INTRODUCTION TO MACHINE LEARNING

Regression: Simple and Linear

Regression Principle

PREDICTORS → REGRESSION → RESPONSE

Example

Shop Data: sales, competition, district size, ...

Data Analyst → **Relationship?**

- Predictors: competition, advertisement, ...
- Response: sales

Shopkeeper → **Predictions!**

Simple Linear Regression

- **Simple:** one *predictor* to model the *response*
- **Linear:** *approximately* linear relationship

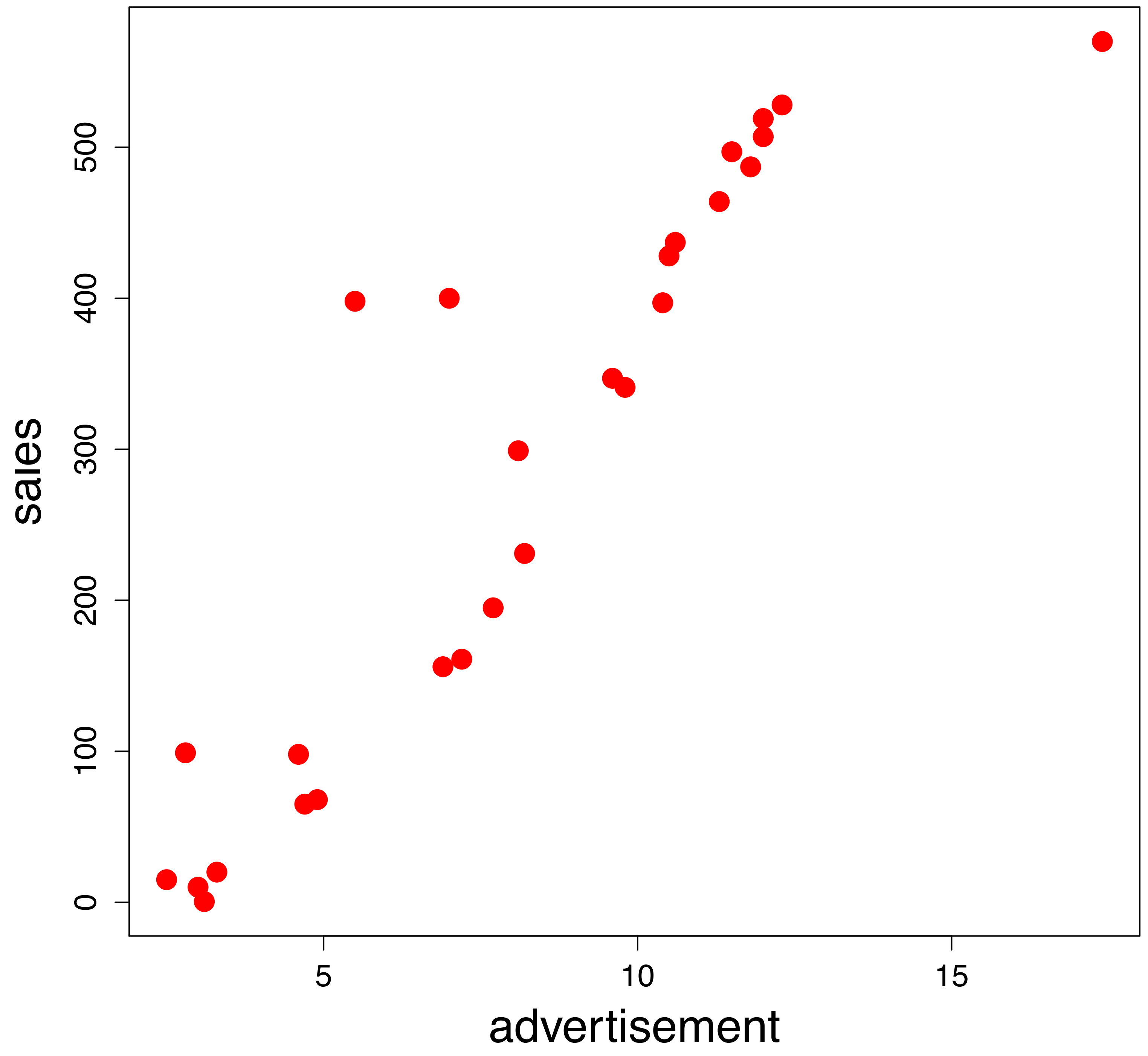
Linearity Plausible? → **Scatterplot!**

Example

- **Relationship:** advertisement → sales
- **Expectation: positively correlated**

Example

- **Observation**: upwards linear trend
- **First Step**: simple linear regression



Model

Fitting a **line**

$$Y = \beta_0 + X\beta_1 + \epsilon$$

- **Predictor:** X
- **Response:** Y
- **Statistical Error:** ϵ
- **Intercept:** β_0
- **Slope:** β_1

Estimating Coefficients

$$\mathrm{res}_i = \underset{\uparrow}{y_i} - (\beta_0 + \underset{\uparrow}{\beta_1} x_i)$$

