Cross Validation and Sample Splitting

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February 22, 2021

Applied Econometrics II

Cross Validation

Cross Validation appears superficially similar to bootstrap but asks a different question.

- Bootstrap tries to construct an empirical analogue to the sampling distribution of $\hat{\theta}$.
- CV tries to measure what the expected out of sample (OOS or EPE) prediction error of a new never seen before dataset.
- The main consideration is to prevent overfitting.
  - In sample fit is always going to be maximized by the most complicated model.
  - OOS fit might be a different story.
  - 1-NN might do really well in-sample, but with a new sample might perform badly.

Sample Splitting/Holdout Method and CV

Cross Validation is actually a more complicated version of sample splitting that is one of the organizing principles in machine learning literature.

Training Set This is where you estimate parameter values.

Validation Set This is where you choose a model- a bandwidth h or tuning parameter λ by computing the error.

Test Set You are only allowed to look at this after you have chosen a model. Only Test Once: compute the error again on fresh data.

- Conventional approach is to allocate 50-80% to training and 10-20% to Validation and Test.
- Sometimes we don't have enough data to do this reliably.

Sample Splitting/Holdout Method

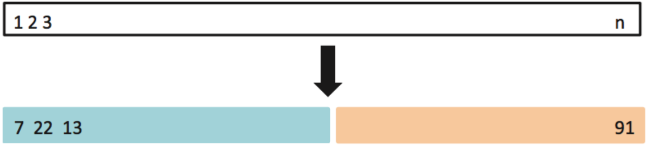

FIGURE 5.1. *A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.*

Challenge with Sample Splitting

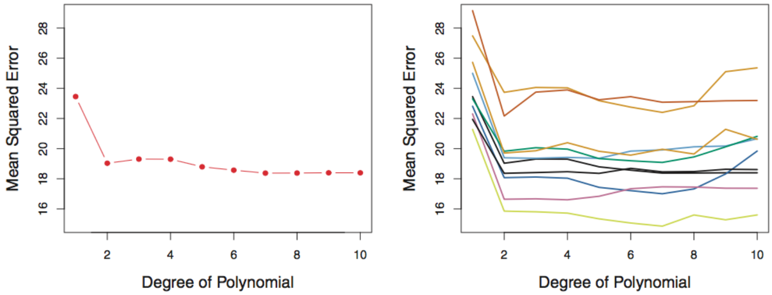

FIGURE 5.2. *The validation set approach was used on the* **Auto** *data set in order to estimate the test error that results from predicting* **mpg** *using polynomial functions of* **horsepower**. Left: *Validation error estimates for a single split into training and validation data sets.* Right: *The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability in the estimated test MSE that results from this approach.*

Cross Validation

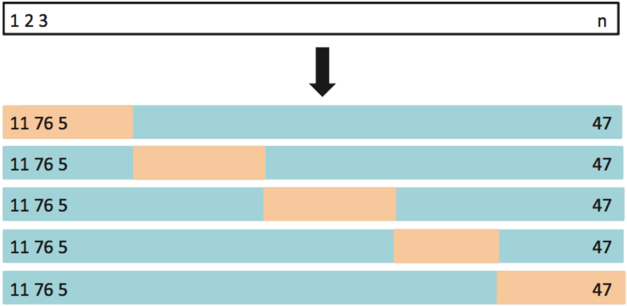

FIGURE 5.5. *A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.*

k-fold Cross Validation

- Break the dataset into k equally sized "folds" (at random).
- Withhold $i = 1$ fold
  - Estimate the model parameters $\hat{\theta}^{(-i)}$ on the remaining $k - 1$ folds
  - Predict $\hat{y}^{(-i)}$ using $\hat{\theta}^{(-i)}$ estimates for the ith fold (withheld data).
  - Compute $MSE_i = \frac{1}{k \cdot N} \sum_j (y_j^{(-i)} - \hat{y}_j^{(-i)})^2$.
  - Repeat for $i = 1, \ldots, k$.
- Construct $\widehat{MSE}_{k,CV} = \frac{1}{k} \sum_i MSE_i$

Leave One Out Cross Validation (LOOCV)

Same as k-fold but with $k = N$.

- Withhold a single observation i
- Estimate $\hat{\theta}_{(-i)}$.
- Predict $\hat{y}_i$ using $\hat{\theta}^{(-i)}$ estimates
- Compute $MSE_i = \frac{1}{N} \sum_j (y_i - \hat{y}_i(\hat{\theta}^{(-i)}))^2$.

Note: this requires estimating the model N times which can be costly.

Cross Validation

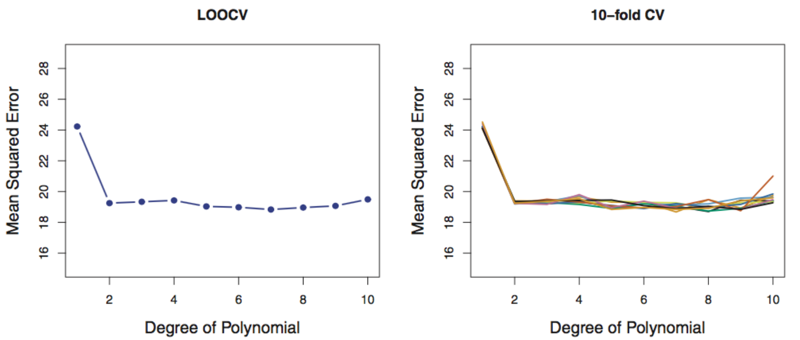

FIGURE 5.4. *Cross-validation was used on the* `Auto` *data set in order to estimate the test error that results from predicting* `mpg` *using polynomial functions of* `horsepower`. Left: *The LOOCV error curve.* Right: 10*-fold CV was run nine separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.*

Cross Validation

- Main advantage of cross validation is that we use all of the data in both estimation and in validation.
    - For our purposes validation is mostly about choosing the right bandwidth or tuning parameter.
- We have much lower variance in our estimate of the OOS mean squared error.
    - Hopefully our bandwidth choice doesn't depend on randomness of splitting sample.

Test Data

- In Statistics/Machine learning there is a tradition to withhold 10% of the data as Test Data.
- This is completely new data that was not used in the CV procedure.
- The idea is to report the results using this test data because it most accurately simulates true OOS performance.
- We don't do much of this in economics.
(Should we do more?)