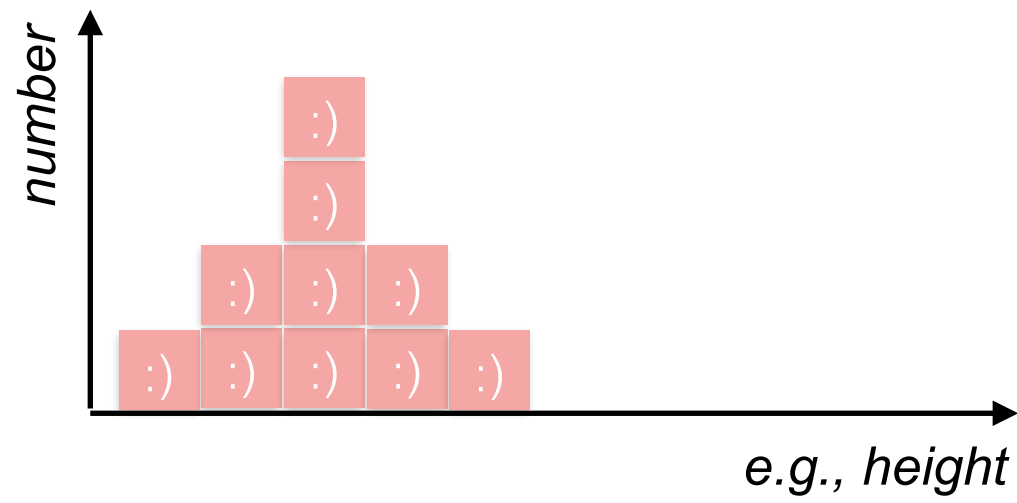


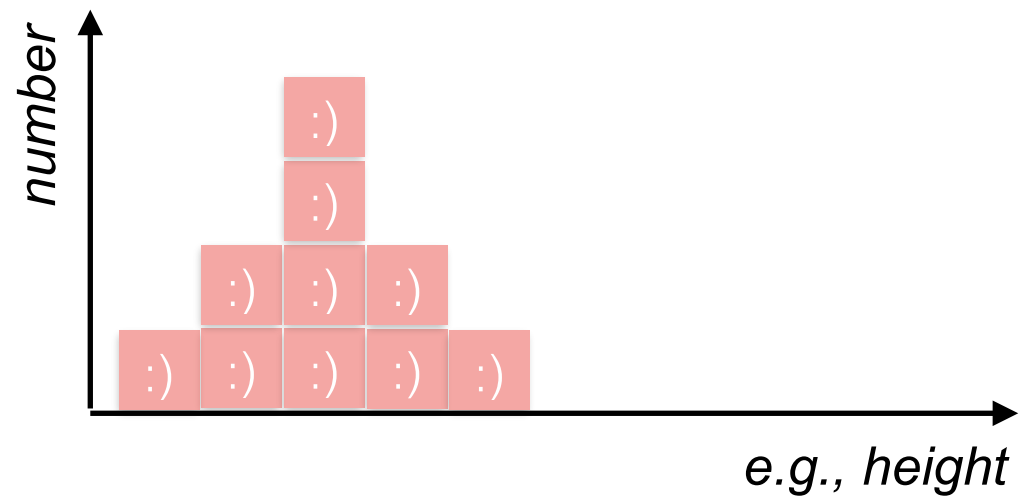
# Model evaluation and comparison

C. Jessica E. Metcalf  
[cmetcalf@princeton.edu](mailto:cmetcalf@princeton.edu)

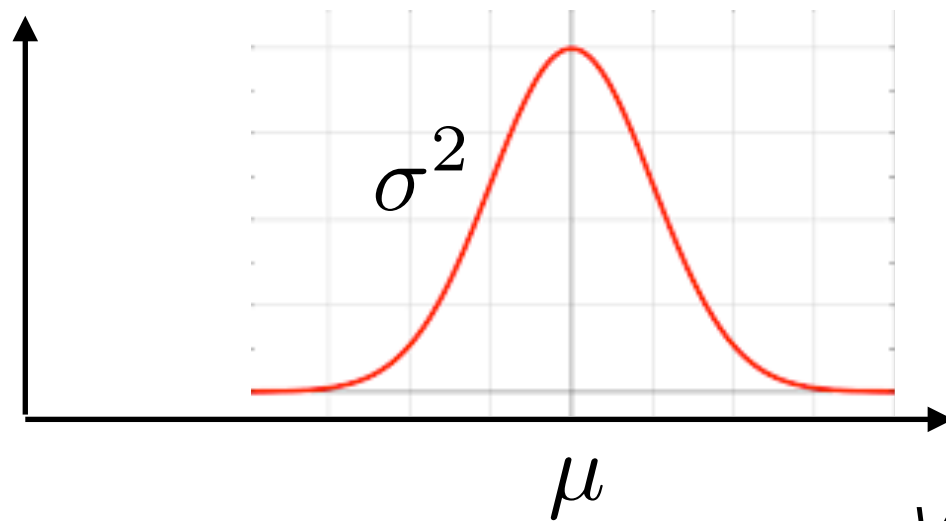
# Data



# Data



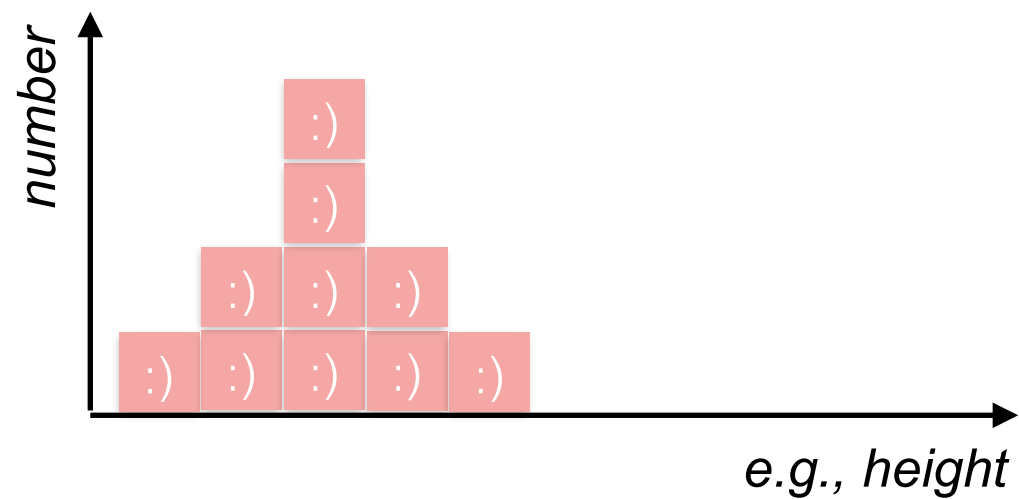
# Likelihood



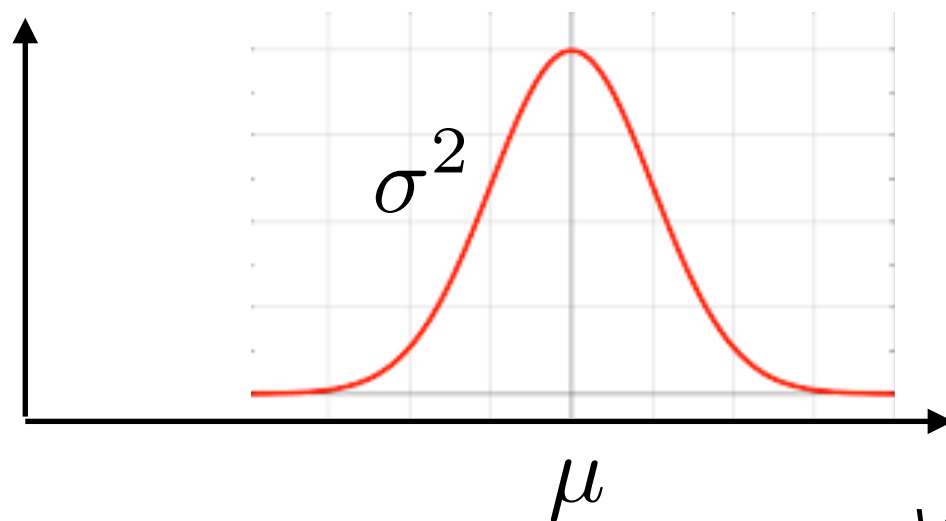
~ the 'probability of seeing the data' given the chosen parameters  
...each individual in the data has a corresponding likelihood... multiply them...

Very low likelihood.

# Data

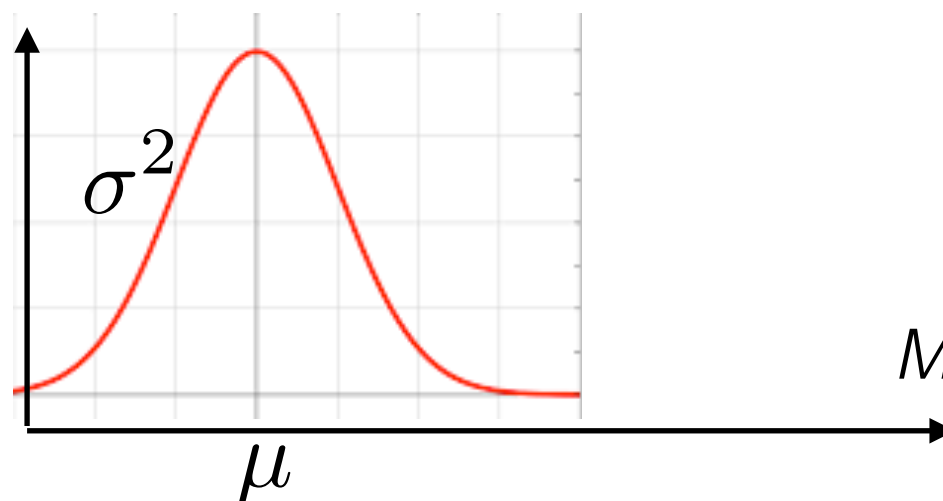


## Likelihood



~ the 'probability of seeing the data' given the chosen parameters  
...each individual in the data has a corresponding likelihood... multiply them...

