STA 35C: Statistical Data Science III

Lecture 14: k-fold Cross-Validation and the Bootstrap

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Announcements

Mid-course survey (Due: tonight)

- Please take 10 minutes to complete the survey on Canvas
- Concrete and detailed feedback and constructive suggestions/requests will be appreciated

Remote lecture next Monday (May 4): More details will be announced on Canvas

Agenda

Recap of model assessment & the bias-variance tradeoff

- Validation set (hold-out) for estimating test MSE
- Leave-one-out cross-validation (LOOCV)

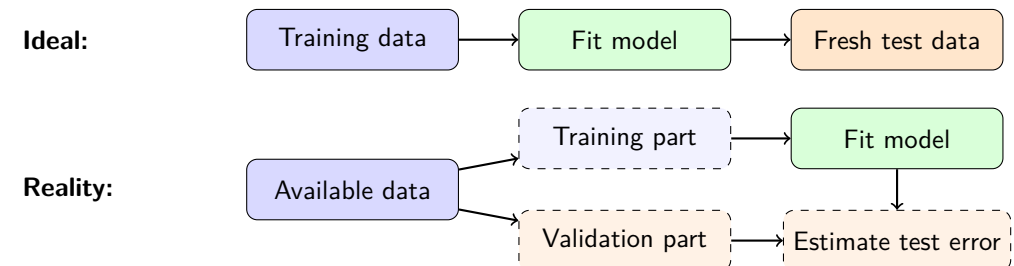
Today:

- k-**fold cross-validation**
- **The bootstrap**: quantifying uncertainty via resampling

Recap: Challenge in estimating test performance

Goal: Choose a model that generalizes well to new data.

- Training performance is not enough: low training error can come from overfitting.
- Ideally, we would evaluate the fitted model on fresh test data.
- In practice, we often only have one available dataset.



Validation data act as a surrogate for fresh test data.

Recap: Validation set approach

Idea: Split available data into a training part and a validation part to estimate test error

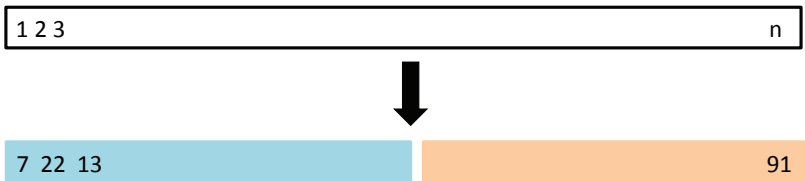


Figure: Splitting n observations into a training set and a validation set. The model is fit on the training set and assessed on the validation set [JWHT21, Figure 5.1]

- **Drawbacks:**
  - Reduced sample size for training $\rightarrow$ reduced efficiency
  - Variability per random split

Recap: Leave-one-out cross-validation (LOOCV)

Key ideas:

- For each i, leave that single point as "validation," train on the remaining $n-1$.
- Repeat for all n points, giving n held-out prediction errors: $\mathrm{MSE}_i = \left(y_i - \hat{f}_i(x_i)\right)^2$.
- Average these n errors to estimate test error: $\widehat{\mathrm{MSE}}_{\mathrm{LOOCV}} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{MSE}_i$.

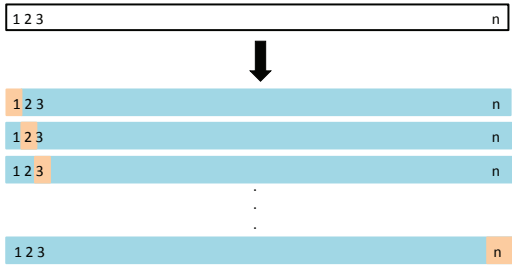


Figure: A set of n data points is repeatedly split into a training set of size $n-1$ and a validation set of size 1. The test error is estimated by averaging the n partial MSEs [JWHT21, Figure 5.3]

Recap: Single validation vs. LOOCV

Validation (single split):

- Enables estimating test MSE from training data alone & widely applicable
- Highly variable across random splits & training is less efficient due to fewer data points in the training subset

LOOCV:

- Removes randomness of splitting; each model is trained on $n - 1$ samples
- Computationally expensive: requires fitting n models

