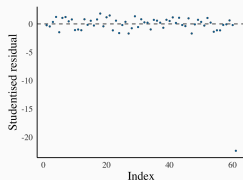
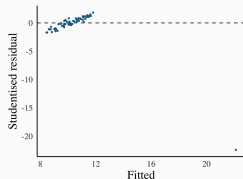
  RESIDUAL <- Observed - Predicted

  R_Student[i] <- RESIDUAL/sd(residuals(SUB_MODEL))
}

head(R_Student)

[1] -0.2406048 -0.4575714  0.3514427  1.2513493 -1.5017222
     1.0782553

R_Student2 <- rstudent(MODEL)
```



```
R_Student <- vector()
for(i in 1:length(x)){
  x_sub <- x[-i]
  y_sub <- y[-i]

  SUB_MODEL <- lm(y_sub ~ x_sub)

  Predicted <- coef(SUB_MODEL)[1] + coef(SUB_MODEL)[2]*x[i]

  Observed <- y[i]

  RESIDUAL <- Observed - Predicted

  R_Student[i] <- RESIDUAL/sd(residuals(SUB_MODEL))
}
```

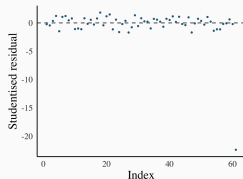
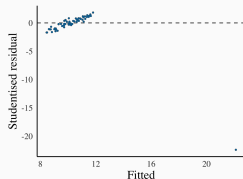
```
head(R_Student)
```

```
[1] -0.2406048 -0.4575714  0.3514427  1.2513493 -1.5017222
     1.0782553
```

```
R_Student2 <- rstudent(MODEL)
```

```
head(R_Student2)
```

```
      1      2      3      4      5      6
-0.2359099 -0.4493959  0.3455835  1.2260592 -1.4704338  1.0566817
```







Both standardised and studentised residuals provide strong evidence to support dropping the outlier.

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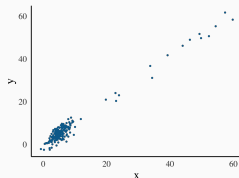
Based on this information, you would then drop the outlier and move forward with your analysis.



Problem: Imagine that, during your data collection, your x values were mostly centered around 5, but every now and then you got a very high value.

Problem: Imagine that, during your data collection, your x values were mostly centered around 5, but every now and then you got a very high value.

```
x <- c(rnorm(180, 5, 2), runif(20, 0, 60))  
y <- linear(x)
```



Problem: Imagine that, during your data collection, your x values were mostly centered around 5, but every now and then you got a very high value.