Very low likelihood.



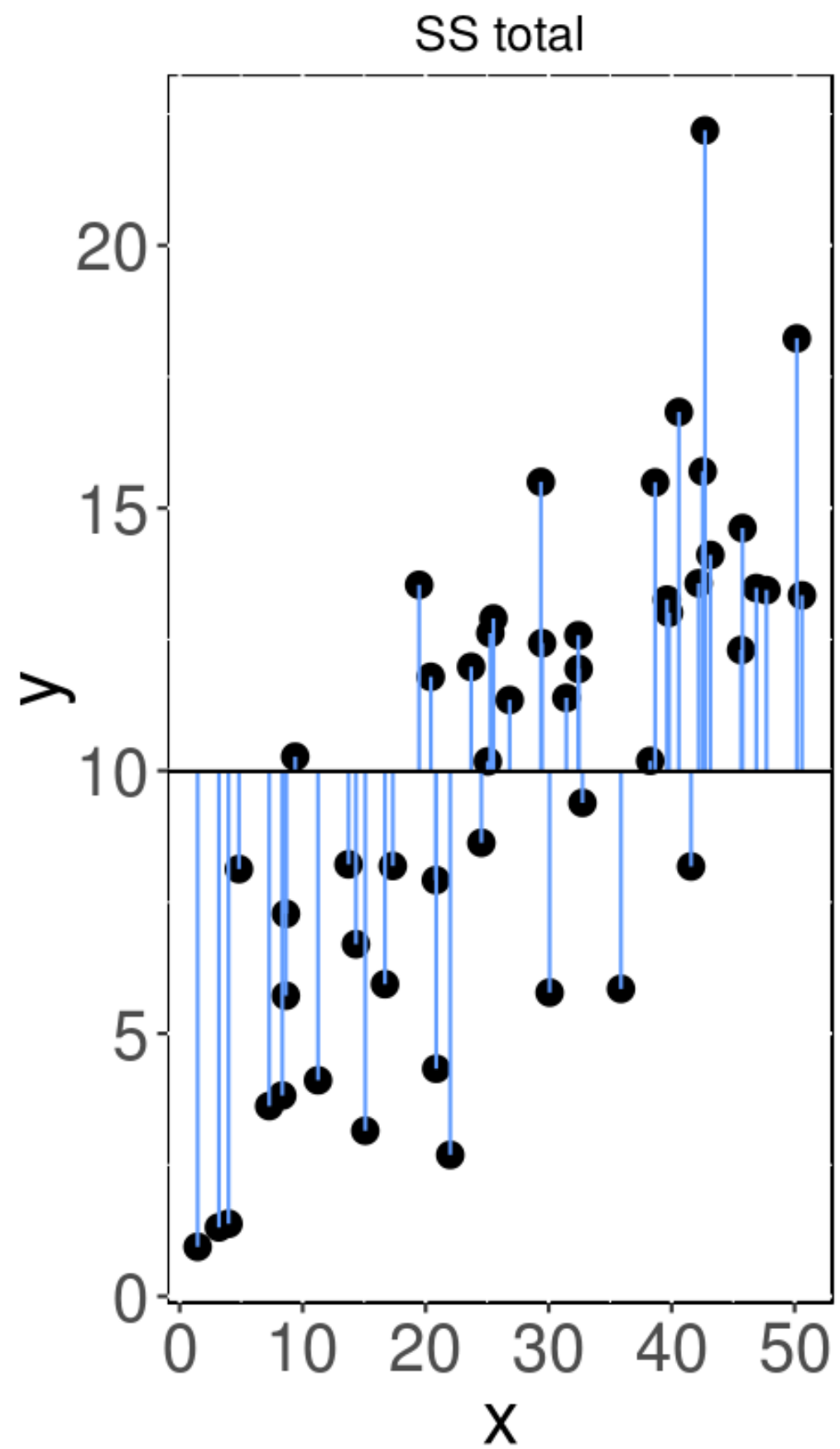
Maximum likelihood

What  $r^2$  tells us

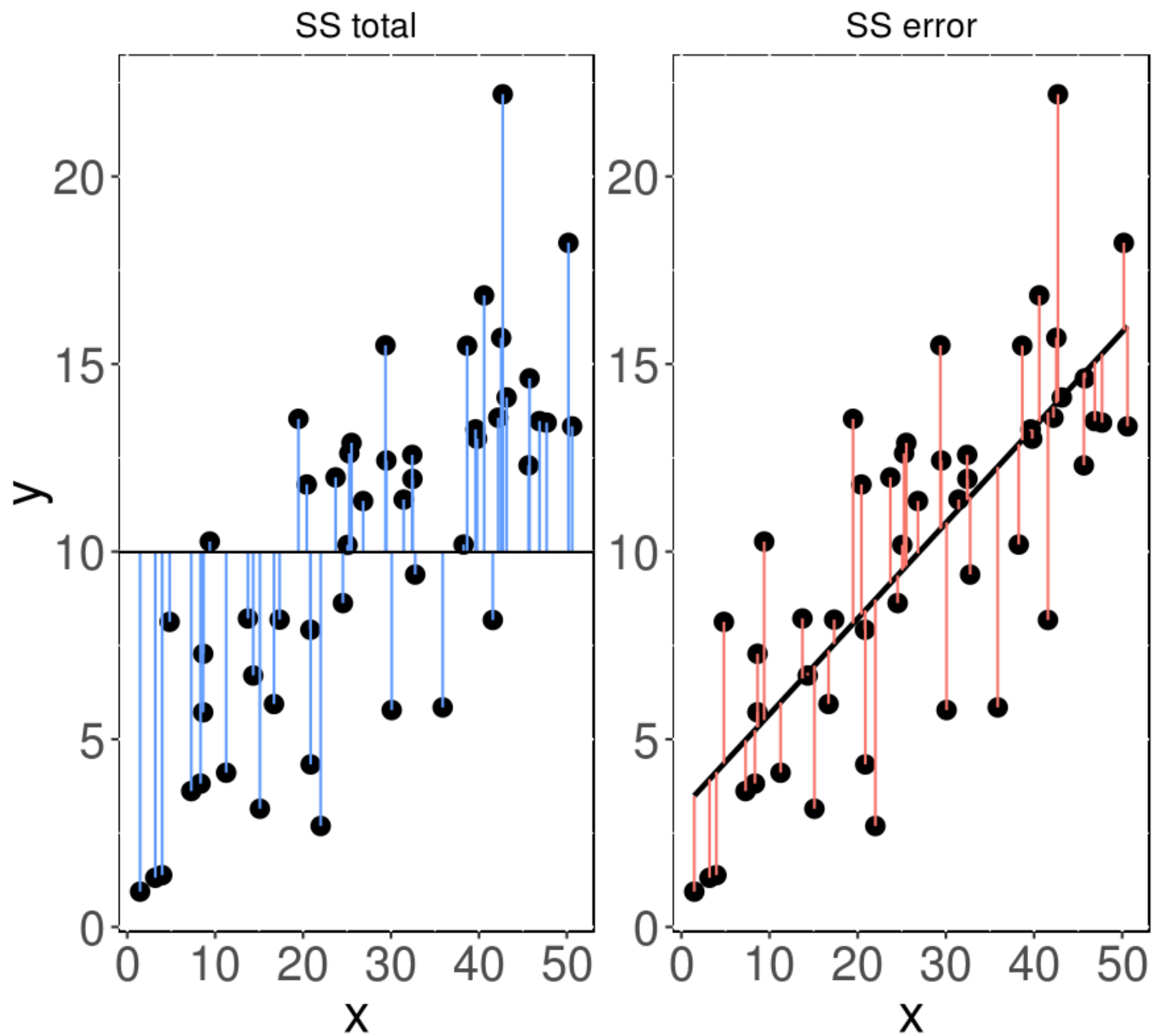
**Parsimony**, under- and over-fitting, and AIC

