Ch 5.1.3-4: k-Fold Cross-Validation

Lecture 13 - CMSE 381

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Mon, Sep 29, 2025

Announcements

Last time:

- Validation Set
- LOOCV

CMSE381_F2025_Schedule : Schedule

	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	M	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	M	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 Sun 10/12
19	M	10/13	PCA	6.3	
20	W	10/15	PCR	6.3	
	F	10/17	***Review***		
	M	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	M	10/27	Step Functions; Basis functions; Start Splines	7.2-7.4	
23	W	10/29	Regression Splines	7.4	

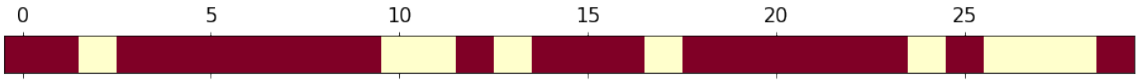
Covered in this lecture

- k-fold CV

Section 1

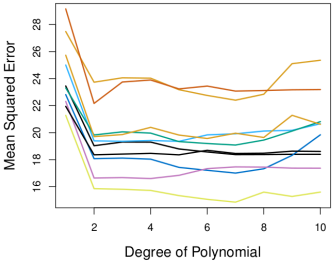
Last time

Validation set approach

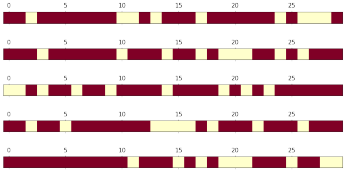


- Divide randomly into two parts:
  - Training set
  - Validation/Hold-out/Testing set
- Fit model on training set
- Use fitted model to predict response for observations in the test set
- Evaluate quality (e.g. MSE)

Problems



Ex. Predict `mpg` using `horsepower`



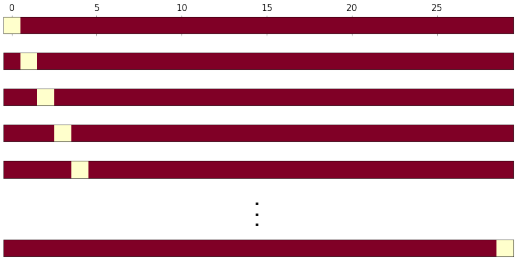
- Highly variable results, no consensus about the error
- Tends to overestimate test error rate

Leave One Out CV (LOOCV)

- Remove (x_1, y_1) for testing.
- Train the model on $n-1$ points: $\{(x_2, y_2), \cdots, (x_n, y_n)\}$
- Calculate $\mathrm{MSE}_1 = (y_1 - \hat{y}_1)^2$

- Remove (x_2, y_2) for testing.
- Train the model on $n-1$ points: $\{(x_1, y_1), (x_3, y_3), \cdots, (x_n, y_n)\}$
- Calculate $\mathrm{MSE}_2 = (y_2 - \hat{y}_2)^2$

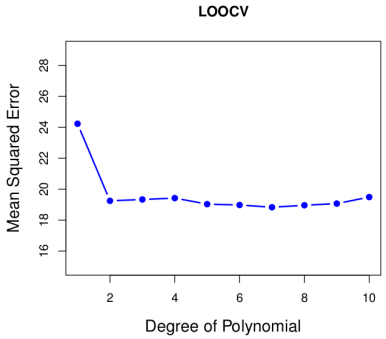
- Rinse and repeat



Return the score:

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

Pros and Cons

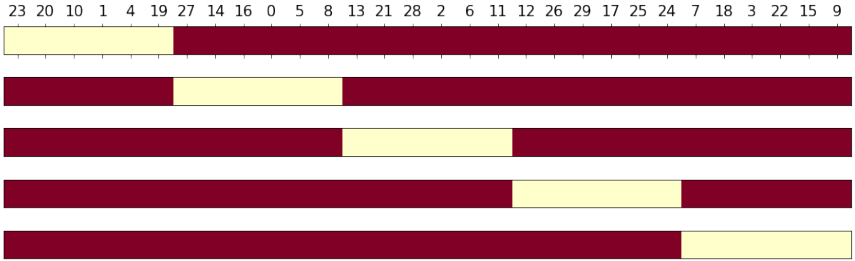


- No variance
- Higher computation cost

Section 2

k-Fold CV

The idea


23 20 10 1 4 19 27 14 16 0 5 8 13 21 28 2 6 11 12 26 29 17 25 24 7 18 3 22 15 9

Mathy version

- Randomly split data into k-groups (folds)
- Approximately equal sized. For the sake of notation, say each set has ℓ points

- Remove ith fold U_i and reserve for testing.
- Train the model on remaining points
- Calculate $\mathrm{MSE}_i = \frac{1}{\ell} \sum_{(x_j, y_j) \in U_i} (y_j - \hat{y}_j)^2$

- Rinse and repeat

Return

$$CV_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \mathrm{MSE}_i$$

Test your understanding: PollEv

By hand first!

There are 10 students in the class, and we have data points for each. They have already been randomly permuted below. Write down the training/testing sets for a 3-fold CV

- Damien
- Alice
- Greta
- Jasmin
- Benji
- Inigo
- Frank
- Carina
- Enrique
- Hubert

Fold 1 **Fold 2** **Fold 3**

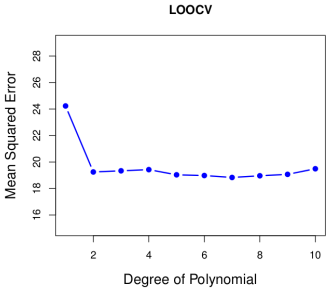
Coding - Building k-fold CV

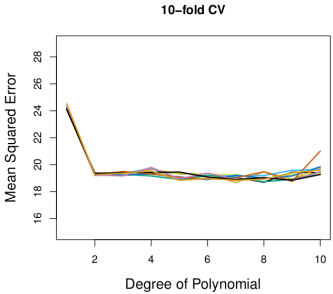
Pros and Cons

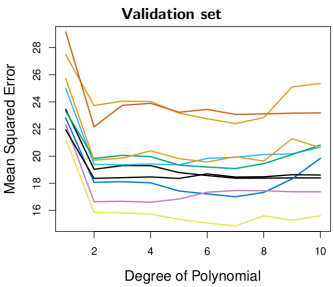
Pros:

Cons:

Comparison


LOOCV
Mean Squared Error
16
18
20
22
24
26
28
2
4
6
8
10
Degree of Polynomial


10–fold CV
Mean Squared Error
16
18
20
22
24
26
28
2
4
6
8
10
Degree of Polynomial


Validation set
Mean Squared Error
16
18
20
22
24
26
28
2
4
6
8
10
Degree of Polynomial

Next time

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