← **Residuals**

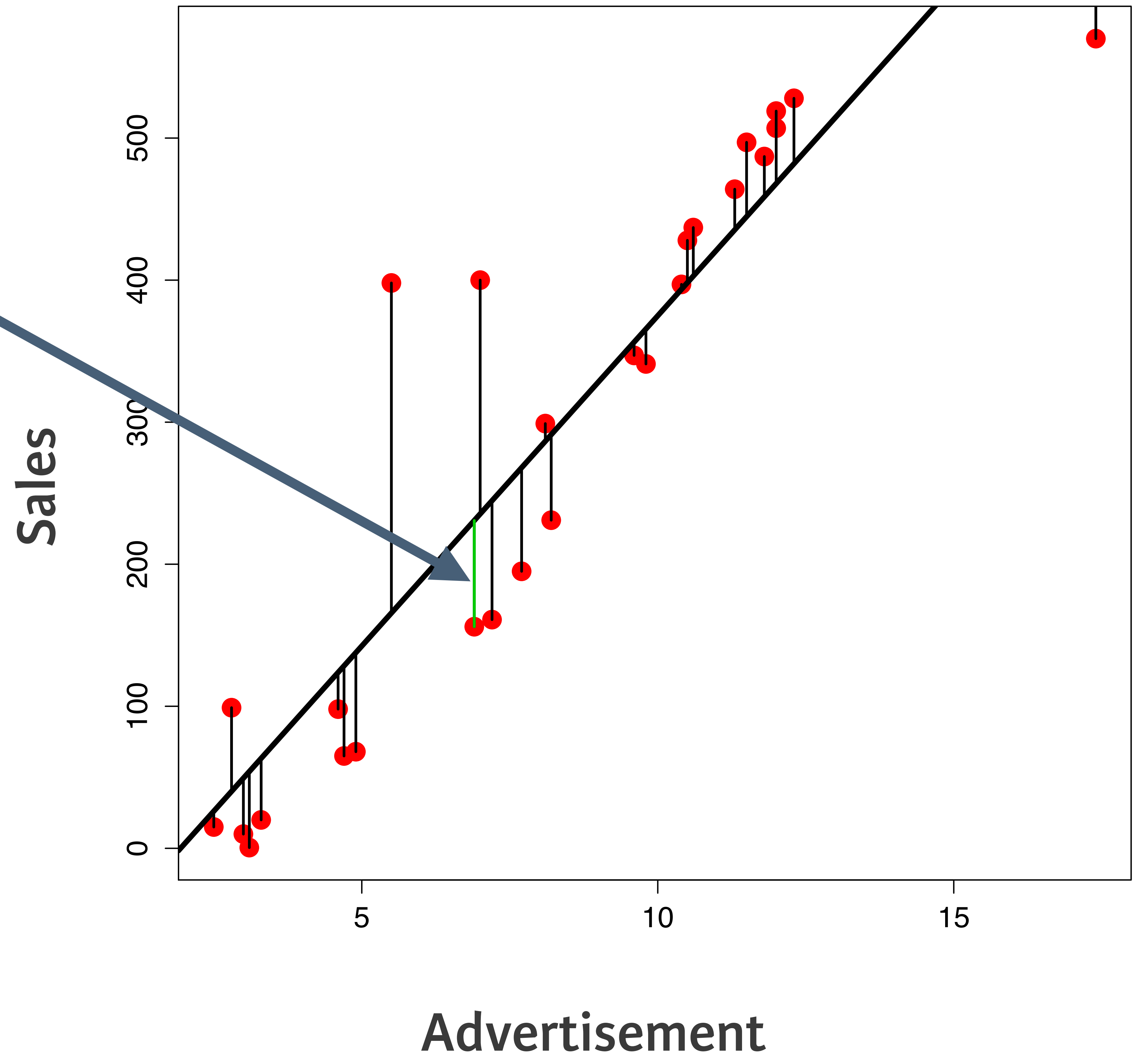
True Response

Fitted Response

#Observations

$$\mathrm{SS}_{\mathrm{res}} = \sum_{i=1}^{N} \mathrm{res}_i^2$$

← **Minimize!**



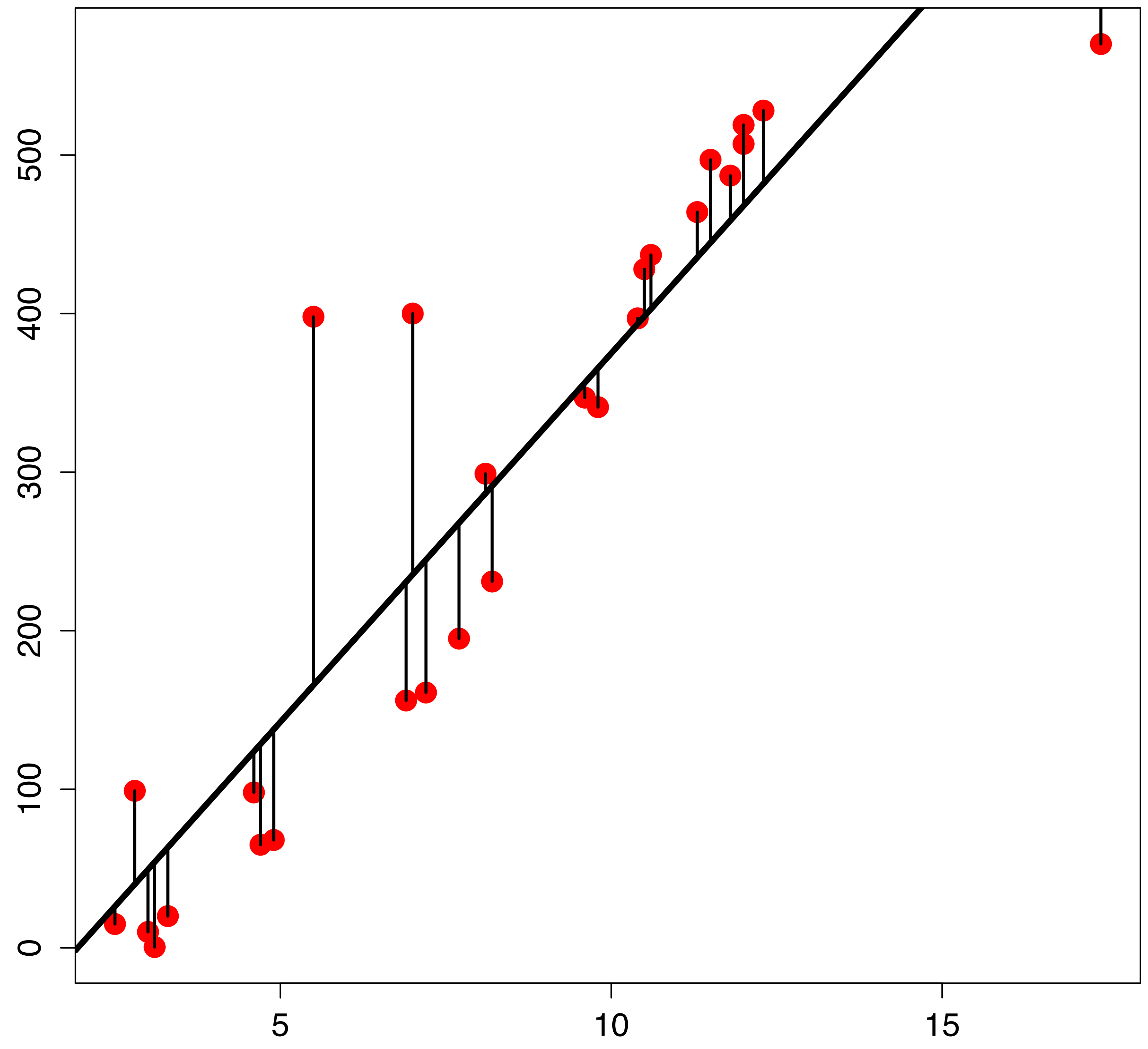
Estimating Coefficients

Response **Predictor**

```
> my_lm <- lm(sales ~ ads, data = shop_data)
```

```
> my_lm$coefficients
```

Returns coefficients



Prediction with Regression

Predicting new outcomes

$$\hat{y}_{new} := \hat{\beta}_0 + \hat{\beta}_1 x_{new}$$

$\hat{\beta}_0, \hat{\beta}_1$ ← Estimated Coefficients

x_{new} ← New Predictor Instance

$\hat{y}_{new}$ ← Estimated Response

Example: Ads: 11.000$ ⟶ Sales: 380.000$

Must be data frame

```
> y_new <- predict(my_lm, x_new, interval = "confidence")
```

Provides confidence interval

Accuracy: RMSE

Measure of **accuracy:**

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$$

Estimated Response

Observations

True Response

Example: **RMSE** = 76.000$ → Meaning?

RMSE has unit + scale → difficult to interpret!

Accuracy: R-squared

Sample mean response

$$\mathrm{SS}_{\mathrm{res}} = \sum_{i=1}^{N} \left(y_i - \hat{y}_i\right)^2 \qquad \mathrm{SS}_{\mathrm{tot}} = \sum_{i=1}^{N} (y_i - \bar{y})^2$$

← **Total SS**

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

← **R-squared**

Interpretation: % explained variance,

R^2 close to 1 → good fit!

```
> summary(my_lm)$r.squared
```

→ **Example: 0.84**

INTRODUCTION TO MACHINE LEARNING

Let’s practice!

