Day 4: Resampling Methods

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Introduction to Statistical Learning

Resampling Methods

- Whenever we have a dataset we can sample subsets thereof - this is what *re*-sampling is. This allows us to rely in a systematic way on training and test datasets.
    - Allows to get a better estimate of the true error
    - Allows to pick the optimal model
- Sampling is computationally taxing but nowadays of little concern - nevertheless, time may be a factor.
- We will look today specifically at two approaches:
    - Cross-validation
    - Bootstrap

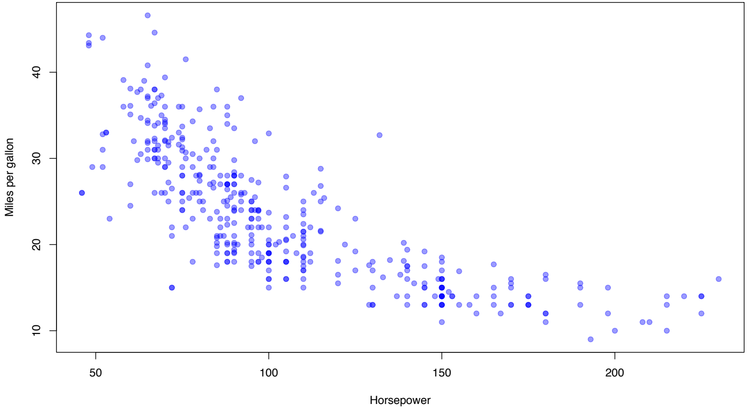
Validation Set Approach

- You want to know the *true* error of a model.
- We can sample from the original dataset and create *training* and *test* dataset.
- You split the data into a *training* and a *test* dataset - you pick the optimal model on the *training* dataset and determine its performance on the *test* dataset.

(James et al, 2013: 177)

Auto Example (James et al, chapter 3)

- Predict `mpg` with horsepower. Problem: How complex is the relationship?



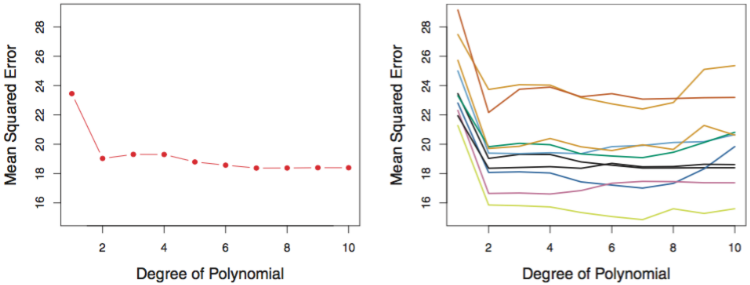
Auto Example (James et al., chapter 3) II

	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6	Model 7
(Intercept)	39.94 ***	56.90 ***	60.68 ***	47.57 ***	-32.23	-162.14 *	-489.06 *
	(0.72)	(1.80)	(4.56)	(11.96)	(28.57)	(71.43)	(189.83)
horsepower	-0.16 ***	-0.47 ***	-0.57 ***	-0.08	3.70 **	11.24 **	33.25 **
	(0.01)	(0.03)	(0.12)	(0.43)	(1.30)	(4.02)	(12.51)
horsepower2		0.00 ***	0.00 *	-0.00	-0.07 **	-0.24 **	-0.85 *
		(0.00)	(0.00)	(0.01)	(0.02)	(0.09)	(0.34)
horsepower3			-0.00	0.00	0.00 **	0.00 *	0.01 *
			(0.00)	(0.00)	(0.00)	(0.00)	(0.00)
horsepower4				-0.00	-0.00 **	-0.00 *	-0.00 *
				(0.00)	(0.00)	(0.00)	(0.00)
horsepower5					0.00 **	0.00 *	0.00 *
					(0.00)	(0.00)	(0.00)
horsepower6						-0.00 *	-0.00
						(0.00)	(0.00)
horsepower7							0.00
							(0.00)
R^2	0.61	0.69	0.69	0.69	0.70	0.70	0.70
RMSE	4.91	4.37	4.37	4.37	4.33	4.31	4.30

*** p < 0.001, ** p < 0.01, * p < 0.05

How many polynomials should be included?