To mitigate the computational burden:

- Use fewer splits to reduce computational cost $\implies$ **k-fold cross-validation**

k-fold cross-validation: 1) Basic ideas

Key ideas:

- Randomly partition the observations into k groups (folds) of roughly equal size
- LOOCV is a special case of k-fold CV with $k = n$
- In practice, common choices are $k = 5$ or $k = 10$

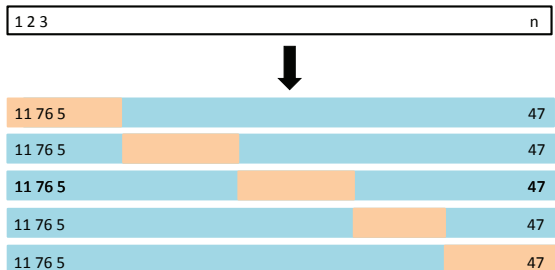


Figure: A schematic of 5-fold CV. The data are split into five non-overlapping groups: one as the validation set and the remainder as the training set [JWHT21, Figure 5.5].

k-fold cross-validation: 2) Procedure

Pseudocode:

- Randomly partition the data into k folds
- **For** each fold $j = 1, \ldots, k$:
  - Take fold j as the validation set
  - Combine the other $k - 1$ folds into a training set and fit the model on it
  - Compute validation error MSE_j on fold j
- Estimate test MSE by averaging:

$$\widehat{\mathrm{MSE}}_{\mathrm{CV}} = \frac{1}{k} \sum_{j=1}^{k} \mathrm{MSE}_j$$

k-fold cross-validation: 3) Example (2-fold, 4 data points)

Example (2-fold CV)

Let our dataset be $\{(5,12),(7,14),(12,17),(16,19)\}$ and choose $k=2$:

- **Fold 1 (Validation):** $(5,12),(12,17)$
- **Fold 2 (Validation):** $(7,14),(16,19)$

Step 1: Train on Fold 2, validate on Fold 1.

$$\text{Training set: } \{(7,14),(16,19)\}.$$

$$\hat{\beta}_1 = \frac{19-14}{16-7} = \frac{5}{9} \approx 0.556, \quad 14 = 0.556 \times 7 + \hat{\beta}_0 \implies \hat{\beta}_0 \approx 10.108.$$

Hence, $\hat{y} = 10.108 + 0.556\,x$.

$$\hat{y}(5) = 10.108 + 0.556 \times 5 = 10.108 + 2.780 \approx 12.888 \quad (\text{actual} = 12),$$
$$\hat{y}(12) = 10.108 + 0.556 \times 12 = 10.108 + 6.672 \approx 16.780 \quad (\text{actual} = 17).$$

$$\text{MSE}_1 = \frac{(12-12.888)^2 + (17-16.780)^2}{2} = \frac{(-0.888)^2 + (0.220)^2}{2} = \frac{0.789 + 0.048}{2} = 0.419.$$

k-fold cross-validation: 3) Example (cont'd)

Example (2-fold CV continued)

Step 2: Train on Fold 1, validate on Fold 2.

$$\text{Training set: } \{(5,12),(12,17)\}.$$

$$\hat{\beta}_1 = \frac{17-12}{12-5} = \frac{5}{7} \approx 0.714, \quad 12 = 0.714 \times 5 + \hat{\beta}_0 \implies \hat{\beta}_0 \approx 8.430.$$

Hence, $\hat{y} = 8.430 + 0.714\,x$.
On the validation points $\{(7,14),(16,19)\}$:

$$\hat{y}(7) = 8.430 + 0.714 \times 7 \approx 13.428 \quad (\text{actual} = 14),$$

$$\hat{y}(16) = 8.430 + 0.714 \times 16 \approx 19.854 \quad (\text{actual} = 19).$$

$$\text{MSE}_2 = \frac{(14-13.428)^2 + (19-19.854)^2}{2} \approx \frac{(0.572)^2 + (-0.854)^2}{2} = \frac{0.327 + 0.729}{2} \approx 0.528.$$