**Sensitivity analysis**

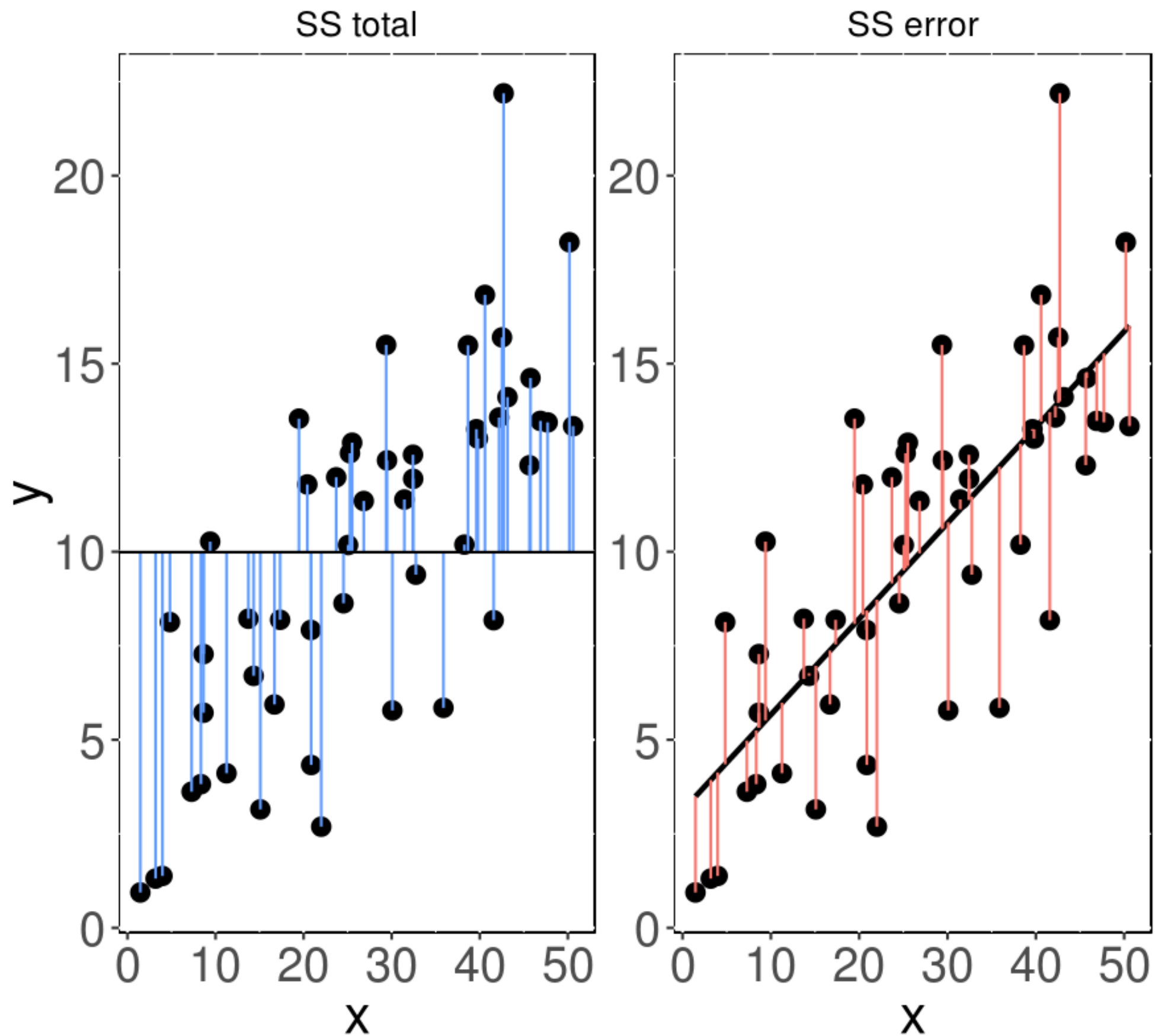
# Definition $r^2$



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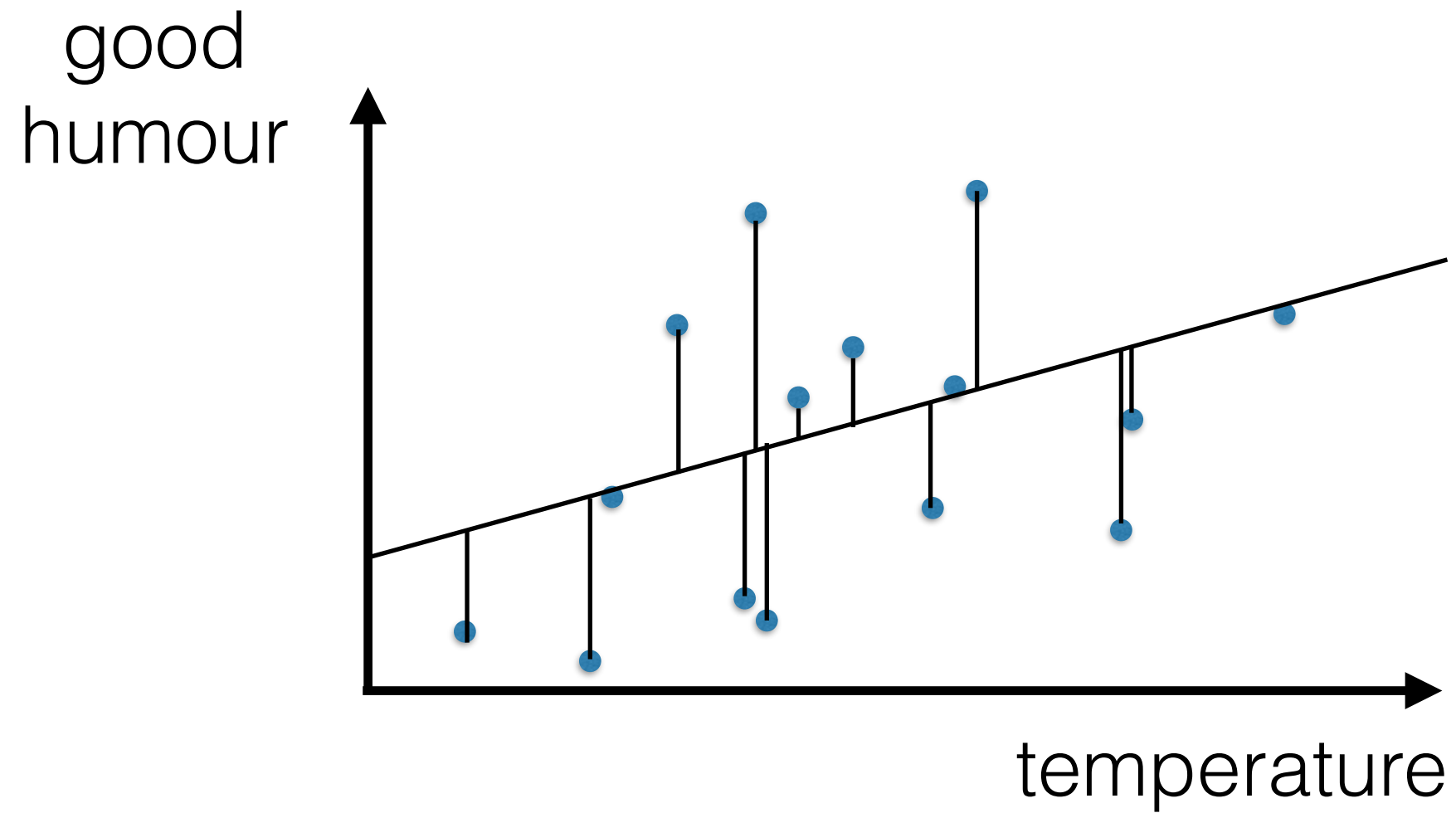
# Definition $r^2$