```
x <- c(rnorm(180, 5, 2), runif(20, 0, 60))
y <- linear(x)
```

```
MODEL <- lm(y ~ x)
```

```
Call:
lm(formula = y ~ x)
```

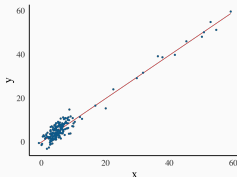
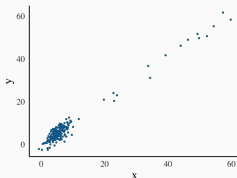
Residuals:

	Min	1Q	Median	3Q	Max
	-5.0696	-1.6995	0.0146	1.7043	6.2317

Coefficients:

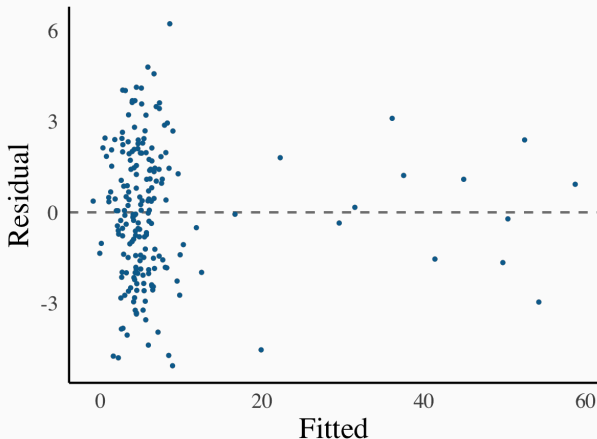
	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-0.06137	0.19602	-0.313	0.755
x	0.99320	0.01617	61.422	<2e-16 ***

Residual standard error: 2.21 on 198 degrees of freedom
Multiple R-squared: 0.9501, Adjusted R-squared: 0.9499
F-statistic: 3773 on 1 and 198 DF, p-value: < 2.2e-16



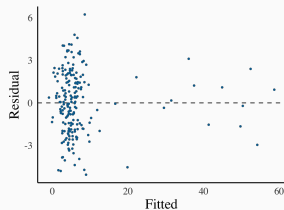


And the residuals on this fit would look like this

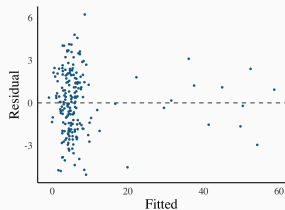




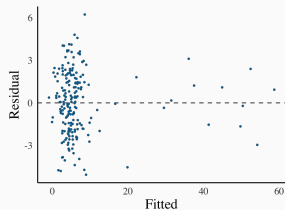
Implications: Sometimes there's actually nothing wrong with your model.



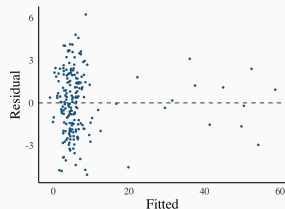
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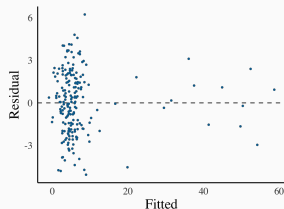


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How to solve the issue:

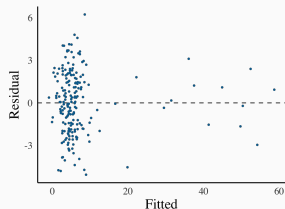
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How to solve the issue:

- If you're lucky, no correction is needed.

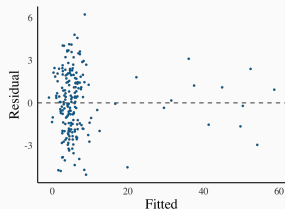
Implications: Sometimes there's actually nothing wrong with your model. Other times, however, an unbalanced x-axis can result in similar problems caused by outliers as we just saw (especially for non-linear relationships). Most of the time you'll find that the model was directionally correct but with inaccurate parameter estimates.



How to solve the issue:

- If you're lucky, no correction is needed.
- The solution to this is almost always to transform your data, typically an explanatory variable.

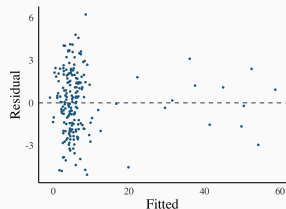
Implications: Sometimes there's actually nothing wrong with your model. Other times, however, an unbalanced x-axis can result in similar problems caused by outliers as we just saw (especially for non-linear relationships). Most of the time you'll find that the model was directionally correct but with inaccurate parameter estimates.



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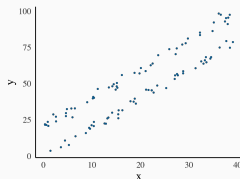
- If you're lucky, no correction is needed.
- The solution to this is almost always to transform your data, typically an explanatory variable.
- If you can, collect more data.
- It's also possible that the model is missing a variable.



Problem: One of the most common reason why a model struggles to fit a particular dataset is that not all the necessary variables have been included. This particular issue results in a wide range of residual structures, and has a lot of possible solutions.

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```
linear_2param <- function(x, x_2) {  
  B_0 <- 0  
  B_1 <- 2  
  B_2 <- 20  
  sig <- 2  
  eps <- rnorm(n = length(x), sd = sig)  
  y <- B_0 + B_1*x + B_2*x_2 + eps  
  y}  
  
x <- runif(100, 0, 40)  
x_2 <- rbinom(100,1,.5)  
y <- linear_2param(x, x_2)
```