INTRODUCTION TO MACHINE LEARNING

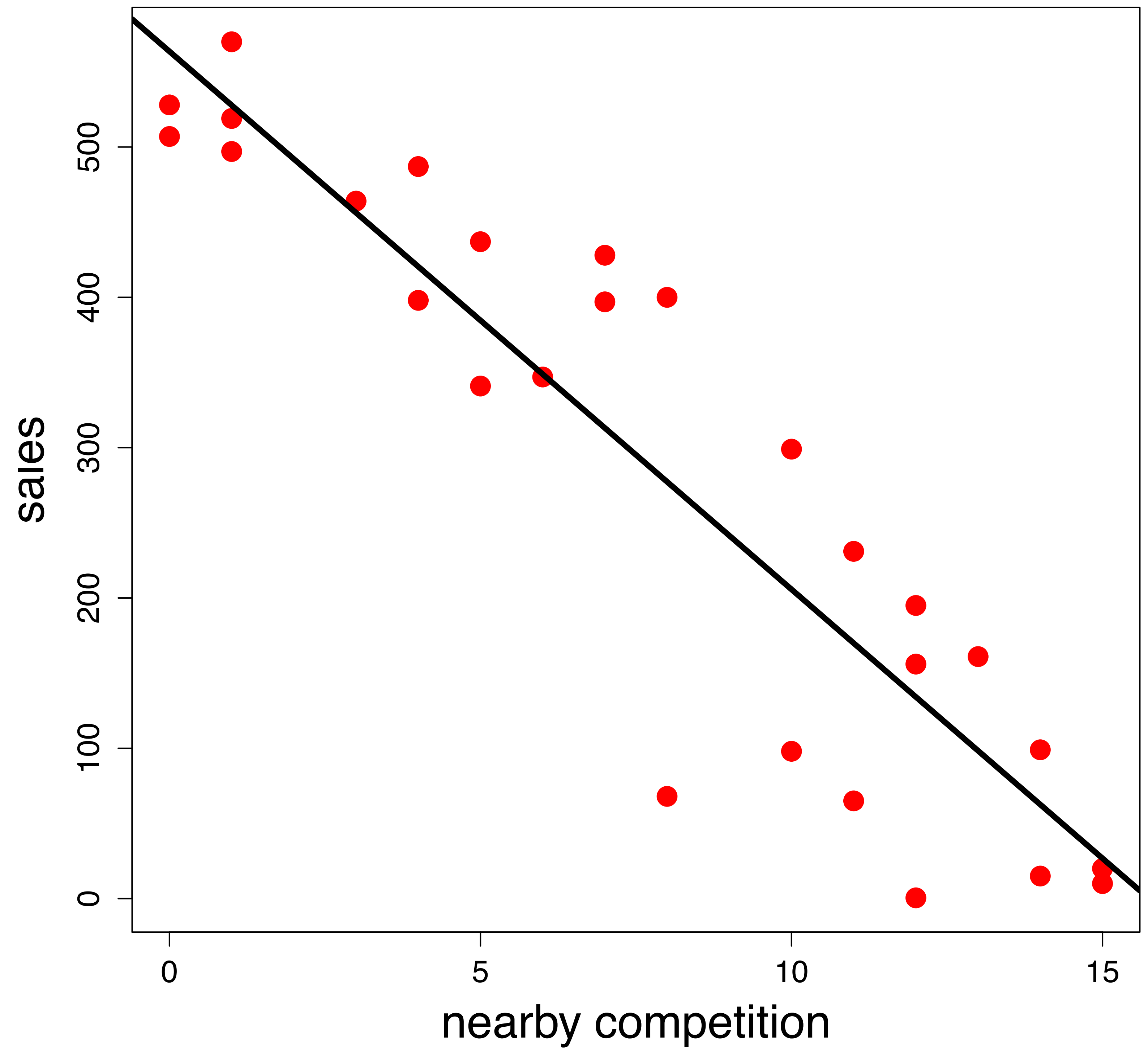
Multivariable Linear Regression

Example

Simple Linear Regression:

```
> lm(sales ~ ads, data = shop_data)
> lm(sales ~ comp, data = shop_data)
```

Loss of information!



Multi-Linear Model

Solution: combine in multi linear model!

- **Higher** predictive power
- **Higher** accuracy

$$\text{Sales} = \beta_0 + \beta_1 \times \text{Competition} + \beta_2 \times \text{Advertisement} + \epsilon$$

Individual Effect

Multi-Linear Regression Model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

- Predictors: X_1, X_2
- Response: Y
- Statistical Error: ϵ
- Coefficients: $\beta_0, \beta_1, \beta_2$

Estimating Coefficients

$$res_i = y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2})$$ ← **Residuals**

↑ True Response

↑ Fitted Response

#Observations

$$SS_{res} = \sum_{i=1}^{n} res_i^2$$ ← **Minimize!**

Extending!

More predictors: total inventory, district size, ...

→ **Extend** methodology to ***p*** predictors:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \epsilon$$

Response

Predictors

```
> my_lm <- lm(sales ~ ads + comp + ..., data = shop_data)
```

RMSE & Adjusted R-Squared

More predictors → { Higher *complexity* and *cost*
Lower *RMSE* and higher *R-squared*

Solution: *adjusted R-squared*

- Penalizes more predictors
- Used to compare

```
> summary(my_lm)$adj.r.squared
```

In Example: 0.819 → 0.906

Influence of predictors

- p-value: indicator influence of parameter
- p-value low — more likely parameter has significant influence

```
> summary(my_lm)

Call:
lm(formula = sales ~ ads + comp, data = shop_data)

Residuals:
     Min        1Q    Median        3Q       Max
-131.920   -23.009    -4.448    33.978   146.486

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  228.740     80.592   2.838 0.009084 **
ads           25.521      5.900   4.325 0.000231 ***
comp         -19.234      4.549  -4.228 0.000296 ***
```