Final 2-fold CV error:

$$\widehat{\text{MSE}}_{\text{CV}} = \frac{\text{MSE}_1 + \text{MSE}_2}{2} \approx \frac{0.419 + 0.528}{2} \approx 0.474.$$

k-fold cross-validation: 4) the `auto` dataset

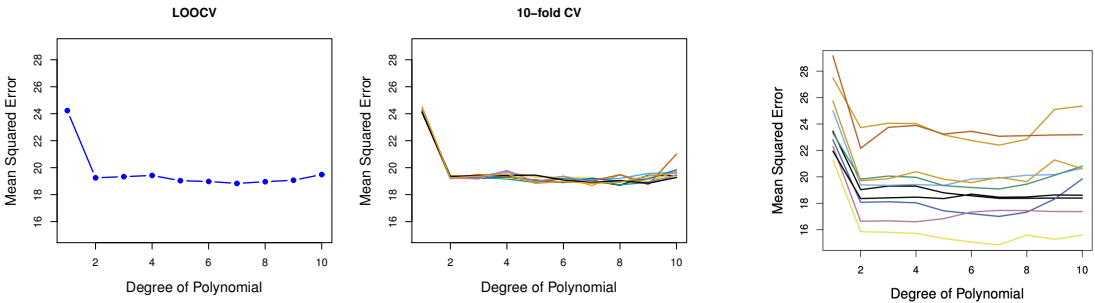


Figure: k-fold CV on the `Auto` dataset for polynomial fits of `mpg` on `horsepower`. **Left:** LOOCV error curve, **Center:** $k = 10$ CV curve, **Right:** single-split validation repeated ten times [JWHT21, Figures 5.2 & 5.4].

- k-fold CV offers a balance between single-split validation and LOOCV

k-fold cross-validation: 5) Pros and cons

Pros:

- Reduced variability compared to a single-split validation
- Fewer models to fit than LOOCV (esp. when $k \ll n$), lowering computational cost
- Each fold uses $\frac{k-1}{k} \cdot n$ points for training

Cons:

- Still computationally more expensive than a single-split approach
- Some randomness persists when compared to LOOCV

Pop-up quiz: k-fold cross-validation

Suppose we have $n = 100$ observations and use 5-fold cross-validation.

Question: Which statement is correct?

A) We fit 100 models, each trained on 99 observations.

B) We fit 5 models, each trained on about 80 observations and validated on about 20.

C) We fit one model on all 100 observations and compute its training MSE.

D) We use the validation folds to estimate the coefficients, and the training folds to estimate test error.

Answer: B. In 5-fold CV, each fold is held out once; each model is trained on the other 4/5 of the data and evaluated on the held-out fold.

Recall: Sampling distribution

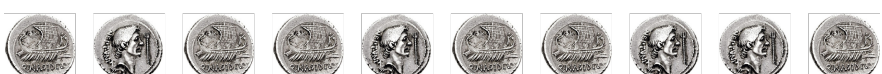
Coin flip example: Suppose we want to estimate $p = \Pr(X = 1)$, the probability of Head

We can flip a coin 10 times and compute $\hat{p} = \bar{X} = \frac{1}{10}\sum_{i=1}^{10} X_i$ to estimate p

Trial 1: 6 Heads, 4 Tails $\Rightarrow \hat{p}_1 = 0.6$

1 0 1 1 0 1 0 0 1 1

Trial 2: 4 Heads, 6 Tails $\Rightarrow \hat{p}_2 = 0.4$



0 1 0 0 1 0 0 1 1 0

$\vdots$

Recall: Sampling distribution

As we repeat many trials, we obtain a distribution of $\hat{p}$ (or equivalently $\bar{X}$):

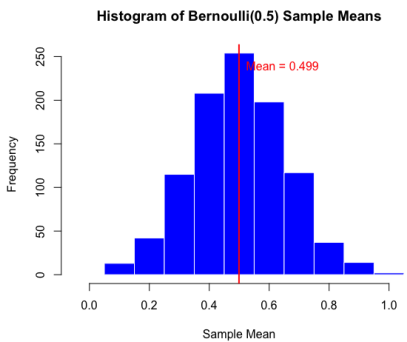


Figure: Histogram of 1000 sample means from 10 coin flips ($p = 0.5$).

