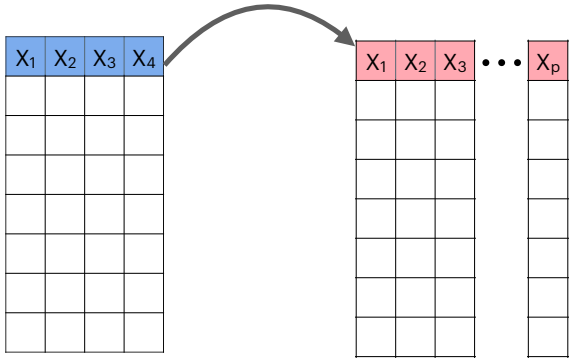
Linear Regression II

Lecture 3

Termeh Shafie

Feature Engineering



when do we do this and why?

Interactions

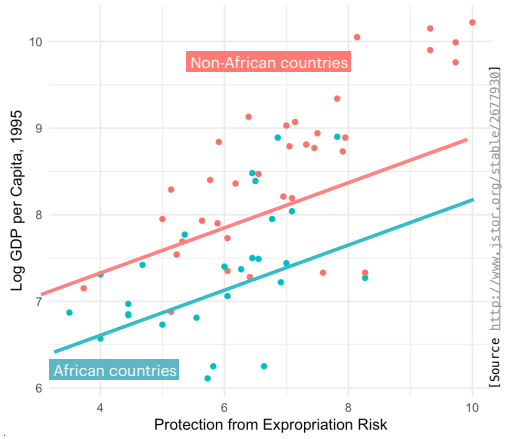
$$Y = \beta_0 + \beta_1 X + \beta_2 Z$$

log GDP | expropriation risk protection | African/Non-African countries

$$Z = 0 \implies Y = \beta_0 + \beta_1 X + \beta_2 Z = \beta_0 + \beta_1 X + \beta_2 \cdot 0 = (\beta_0) + (\beta_1) X$$

$$Z = 1 \implies Y = \beta_0 + \beta_1 x_1 + \beta_2 Z = \beta_0 + \beta_1 X + \beta_2 \cdot 1 = (\beta_0 + \beta_2) + (\beta_1) X$$

different intercepts | same slope



Interactions

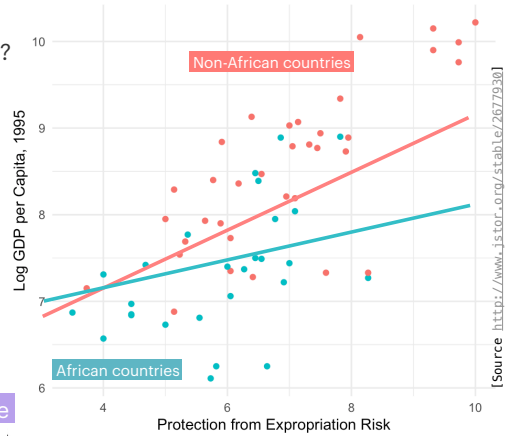
Is the relationship between **X** and **Y** different when you consider values of **Z**?

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ$$

$$Z = 0 \implies Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 ZX = \beta_0 + \beta_1 X + \beta_2 \cdot 0 + \beta_3 \cdot 0 = (\beta_0) + (\beta_1) X$$

$$Z = 1 \implies Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 ZX = \beta_0 + \beta_1 X + \beta_2 \cdot 1 + \beta_3 \cdot 1 \cdot X = (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X$$

different intercepts | different slope



Interactions

Income	Limit	Rating	Cards	Age	Education	Own	Student	Married	Region	Balance
14.891	3606	283	2	34	11	No	No	Yes	South	333
106.025	6645	483	3	82	15	Yes	Yes	Yes	West	903
104.593	7075	514	4	71	11	No	No	No	West	580
148.924	9504	681	3	36	11	Yes	No	No	West	964
55.882	4897	357	2	68	16	No	No	Yes	South	331
80.180	8047	569	4	77	10	No	No	No	South	1151

[Source: First six rows of dataset "Credit", ISLR2]

