

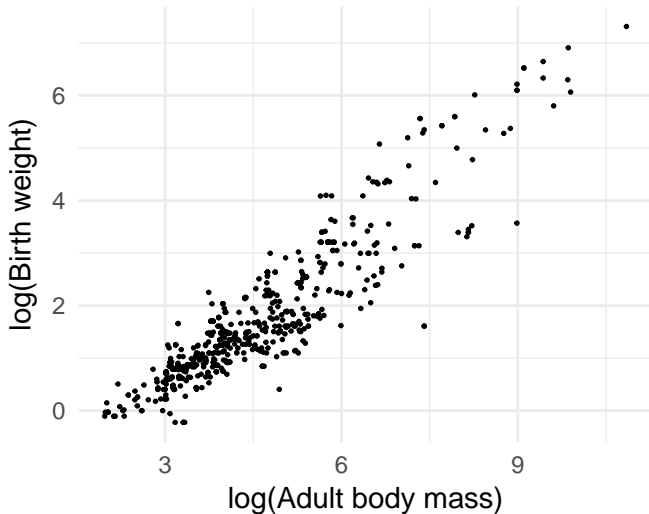
Parameter uncertainty and model criticism for linear regression

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Recap

How to predict birth weight?



Assumptions

1. Linear relationship between x and y :

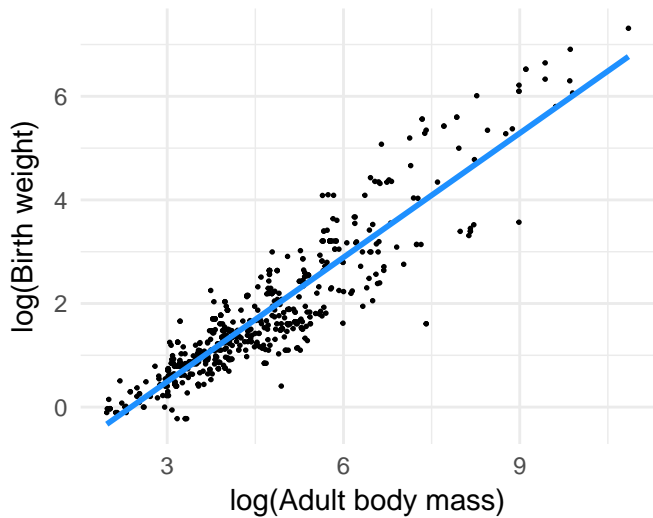
$$\hat{y}_i = \beta_0 + \beta_1 x_i$$

2. Normal error in y (variation around line):

$$y_i \sim \text{Normal}(\hat{y}_i, \sigma)$$

3. Homoskedasticity (errors have constant variance)
4. Observations are independent:

$$-\log(L(y; \beta_0, \beta_1, \sigma)) = -\sum_{i=1}^n \log(p(y_i; \beta_0, \beta_1, \sigma))$$



Today: parameter uncertainty and model criticism

1. How uncertain are our estimates?
2. How much can the model explain?
3. Evaluating linearity
4. Evaluating homoskedasticity

Evaluating uncertainty

Standard error

$$SE = \sqrt{\text{diag}(H^{-1})}$$

Hessians

18th century German auxiliaries

- ▶ contracted for military service by the British government
- ▶ $\approx 25\%$ of British forces in American Revolutionary War
- ▶ from the German state of Hesse-Kassel



But what is a Hessian really?

A square matrix of second-order partial derivatives

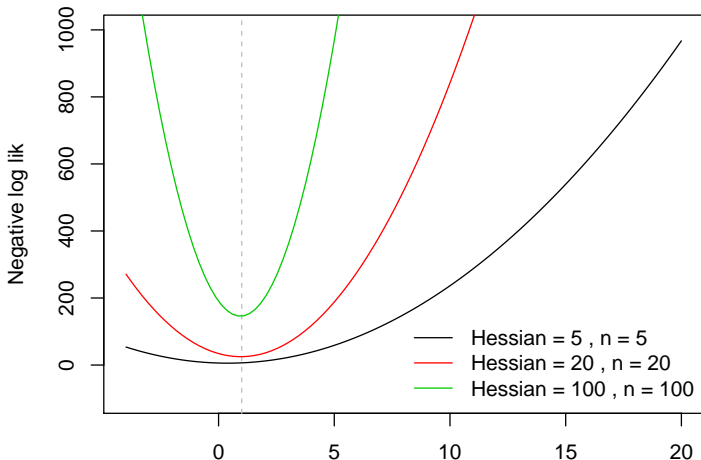
$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_p} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_p} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_p \partial x_1} & \frac{\partial^2 f}{\partial x_p \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_p^2} \end{bmatrix}$$

What is a Hessian graphically?

Curvature of the log likelihood

→ how much information do we have?