This is called the **sampling distribution** of $\hat{p}$

- The estimate $\hat{p}$ from a random sample is itself a random variable!
- Its variance reflects the uncertainty in $\hat{p}$

$$\mathrm{SE}(\hat{p}) = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}(\hat{p}_b - \bar{p})^2}$$

- In this example (see left), $B = 1000$, $\bar{p} = \frac{1}{1000}\sum \hat{p}_i = 0.499$
- This calculation requires 1000 *fresh* samples! (which we usually do not have)

Challenge: We have only "one" sample in practice

In most practical scenarios, we only have a single sample (=dataset)

Trial 1: 6 Heads, 4 Tails $\Rightarrow \hat{p}_1 = 0.6$

Question: How can we approximate the sampling distribution and estimate $\mathrm{SE}(\hat{p})$, using *only* this single sample?

Answer: The bootstrap
We can *"sample" from this given dataset* to generate fresh, synthetic samples

The Bootstrap: 1) Motivation

Reasoning behind the bootstrap:

- We often want to measure the uncertainty of an estimate (mean, regression coefficients, etc.)
- Some estimates have known standard error formulas (like the sample mean in a simple scenario), but these rely on assumptions that may fail
- In more complex settings, we may not have a closed-form standard error formula for the estimator

Goal: Estimate uncertainty *without* strong parametric assumptions, by reusing our one dataset as if it were the population

Question: How do we resample to create synthetic samples from our data?

The Bootstrap: 2) (Re-)sampling with replacement

Core idea: Treat our dataset as an empirical approximation of the population

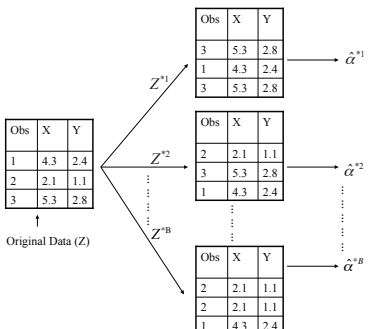


Figure: Illustration of the bootstrap for $n = 3$ observations. Each bootstrap dataset yields an estimate of α [JWHT21, Figure 5.11].

- Draw *resamples* of size *n with replacement* from the dataset
- Compute the statistic (mean, regression coefficient, etc.) each time
- The spread of these "bootstrap statistics" approximates the sampling distribution (and hence the SE)

The Bootstrap: 3) Procedure

Pseudocode: To estimate the uncertainty of an estimator $\hat{\alpha} = T(Z)$ (e.g., sample mean, slope),

- Let $Z = \{Z_1, Z_2, \ldots, Z_n\}$ be our observed data (of size n)
- **For** $b = 1$ to B:
  - Sample n observations *with replacement* from Z, call that Z_b^*
  - Compute the bootstrap estimate $\hat{\alpha}_b^* = T(Z_b^*)$

Bootstrap SE formula:

$$\mathrm{SE}_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}\left(\hat{\alpha}_b^* - \overline{\hat{\alpha}^*}\right)^2} \qquad \text{where} \qquad \overline{\hat{\alpha}^*} = \frac{1}{B}\sum_{b=1}^{B}\hat{\alpha}_b^*$$

- Note that this is simply the sample standard deviation of $\{\hat{\alpha}_1^*, \ldots, \hat{\alpha}_B^*\}$

Bootstrap: 4) An example of sample mean

Observed dataset (n=5):

$$x = \{2.1,\ 3.5,\ 1.8,\ 2.7,\ 3.2\}.$$

We want to estimate $\mu = \mathbb{E}[X]$ and its uncertainty, namely, $\mathrm{SE}(\hat{\mu})$.

- **Original sample mean:**

$$\bar{x} = \frac{2.1 + 3.5 + 1.8 + 2.7 + 3.2}{5} \approx 2.66$$

- **Bootstrap replicates ($B = 1000$):**
  - Draw 5 points *with replacement* from x to form each x_b^*.
  - Compute $\bar{x}_b^*$ for each.
  - For example,
    - Sample 1: $\{2.1, 2.1, 3.5, 2.7, 3.2\} \implies \bar{x}_1^* = 2.72$
    - Sample 2: $\{3.5, 1.8, 1.8, 3.2, 3.2\} \implies \bar{x}_2^* = 2.70$
- **Distribution of $\bar{x}_b^*$:** Yields an approximate sampling distribution for $\bar{x}$.

