Regression

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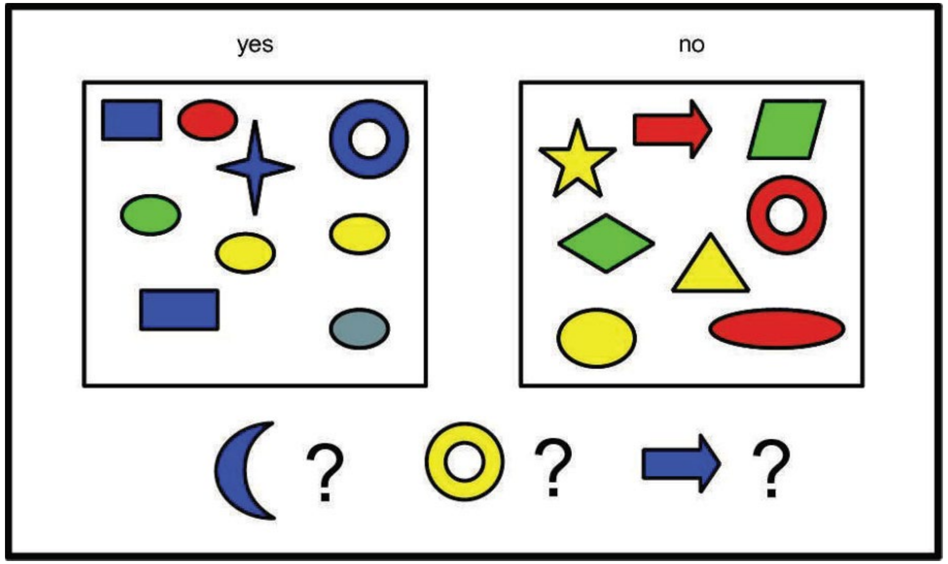
Supervised Learning

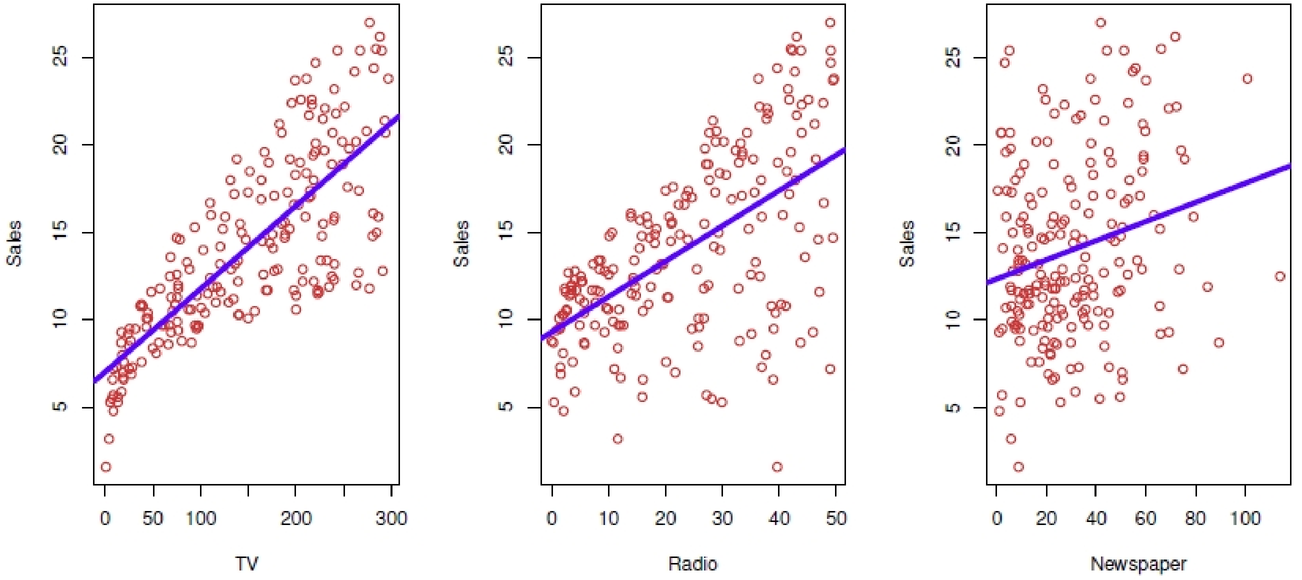
- Given: Training data as labeled instances $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$
- Goal: Learn a rule $(f: x \rightarrow y)$ to predict outputs y for new inputs x
- Example)
  - Data: ((Blue, Square, 10), yes), . . . ((Red, Ellipse, 20.7), yes)
  - Task: For new inputs (Blue, Crescent, 10), (Yellow, Circle, 12), are they yes/no?



Color	Shape	Size	Label
Blue	Square	10	1
Red	Ellipse	2.4	1
Red	Ellipse	20.7	0
Blue	Crescent	10	?
Yellow	Circle	12	?

Supervised Learning

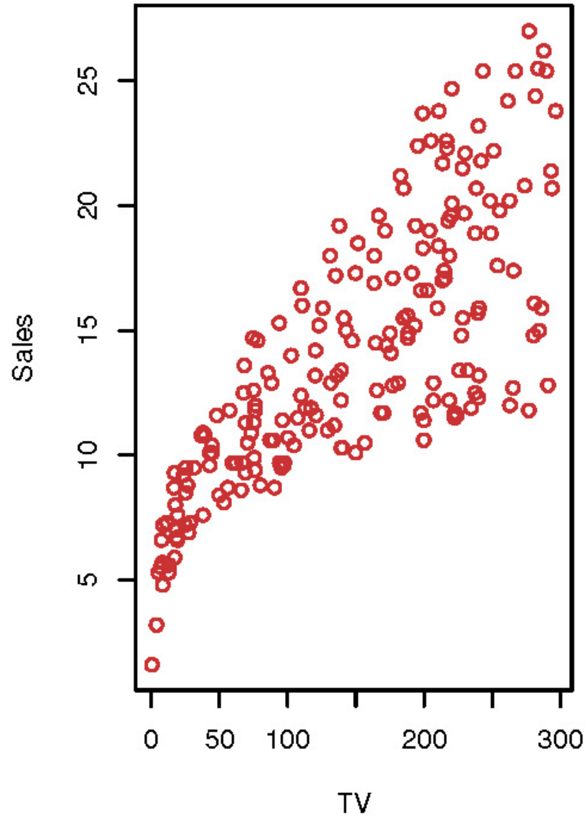
- Regression: Real-valued outputs
- Example)
  - Data: Advertising budgets and sales {(TV, Radio, Newspaper), Sales}
  - Task: Predict sales given new advertising budgets
  - Method: Fitting a line or non-linear curve



SIMPLE LINEAR REGRESSION

Problem

- Data: Advertising budgets and sales {TV, Sales}
- Task: Predict sales given new advertising TV budget



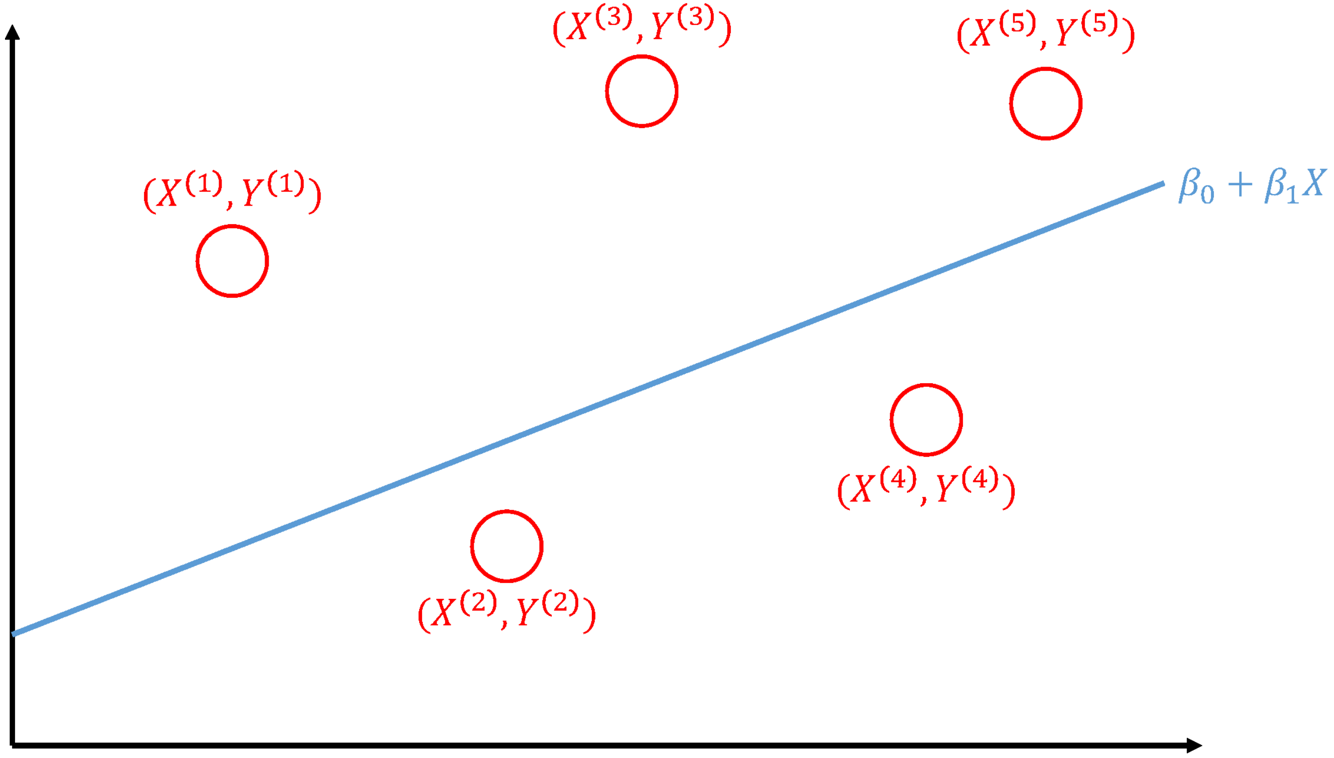
Data

- N: # training data
- X: TV ad budget (input variable, features)
- Y: sales (output variable, response variable)
- (x, y): one training data
- $(x^{(i)}, y^{(i)})$: i-th training data

