Resampling Methods Exercises

Slides on Introduction to Statistical Learning, Chapter 5

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Using basic statistical properties of the variance, as well as single- variable calculus, derive (5.6). In other words, prove that α given by (5.6) does indeed minimize $Var(\alpha X + (1-\alpha)Y)$. (5.6) is:

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}.$$

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Answer Simply note that

$$\begin{aligned} \operatorname{Var}(\alpha X + (1 - \alpha)Y) &= \alpha^2 \sigma_X^2 + (1 - \alpha)^2 \sigma_Y^2 + 2\alpha (1 - \alpha) \sigma_{XY} \\ &= A\alpha^2 + B\alpha + C \\ &= A\left(\alpha + \frac{B}{2A}\right)^2 + \tilde{C} \end{aligned}$$

where
$$A=\sigma_X^2+\sigma_Y^2-2\sigma_{XY}$$
 and $B=-2\sigma_Y^2+2\sigma_{XY}$, QED.

We will now derive the probability that a given observation is part of a bootstrap sample. Suppose that we obtain a bootstrap sample from a set of n observations.

- (a) What is the probability that the first bootstrap observation is not the jth observation from the original sample? Justify your answer.
- (b) What is the probability that the second bootstrap observation is not the jth observation from the original sample?
- (c) Argue that the probability that the jth observation is not in the bootstrap sample is $\left(1-\frac{1}{n}\right)^n$.

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Answer

- (a) $1 \frac{1}{n}$ since the bootstrap observation is uniformly randomly chosen.
- (b) Its sampling with replacement, so $1 \frac{1}{n}$.
- (c) $\mathbb{P}(j\text{th obs not in boot sample})$ is the product as each bootstrap sample is independent.

- (d) When n=5, what is the probability that the jth observation is in the bootstrap sample?
- (e) When n=100, what is the probability that the jth observation is in the bootstrap sample?
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Answer

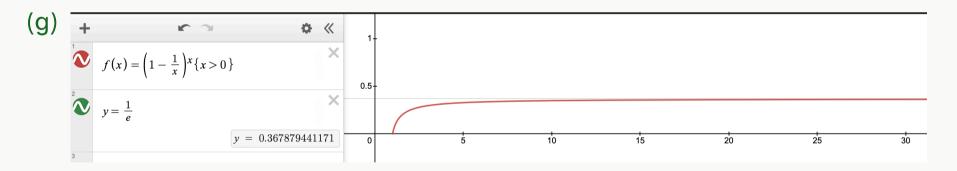
(d)
$$\left(1 - \frac{1}{5}\right)^5 \approx 0.3276800000000002$$

(e)
$$\left(1 - \frac{1}{100}\right)^{100} \approx 0.3660323412732289$$
.

(g) Create a plot that displays, for each integer value of n from 1 to $100\,000$, the probability that the jth observation is in the bootstrap sample. Comment on what you observe.

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Answer



(see Desmos plot.) I observe convergence to $\frac{1}{e}$. Of course, this is because

$$\left(1-\frac{1}{n}\right)^n = e^{n\log(1-\frac{1}{n})} = e^{n\left(-\frac{1}{n}-\frac{1}{2n^2}+O\left(\frac{1}{n^3}\right)\right)} = e^{-1-\frac{1}{2n}+O\left(\frac{1}{n^2}\right)} = \frac{1}{e} - \frac{1}{2en} + O\left(\frac{1}{n^2}\right).$$

(h) We will now investigate numerically the probability that a bootstrap sample of size n=100 contains the jth observation. Here j=4. We first create an array store with values that will subsequently be overwritten using the function <code>np.empty()</code>. We then repeatedly create bootstrap samples, and each time we record whether or not the fifth observation is contained in the bootstrap sample.

```
rng = np.random.default_rng(10)
store = np.empty(10000)
for i in range(10000):
    store[i] = np.sum(rng.choice(100, size=100, replace=True) == 4) > 0
np.mean(store)
```

(NB typo corrected) Comment on the results obtained.

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(NB typo corrected) Comment on the results obtained.

Answer We get 0.6362. The bootstrap sample size is $10\,000$, so the true probability is 1-0.36786104643302414=0.6321389535669759 which is consistent.

We now review k-fold cross-validation.

- (a) Explain how k-fold cross-validation is implemented.
- (b) What are the advantages and disadvantages of k-fold cross-validation relative to:
 - i. The validation set approach?
 - ii. LOOCV?

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Answer

- (a) Split the data randomly into k bins. For each bin, train on the other k-1 bins and then test on the kth bin. Then report the average test error across bins $CV_{(k)} = \frac{1}{k} \sum_{i=1}^k MSE_i$.
- (b) i. Pros Helps prevent fitting to the particular splitCons not repeatable (unless seed fixed), more compute needed
 - ii. **Pros** usually less compute needed, less variance (for small k) **Cons** not repeatable, higher bias

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Answer We use the bootstrap. First we use our method to make some small number n of predictions Y_i . Then we use these to create $N\gg n$ bootstrap samples $Y_i^*=(Y_{i1}^*,...,Y_{in}^*)$. Finally, our estimate for the standard deviation is the average of the bootstrap standard deviations,

$$\sigma_Y \approx \frac{1}{N} \sum_{i=1}^N \sigma_{Y_i^*} = \frac{1}{N} \sum_{i=1}^N \sqrt{\frac{1}{n} \sum_{j=1}^n Y_{ij}^{*2} - \left(\frac{1}{n} \sum_{j=1}^n Y_{ij}^*\right)^2}.$$