Validation approach applied to Auto



(James et al, 2013: 178)

- Validation approach: highly variable results (right plot)
- Validation approach may tend to over-estimate test error due to small sample for training data.

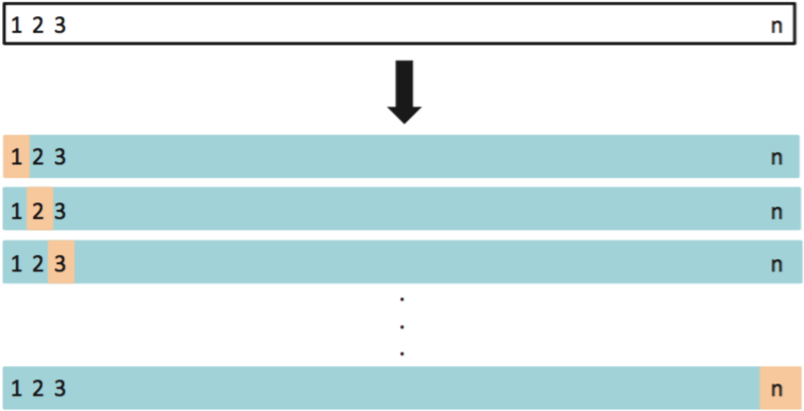
LOOCV 1

- Disadvantage 1: The error rate is highly variable
- Disadvantage 2: A large part of the data are not used to train the model

Alternative approach: Leave-one-out-cross-validation

- Leave on out and estimate model, assess the error rate (MSE_i)
- Average over all n steps, $CV_n = \frac{1}{n} \sum_{i=1}^{n} MSE_i$

LOOCV 2



(James et al, 2013: 179)

LOOCV 3

For LS linear or polynomial models there is a shortcut for LOOCV:

$$CV_{LOOCV} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2$$

Advantages:

- Less bias than validation set approach - will not over-estimate the test error.
- The *MSE* of LOOCV does not vary over several attempts.

Disadvantage:

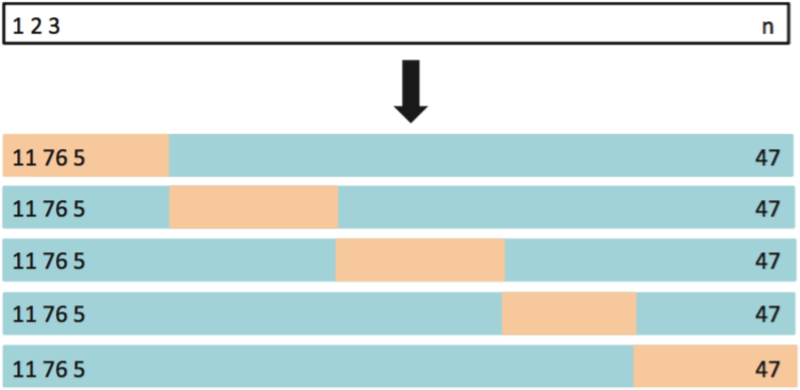
- One has to estimate the model n times.

k-fold Validation

- Compromise between validation set and LOOCV is k-fold validation.
- We divide the dataset into k different folds, whereas $k = 5$ or $k = 10$.
- We then estimate the model on $d - 1$ folds and use the kth fold as test dataset:

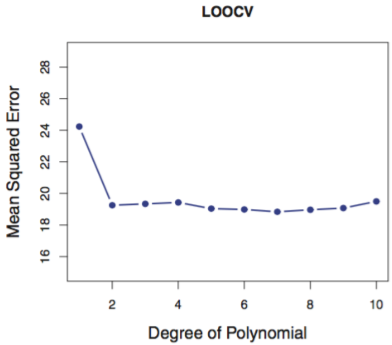
$$CV_k = \frac{1}{k} \sum_{i=1}^{K} MSE_i$$

k-fold validation



(James et al, 2013: 181)