X	Y
230.1	22.1
44.5	10.4
17.2	9.3
151.5	18.5
180.8	12.9
8.7	7.2
57.5	11.8
$\vdots$	$\vdots$

Linear Regression

- Data: N TV advertising budgets and sales (X, Y)
- Task: Predict sales $y^{(test)}$ given new advertising TV budget $x^{(test)}$
- Model: $Y \approx \beta_0 + \beta_1 X$

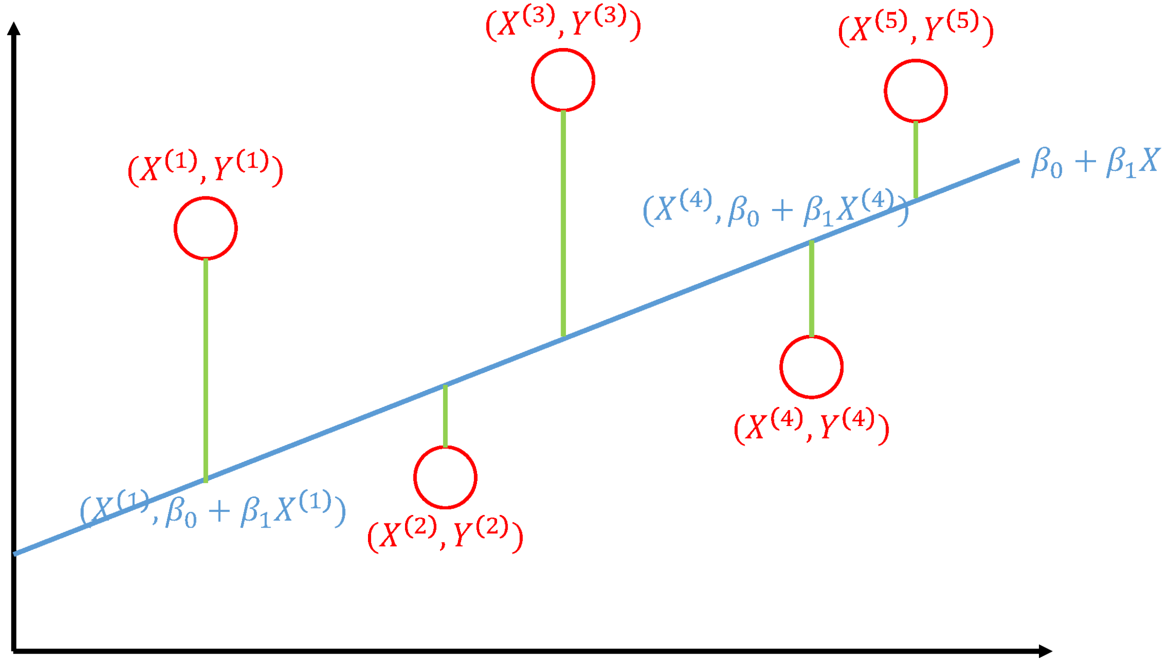


Linear Regression

- Data: N TV advertising budgets and sales (X, Y)
- Task: Predict sales $y^{(test)}$ given new advertising TV budget $x^{(test)}$
- Model: $Y \approx \beta_0 + \beta_1 X$
- New problem: Find the best β_0 and β_1
- A question: What are the best β_0 and β_1?
- Possible answer: Given a data $x^{(i)}$, no difference between
  - $\hat{y}^{(i)}$: output of the model with β_0 and β_1
  - $y^{(i)}$: real data output

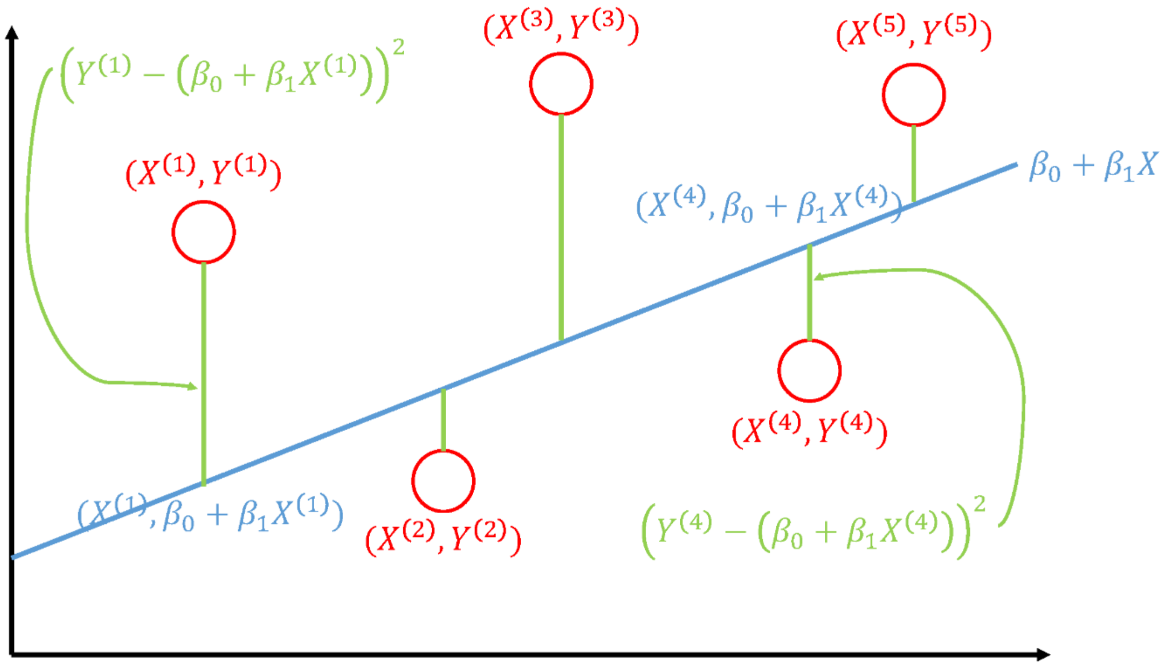
Linear Regression

- Data: N TV advertising budgets and sales (X, Y)
- Task: Predict sales $y^{(test)}$ given new advertising TV budget $x^{(test)}$
- Model: $Y \approx \beta_0 + \beta_1 X$
- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$



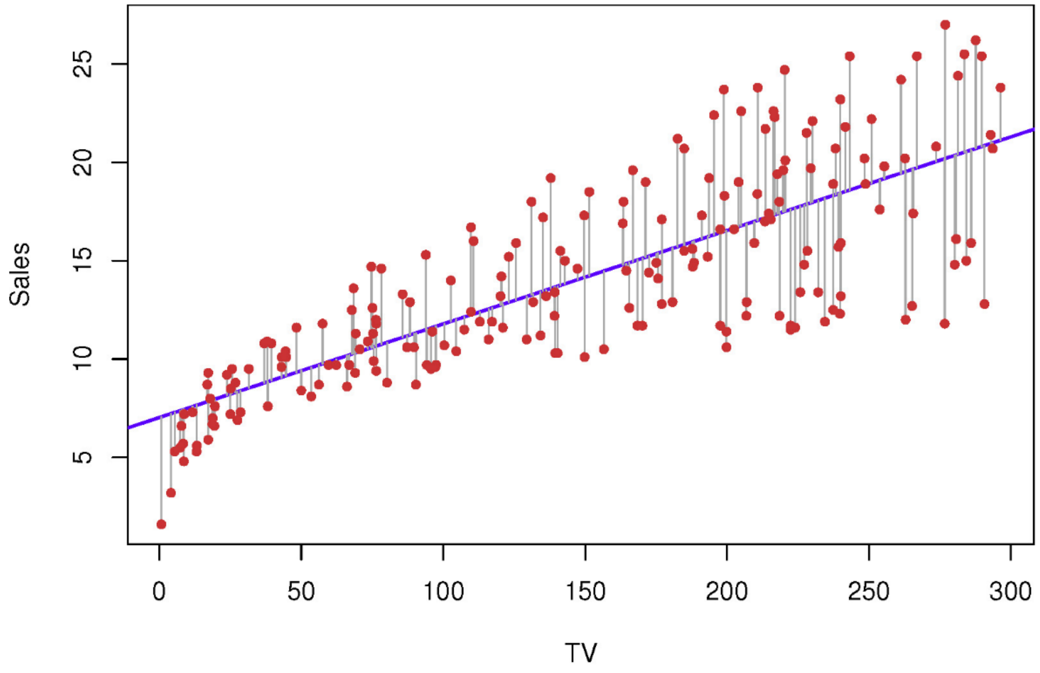
Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X$
- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$
- Difference: $\left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)}\right)\right)^2$



Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X$
- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$
- All data difference: $\sum_i^N \left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)}\right)\right)^2$



Linear Regression

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- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$
- All data difference: $\sum_i^N \left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)}\right)\right)^2$
- Method: Find the best β_0 and β_1 that minimize the all data difference

$$\underset{\beta_0, \beta_1}{\arg\min} \sum_i^N \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)}\right)\right)^2$$

Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X$
- Parameters: β_0, β_1
- Loss function

$$\mathrm{L}(\beta_0, \beta_1) = \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)}\right)\right)^2$$

- Task

$$\underset{\beta_0, \beta_1}{\arg\min} \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)}\right)\right)^2$$