Problem: One of the most common reason why a model struggles to fit a particular dataset is that not all the necessary variables have been included. This particular issue results in a wide range of residual structures, and has a lot of possible solutions.

```
linear_2param <- function(x, x_2) {  
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  y}
```

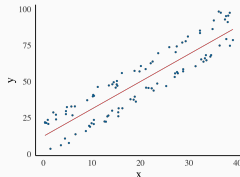
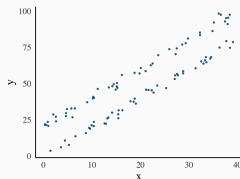
```
x <- runif(100, 0, 40)  
x_2 <- rbinom(100,1,.5)  
y <- linear_2param(x, x_2)
```

```
MODEL <- lm(y ~ x)
```

Coefficients:

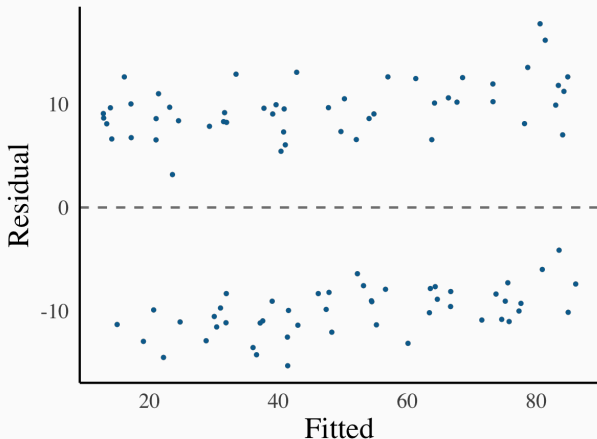
	Estimate	Std. Error	t value	Pr(>t)
(Intercept)	7.69031	2.11970	3.628	0.000456 ***
x	2.10136	0.09428	22.288	< 2e-16 ***

Residual standard error: 10.41 on 98 degrees of freedom
Multiple R-squared: 0.8352, Adjusted R-squared: 0.8335
F-statistic: 496.7 on 1 and 98 DF, p-value: < 2.2e-16
Biol 520C: Statistical modelling for biological data



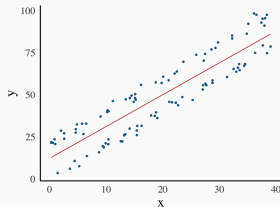


And the residuals on this fit would look like this

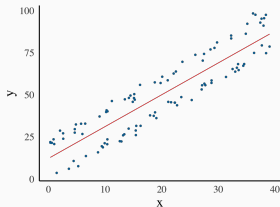




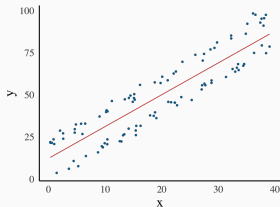
Implications: Notice how the slope is still accurate, but the estimated intercept is both off, and significant.



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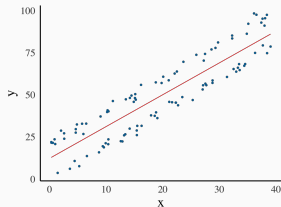


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How to solve the issue:

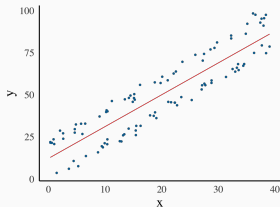
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How to solve the issue:

- Even though this approach wouldn't work in this example, it's worth attempting to transform a variable.

Implications: Notice how the slope is still accurate, but the estimated intercept is both off, and significant. The model isn't completely worthless, but it's definitely not as good as if you had all the variables you needed.