P-Values

Example

- Want 95% confidence — p-value <= 0.05
- Want 99% confidence — p-value <= 0.01

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  228.740     80.592   2.838 0.009084 **
ads           25.521      5.900   4.325 0.000231 ***
comp         -19.234      4.549  -4.228 0.000296 ***
```

P-Values

Note: Do not mix up R-squared with p-values!

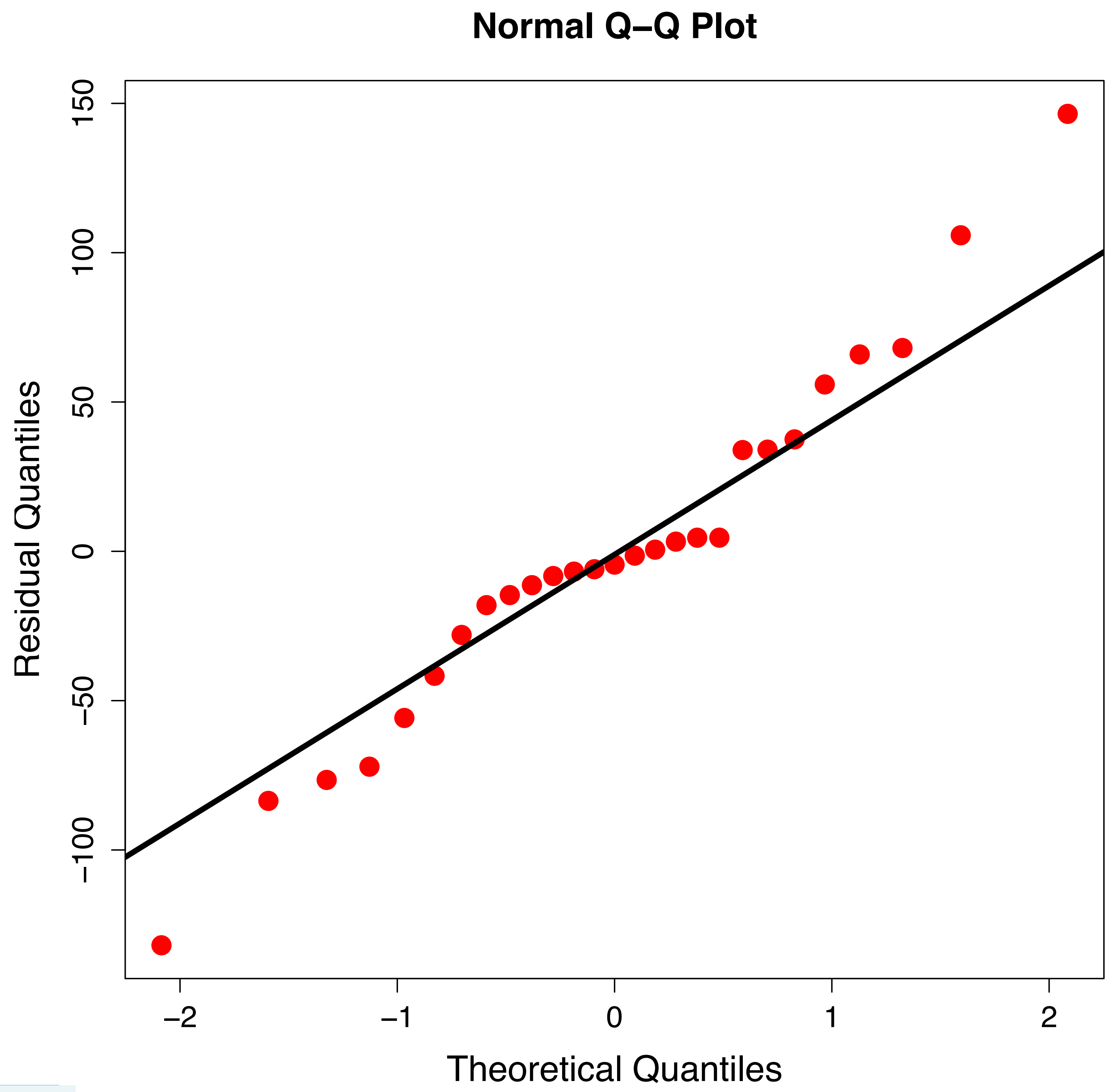
Assumptions

- Just make a model, make a summary and look at p-values?
- Not that simple!
- We made some implicit assumptions

Verifying Assumptions

Residuals:

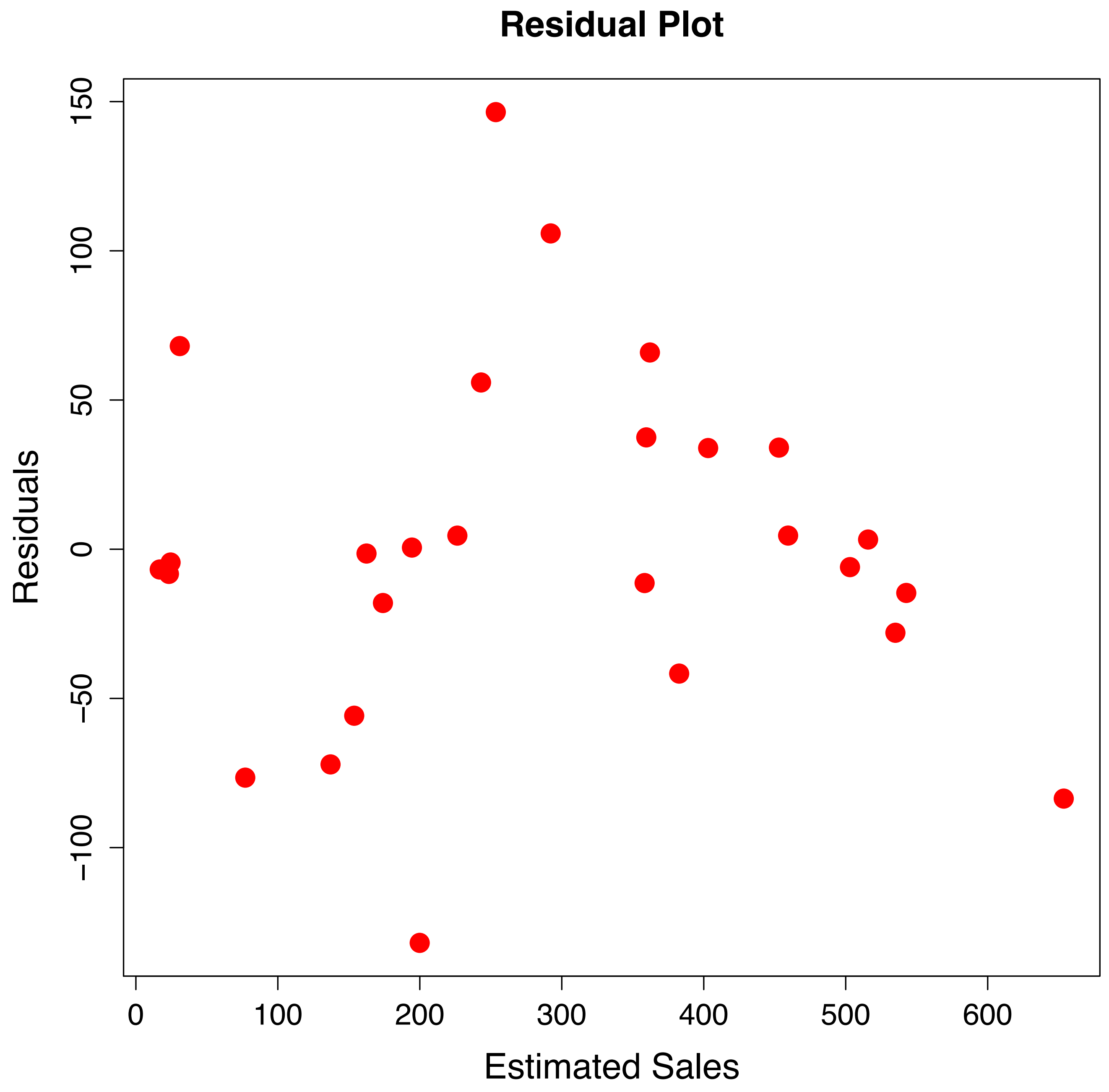
- Independent: No pattern?
- Identical Normal: Approximately a line?

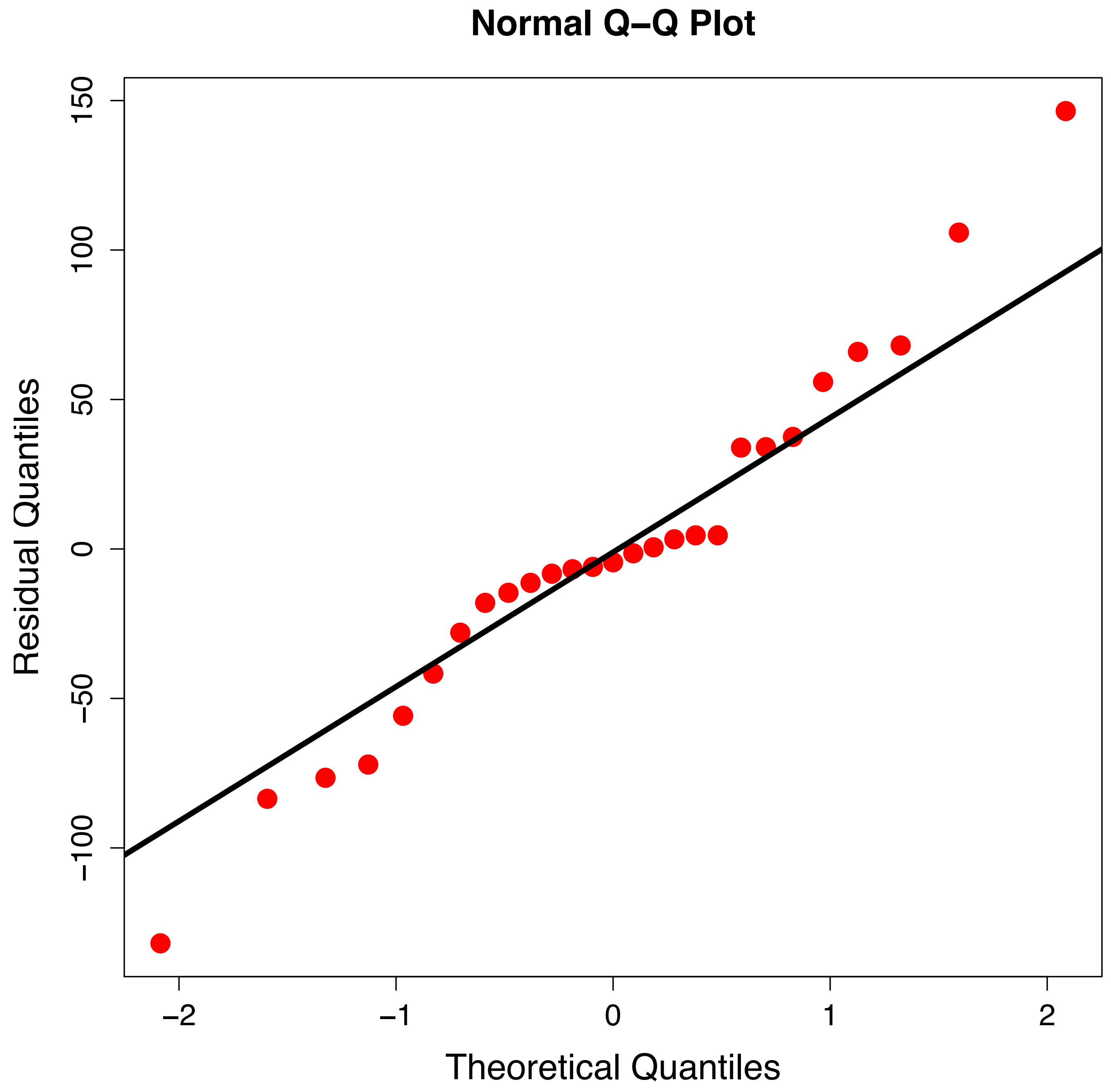