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 (X_1 \times X_2)$$

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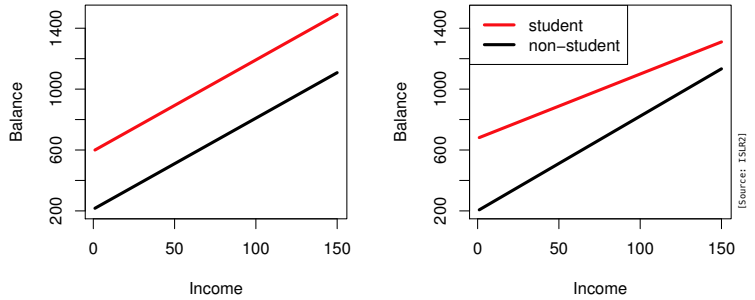
Interactions



$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 (X_1 \times X_2)$$

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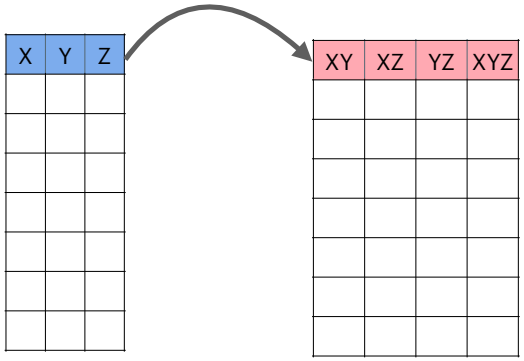
Interactions



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Dummy Variables: Adding a Bivariate Covariate

"one-hot encoding"

Income	Limit	Rating	Cards	Age	Education	Own	Student	Married	Region	Balance
14.891	3606	283	2	34	11	No	No	Yes	South	333
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[Source: First six rows of dataset "Credit", ISLR2]

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

0/1 -1/1

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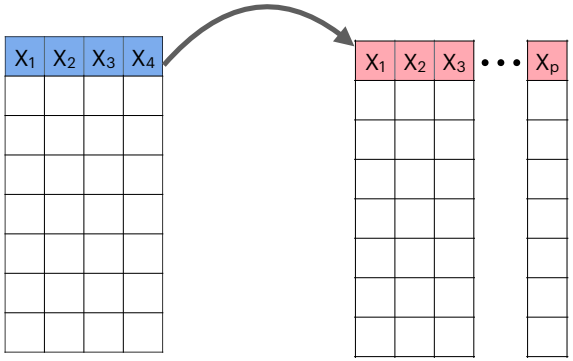
Feature Engineering



we'll return to feature engineering in our lecture on "non-liner" linear regression

Estimate $\hat{f}$ = Learn $\hat{f}$

$$Y = f(\boldsymbol{X}) + \varepsilon$$

sources of error:
irreducible error ε
reducible error $\hat{f}$

the squared error for a given estimate $\hat{f}$ is

$$E(\text{actual} - \text{predicted})^2 = E(Y - \hat{Y})^2$$

which factors as

$$E[f(\boldsymbol{X}) + \varepsilon - \hat{f}(\boldsymbol{X})]^2$$

$$\underbrace{[f(\boldsymbol{X}) - \hat{f}(\boldsymbol{X})^2]}_{\text{reducible}} + \underbrace{\text{Var}(\varepsilon)}_{\text{irreducible}}$$

until now, training data was the only data we considered
we compute reducible error (e.g. MSE) on the same data used to learn $\hat{f}$
let's change that!

Training

training data set

$$\{(y_1, x_1,), \ldots, (y_n, x_n))\}$$

used to find function q that minimizes **Training MSE**

$$\hat{f} = \arg\min_q MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - q(x_i))^2$$

Testing

testing data sets (unseen)