$$R^2 = 1 - \frac{SSE_p}{SST}$$

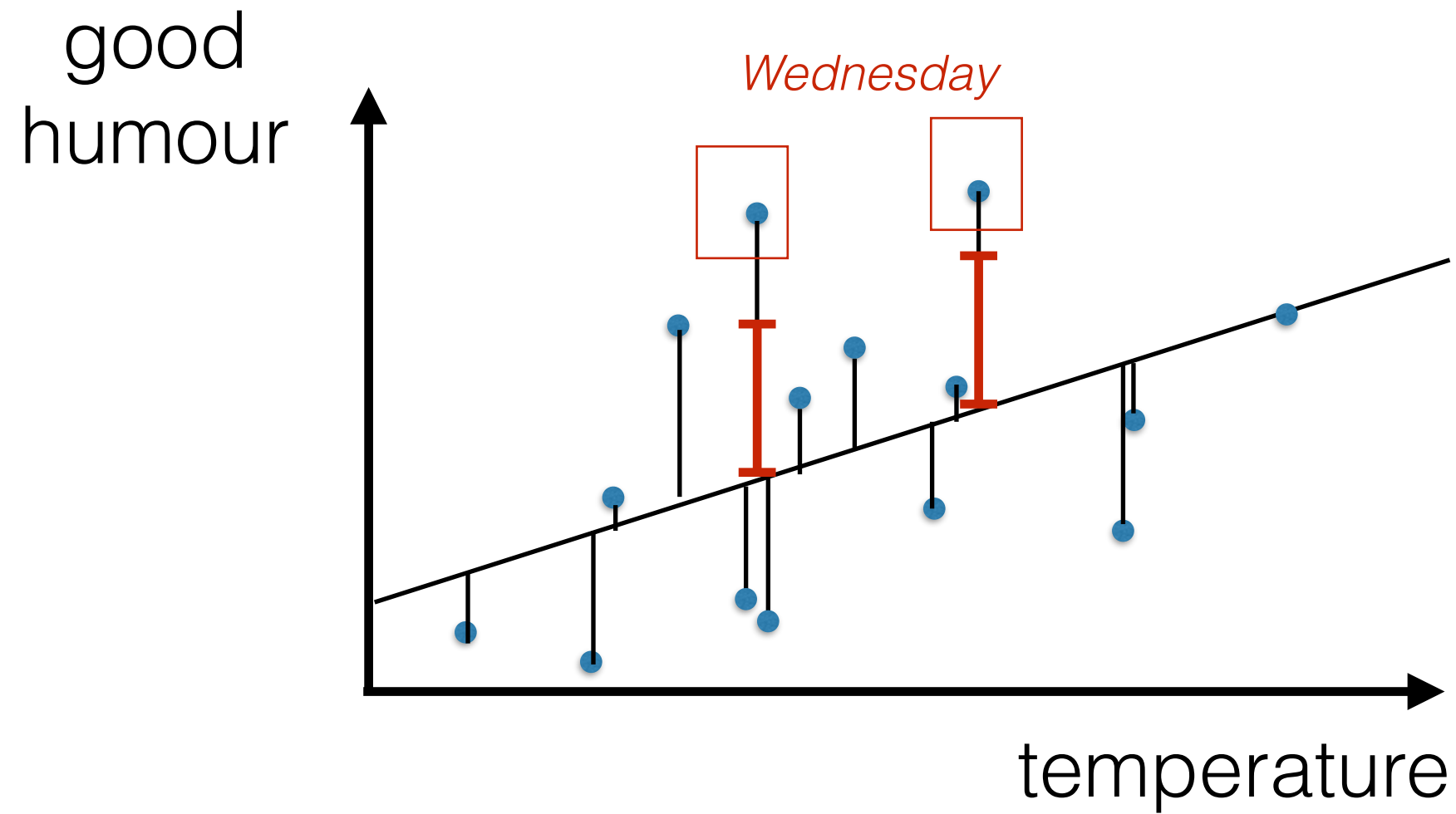


# Adding covariates and $R^2$



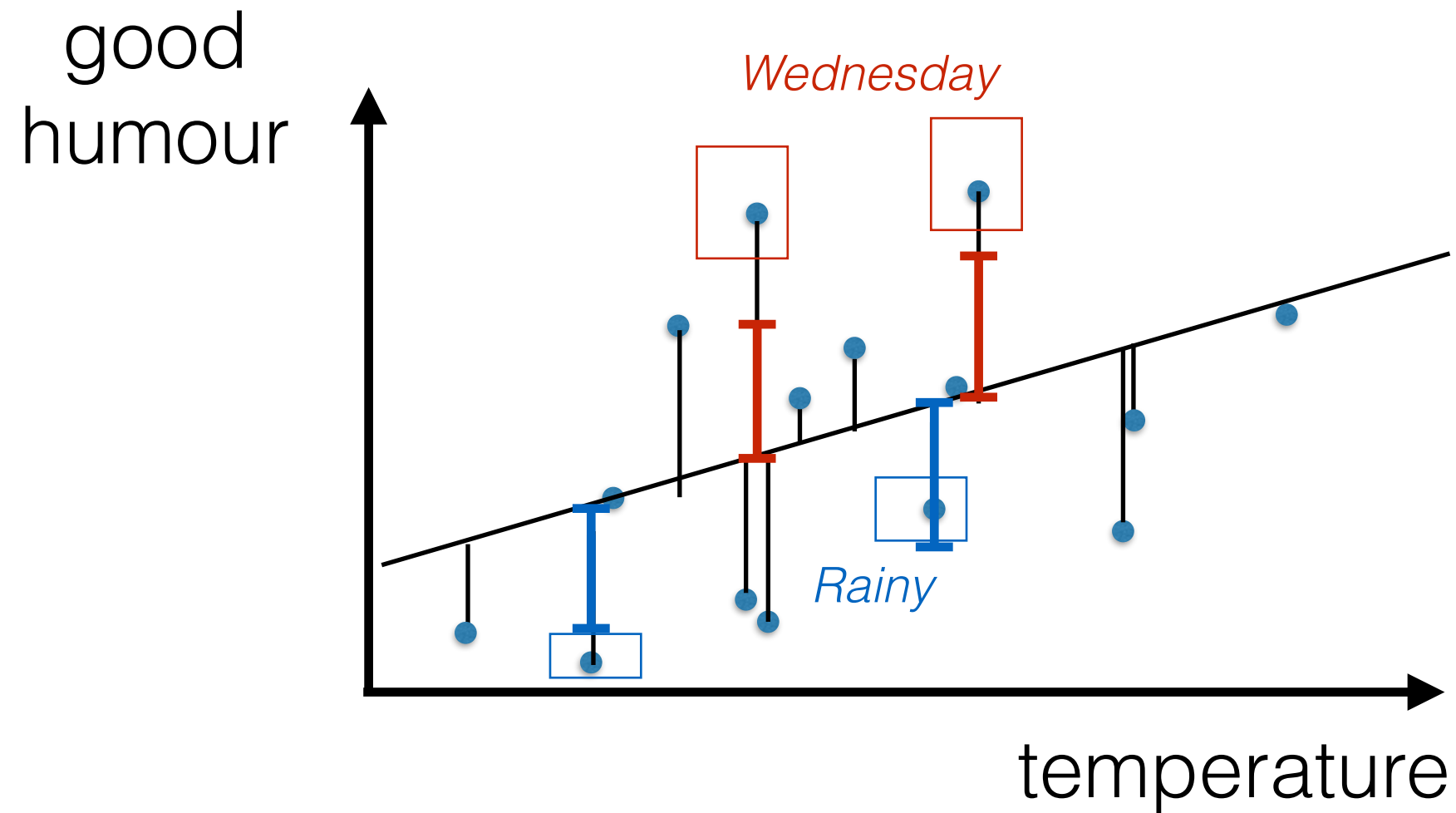
$$\text{humour} = b_0 + b_1 \text{temperature} + \text{Error}$$

# Adding covariates and $R^2$



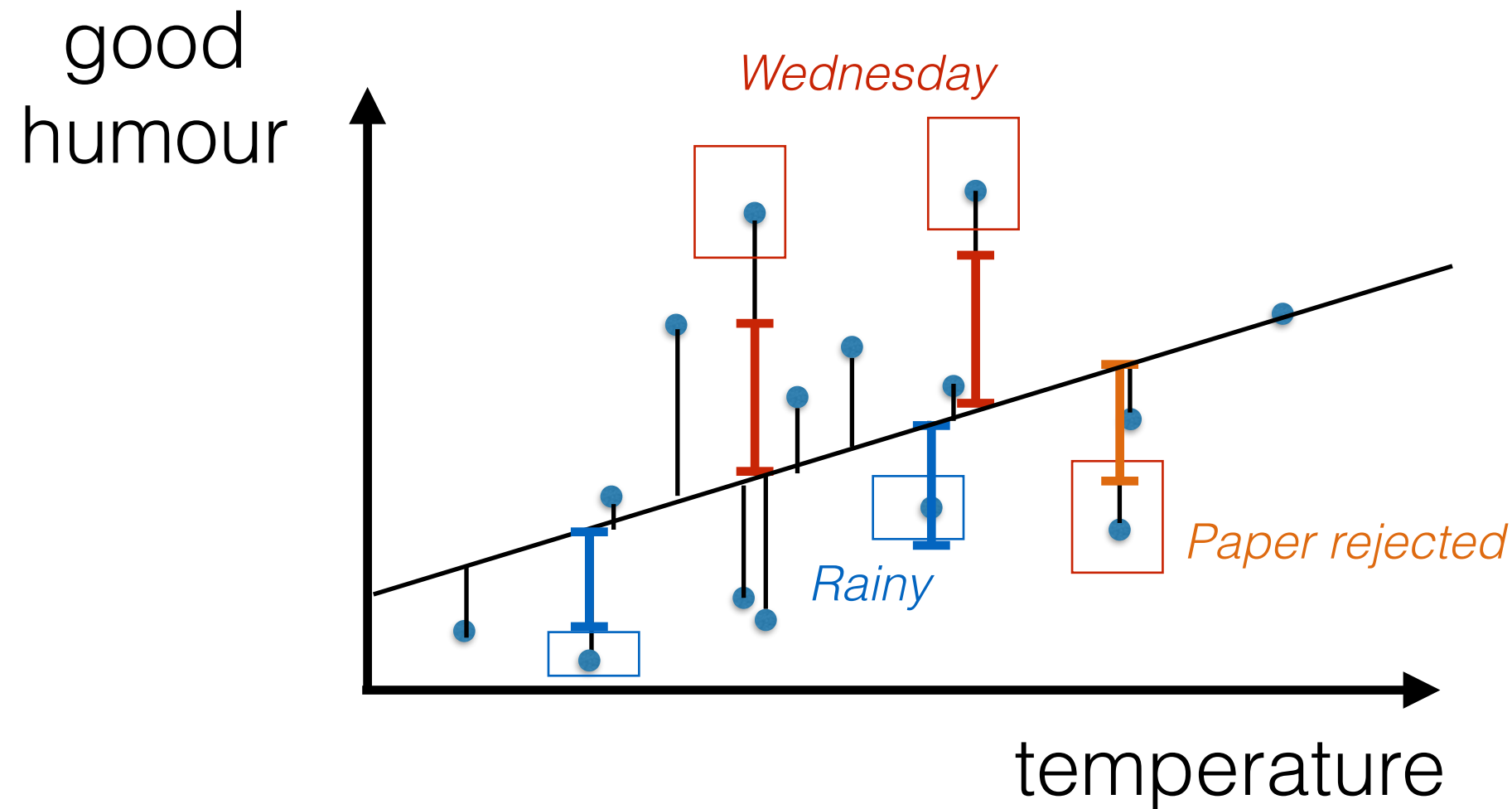
$$\text{humour} = b_0 + b_1\text{temperature} + b_2\text{Wednesday} + \text{Error}$$