Bootstrap: 4) An example of sample mean (R script)

```r
# Define the observed dataset
x <- c(2.1, 3.5, 1.8, 2.7, 3.2)
n <- length(x)

# Number of bootstrap reps
B <- 1000

# Compute the original sample mean
original_mean <- mean(x)

# Initialize a vector
boot_means <- numeric(B)

# Perform the bootstrap
for (b in 1:B) {
  x_star <- sample(x, n, replace=TRUE)
  boot_means[b] <- mean(x_star)
}
```

```r
# Plot histogram of bootstrap means
hist(boot_means,
     main="Bootstrap Sample Means",
     xlab="Bootstrapped Mean",
     col="skyblue",
     border="white")

# Add vertical line for original mean
abline(v=original_mean, col="red", lwd=2)

# Label original mean
text(x=original_mean,
     y=par("usr")[4]*0.9,
     labels=paste("Original mean:",
                  round(original_mean,3)),
     pos=4,
     col="red")
```

- Alternatively, use `boot()` in the "boot" package for built-in methods; see [JWHT21, Ch 5.3.4].

Bootstrap: 4) An example of sample mean (histogram)

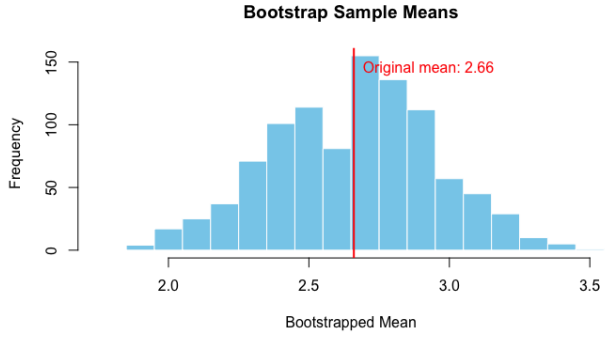


Figure: Histogram of 1000 bootstrap sample means for the example dataset.

Interpretation:

- The center is near $\bar{x} \approx 2.66$
- The spread approximates how $\bar{x}$ might vary across repeated samples from the population

Bootstrap: 5) Pros and Cons

Pros:

- Requires minimal assumptions about the population distribution
- Straightforward to implement for many statistics (means, regression coefficients, etc.)
- Flexible for constructing confidence intervals via percentile methods, etc.

Cons:

- Potentially expensive for large n or complex models (because B can be large)
- Relies on the observed sample being representative of the true population (garbage in, garbage out)
- Less straightforward if data are highly dependent or from complex sampling designs

Pop-up quiz: Bootstrap vs. cross-validation

Suppose we have one dataset and fit a regression model. We want to estimate the uncertainty of the fitted slope $\hat{\beta}_1$.

Question: Which approach is most appropriate?

A) Use k-fold cross-validation, because it estimates the standard error of $\hat{\beta}_1$.

B) Use the bootstrap: resample observations with replacement, refit the model many times, and examine the spread of the bootstrapped slopes.

C) Use the training MSE, because low training error implies low uncertainty in $\hat{\beta}_1$.

D) Split the data once into training and validation sets; the validation MSE is the standard error of $\hat{\beta}_1$.

Answer: B. Cross-validation estimates predictive performance, while the bootstrap estimates uncertainty by approximating the sampling distribution of an estimator.

Wrap-up & Takeaways

- **Validation & Cross-Validation**:
  - Single-split validation is simple but can vary a lot with random splits
  - LOOCV removes randomness and uses almost all observations for training but can be computationally expensive
  - k-fold CV is a practical compromise: fewer fits than LOOCV and more stable than a single validation split
- **Bootstrap**:
  - Resamples from dataset to approximate the sampling distribution of an estimate
  - Widely used to get SEs and confidence intervals with minimal assumptions
  - Flexible and particularly helpful for complex or unknown distributions
  - Relies on the observed sample being representative of the true population

References


Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani.
An Introduction to Statistical Learning: with Applications in R, volume 112 of *Springer Texts in Statistics*.
Springer, New York, NY, 2nd edition, 2021.