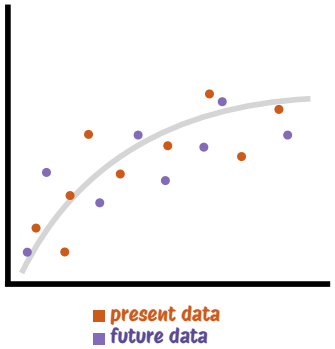
$$(y_0, x_0)$$

used to compute **Test MSE**

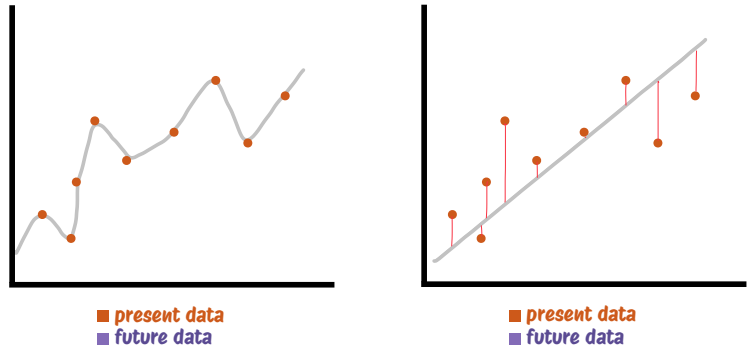
$$E[y_0 - \hat{f}(x_0)^2]$$

`often not so closely related`

Training and Testing



Training and Testing



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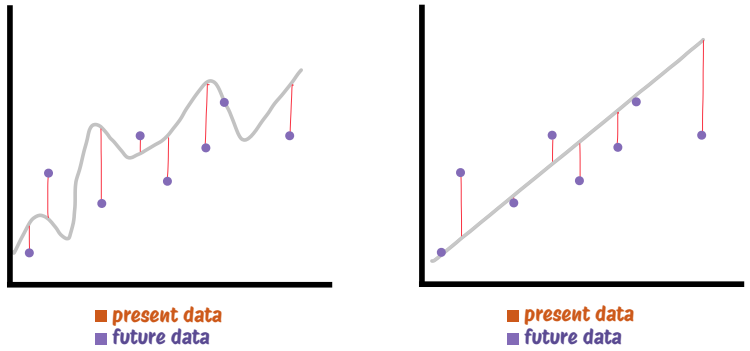
Training and Testing



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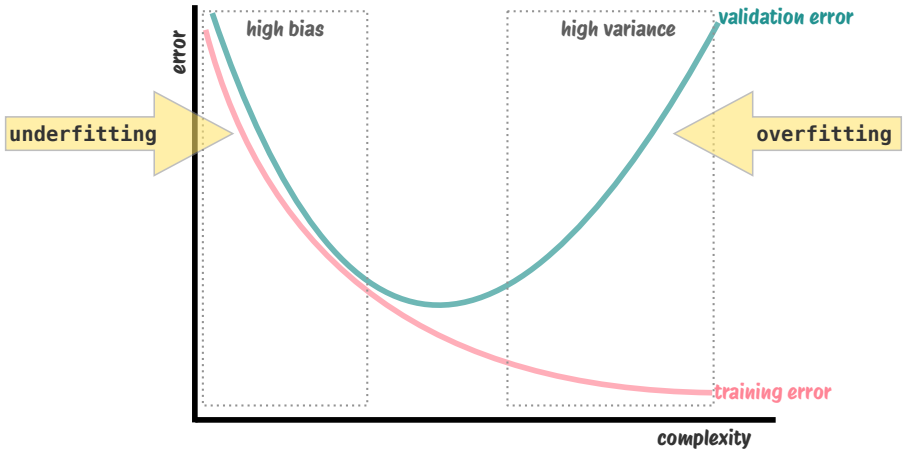
Bias Variance Trade-Off



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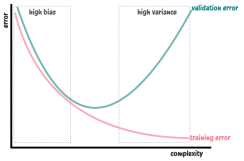
Formalizing Bias Variance Trade-Off



$$Y = f(X) + \varepsilon$$

Sources of Error:

1. Irreducible: ε
2. Reducible: $\hat{f}(x)$ not similar to $f(x)$

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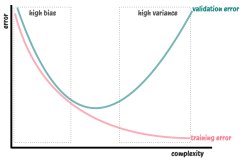
Formalizing Bias Variance Trade-Off