```
> plot(lm_shop$fitted.values,  lm_shop$residuals)
> qqnorm(lm_shop$residuals)
```

← **Draws normal Q-Q plot**

Verfiying Assumptions





- Important to avoid mistakes!
- Alternative tests exist

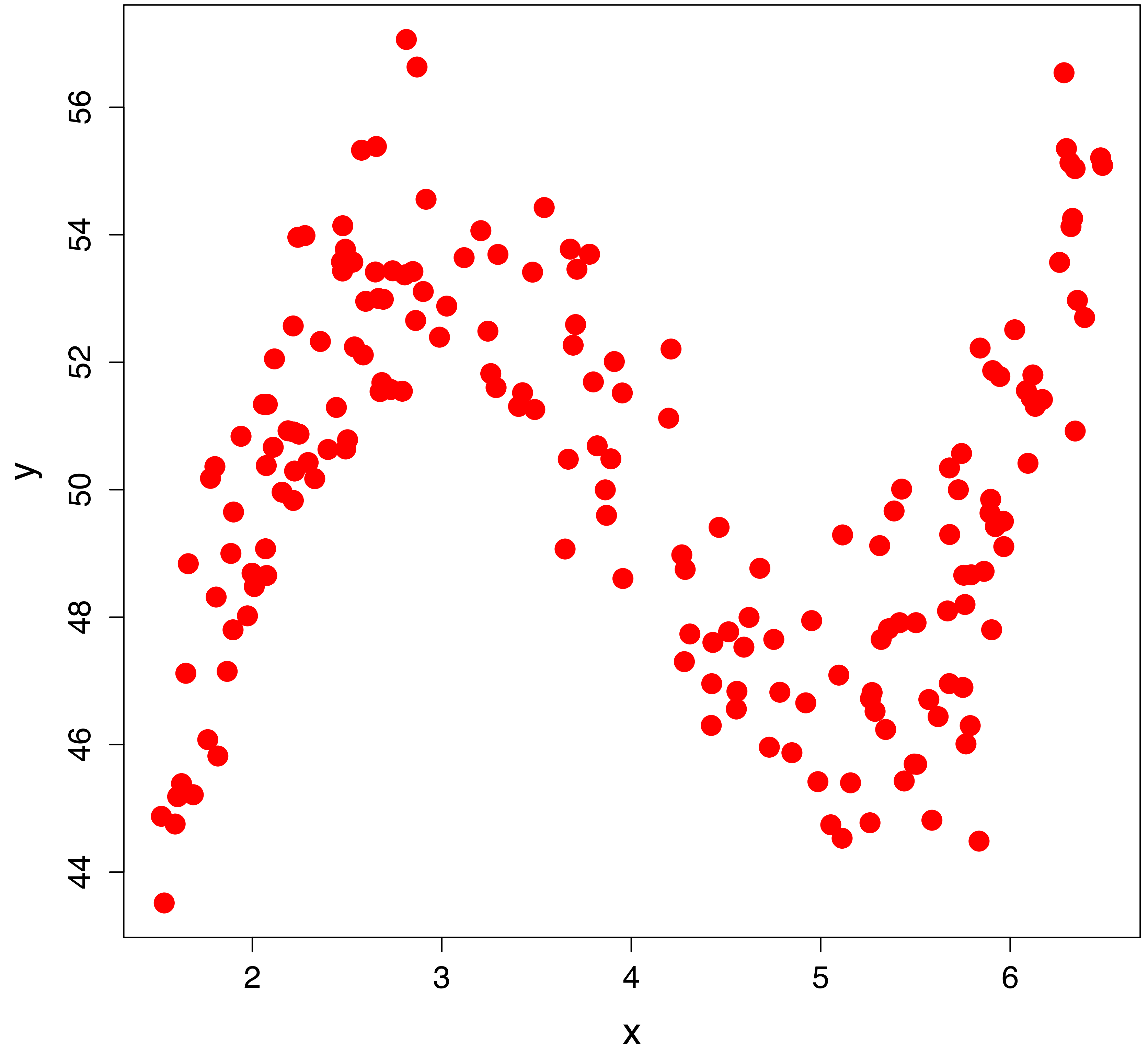
Let's practice!

INTRODUCTION TO MACHINE LEARNING

k-Nearest Neighbors and Generalization

Non-Parametric Regression

Problem: Visible pattern, but not linear



Non-Parametric Regression

Problem: Visible pattern, but not linear

Solutions:

- Transformation ← **Tedious**
- Multi-linear Regression ← **Advanced**
- non-Parametric Regression ← **Doable**

Non-Parametric Regression