Linear Regression

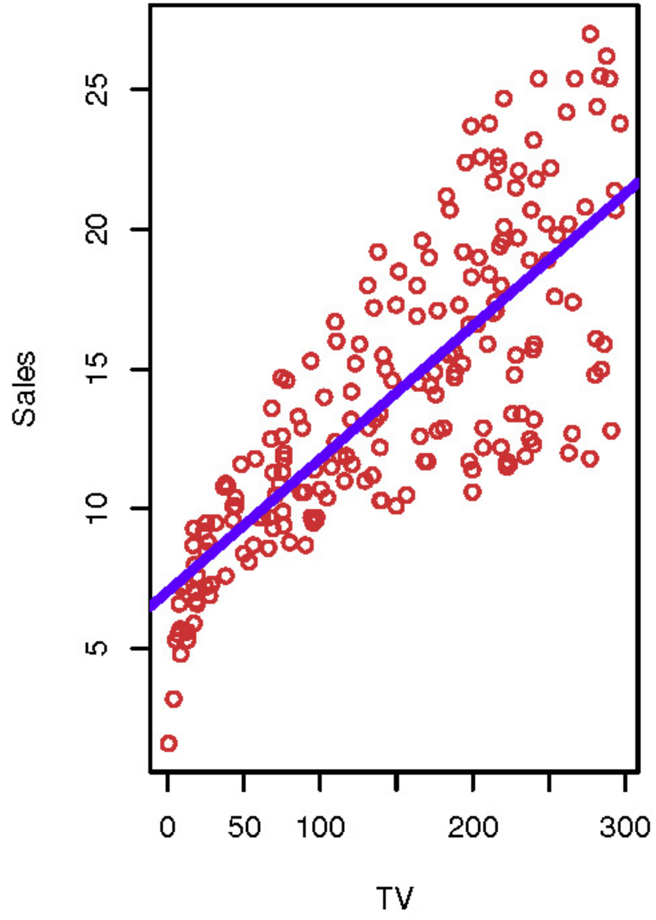
- Model: $Y \approx \beta_0 + \beta_1 X$
- Parameters: β_0, β_1
- Loss function

$$\mathrm{L}(\beta_0, \beta_1) = \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)} \right) \right)^2$$

- Task

$$\underset{\beta_0, \beta_1}{\arg\min} \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)} \right) \right)^2$$

- Algorithm: Gradient-descent algorithm



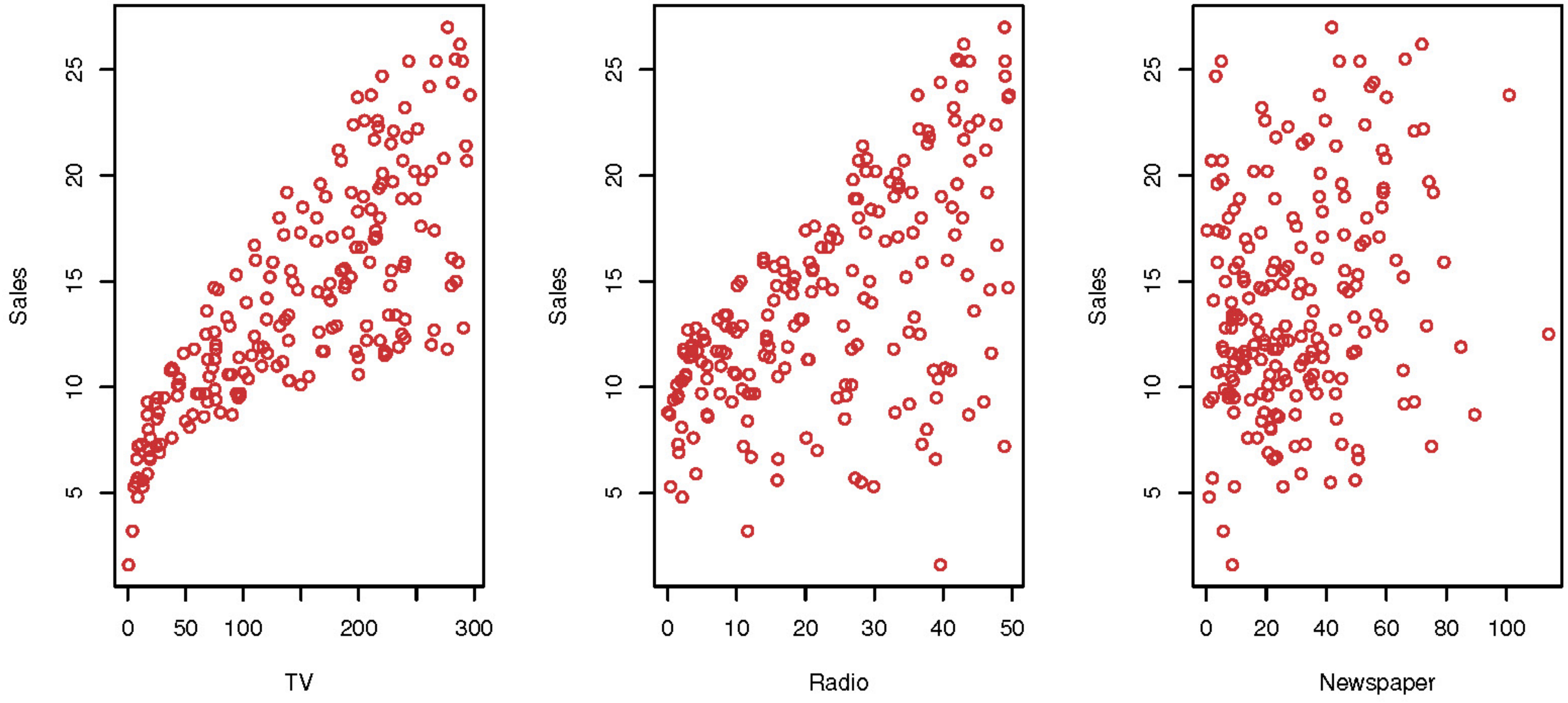
Supervised Learning

- Problem: Predict outputs y for new inputs x based on a rule $(f: x \rightarrow y)$
- Data: Labeled instances $\{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$
- Model: Supervised model (e.g. linear regression)
- Parameters: Unknown values of the model
- Loss function: Difference between the outputs of the model and the data
- Task: Find the parameters that minimize the loss function
- Algorithm: Various algorithms

MULTIPLE LINEAR REGRESSION

Problem

- Data: Advertising budgets and sales {(TV, Radio, Newspaper), Sales}
- Task: Predict sales given new advertising budgets



Data

- N: # training data
- X_1, X_2, X_3: (TV, Radio, Newspaper) AD budgets
- Y: sales
- (x_1, x_2, x_3, y): one training data
- $(x_1^{(i)}, x_2^{(i)}, x_3^{(i)}, y^{(i)})$: i-th training data

X_1	X_2	X_3	Y
230.1	37.8	69.2	22.1
44.5	39.3	45.1	10.4
17.2	45.9	69.3	9.3
151.5	41.3	58.5	18.5
180.8	10.8	58.4	12.9
8.7	48.9	75	7.2
57.5	32.8	23.5	11.8
⋮	⋮	⋮	⋮

Linear Regression

- Data: N advertising budgets and sales (X_1, X_2, X_3, Y)
- Task: Predict sales $y^{(test)}$ given new ad budgets $x_1^{(test)}, x_2^{(test)}, x_3^{(test)}$
- Model: $Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$
- New problem: Find the best $\beta_0, \beta_1, \beta_2$ and β_3
- A question: What are the best βs?
- Possible answer: Given a data $x^{(i)}$, no difference between
  - $\hat{y}^{(i)}$: output of the model with $\beta_0, \beta_1, \beta_2$ and β_3
  - $y^{(i)}$: real data output

Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$
- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$
- Difference: $\left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \beta_3 x_3^{(i)}\right)\right)^2$

Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$
- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$
- All data difference

$$\sum_{i}^{N} \left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \beta_3 x_3^{(i)}\right)\right)^2$$

Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$
- Idea: Given a data $x^{(i)}$, minimize the difference between $\hat{y}^{(i)}$ and $y^{(i)}$
- All data difference

$$\sum_{i}^{N} \left(y^{(i)} - \hat{y}^{(i)}\right)^2 = \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \beta_3 x_3^{(i)}\right)\right)^2$$

- Method: Find the best βs that minimize the all data difference

$$\underset{\beta_0, \beta_1, \beta_2, \beta_3}{\arg\min} \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \beta_3 x_3^{(i)}\right)\right)^2$$

Linear Regression

- Model: $Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$
- Parameters: $\beta_0, \beta_1, \beta_2, \beta_3$
- Loss function

$$\mathrm{L}(\beta_0, \beta_1, \beta_2, \beta_3) = \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \beta_3 x_3^{(i)} \right) \right)^2$$