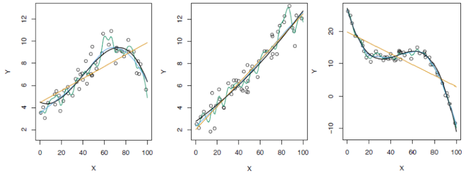
k-fold validation vs LOOCV



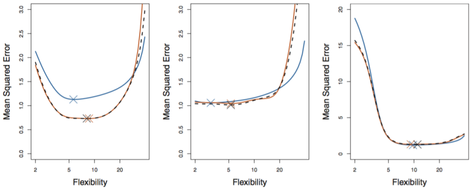
(James et al, 2013: 180)

Note: Similar error rates, but 10-fold CV is much faster.

k-fold validation vs LOOCV



(James et al, 2013: ch2)



blue: true MSE
black: LOOCV MSE
brown: 10-fold CV

(James et al, 2013: 182)

Variance-Bias Trade-Off

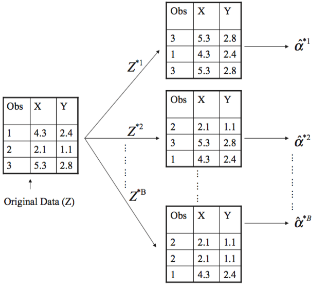
- LOOCV and k-fold CV lead to estimates of the test error.
- LOOCV has almost no bias, k-fold CV has small bias (since not $n-1$ but only $(k-1)/k \cdot n$ observations used for estimation).
- But, LOOCV has higher variance since all n data subsets are highly similar and hence the estimates are stronger correlated than for k-fold CV.
- Variance-Bias trade-off: We often rely on k-form for $k=5$ or $k=10$.

CV Above All Else?

- CV is fantastic but not a silver bullet.
- It has been shown that CV does not necessarily work well for hierarchical data:
  - One problem is to create independent folds (see Chu and Marron, 1991 and Alfons, 2012)
  - CV not well suited for model comparison of hierarchical models (Wang and Gelman, 2014)
- One alternative: Ensemble Bayesian Model Averaging (Montgomery et al., 2015 and see for MLM Broniecki et al., 2017).

Bootstrap

- Bootstrap allows us to assess the certainty/uncertainty of our estimates with one sample.
- For standard quantities like $\hat{\beta}$ we know how to compute $se(\hat{\beta})$. What about other non-standard quantities?
- We can re-sample from the original samples:



(James et al, 2013: 190)

Bootstrap (2)

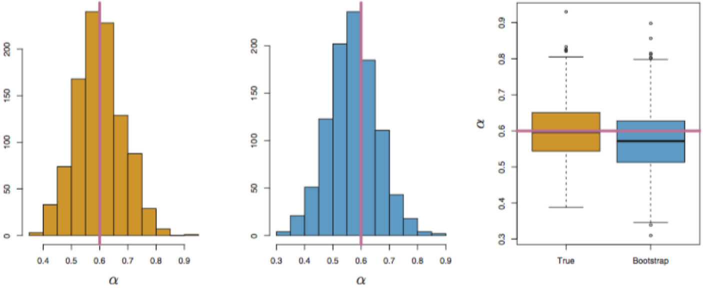
```
> m1 <- lm(mpg ~ year, data=Auto)
> summary(m1)

Residuals:
     Min       1Q   Median       3Q      Max 
-12.0212  -5.4411  -0.4412   4.9739  18.2088 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept) -70.01167    6.64516  -10.54   <2e-16 ***
year          1.23004    0.08736   14.08   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

> set.seed(112)
> n.sim <- 10000
> beta.catcher <- matrix(NA,n.sim,2)
> for (i in 1:n.sim){
+   rows.d1 <- sample(c(1:392),392,replace = TRUE)
+   d1 <- Auto[rows.d1,]
+   beta.catcher[i,] <- coef(lm(mpg ~ year, data=d1))
+ }
>
> sqrt(var(beta.catcher[,1]))
[1] 6.429225
```

Bootstrap (3)



yellow: 1,000 datasets
blue: 1,000 bootstrap samples

(James et al, 2013: 189)

Lab

- Cross-validation (LOOCV, and k-fold)
- Bootstrap
- CV applied to classification