Problem: Visible pattern, but not linear

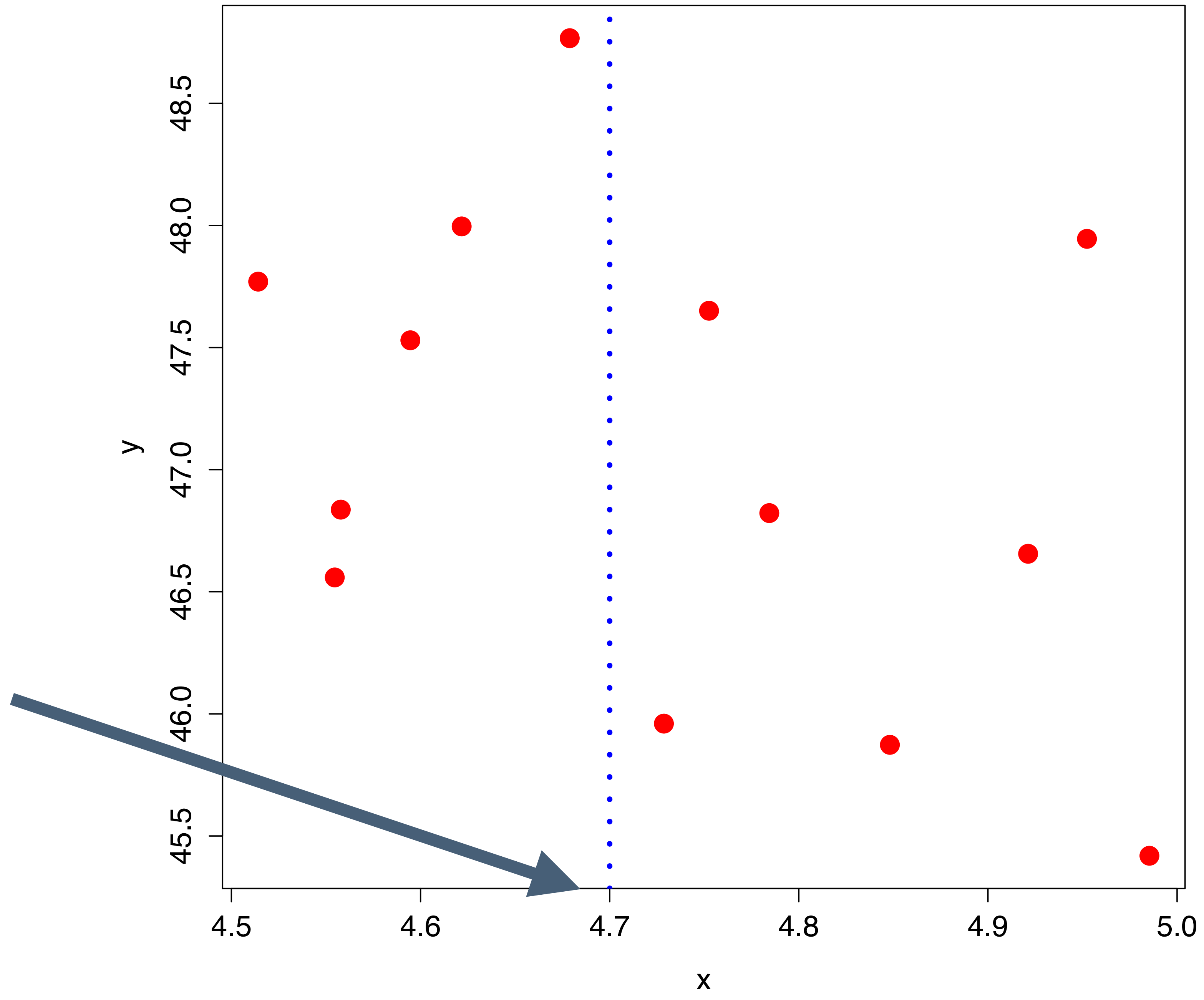
Techniques:

- k-Nearest Neighbors
- Kernel Regression
- Regression Trees
- ...

No parameter estimations required!

k-NN: Algorithm

Given a *training set* and a *new observation:*

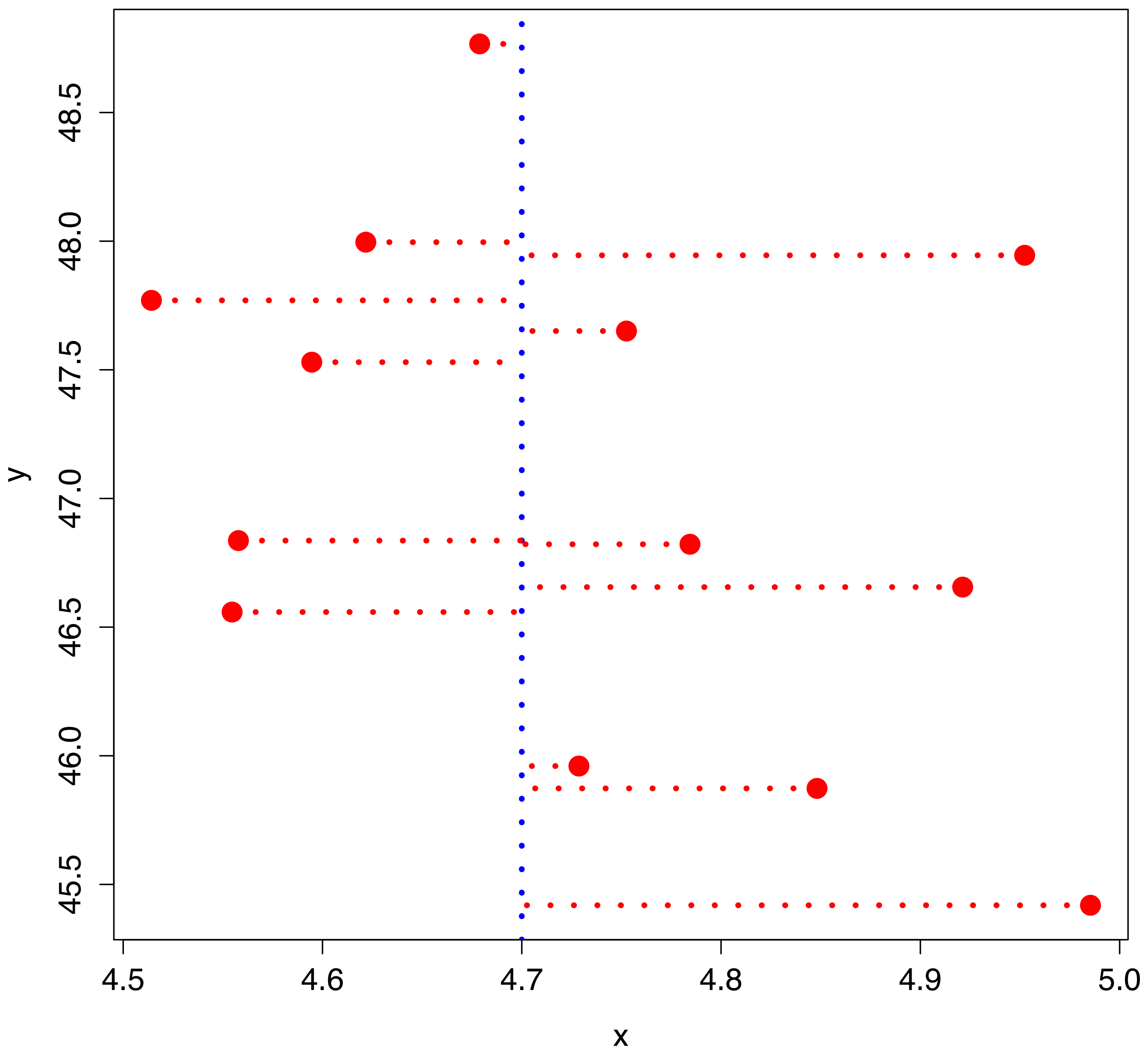


New observation

k-NN: Algorithm

Given a *training set* and a *new observation:*

1. Calculate the distance in the predictors

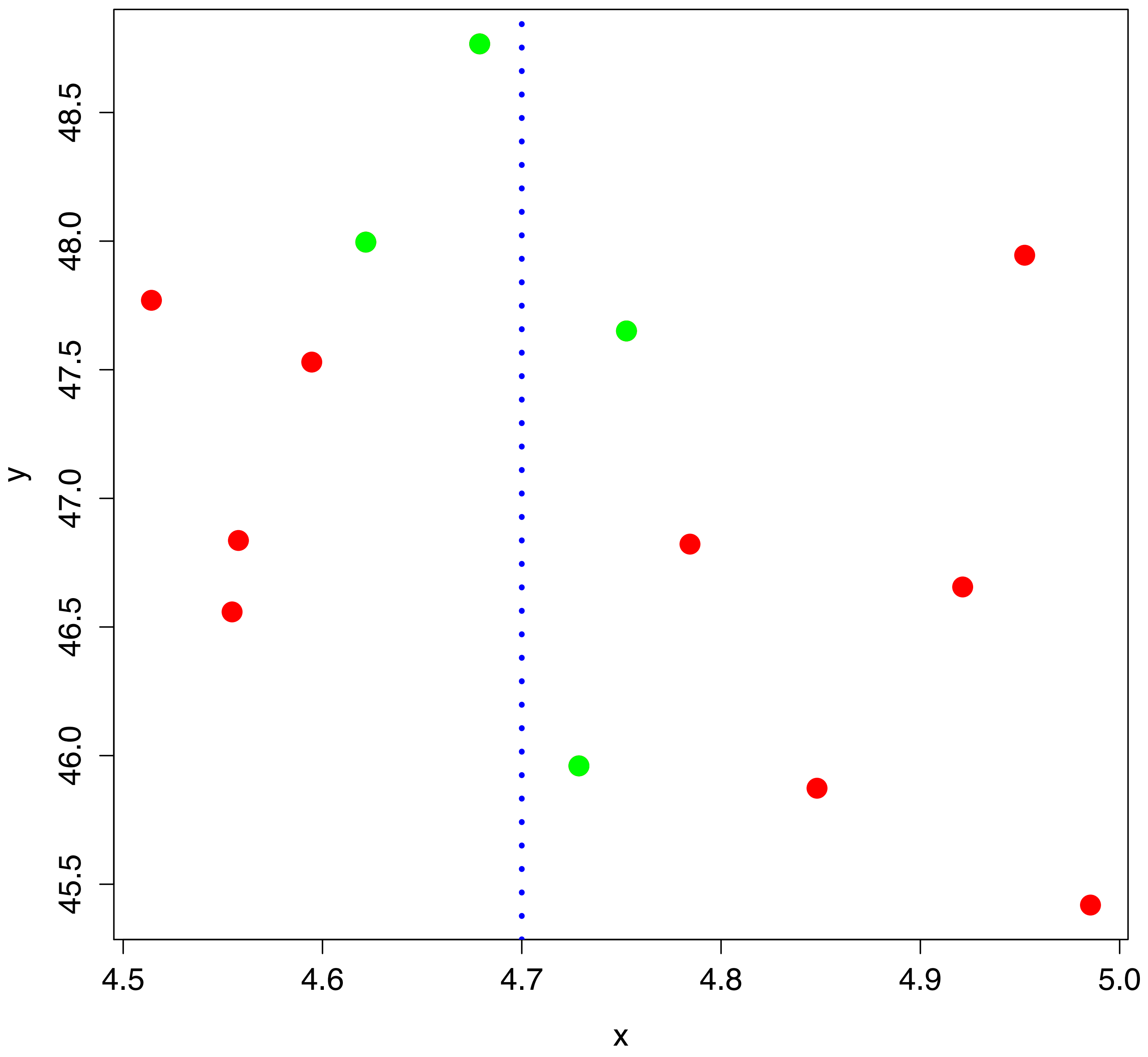


k-NN: Algorithm

Given a *training set* and a *new observation:*

2. Select the **k** nearest

k = 4 →

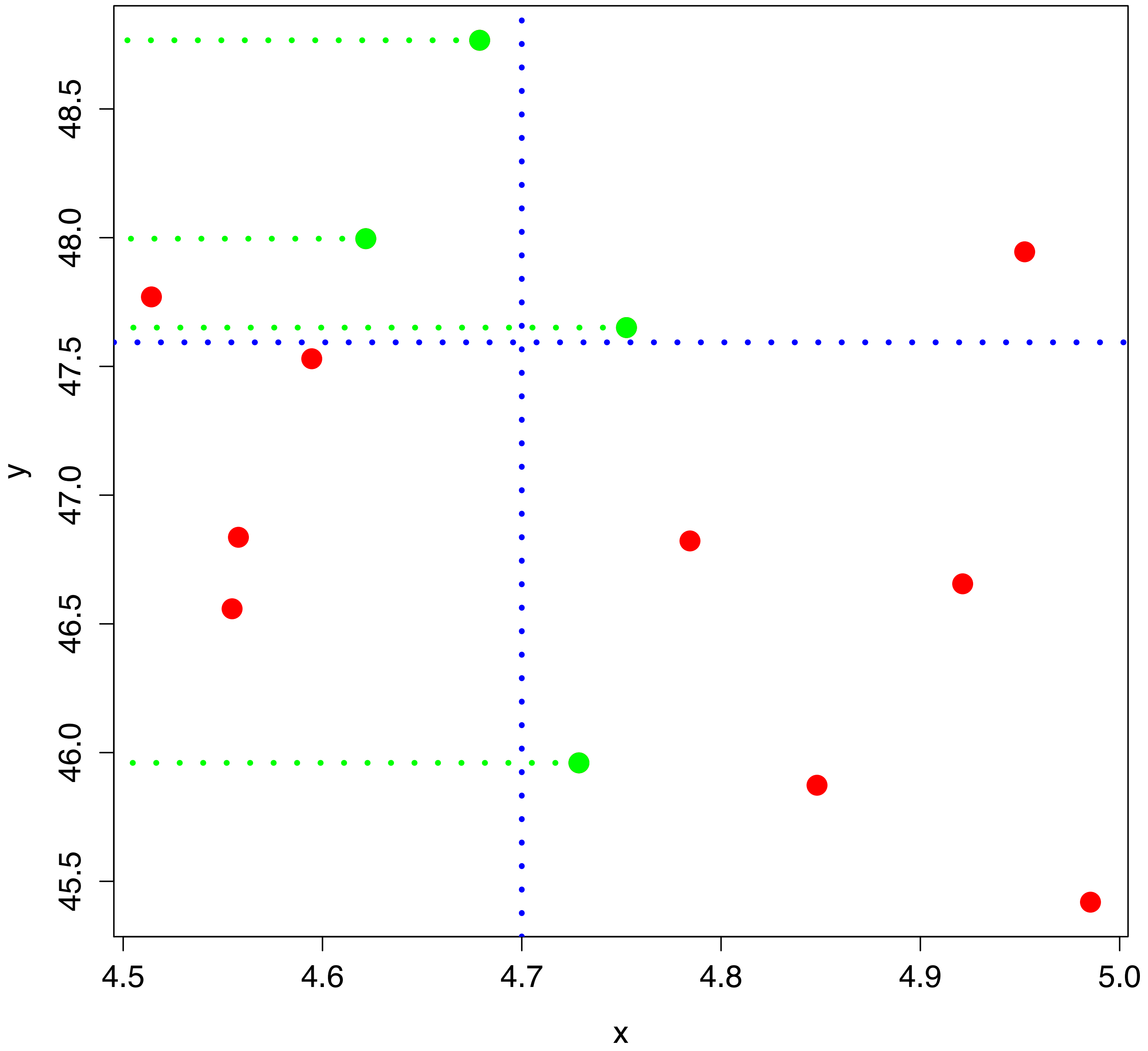