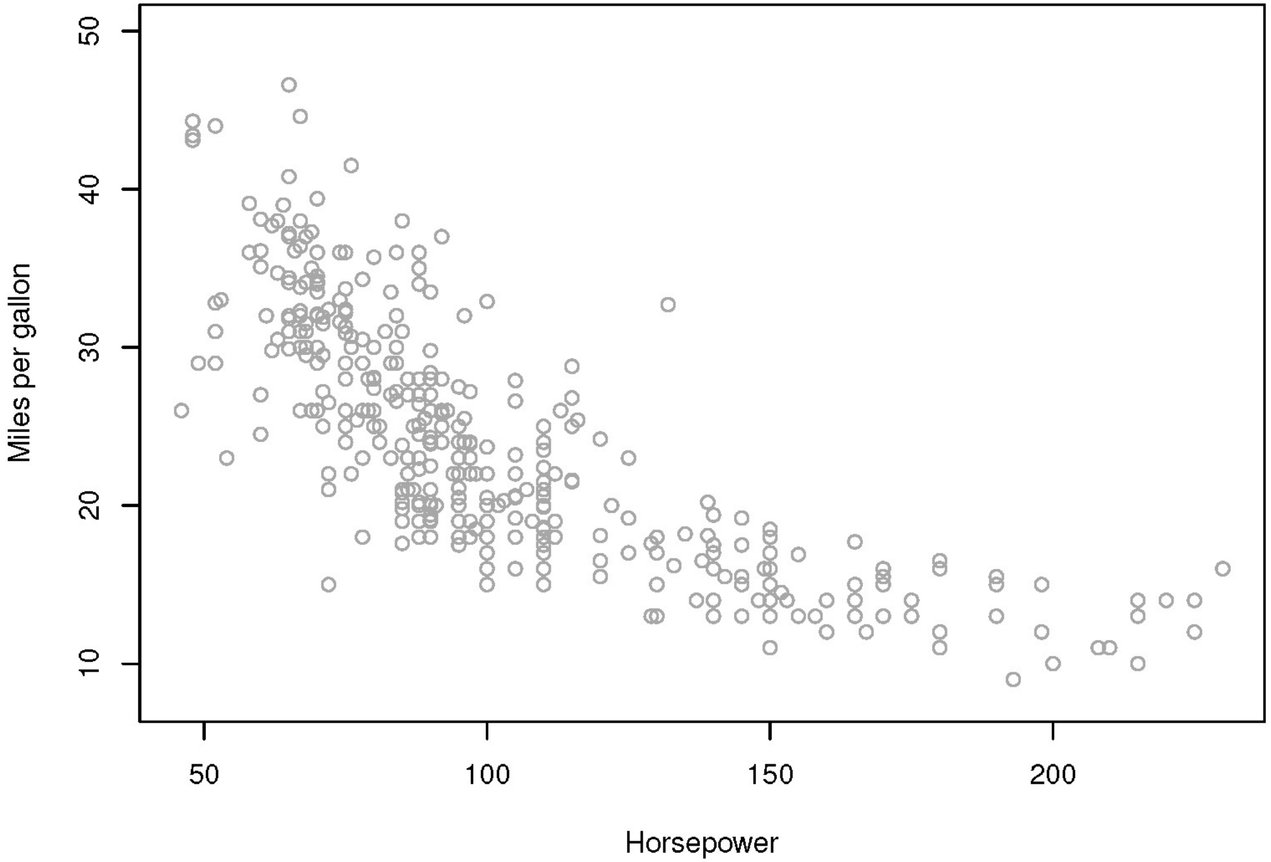
- Task

$$\underset{\beta_0, \beta_1, \beta_2, \beta_3}{\arg\min} \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x_1^{(i)} + \beta_2 x_2^{(i)} + \beta_3 x_3^{(i)} \right) \right)^2$$

POLYNOMIAL REGRESSION

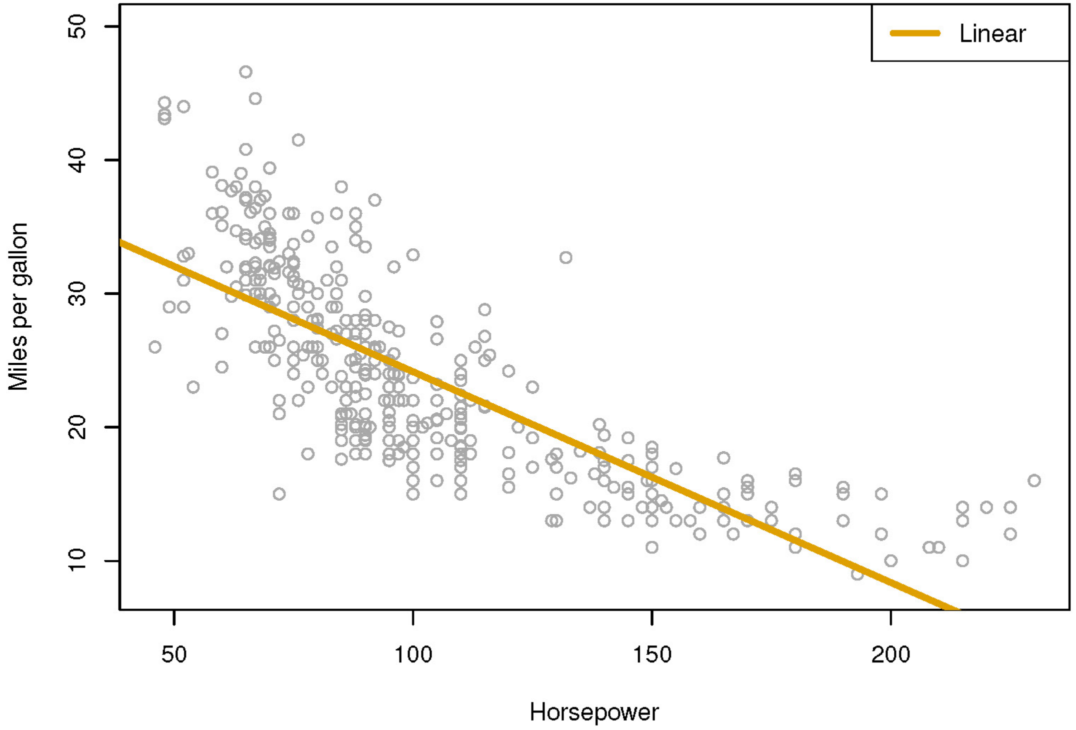
Problem

- Data: Car engine horsepower and miles/gallon {Horsepower, Miles/gallon}
- Task: Predict miles/gallon given a new car engine



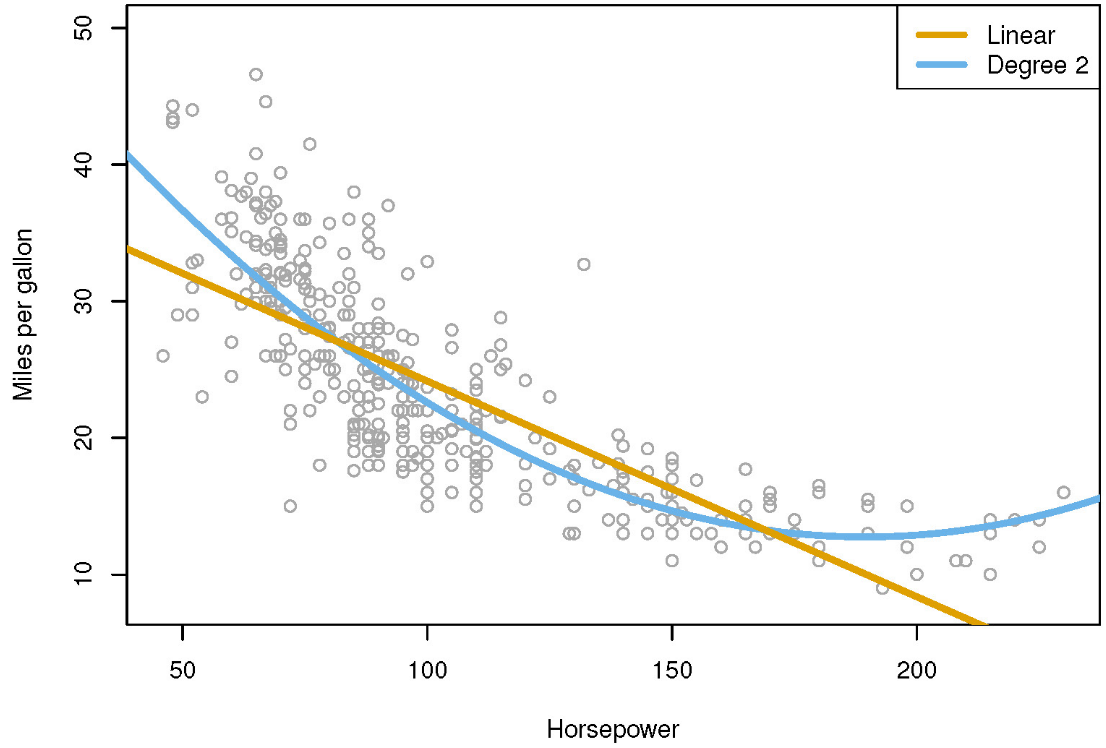
Linear Regression

- Data: Car engine horsepower and miles/gallon {Horsepower, Miles/gallon}
- Task: Predict miles/gallon given a new car engine
- Model: Simple Linear Regression $Y \approx \beta_0 + \beta_1 X$



Polynomial Regression

- Data: Car engine horsepower and miles/gallon {Horsepower, Miles/gallon}
- Task: Predict miles/gallon given a new car engine
- Model: $Y \approx \beta_0 + \beta_1 X + \beta_2 X^2$



Polynomial Regression

- Model: $Y \approx \beta_0 + \beta_1 X + \beta_2 X^2$
- Parameters: $\beta_0, \beta_1, \beta_2$
- Loss function

$$\mathrm{L}(\beta_0, \beta_1, \beta_2) = \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)} + \beta_2 (x^{(i)})^2 \right) \right)^2$$