**Negative log likelihood profiles
for the mean**



Recap

Hessian tell us about curvature

SE tells us about uncertainty

Computing confidence intervals from SE

Approximation:

$$CI(\theta) \pm \theta_{MLE} + t_{\alpha/2} SE(\theta)$$

```
# e.g., 95% confidence interval
```

```
params <- fit$par
```

```
sample_size <- length(y)
```

```
n_params <- length(params)
```

```
crit_t <- qt(0.025, sample_size - n_params)
```

```
lower_ci <- params[1] + crit_t * SE[1]
```

```
upper_ci <- params[1] - crit_t * SE[1]
```

Assumption (big one)

The log likelihood profile is quadratic

- ▶ more reliable for large n

Confidence interval demo

Questions?

$$SE = \sqrt{\text{diag}(H^{-1})}$$

$$\text{CI}(\theta) \pm \theta_{\text{MLE}} + t_{\alpha/2} \text{SE}(\theta)$$

Deep connections to least squares

Minimizing this:

$$-\log(L(y; \beta_0, \beta_1, \sigma)) = -\sum_{i=1}^n \log(p(y_i; \beta_0, \beta_1, \sigma))$$

Is almost the same as minimizing this:

$$\sum_{i=1}^n (y_i - \hat{y}_i)^2$$

Comparing our estimates

Residual sum of squares

Variation in y **around the line**

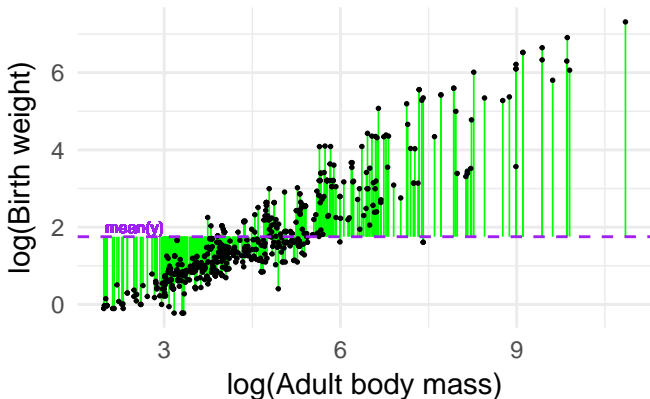
$$SS_R = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$



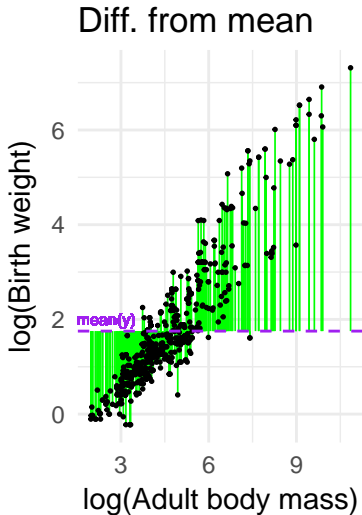
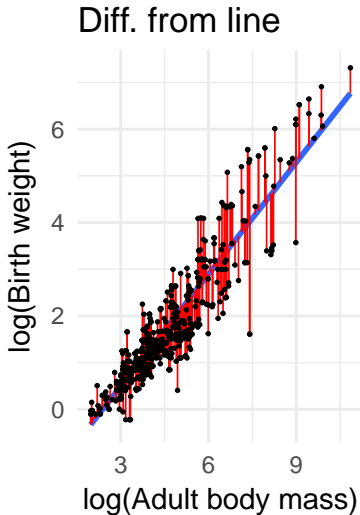
Total sum of squares

Variation in y **relative to the sample mean**

$$SS_T = \sum_{i=1}^n (y_i - \bar{y})^2, \text{ where } \bar{y} = \frac{\sum_{i=1}^n y_i}{n}$$



Residual vs. total sum of squares



Residual vs. total sum of squares

$$SS_R = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

$$SS_T = \sum_{i=1}^n (y_i - \bar{y})^2$$

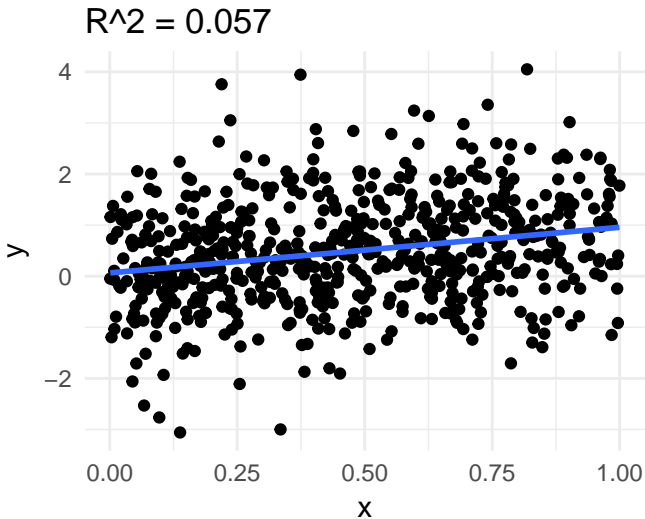
*demo

How much can our model explain?