Expected **test MSE**

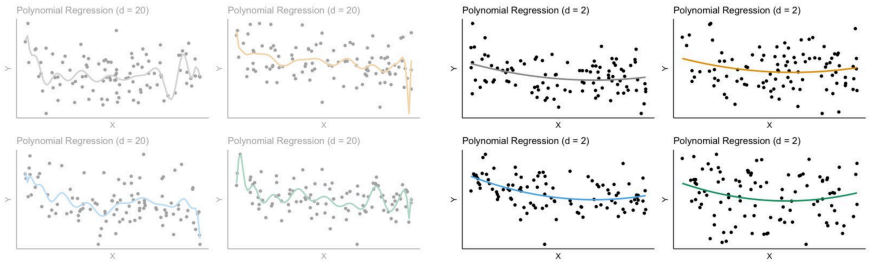


$$\underbrace{E\left(y_0 - \hat{f}(x_0)\right)^2}_{\text{expected MSE at } x_0 \text{ if we repeatedly estimated } f(x) \text{ with different training sets}} = \text{Var}(\hat{f}(x_0)) + \left[\text{bias}(\hat{f}(x_0))\right]^2 + \underbrace{\text{Var}(\varepsilon)}_{\text{irreducible error}}$$

Formalizing Bias Variance Trade-Off

Expected **test MSE**

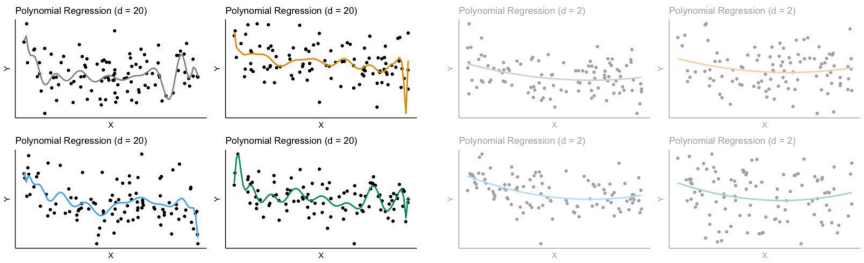
$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + \left[\text{bias}(\hat{f}(x_0))\right]^2 + \text{Var}(\varepsilon)$$



Formalizing Bias Variance Trade-Off

Expected **test MSE**

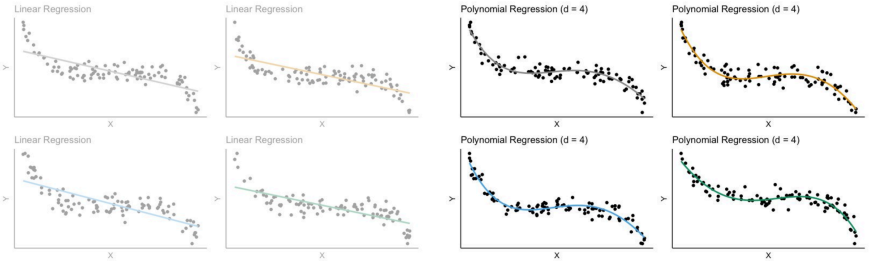
$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + \left[\text{bias}(\hat{f}(x_0))\right]^2 + \text{Var}(\varepsilon)$$



Formalizing Bias Variance Trade-Off

Expected **test MSE**

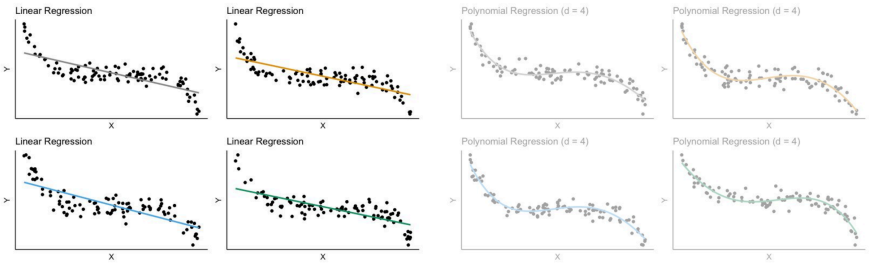
$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + \left[\text{bias}(\hat{f}(x_0))\right]^2 + \text{Var}(\varepsilon)$$