# Adding covariates and R<sup>2</sup>



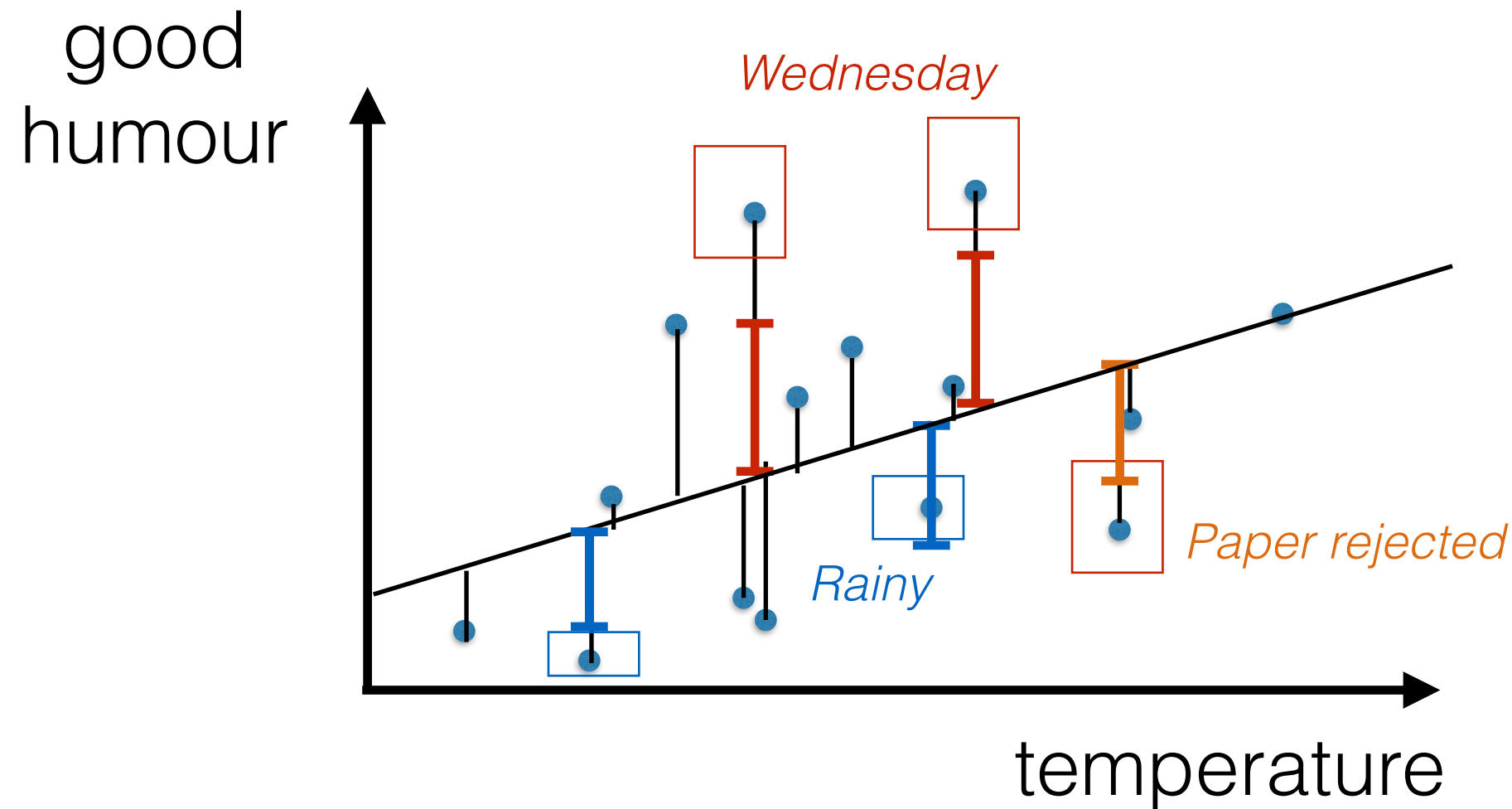
$$\text{humour} = b_0 + b_1\text{temperature} + b_2\text{Wednesday} + b_3\text{rain} + \text{Error}$$

# Adding covariates and R<sup>2</sup>



$$\text{humour} = b_0 + b_1\text{temperature} + b_2\text{Wednesday} + b_3\text{rain} + b_4\text{rejection} + \text{Error}$$

# Adding covariates and $R^2$



Adding covariates almost always increases the  $R^2$  - so a key question is when to stop.

What  $r^2$  tells us

**Parsimony**, under- and over-fitting, and AIC

**Sensitivity analysis**

# Parsimony, or Occam's razor

William of Occam, 1288-1348

All else being equal, the simplest explanation is the best.

*... model with fewest parameters is the best - as long as it can actually predict reasonably!*



# Interpreting covariates

$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

but if  $x_1$  is very similar to  $x_2$

$$y \sim \alpha + (\beta_1 + \beta_2)x_1 + \epsilon$$

so?



# Interpreting covariates

$$y = \alpha + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

but if  $x_1$  is very similar to  $x_2$

$$y \sim \alpha + (\beta_1 + \beta_2)x_1 + \epsilon$$

so?

hard to interpret *mechanistically*  
hard to extrapolate across *contexts*

A good model should be:

- Parsimonious
- Conform to data
- Balance conformity to data and parsimony

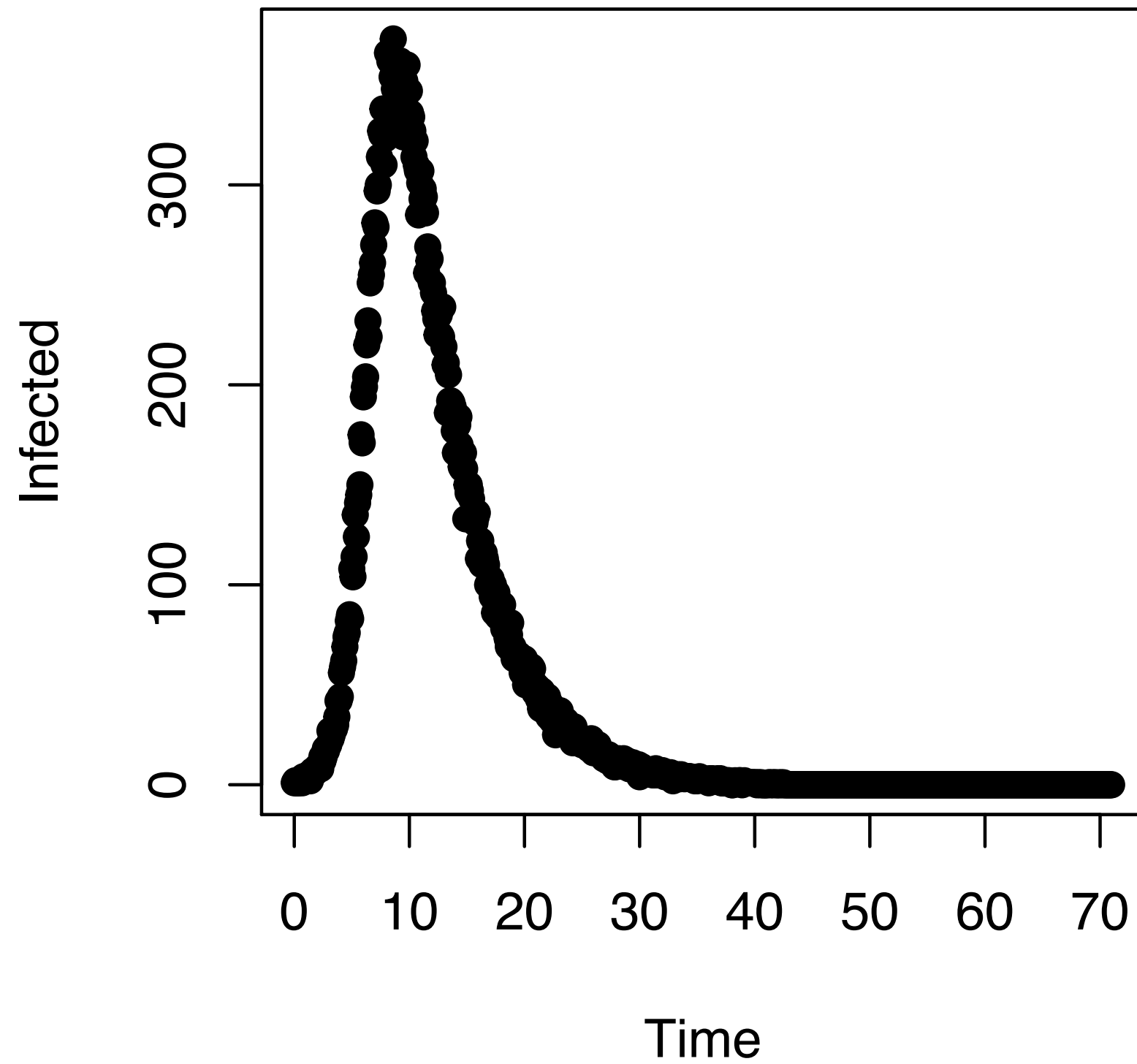
# A good model should be:

- Parsimonious
- Conform to data
- Balance conformity to data and parsimony
- Not under-fitted - introduces *biases*  
(=missing key variables or effects)
- Not over-fitted - introduces *high variability*  
(=unnecessarily complex)

A good model should be:

- Parsimonious
- Conform to data
- Balance conformity to data and parsimony
- Not under-fitted - introduces *biases*  
(=missing key variables or effects)
- Not over-fitted - introduces *high variability*  
(=unnecessarily complex)
- Easily generalizable