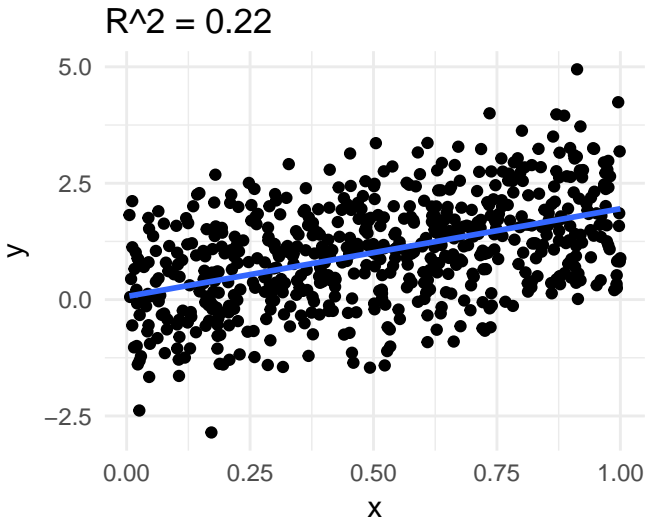
Coefficient of determination

$$R^2 = 1 - \frac{SS_R}{SS_T}$$

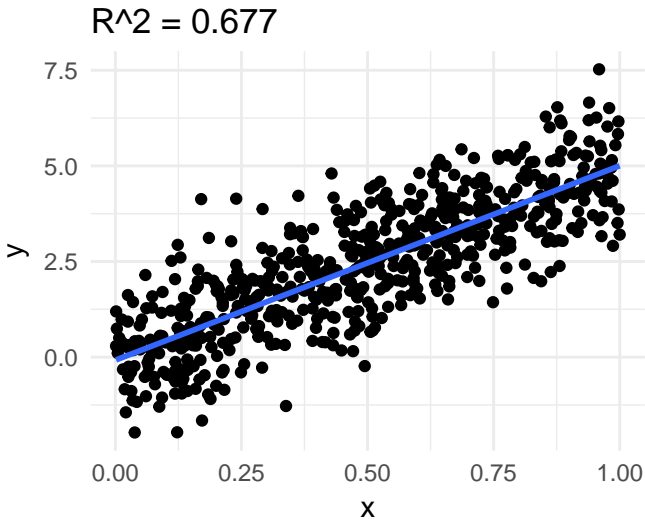
Visualizing R^2



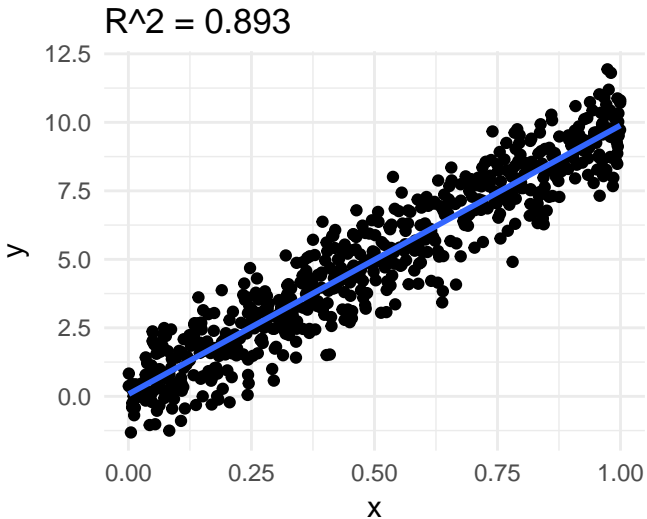
Visualizing R^2



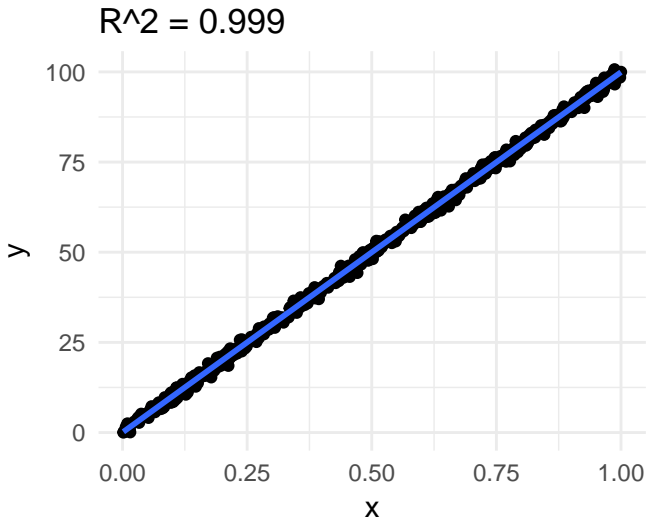
Visualizing R^2



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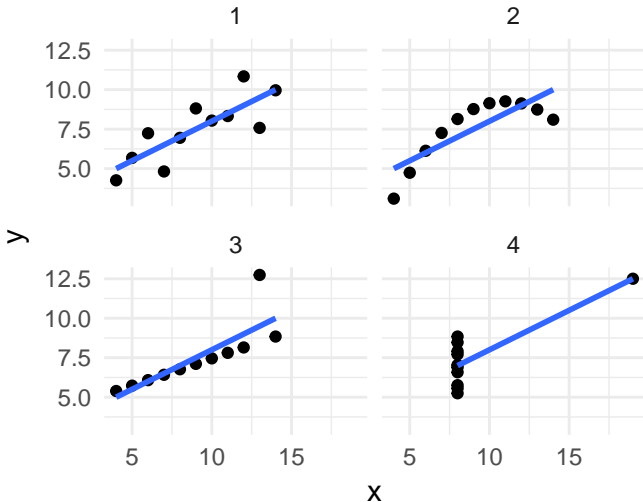


Visualizing R^2



Beware R^2

$R^2 = 0.666$ for each of these



Computing R^2 demo

Summary: R^2

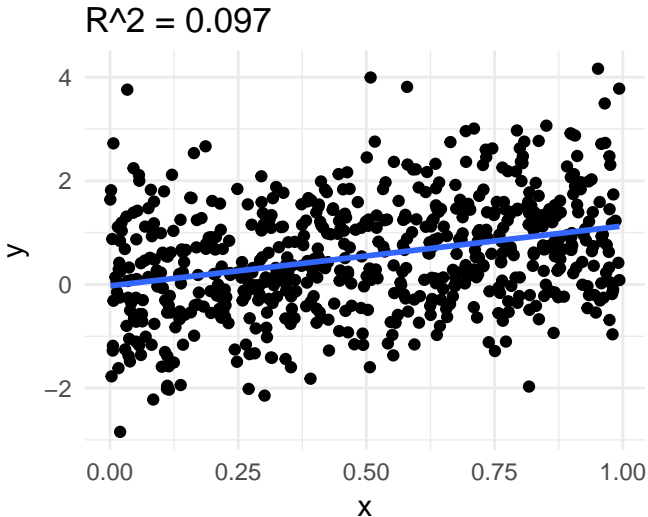
$$R^2 = 1 - \frac{SS_R}{SS_T}$$

- ▶ how well the line approximates the data
- ▶ bounded between 0 and 1

Problems with R^2

1. Sensitive to the range of x

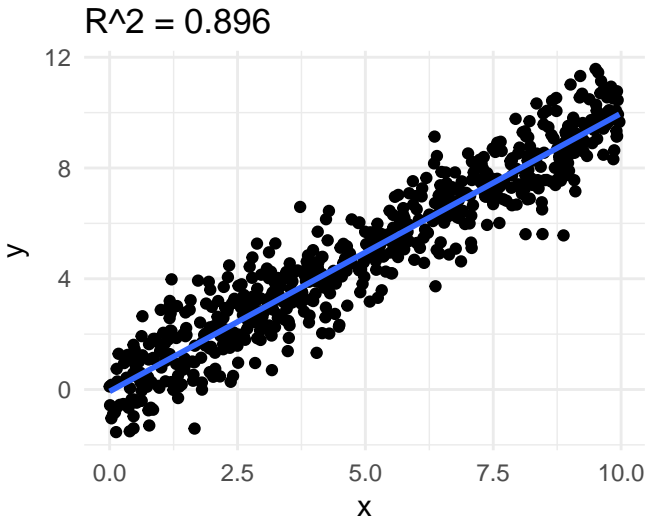
$$y \sim \text{Normal}(0 + x, 1)$$



Problems with R^2

$y \sim \text{Normal}(0 + x, 1)$

1. Sensitive to the range of x



Problems with R^2

1. Sensitive to the range of x
 2. Does not measure prediction error
- ▶ only measures fit to the **training** data

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Problems with R^2

1. Sensitive to the range of x
 2. Does not measure prediction error
 3. Not comparable among models with different y
 4. We get the same R^2 by regressing x on y
 5. Can calculate R^2 for silly models
- e.g., <http://tylervigen.com/spurious-correlations>

Recap for today

1. Quantifying uncertainty in parameters

- ▶ reviewed Hessians, standard error, and confidence intervals

2. Introducing R^2 (coefficient of determination)

- ▶ how to calculate from sums of squares
- ▶ some shortcomings