k-NN: Algorithm

Given a *training set* and a *new observation:*

3. Aggregate the response of the **k** nearest

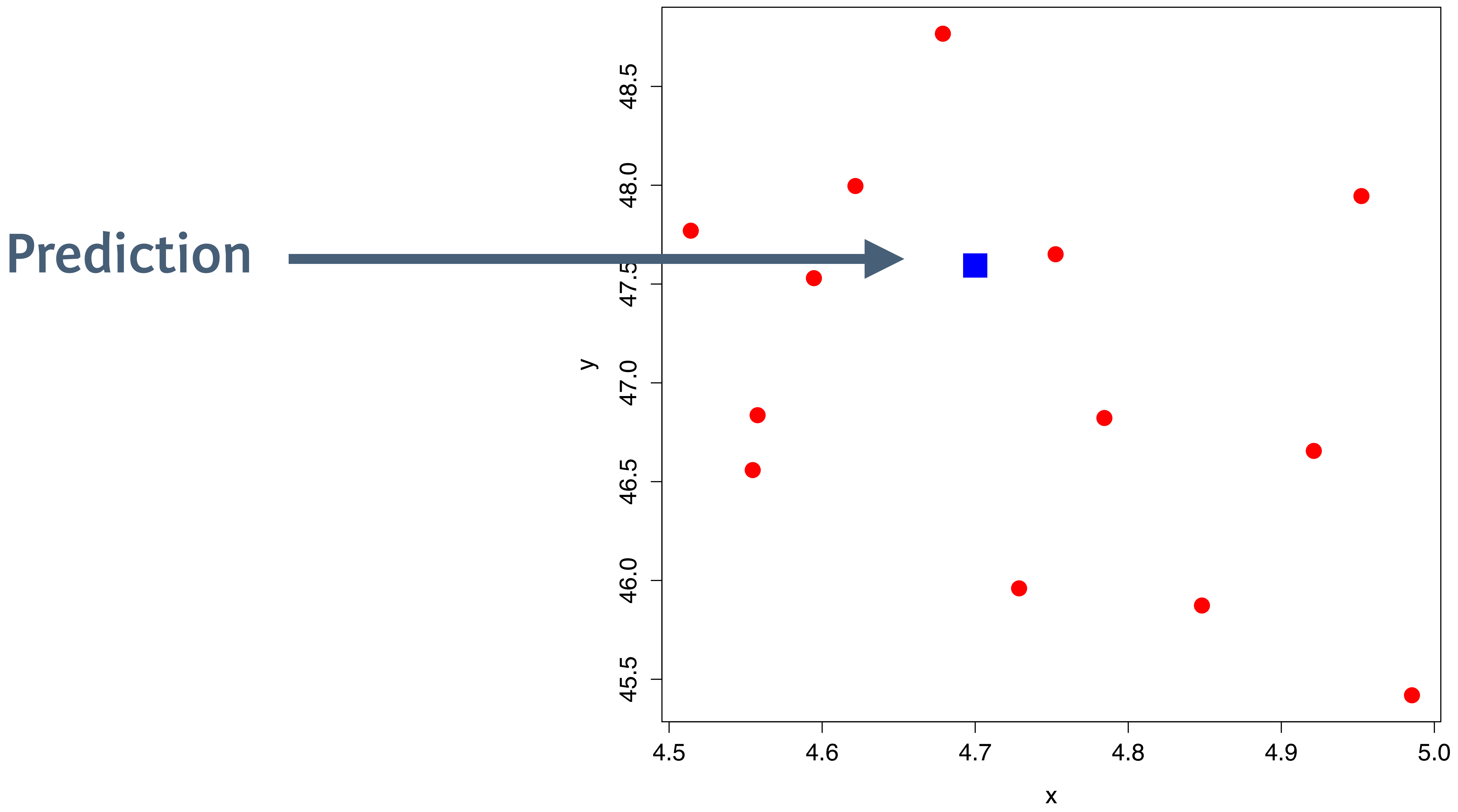
Mean of 4 responses



k-NN: Algorithm

Given a *training set* and a *new observation:*

4. The outcome is your prediction



Choosing k

- k = 1: Perfect fit on training set but poor predictions
- k = #obs in training set: Mean, also poor predictions

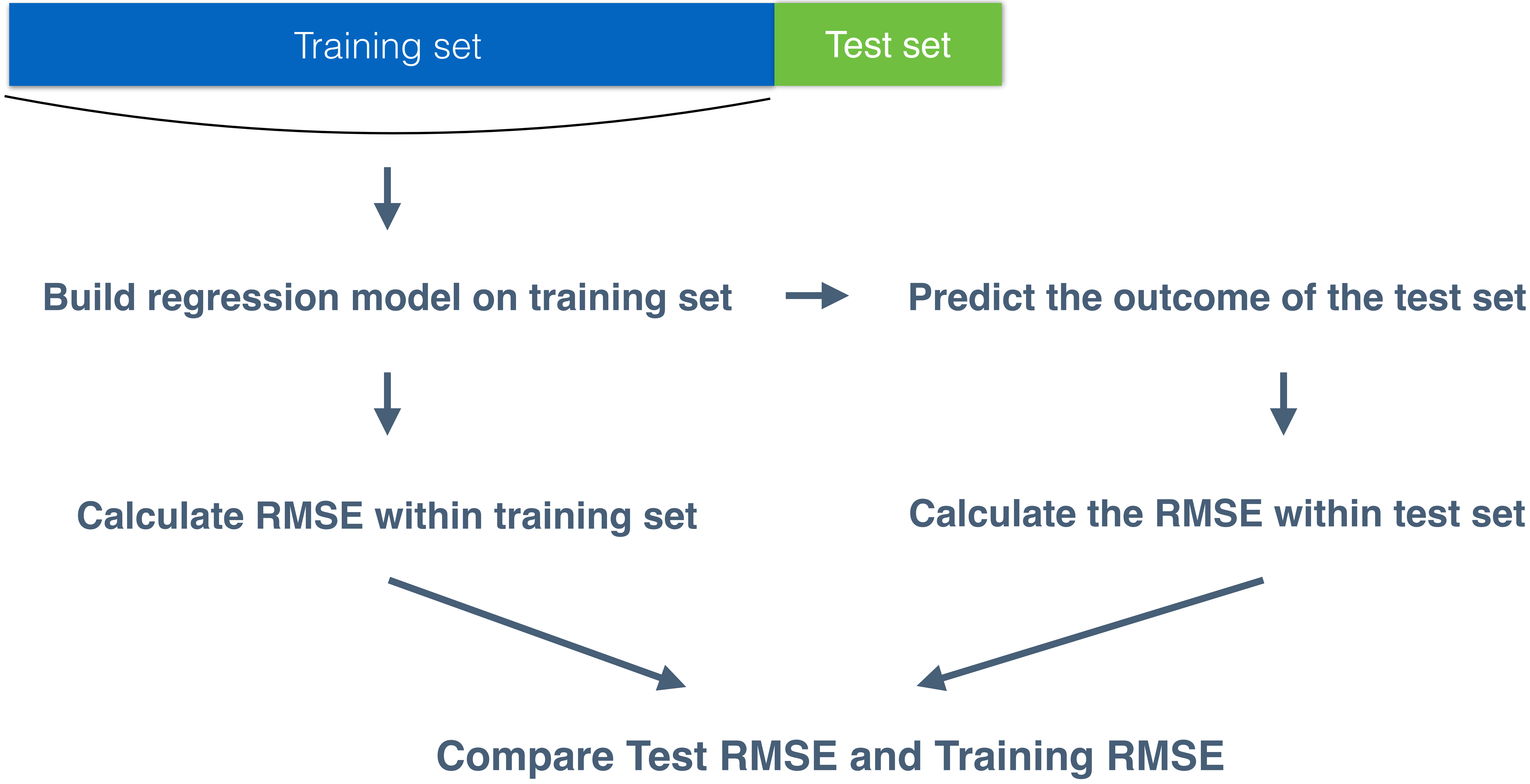
Bias - Variance trade off!

Reasonable: k = 20% of #obs in training set

Generalization in Regression

- Built your own regression model
- Worked on training set