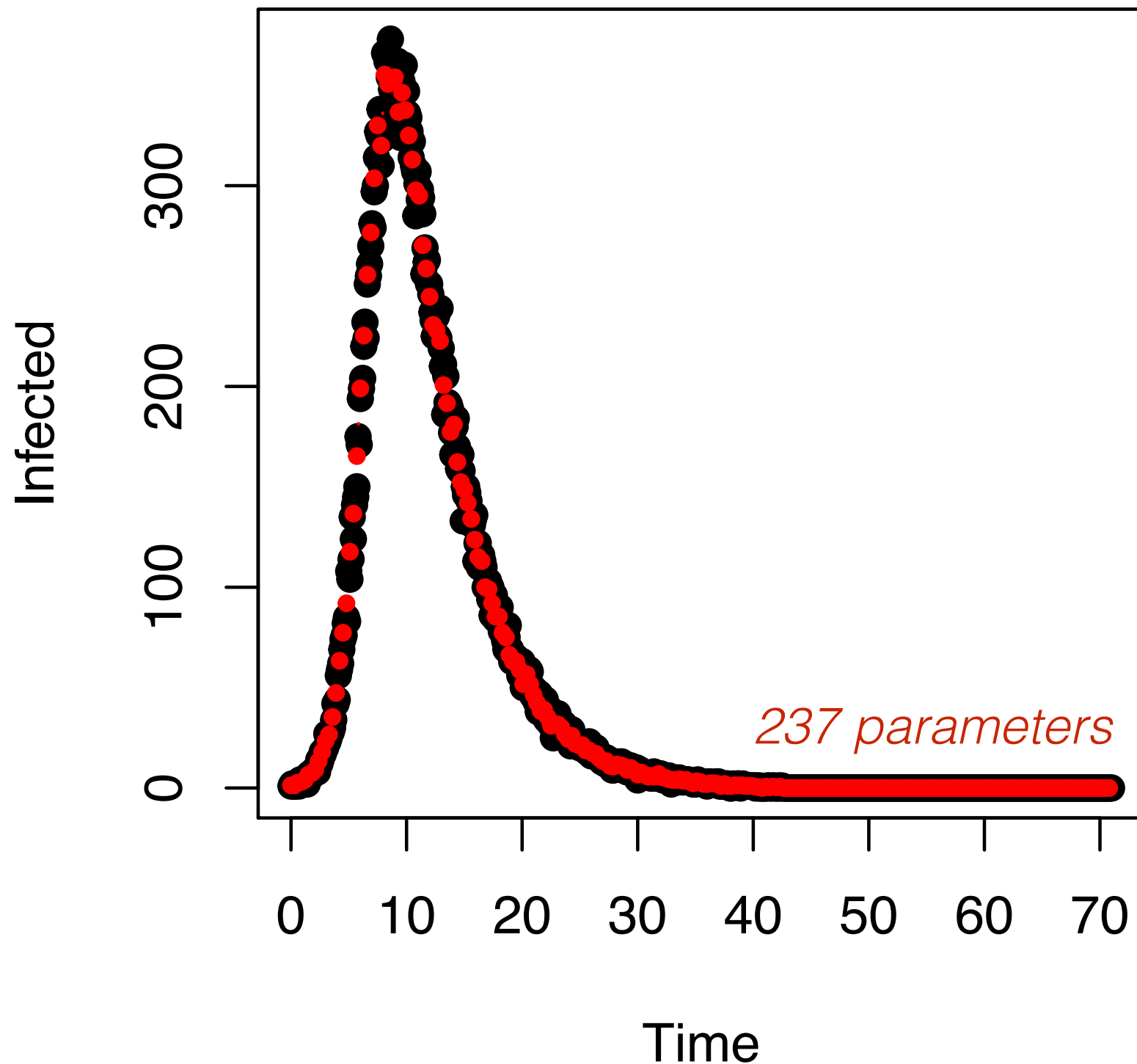
# An outbreak



# Over-fitting

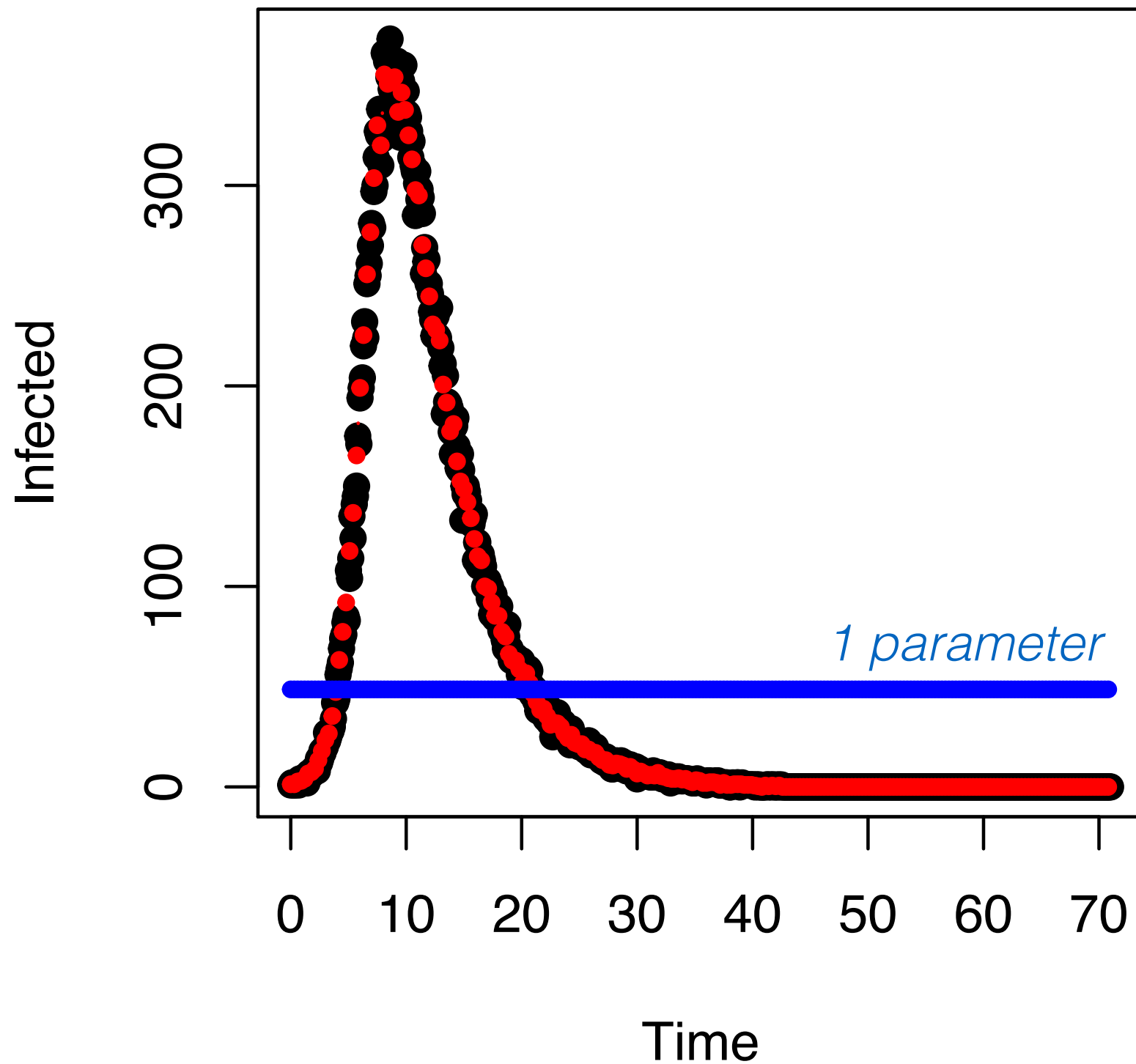
Here, get the mean per three data-points.

In the extremes, one parameter per data-point.