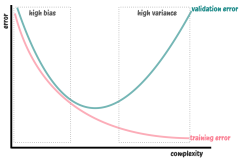
Formalizing Bias Variance Trade-Off

Expected **test MSE**

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + \left[\text{bias}(\hat{f}(x_0))\right]^2 + \text{Var}(\varepsilon)$$



Formalizing Bias Variance Trade-Off

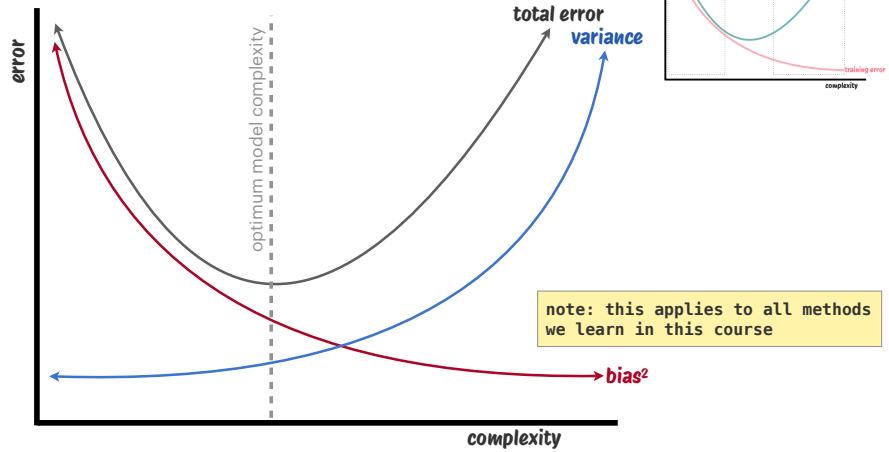


Expected **test MSE**

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \underbrace{\text{Var}(\hat{f}(x_0))}_{\text{variance increases with complexity}} + \underbrace{\left[\text{bias}(\hat{f}(x_0))\right]^2}_{\text{bias decreases with complexity}} + \text{Var}(\varepsilon)$$

[try it out: https://floswald.shinyapps.io/bias_variance/

Bias Variance Trade-Off



note: this applies to all methods we learn in this course

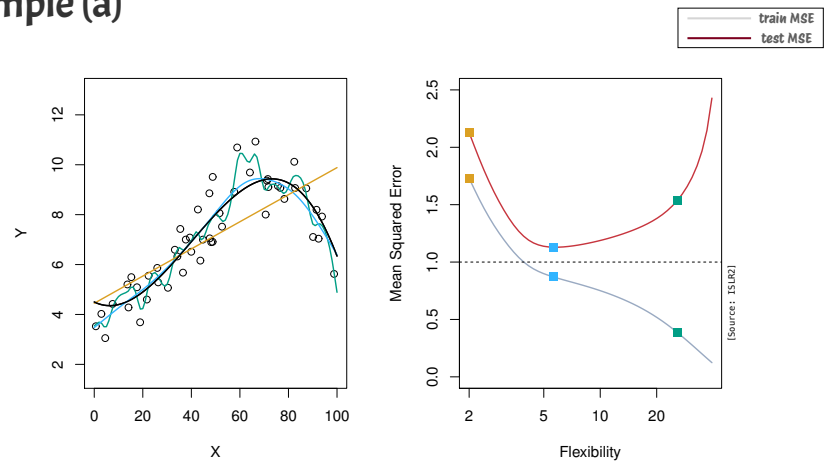
Bias Variance Trade-Off

There commonly used methods for finding the optimal model between simple and complicated are

- regularization
- boosting
- bagging

(the key here is **model validation**)

Example (a)



