Linear Regression II

Lecture 3

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Assessing Model Fit

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

signal noise

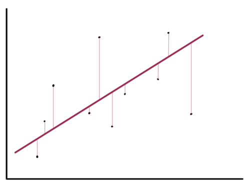
Loss Function

a metric for model performance, lower values are better

(for now we pretend that we have never heard of or seen cross-validation)

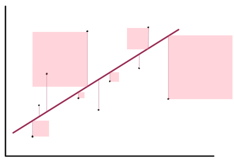
Assessing Model Fit

$$\text{MAE} = \frac{1}{n}\sum_i |\text{actual}_i - \text{predicted}_i|$$



Assessing Model Fit

$$\text{MSE} = \frac{1}{n}\sum_i (\text{actual}_i - \text{predicted}_i)^2$$

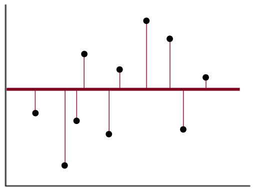


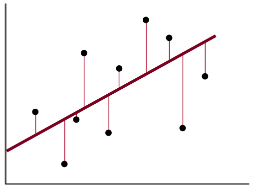
$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_i (\text{actual}_i - \text{predicted}_i)^2}$$

...what about a measure that is always on the same scale?

Assessing Model Fit

$$R^2 = 1 - \frac{\sum_i (\text{actual}_i - \text{predicted}_i)^2}{\sum_i (\text{actual}_i - \text{average})^2}$$





Assessing Model Fit

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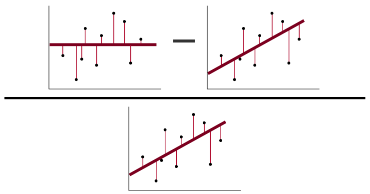

Assessing Model Fit

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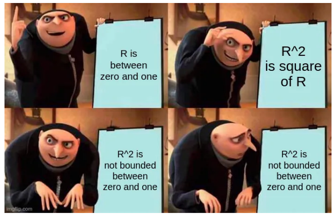
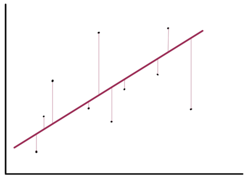


Assessing Model Fit

$$\text{MAPE} = \frac{1}{n}\sum_i \left| \frac{\text{actual}_i - \text{predicted}_i}{\text{actual}_i} \right|$$



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

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

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

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

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

until now, training data was the only data we considered
we compute reducible error (or 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)

