IFI 9000 Analytics Methods Resampling and Boosting

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Review of Cross Validation

• As mentioned earlier, model selection based on the RSS or R^2 statistics can be misleading, since the training error is not a good representative of the actual test error



- Instead through a process of splitting the data into training and validation sets, we were able to use LOOCV or *K*-fold CV as estimates of the test error
- The *K*-fold cv is more desirable estimate, computationally and statistically

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Bootstrap

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- The bootstrap is a flexible and very powerful statistical tool that can be used to **quantify the uncertainty** with a given estimator or statistical learning method
- It can provide an estimate of the standard error of a coefficient, or a **confidence interval for that coefficients**, regardless of how complex the derivation of that coefficient is

- Lets explain bootstrap via an example, Best investment allocation
- Suppose that we wish to invest a fixed sum of money in two financial assets that yield returns of X and Y (random quantities)
- We will invest α shares in X, and will invest the remaining $1-\alpha$ in Y
- To minimize the risk, we want to minimize $var(\alpha X + (1 \alpha)Y)$
- We can show that the minimizer is

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

where
$$\sigma_{XY}^2 = cov(X,Y)$$
 and $\sigma_Y^2 = var(Y)$

- In practice, σ_X^2, σ_Y^2 and σ_{XY} are unknown
- Suppose we are given a data set containing pairs of X and Y. We can estimate σ_X^2, σ_Y^2 and σ_{XY} from the sample set and get an estimate $\hat{\alpha}$ for the optimal share
- Ideally, we can generate these sample sets many times, and estimate an $\hat{\alpha}$ for each and look into the histogram
- However, in practice we only have one sample set to use
- Bootstrap yet allows us to generate good estimates of α using only one sample set

Bootstrap via an Example

To see how nicely bootstrap works, let's compare its outcome with the case that α is generated from many synthetic sample generations

- We generate 1,000 sample sets each containing 100 pairs of X and Y
- For the synthetic data generated $\sigma_X^2 = 1, \sigma_Y^2 = 1.25$ and $\sigma_{XY}^2 = 0.5$ which yield an optimal value of $\alpha = 0.6$



• To get the left panel we generate 1,000 synthetic sample sets, for each obtain $\hat{\alpha}$ and plot the histogram and calculate

$$\bar{\alpha} = \frac{1}{1000} \sum_{i=1}^{1} 000 \hat{\alpha}_i = 0.5996$$

$$SE(\alpha) = \sqrt{\frac{1}{1000 - 1} \sum_{i=1}^{1} 000(\hat{\alpha}_i - \bar{\alpha})^2} = 0.083$$

- For the bootstrap we only use one of the sample sets and regenerate new sample set by **sampling with replacement**
- Surprisingly, the results are very close to $\alpha = 0.6$

Bootstrap via an Example

• Surprisingly, the results are very close to $\alpha = 0.6$



Left: A histogram of the estimates of α obtained by generating 1,000 simulated data sets from the true population. **Center**: A histogram of the estimates of obtained from 1,000 bootstrap samples from a single data set. **Right**: The estimates of displayed in the left and center panels are shown as boxplots. In each panel, the pink line indicates the true value of α .

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Resampling and Boosting

- Suppose a black-box calculates $\hat{\alpha}$ from a sample set, e.g., a coefficient in linear or logistic regression
- We are interested in estimating the variability of $\hat{\alpha}$ without examining many new sample sets
- Denoting the first bootstrap data set by Z^{*1} , we use Z^{*1} to produce a new bootstrap estimate for α , which we call $\hat{\alpha}^{*1}$
- This procedure is repeated B (say 100 or 1,000) times, in order to produce B different bootstrap data sets, Z^{*1}, Z^{*2}, · · · , Z^{*B}, and the corresponding α estimates â^{*1}, · · · , â^{*B}

Bootstrap General Framework



• We estimate the standard error (SE) of these bootstrap estimates using the formula

$$\mathcal{SE}_B(\hat{\alpha}) = \sqrt{rac{1}{B-1}\sum_{r=1}^B (\hat{lpha}^{*r} - \bar{\hat{lpha}})^2}, \quad ext{where} \quad \bar{\hat{lpha}} = rac{1}{B}\sum_{r=1}^B \hat{lpha}^{*r}$$

• This serves as an estimate of the standard error of α estimated from the original data set

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