How to solve the issue:

- Even though this approach wouldn't work in this example, it's worth attempting to transform a variable.
- If that doesn't work, though, you probably need to deal with the missing variable problem.



Attempting a fix: Let's add a second parameter to our model.

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```
MODEL2 <- lm(y ~ x + x_2)
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Call:

```
lm(formula = y ~ x + x_2)
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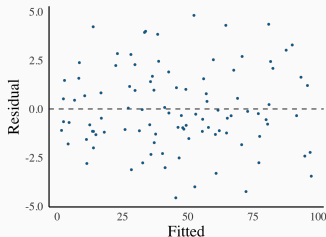
Residuals:

Min	1Q	Median	3Q	Max
-5.2565	-1.4237	0.1298	1.3260	4.3949

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-0.45906	0.45905	-1.0	0.32
x	2.00473	0.01754	114.3	<2e-16 ***
x_2	20.38987	0.41025	49.7	<2e-16 ***

Residual standard error: 2.029 on 97 degrees of freedom
Multiple R-squared: 0.9934, Adjusted R-squared: 0.9933
F-statistic: 7349 on 2 and 97 DF, p-value: < 2.2e-16



Attempting a fix: Let's add a second parameter to our model.

```
MODEL2 <- lm(y ~ x + x_2)
```

Call:

```
lm(formula = y ~ x + x_2)
```

Residuals:

Min	1Q	Median	3Q	Max
-5.2565	-1.4237	0.1298	1.3260	4.3949

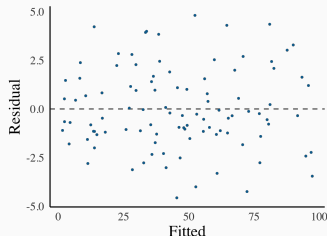
Coefficients:

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Residual standard error: 2.029 on 97 degrees of freedom

Multiple R-squared: 0.9934, Adjusted R-squared: 0.9933

F-statistic: 7349 on 2 and 97 DF, p-value: < 2.2e-16



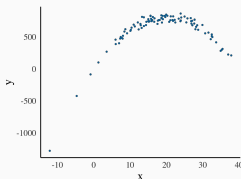
The parameter estimates match the model we simulated from, and fitted model makes far more accurate predictions because it's able to take into account the additional information from x_2



Problem: Imagine a situation where y tends to be small at small values of x , large and intermediate values of x , but then small again at the largest values of x . This scenario represents a non-linear relationship between x and y , which ends up being very common in practice.

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quad <- function(x) {  
  B_0 <- 0  
  B_1 <- 80  
  B_2 <- -2  
  sig <- 40  
  eps <- rnorm(n = length(x), sd = sig)  
  y <- B_0 + B_1*x + B_2*x^2 + eps  
  y}  
  
x <- rnorm(100, mean = 20, 10)  
y <- quad(x)
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x <- rnorm(100, mean = 20, 10)
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```
MODEL <- lm(y ~ x)
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	478.594	67.807	7.058	2.44e-10 ***
x	5.247	3.175	1.653	0.102

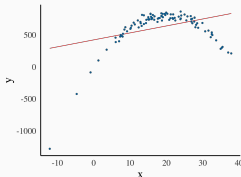
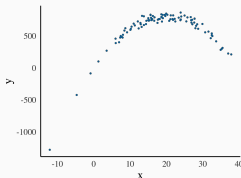
Residual standard error: 330.8 on 98 degrees of freedom

Multiple R-squared: 0.02712, Adjusted R-squared:

0.01719

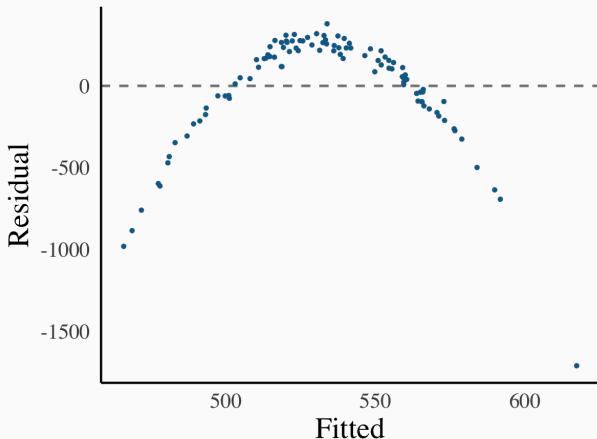
F-statistic: 2.732 on 1 and 98 DF, p-value: 0.1016

Biol 520C: Statistical modelling for biological data



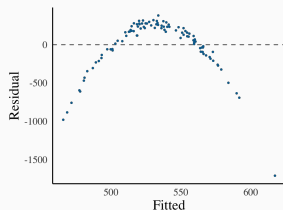


And the residuals on this fit would look like this

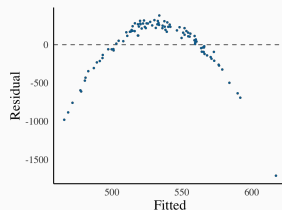




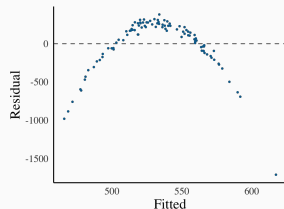
Implications: If your model is off, as in the example above, your predictions will be effectively worthless. In situations like this the model is doing very little to explain any relationship between x and y . You can see this by the fact that the residuals (i.e., what's left after the model has made a prediction) look exactly like the data.



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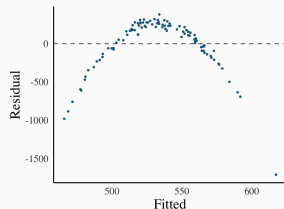


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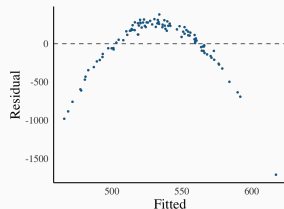
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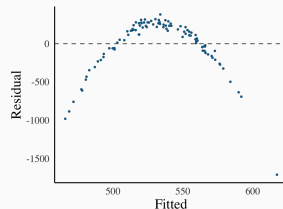
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How to solve the issue:

- Sometimes patterns like this indicate that a variable needs to be transformed.
- If the pattern is actually as clear as this example, you probably need to add a non-linear term.
- Or, as always, it's possible that the issue is a missing variable.



Attempting a fix: You might notice that the shape here is typically associated with a quadratic formula: $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2$

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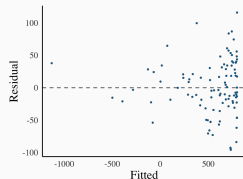
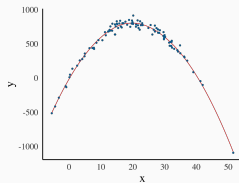
Residuals:

	Min	1Q	Median	3Q	Max
	-88.31	-29.03	-6.62	33.34	95.89

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	2.82349	11.09741	0.254	0.8
x	80.22120	1.10150	72.829	<2e-16 ***
I(x^2)	-2.02119	0.02742	-73.706	<2e-16 ***

Residual standard error: 44.04 on 97 degrees of freedom
Multiple R-squared: 0.9829, Adjusted R-squared: 0.9826
F-statistic: 2793 on 2 and 97 DF, p-value: < 2.2e-16



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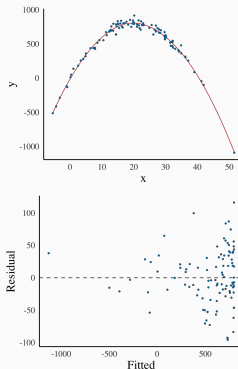
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The residuals are slightly unbalanced, but otherwise decent looking.



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Deviations from this expectation provide you with clues on how you might be able to improve the fit of your model.