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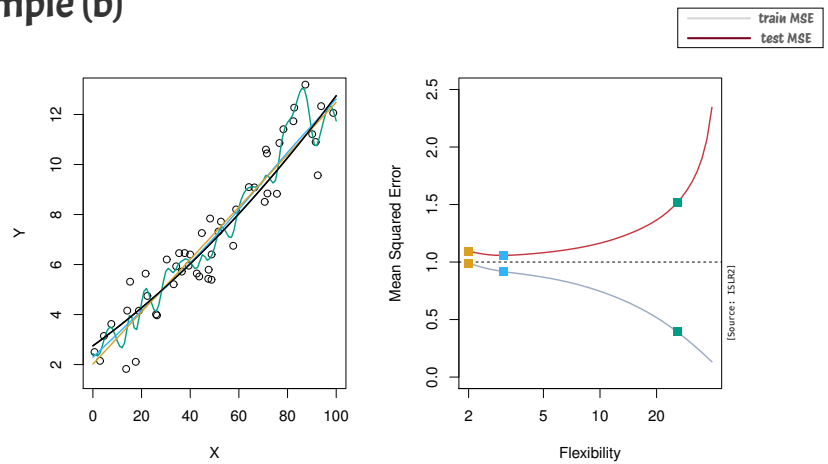
Example (b)



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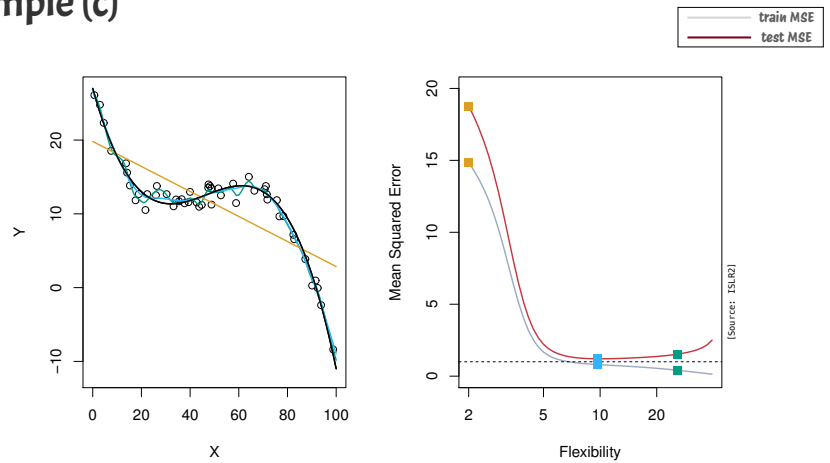
Example (c)



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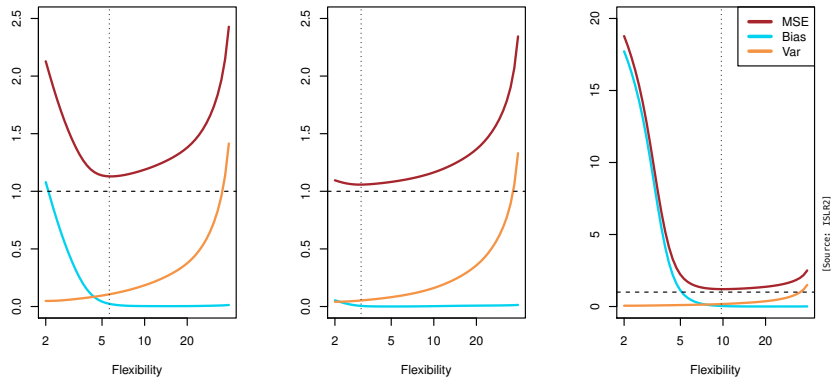
Example (a)-(c): Bias Variance Trade-Off



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A Simulation Example

Estimate the conditional mean of Y given $\boldsymbol{X}$

$$Y = f(\boldsymbol{X}) + \varepsilon$$

Assume probability model:

$$Y = 1 - 2x - 3x^2 + 5x^3 + \varepsilon$$

where $\varepsilon \sim \mathrm{N}(0,\sigma^2)$

Alternatively:

$$Y \mid X \sim \mathrm{N}(1 - 2x - 3x^2 + 5x^3, \sigma^2) \quad \text{or}$$

$$\mu(x) = E[Y \mid \boldsymbol{X} = \boldsymbol{x}] = 1 - 2x - 3x^2 + 5x^3$$

conditional mean is a **linear combination of the feature variables**

note: the true probability model and thus also $\mu(x)$ are often not known!