- Task

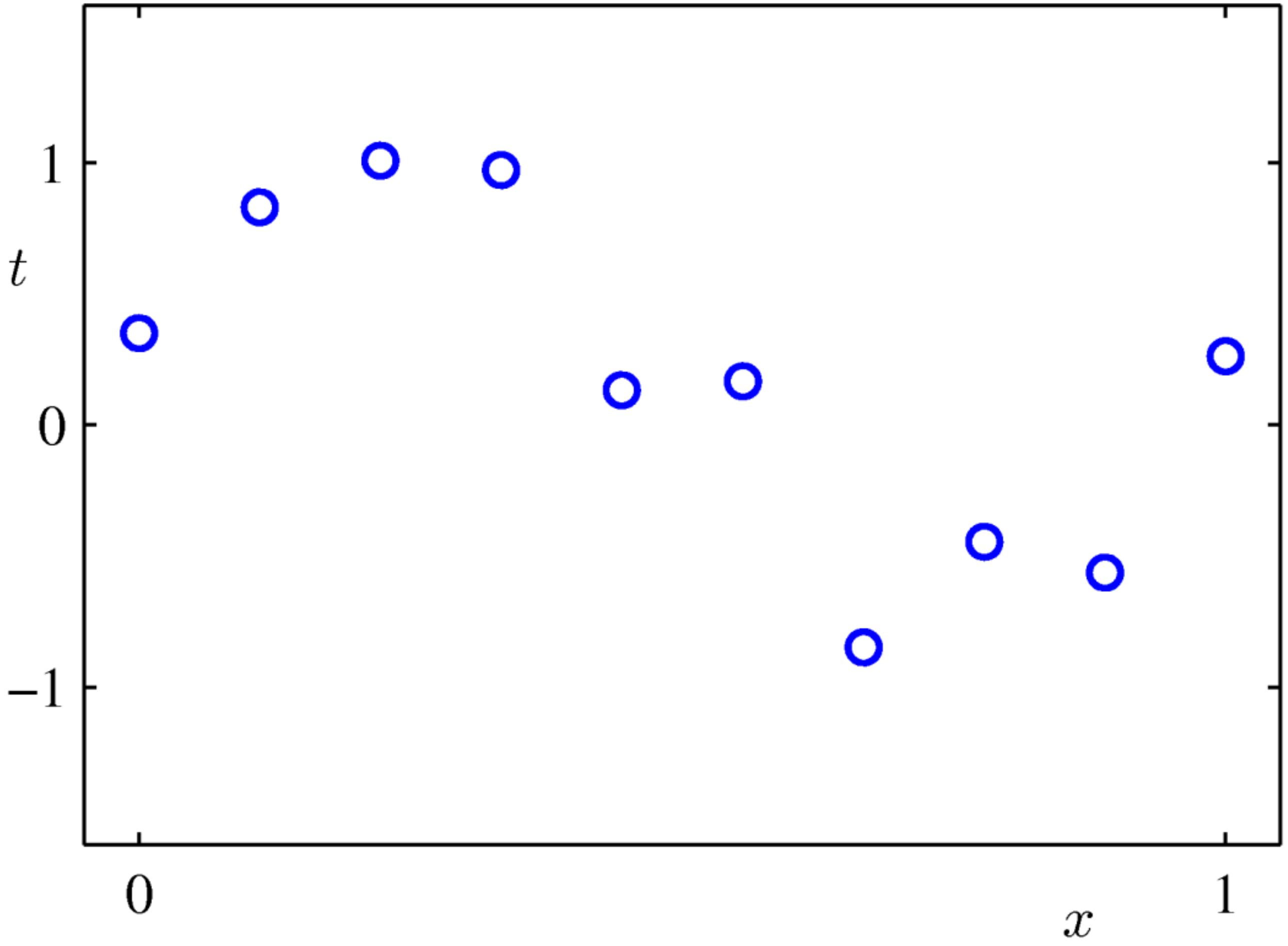
$$\underset{\beta_0, \beta_1}{\arg\min} \sum_{i}^{N} \left(y^{(i)} - \left(\beta_0 + \beta_1 x^{(i)} + \beta_2 (x^{(i)})^2 \right) \right)^2$$

- Algorithm: Gradient-descent algorithm

OVERFITTING & GENERALIZATION

Goodness of Fit

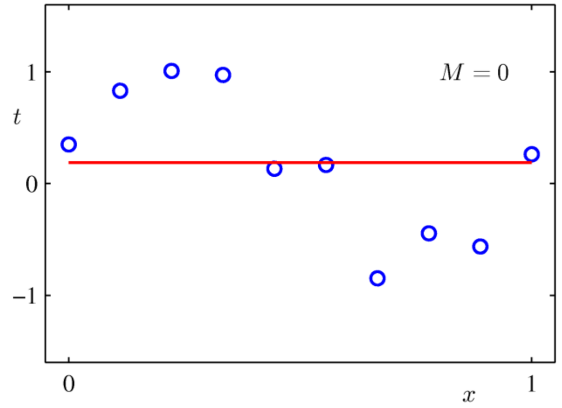
Of Which order polynomial will be best for the data?



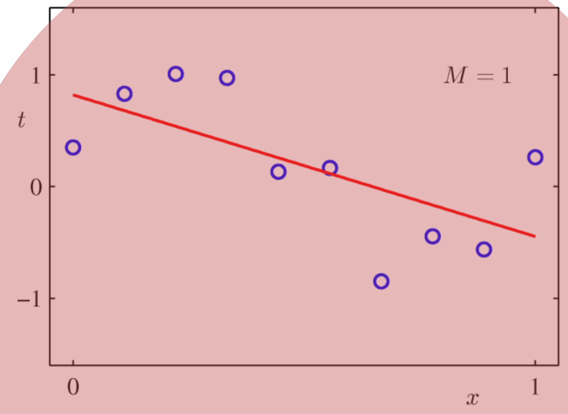
Overfitting vs Generalization

Of Which order polynomial will be best for the data?

The model which has the least error as much as possible



0^{th} order polynomial regression



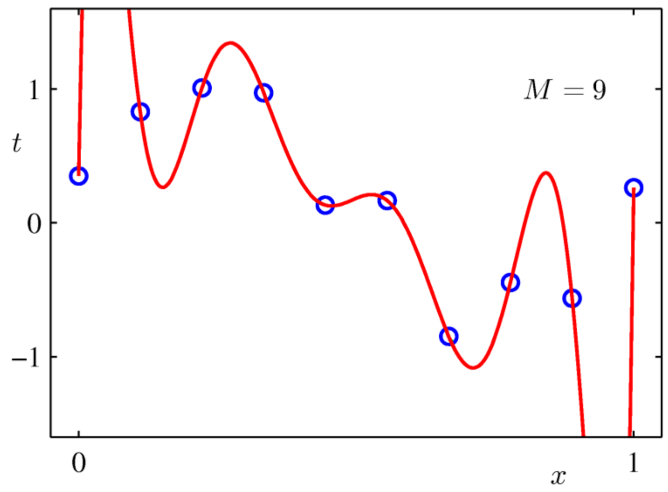
1^{st} order polynomial regression

This is better because it has less error

Overfitting vs Generalization

Of Which order polynomial will be best for the data?

- What about this?



9^{th} order polynomial regression

- This may be the BEST because the error is ZERO!!

Do you agree with this?

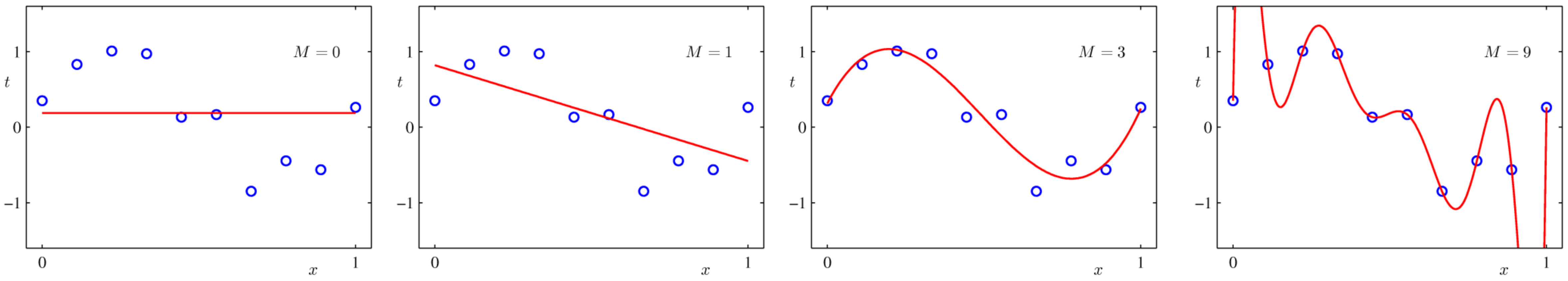
Overfitting vs Generalization

What is the purpose of Machine Learning?

Learning the given data as exactly as possible

vs

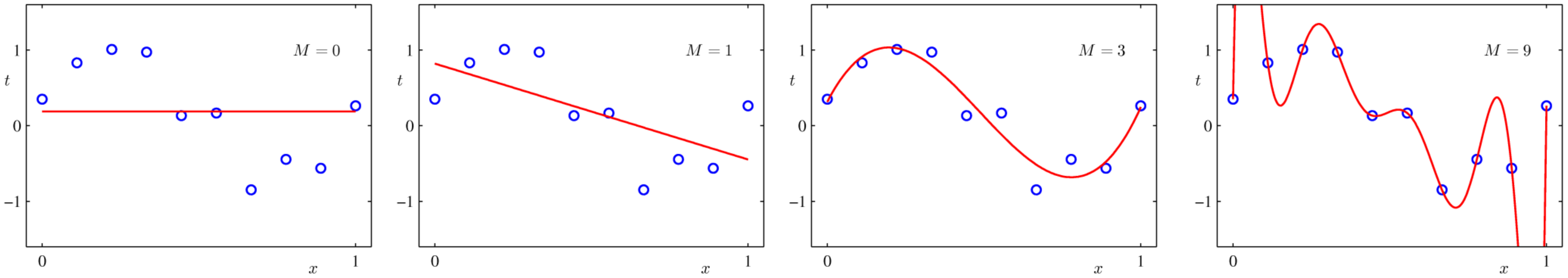
Predict the unknown data as exactly as possible based on the given data



Overfitting vs Generalization

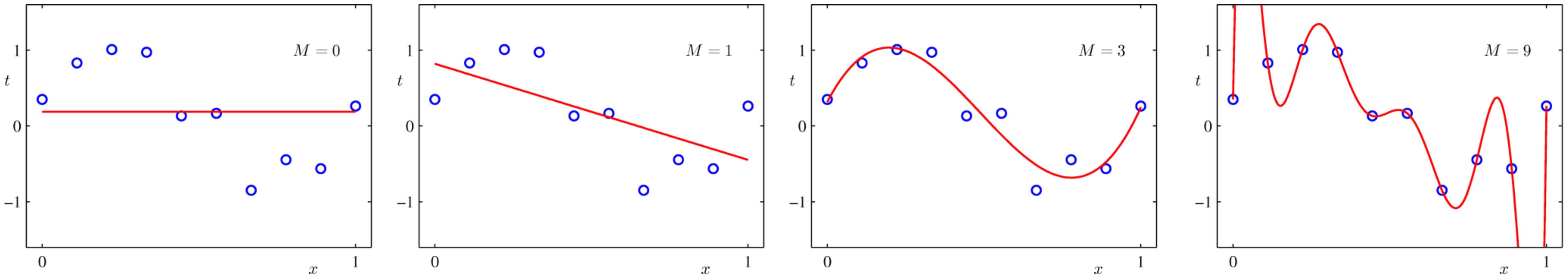
Then, which one looks best?