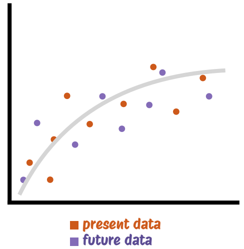
$$(y_0, x_0)$$

used to compute **Test MSE**

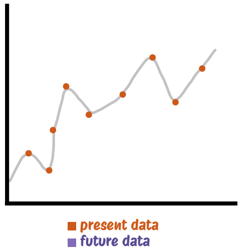
$$E[y_0 - \hat{f}(x_0)^2]$$

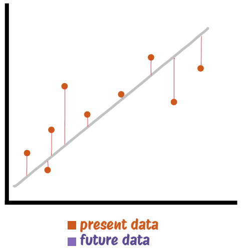
often not so closely related

Training and Testing

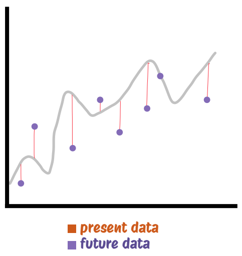


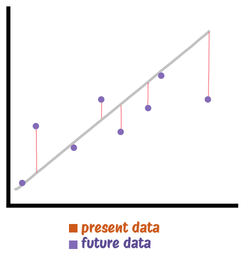
Training and Testing



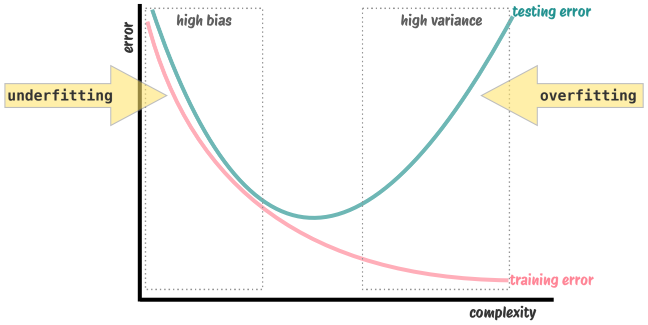


Training and Testing

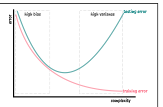




Bias Variance Trade-Off



Formalizing Bias Variance Trade-Off

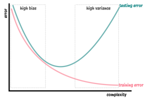


Expected test MSE

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

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

Formalizing Bias Variance Trade-Off

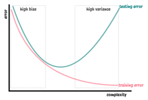


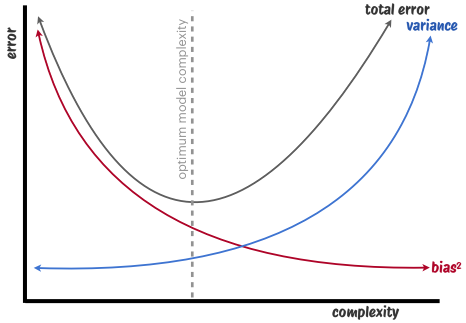
Expected **test MSE**

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

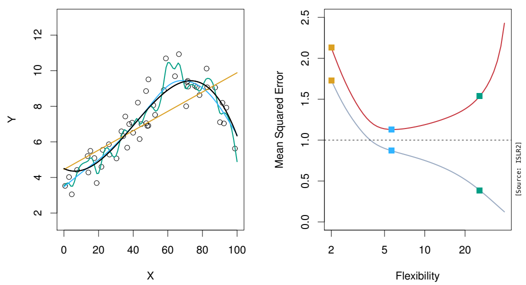
[try it out: https://floswald.shinyapps.io/bias_variance/]

Bias Variance Trade-Off

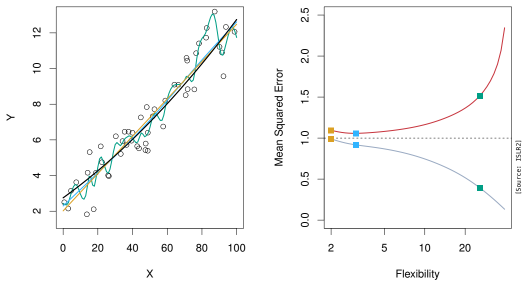




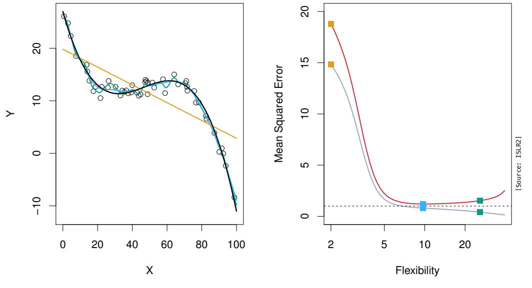
Example (a)



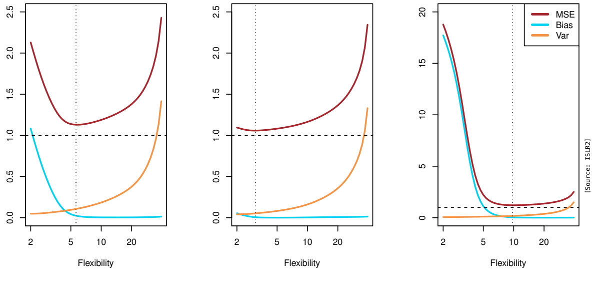
Example (b)



Example (c)



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



A Simulation Example

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

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

Assume probability model:

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

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

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

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

2. Fit three models to data:

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

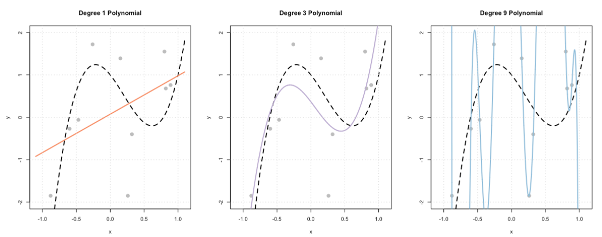
   II. Degree 3 Polynomial $\mu(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

   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

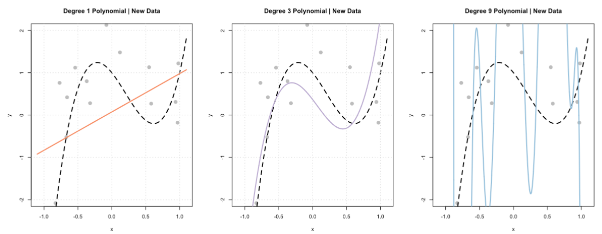
A Simulation Example

- 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?



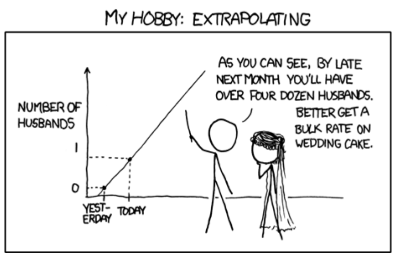
A Simulation Example

Generate new data and check...

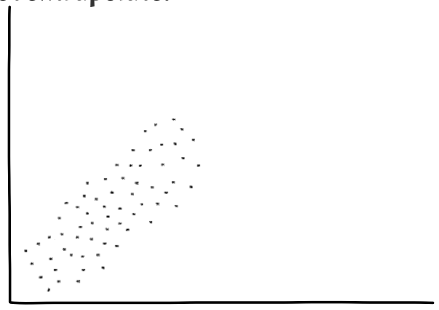


Some Do Not's!

Extrapolation



Do not extrapolate!



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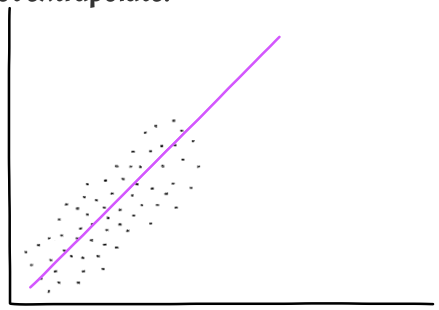

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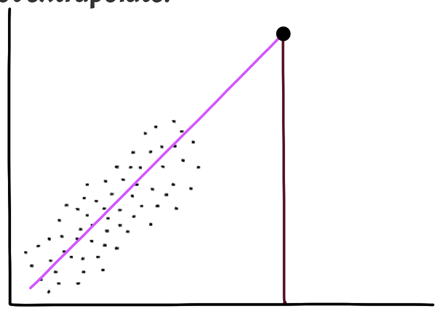

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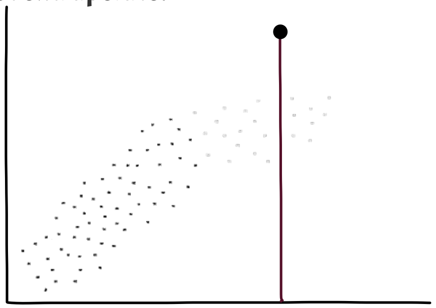

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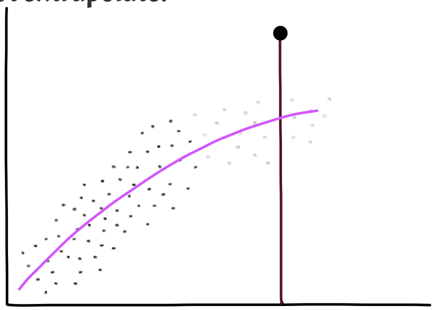

Do not fit model on test data!

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

This Week's Practical

Linear Regression: Evaluate Model Performance