- Does it generalize well?!
- Two techniques
    - Hold Out: simply split the dataset ←
    - K-fold cross-validation

Hold Out Method for Regression



Training set

Test set

Build regression model on training set

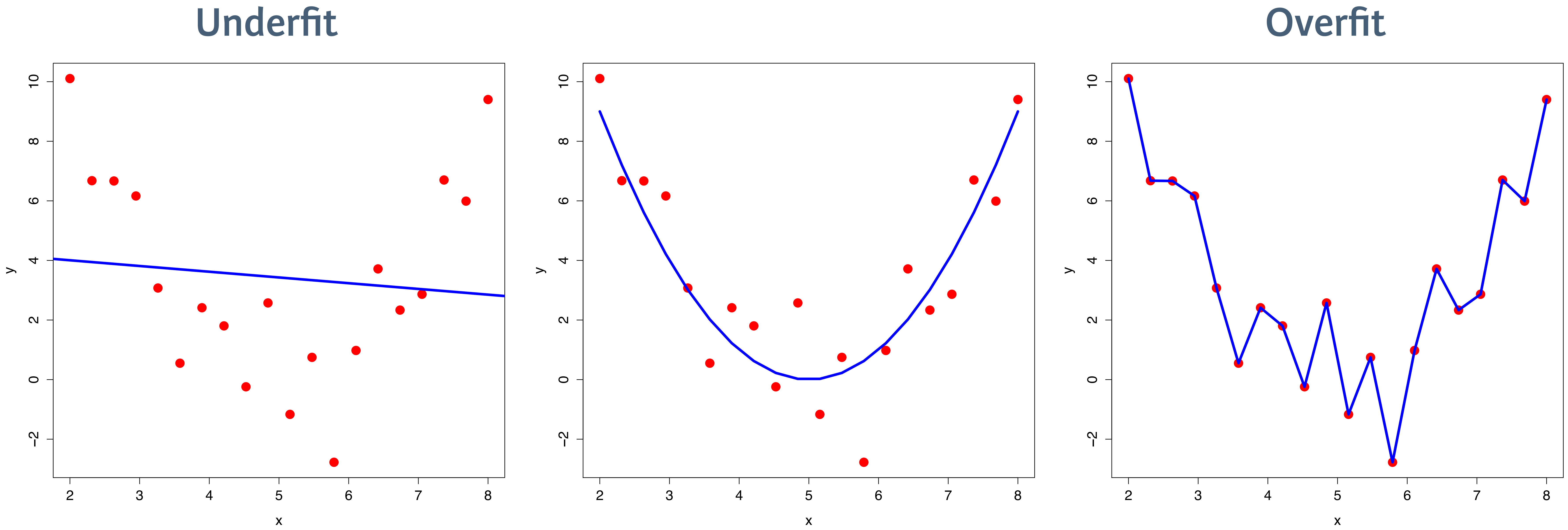
Predict the outcome of the test set

Calculate RMSE within training set

Calculate the RMSE within test set

Compare Test RMSE and Training RMSE

Under and Overfitting


Underfit

Overfit

- Fit: ✗
- Generalize: ✓
- Prediction: ✗

- Fit: ✓
- Generalize: ✓
- Prediction: ✓

- Fit: ✓
- Generalize: ✗
- Prediction: ✗

INTRODUCTION TO MACHINE LEARNING

Let’s practice!