- As the order (M) increases,
  - the complexity of model increases
- As the complexity of model increases,
  - the model can more exactly learn the given data
  - However, the prediction accuracy does not necessarily increase



Model Evaluation

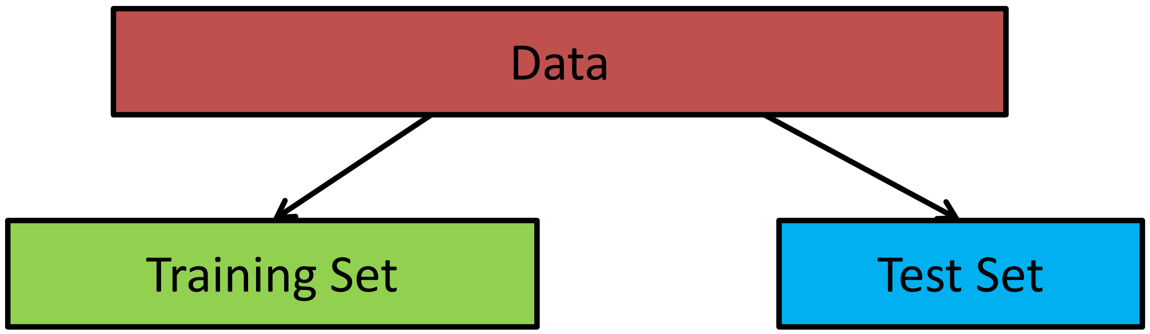
- Which model is best?
  - You may try several approaches and need to choose one
  - You may try several different parameters of a model and need to choose one
- Model Evaluations
  - Based on Training & Testing data set
  - Cross-Validation



Training Set and Test Set

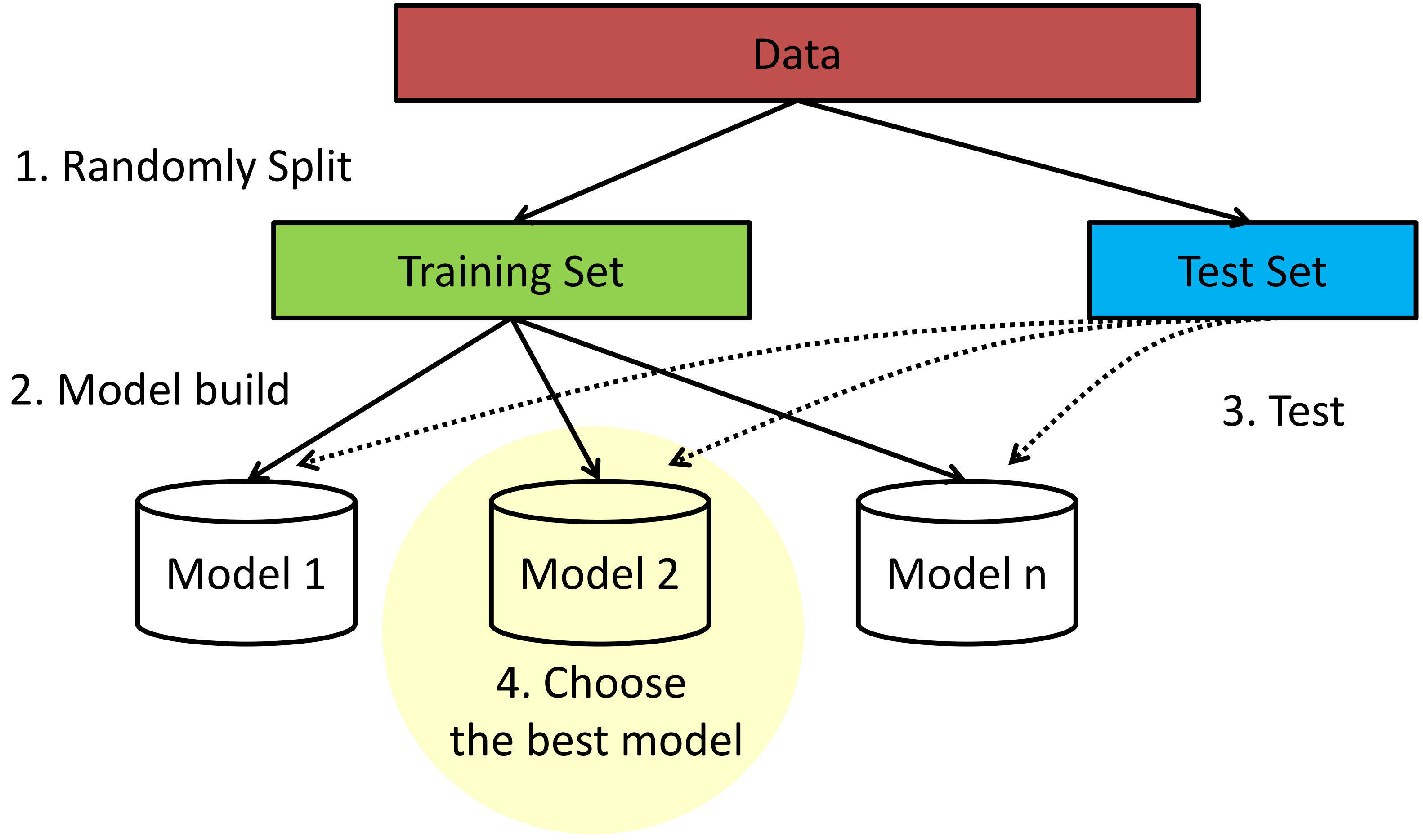
How to choose a good model

- Divide the given data into TRAINING set and TEST set
  - Training set and Test set should NOT overlap each other!!
  - Both need to be independent as much as possible
- With Training set, build various models
- With Test set, evaluate each model
- Choose the model which shows the best performance with Test set



