Ch 5.1.1-2: Leave One Out Cross-validation Lecture 12 - CMSE 381

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:

Dept of Computational Mathematics, Science & Engineering

Friday, Sep 26, 2025

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Announcements

Last time:

Exam

Announcements:

- Exam 1 grades.... hopefully soon
- HW #4 will be posted later next week.
 - Changed Deadline! Due Sunday Oct 12

CMSE381 F2025 Schedule : Schedule

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	M	9/22	Project Day & Review						
	W	9/24	Midterm #1						
12	F	9/26	Leave one out CV	5.1.1, 5.1.2					
13	М	9/29	k-fold CV	5.1.3					
14	W	10/1	More k-fold CV	5.1.4-5					
15	F	10/3	k-fold CV for classification	5.1.5					
16	М	10/6	Subset selection	6.1					
17	W	10/8	Shrinkage: Ridge	6.2.1					
18	F	10/10	Shrinkage: Lasso	6.2.2	HW #4 Due				
19	М	10/13	PCA	6.3	Sun 10/12				
20	W	10/15	PCR	6.3					
	F	10/17	Review						
	М	10/20	Fall Break						
	W	10/22	Midterm #2						
21	F	10/24	Polynomial & Step Functions	7.1-7.2	HW #5 Due Sun 10/28				
22	М	10/27	Step Functions; Basis functions; Start Splines	7.2-7.4					
23	W	10/29	Regression Splines	7.4					

2/21

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Covered in this lecture

- Validation Set
- LOO CV

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Section 1

Validation set

What's the problem?

- How well is my ML method doing? *Model Assessment*
- Which method is best for our data?
- How many features should I use? Which ones? Model selection
- What is the uncertainty in the learned parameters?

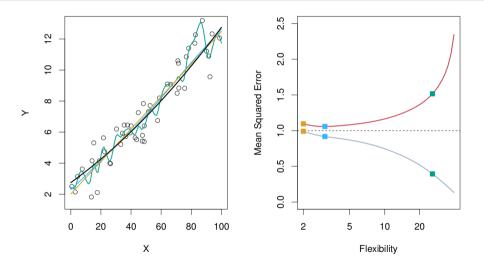
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Training Error vs Testing Error

Training Error

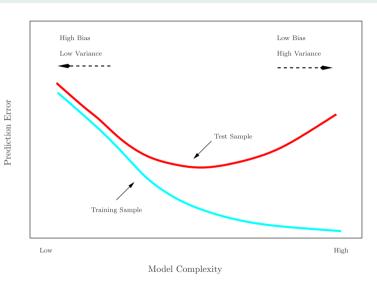
Testing Error

Throw-back



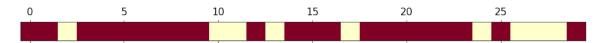
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Model tradeoffs



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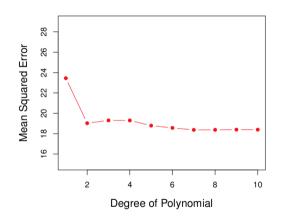
Validation set approach



- Divide randomly into two parts:
 - Training set
 - Validation/Hold-out/Testing set
- Fit model on training set
- Use fitted model to predict response for observations in the test set
- Evaluate quality (e.g. MSE)

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Example with the auto data



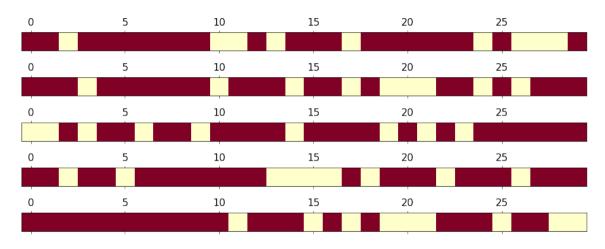
Predicting mpg using horsepower:

$$mpg = \beta_0 + \beta_1 hp + \beta_2 hp^2 + \dots + \beta_p hp^p$$

10 / 21

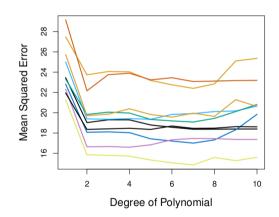
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Rinse and repeat



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Again example with auto data



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Coding example in jupyter notebook

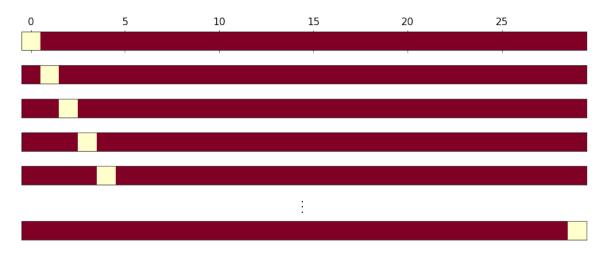
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Section 2

Leave-One-Out Cross-Validation (LOOCV)

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The idea



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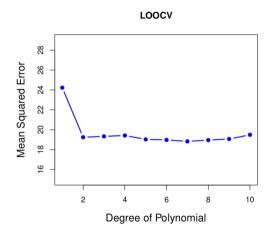
The idea in mathy words

- Remove (x_1, y_1) for testing.
- Train the model on n-1 points: $\{(x_2, y_2), \dots, (x_n, y_n)\}$
- Calculate $MSE_1 = (y_1 \hat{y}_1)^2$
- Remove (x_2, y_2) for testing.
- Train the model on n-1 points: $\{(x_1, y_1), (x_3, y_3), \dots, (x_n, y_n)\}$
- Calculate $MSE_2 = (y_2 \hat{y}_2)^2$
- Rinse and repeat

Return the score:

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \mathrm{MSE}_{i}$$

Again example with auto data



Do the LOOCV coding section

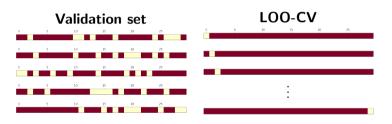
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LOOCV Pros and Cons

Advantages:

Disadvantages:

TL;DR



LOO-CV Score

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \text{MSE}_i$$

20 / 21

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Next time

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