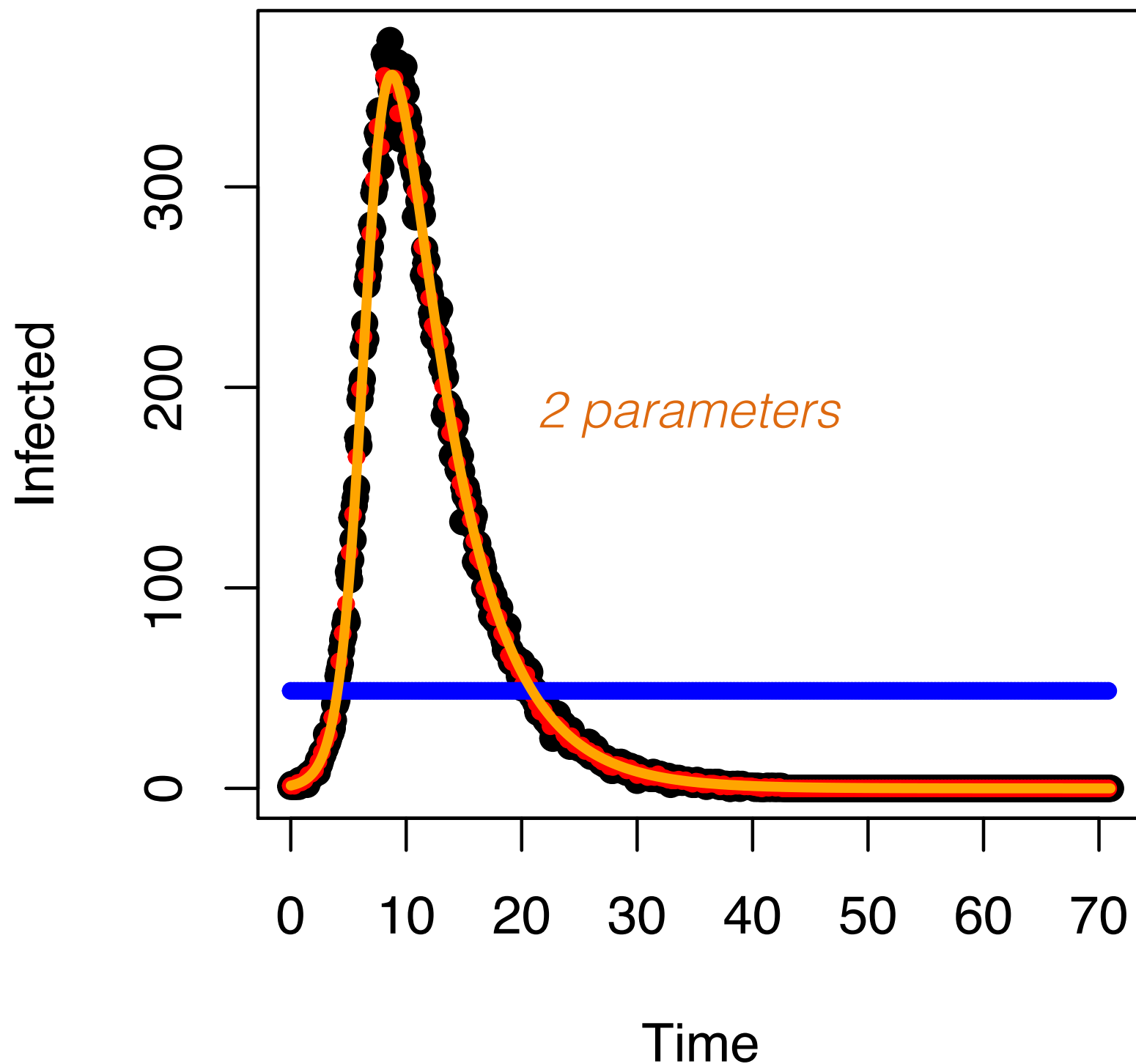
# Under-fitting

Here, one mean for all data points



# Likelihood fitting

Here, a mechanistic (SI) model, i.e., two parameters.



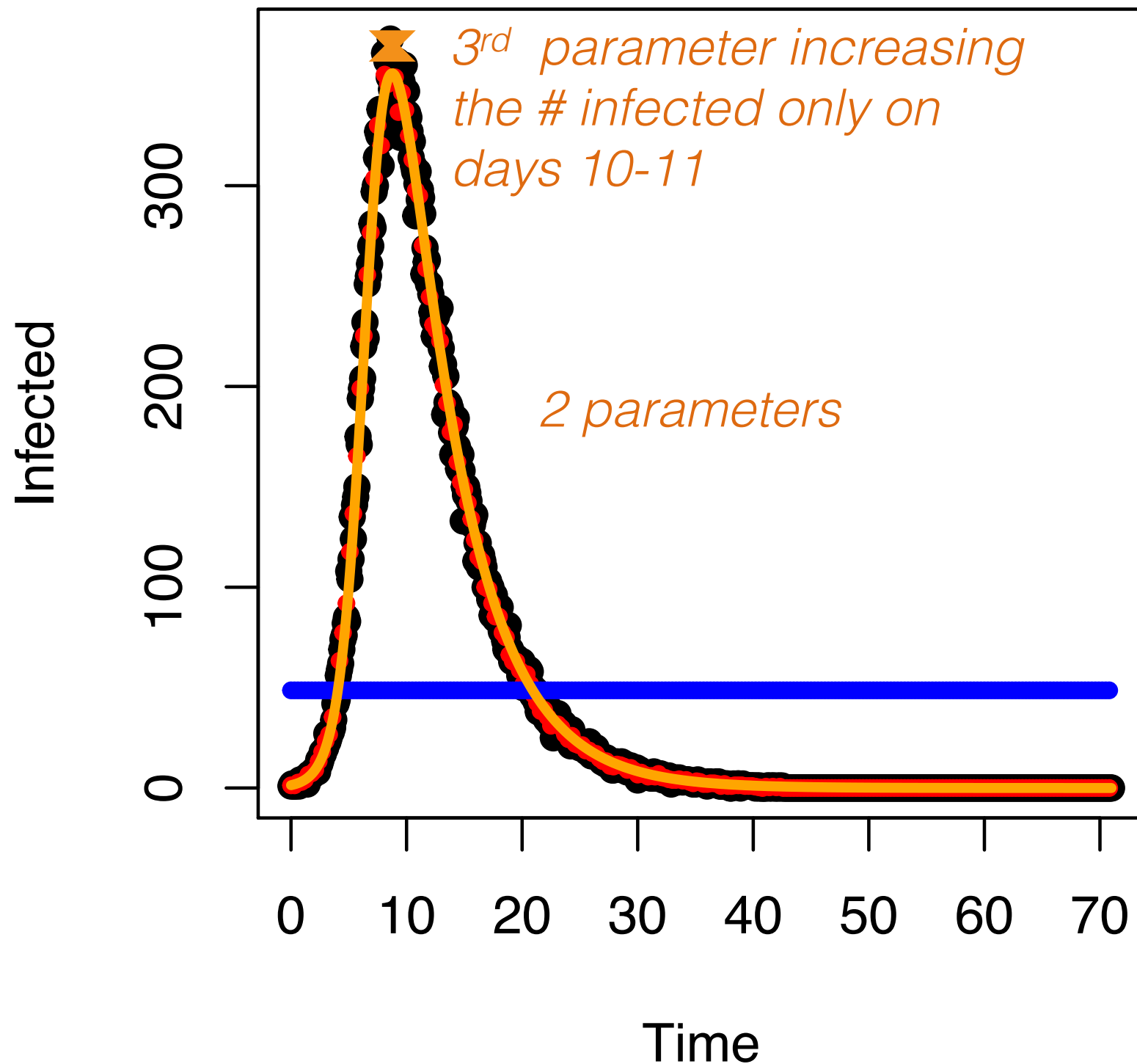
$$\frac{dS(t)}{dt} = -\beta S(t)I(t)$$

$$\frac{dI(t)}{dt} = \beta S(t)I(t) - \gamma I(t)$$



# Likelihood fitting

Here, a mechanistic (SI) model, i.e., two parameters.



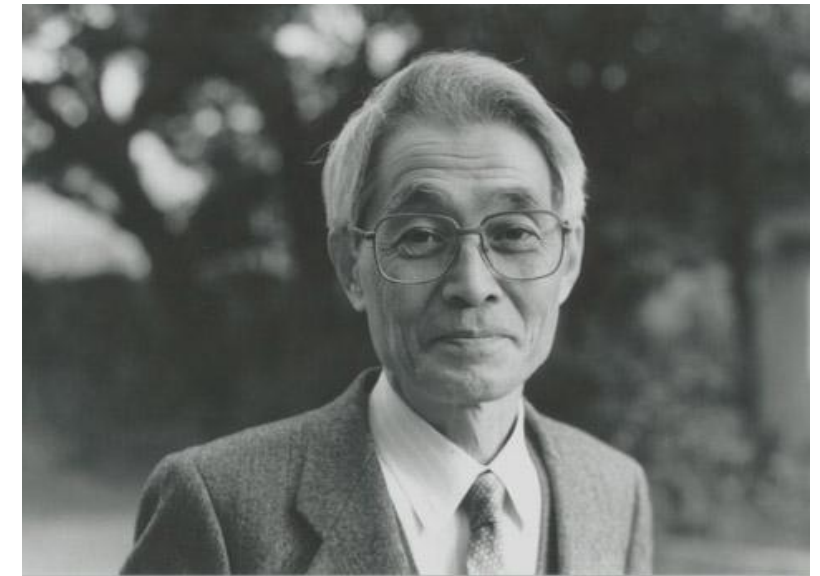
$$\frac{dS(t)}{dt} = -\beta S(t)I(t)$$

$$\frac{dI(t)}{dt} = \beta S(t)I(t) - \gamma I(t)$$

# Akaike's Information Criteria

Hirotsugu Akaike, 1927-2009.

In the 1970s he used **information theory** to build a numerical equivalent of Occam's razor.



$$AIC = 2K - 2\log L$$

K is the number of **parameters** ('penalty')

$\log L$  is the **log Likelihood** ('goodness of fit')

The model with **the lowest AIC is the preferred.**

# Akaike's Information Criteria

## **Advantages:**

Does not require one candidate model to be correct  
Can compare nested and un-nested models  
Can compare models of different families of probability distributions