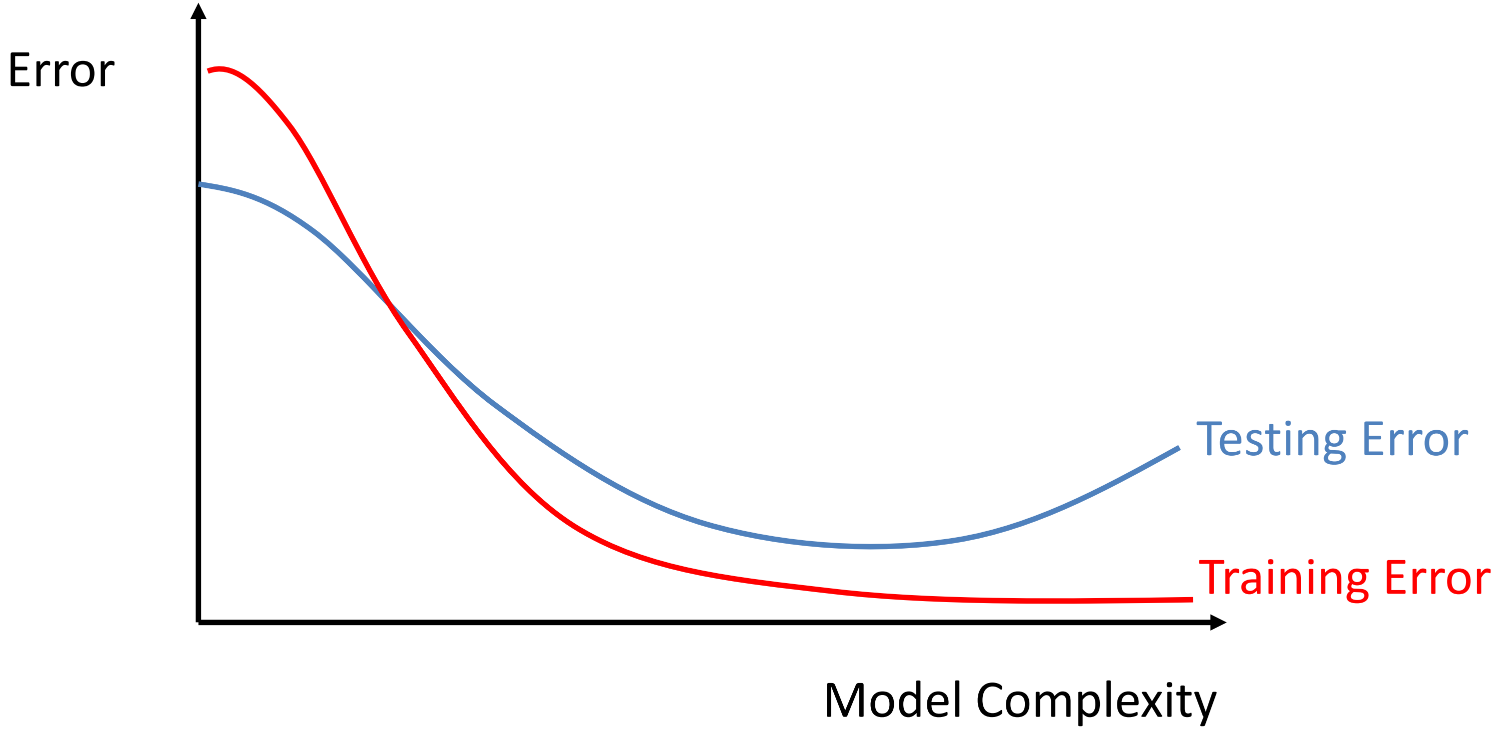
Training Set and Test Set

How to choose a good model



Training Set and Test Set

Performance Graph

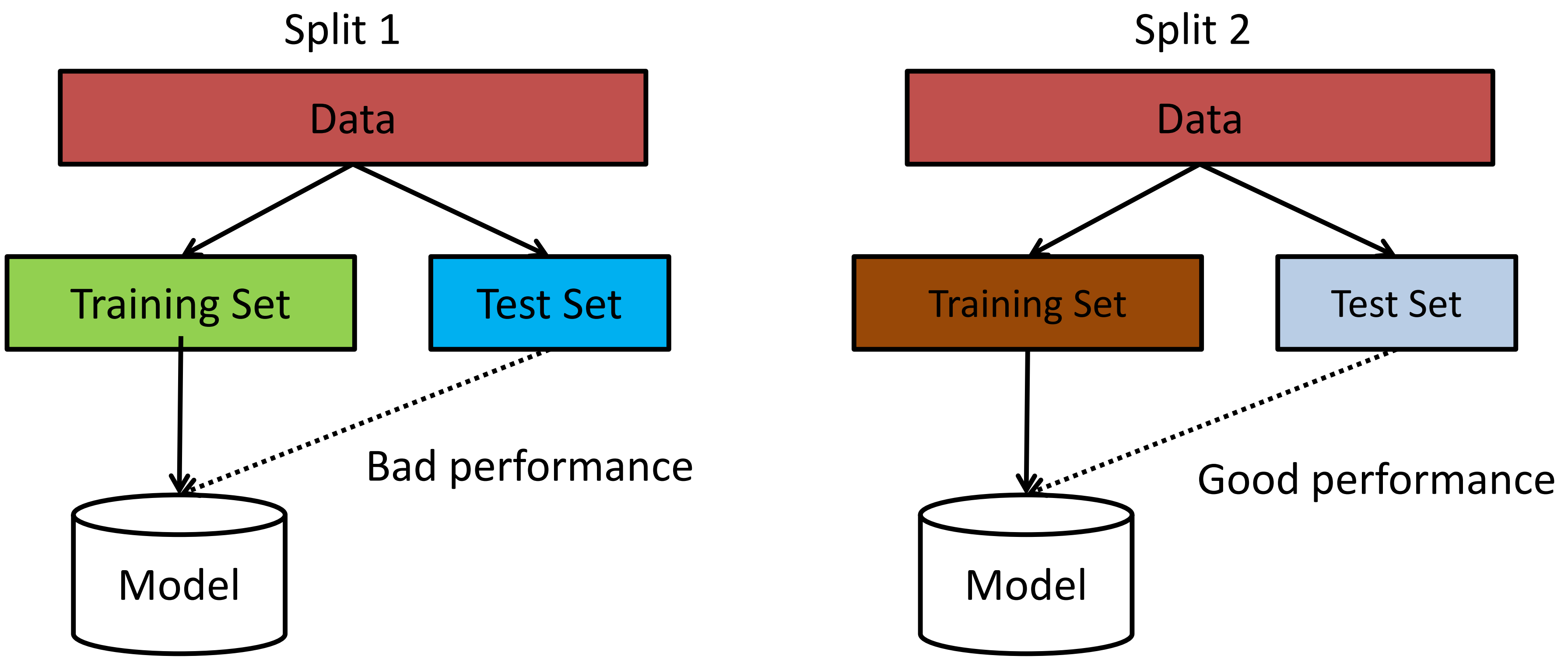


Training Set and Test Set

- Size of test set
  - 50~30% of given data
- Advantage
  - Simple & easy
- Disadvantage
  - Test set is not used for modeling building
  - Data is randomly split
    - Evaluation can be significantly different depending on data split

Training Set and Test Set

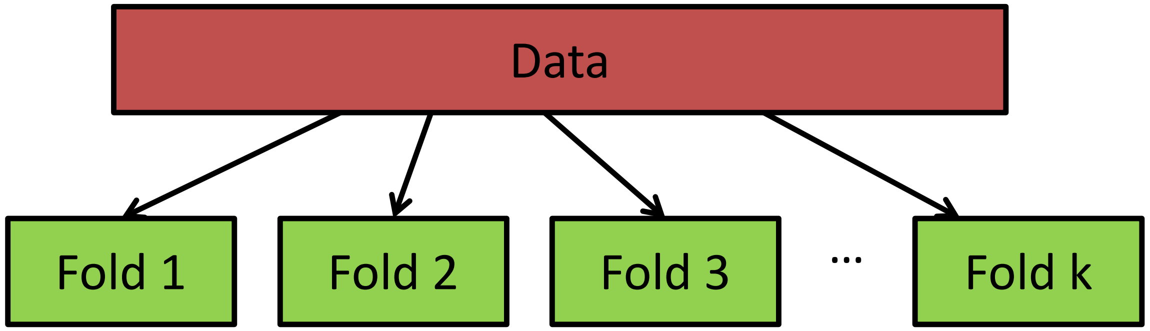
Data Waste & Random Split



Cross Validation

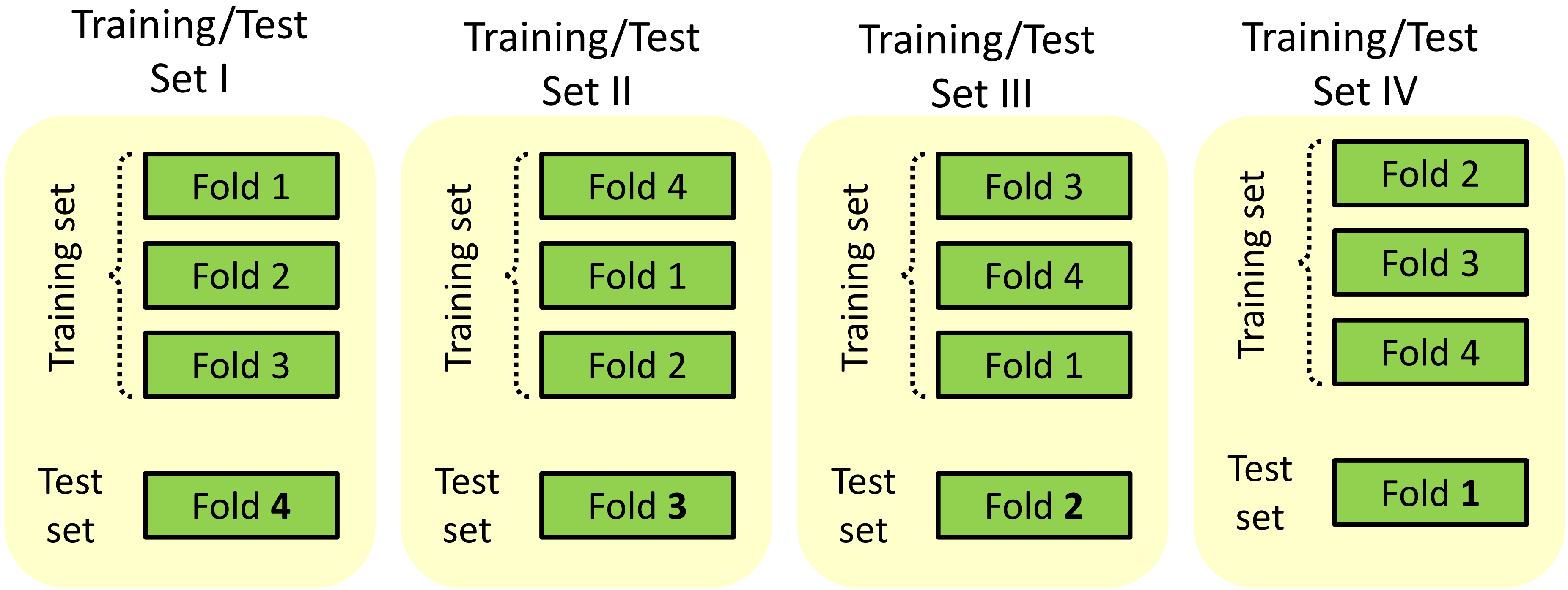
K-fold Cross Validation

- Split given data into *K* folds
- Folds should not overlap with each other
- Compose *k-1* training set and 1 test set with k folds
- Can reduce statistical variance