A Simulation Example

1. Simulate data from assumed probability model

$$Y = 1 - 2x - 3x^2 + 5x^3 + \varepsilon$$

2. Fit three models to data:

I. Degree 1 Polynomial $\mu(x) = \beta_0 + \beta_1 x$

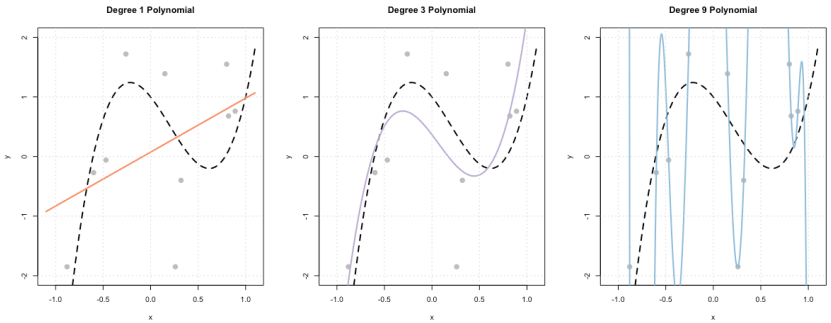
II. Degree 3 Polynomial $\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

III. Degree 9 Polynomial $\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \ldots + \beta_9 x^9$

ENTER R

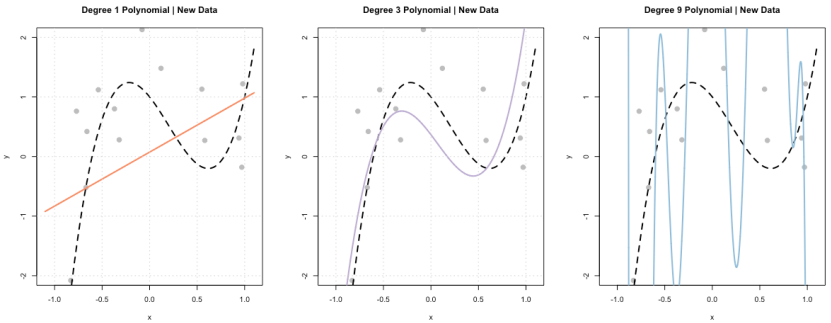
A Simulation Example

- How close is the estimated regression (mean) function to the data?
- How close is the estimated regression (mean) function to the true regression (mean) function?



A Simulation Example

Generate new data and check...



Some Do Not's!

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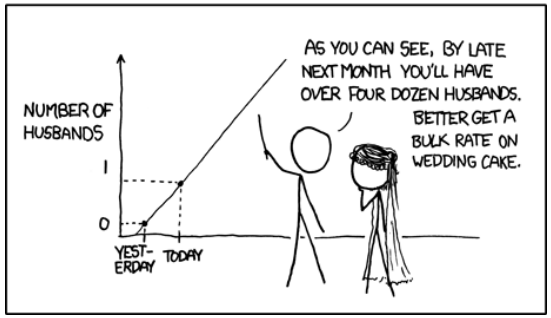
Extrapolation



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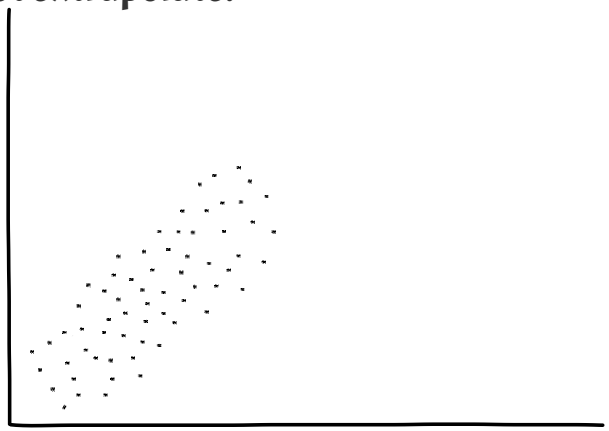
Do not extrapolate!