## **Disadvantages:**

Needs reasonable amounts of data

What  $r^2$  tells us

**Parsimony**, under- and over-fitting, and AIC

**Sensitivity analysis**

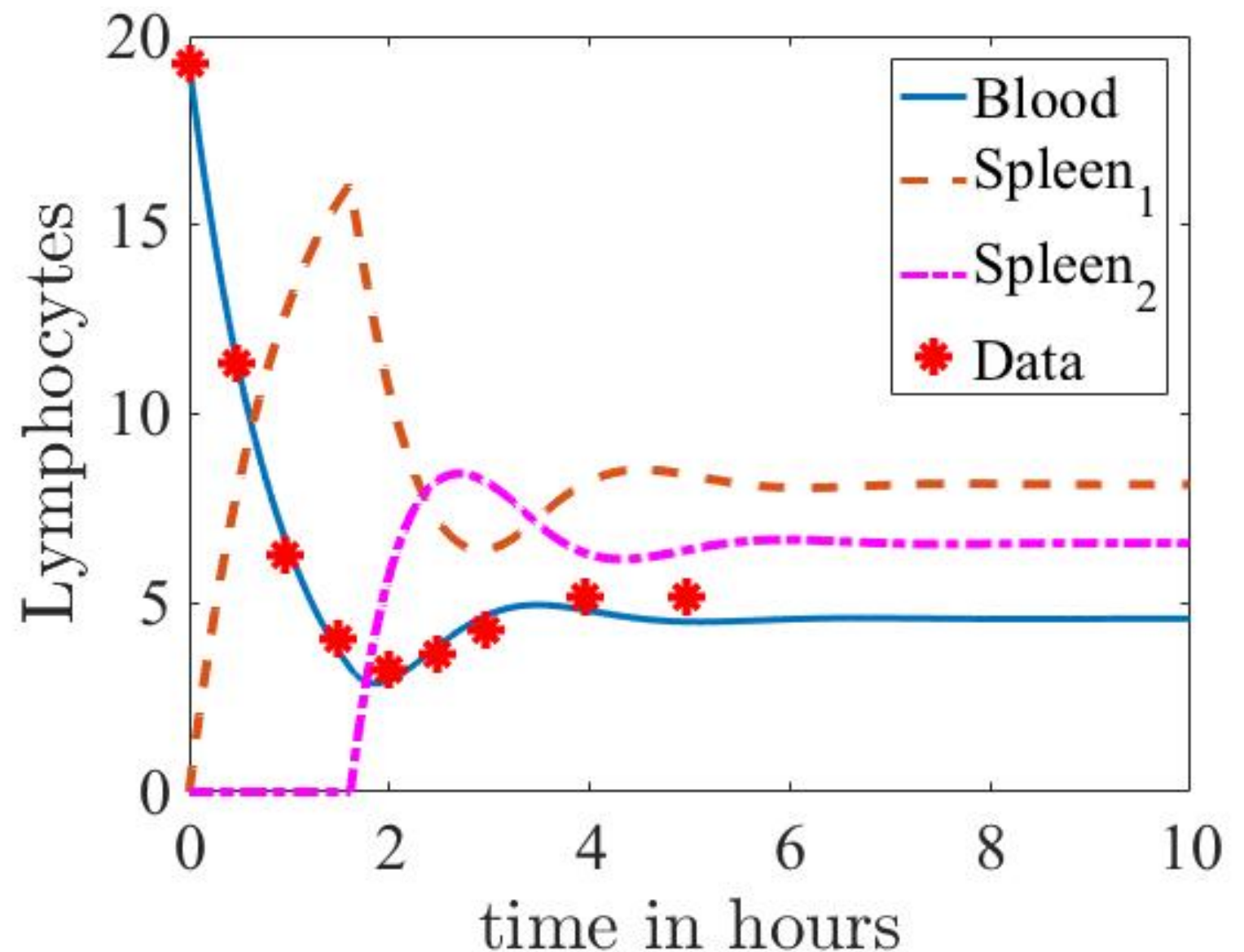
# Sensitivity analysis

- Identifying parameters to which output is **sensitive**
- Identifying **intervention** parameters
- Testing **robustness** of model **predictions**
- Explore **uncertainty** in parameters
- Model **simplification**
- Explore **associations** between parameters

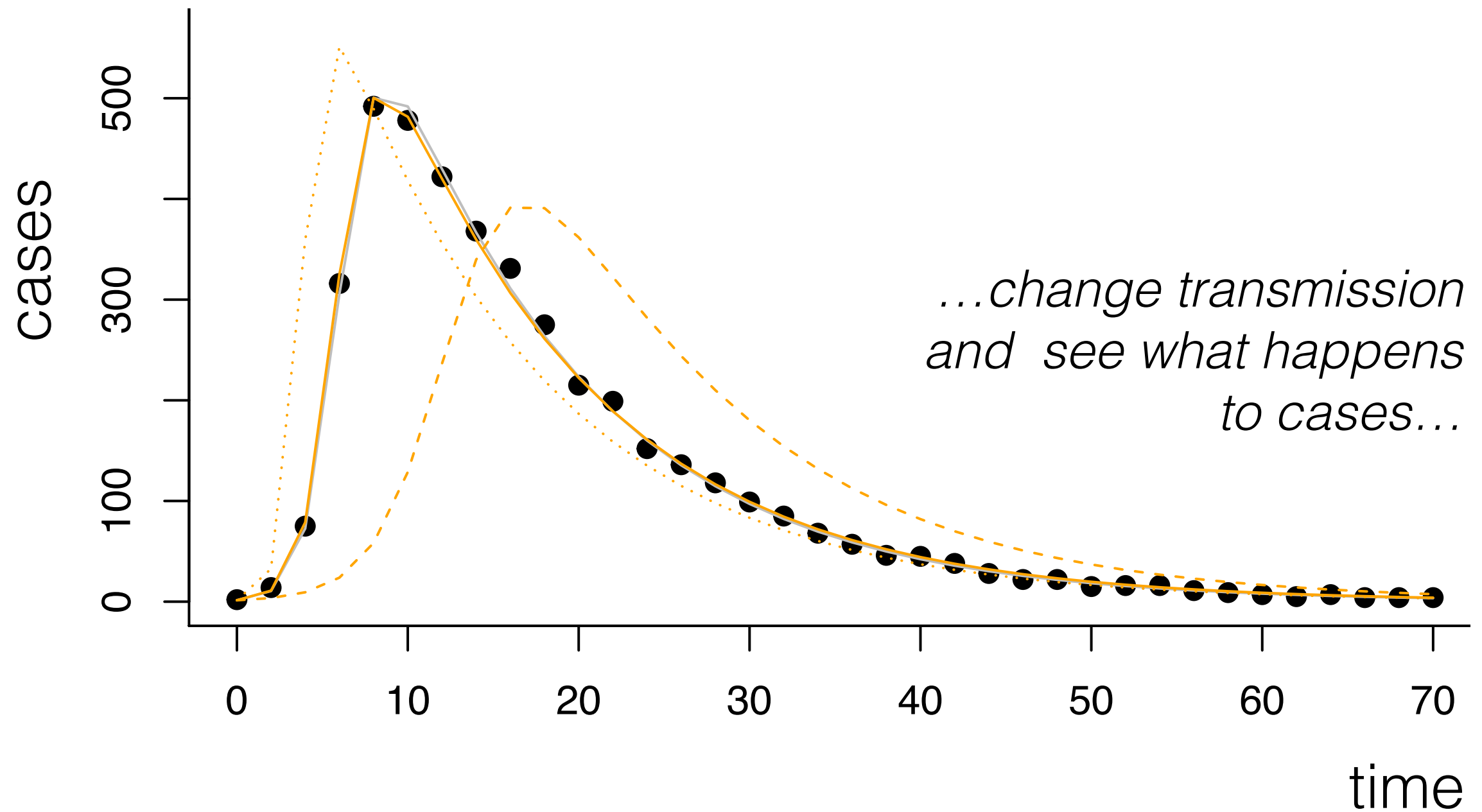
# Example: lymphocyte migration between blood & spleen

$$\begin{aligned}\frac{dB}{dt} &= p_3 S_2 - p_1 B \\ \frac{dS_1}{dt} &= p_1 B - p_2 S_1 \\ \frac{dS_2}{dt} &= p_2 S_1 - p_3 S_2\end{aligned}$$

$$\begin{aligned}p_1 &= 1.0967 \\ p_2 &= 0.7638 \\ p_3 &= 0.7638\end{aligned}$$



# Example: changing the magnitude of transmission



# Global sensitivity analysis

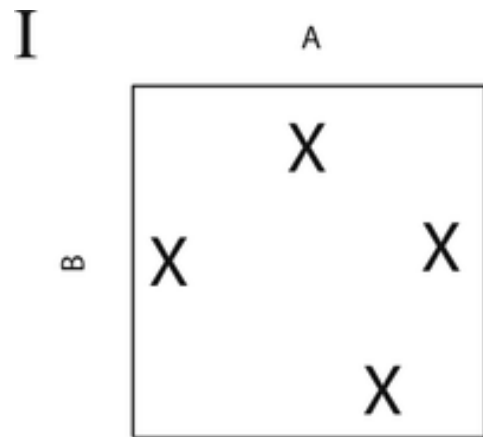
Evaluate impact of values across the full range possible for all parameters.



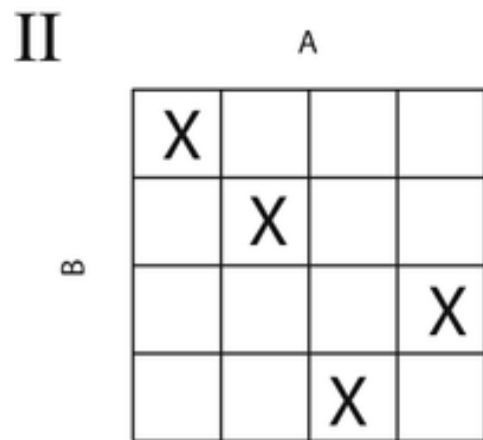


# Global sensitivity analysis

Evaluate impact of values across the full range possible for all parameters.



Random sampling



Latin hypercube sampling

Decide on # sample points; then get one sample in each row & column

# Conclusions

A good model should balance **conformity to data** and **parsimony**

**R<sup>2</sup>** tells us how well models fit ('conformity'), but increases with the number of covariates

Metrics such as **AIC** provide a means to evaluate model parsimony

**Sensitivity analysis** is key to understanding the larger context of parameters (generalizability, etc) and tools exist to do it efficiently (LHS)

# Conclusions

Un bon modèle devrait équilibrer **conformité aux données, et la parcimonie**

**R<sup>2</sup>** nous décrit la capture des données - mais augmente toujours avec le nombre de covariés

Des metrics tel le **AIC** nous donne le moyen d'évaluer la parcimonie d'un modèle relatif a d'autres modèles.

L'analyse de la **sensibilité** est clef pour comprendre les paramètres dans un context plus large (si ils décrivent le cas general, etc) et des outils existent pour le faire efficacement.