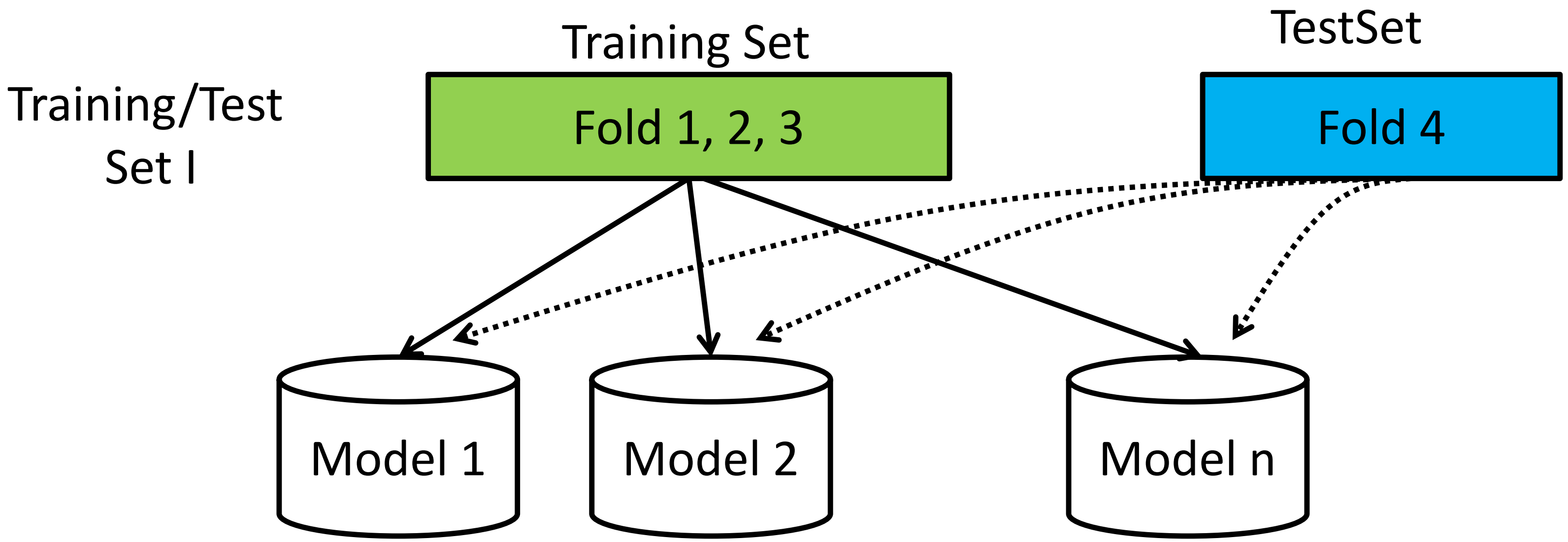
Cross Validation

Example: 4 fold cross validation



Choose a model by the average performance of 4 sets

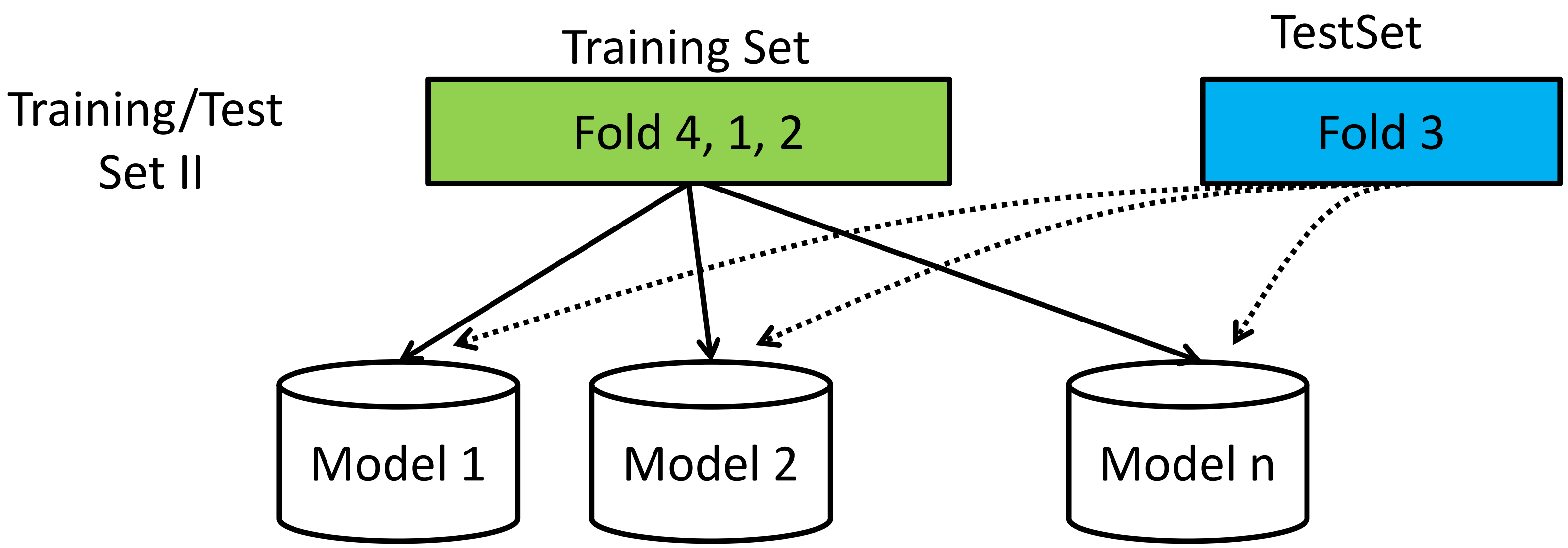
Cross Validation



Set I	3	4	…	5
Set II			…	
Set III			…	
Set IV			…	

Performance

Cross Validation

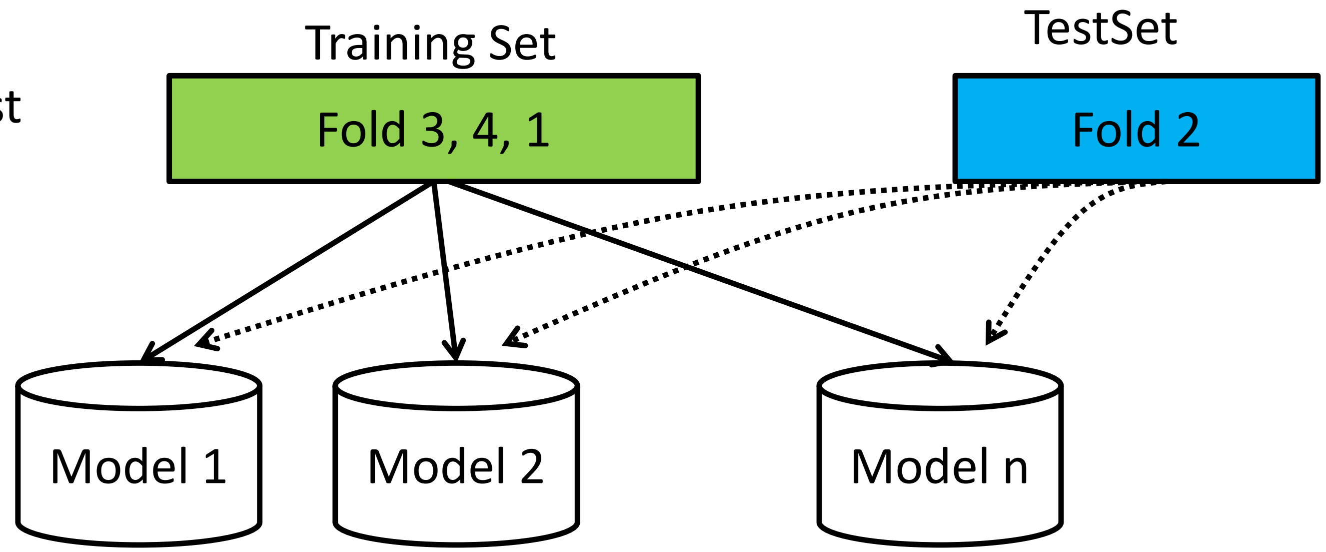


Set I	3	4	…	5
Set II	4	1	…	2
Set III			…	
Set IV			…	

Performance

Cross Validation

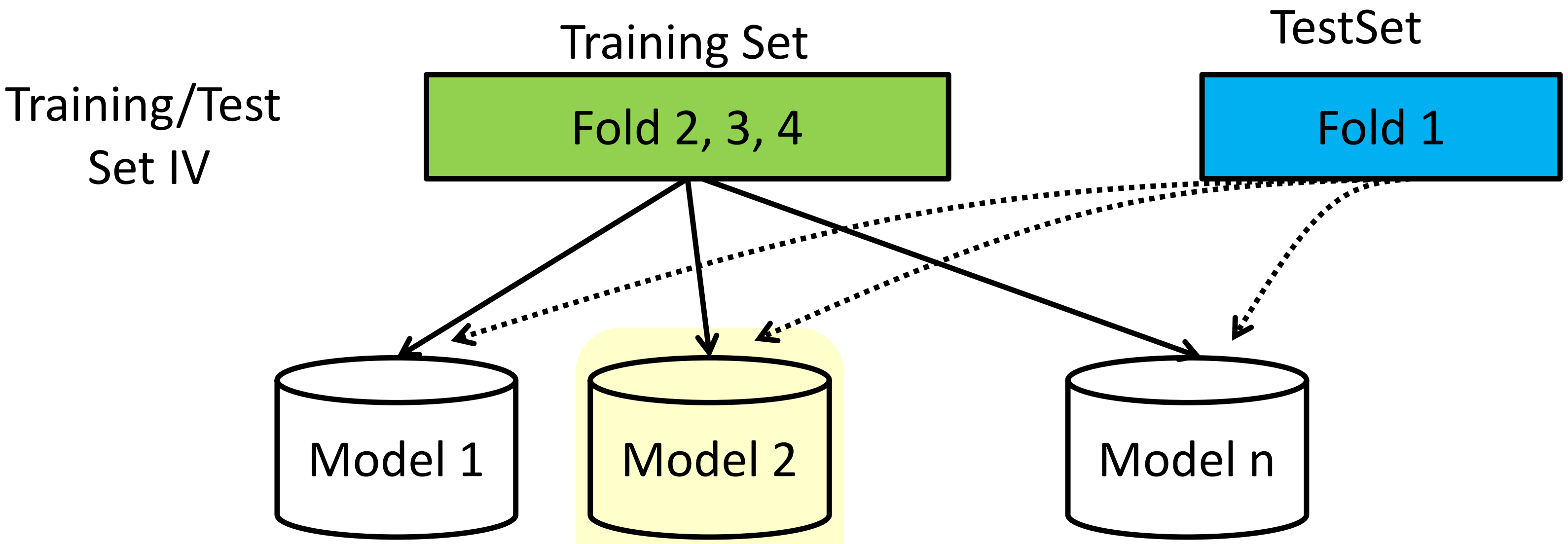
Training/Test
Set III



Set I	3	4	…	5
Set II	4	1	…	2
Set III	5	2	…	3
Set IV			…	

Performance

Cross Validation



Set I	3	4	…	5
Set II	4	1	…	2
Set III	5	2	…	3
Set IV	4	3	…	2

Performance

Cross Validation

- Summary
  - The data set is divided into *k* subsets, and the holdout method is repeated *k* times.
  - Each time, one of the *k* subsets is used as the test set and the other *k-1* subsets are put together to form a training set.
  - Then the average error across all *k* trials is computed.
  - The variance is reduced as *k* is increased.
- Advantage
  - Less dependent on how the data gets divided.
  - Every data point gets to be in a test set exactly once, and gets to be in a training set k-1 times.
- Disadvantage
  - Time