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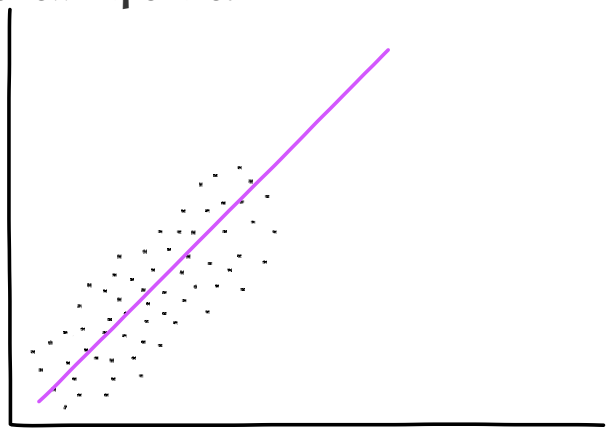
Do not extrapolate!



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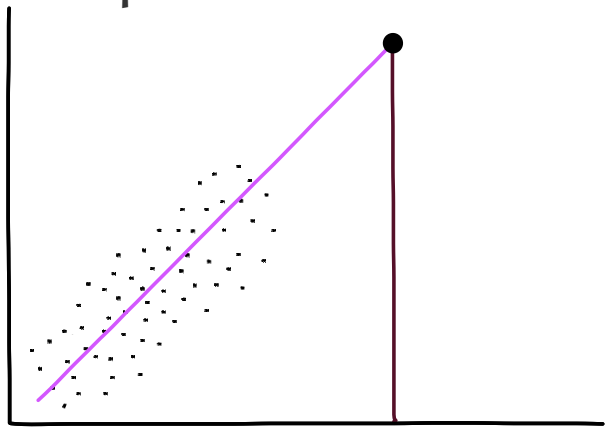
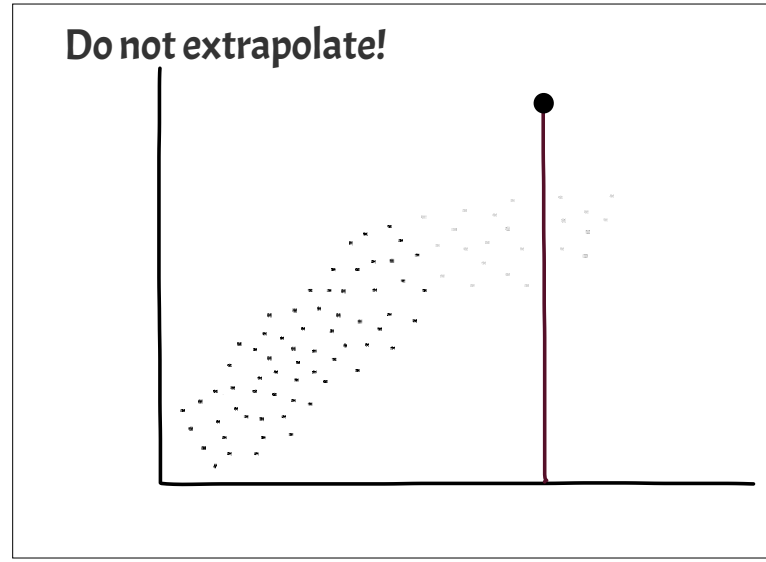
Do not extrapolate!





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Do not extrapolate!

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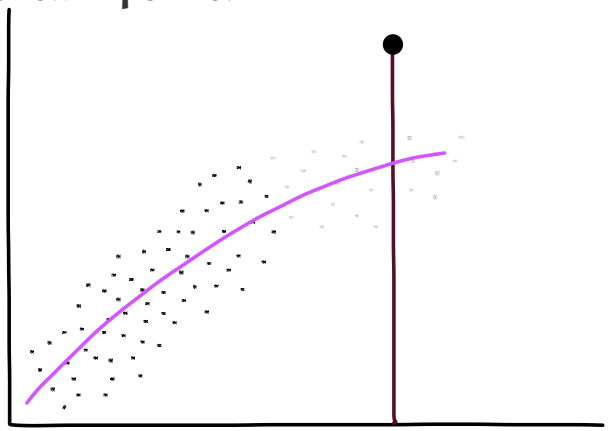
Do not extrapolate!



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Do not fit model on test data!

In addition to the train-test split,
we will later split the data into validation set

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This Week's Practical

Linear Regression: Evaluate Model Performance