Statistics for Data Science

Lesson 27 - Bootstrap and resampling methods

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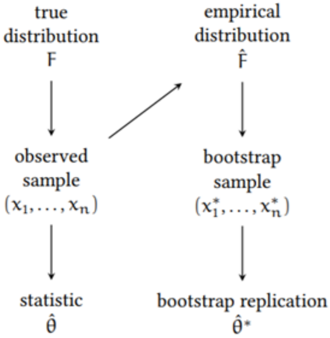
Bootstrap principle

- Let $X_1, \dots, X_n \sim F$ be a random sample
  - with *unknown distribution F*
- Estimator $T = h(X_1, \dots, X_n)$, e.g., $\bar{X}_n = (X_1 + \dots + X_n)/n$
- From a dataset $x_1, \dots, x_n$, we can
  - derive a point estimate $\hat{\theta} = h(x_1, \dots, x_n)$
  - or, derive an estimate $\hat{F}$ of F
- From $\hat{F}$ we can generate (a lot of) *bootstrap samples* $x_1^*, \dots, x_n^*$
  - as realizations of $X_1^*, \dots, X_n^* \sim \hat{F}$

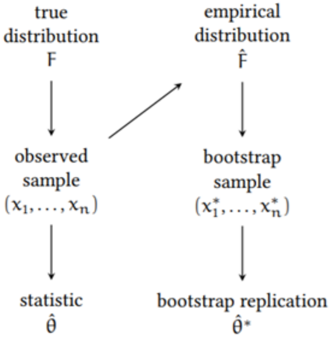
  and then (a lot of) bootstrap point estimates $\hat{\theta}^* = h(x_1^*, \dots, x_n^*)$



- By the **Glivenko-Cantelli Thm**, the empirical distribution of $\hat{\theta}^*$ will approximate the distribution of $T^* = h(X_1^*, \dots, X_n^*)$ and then of T

> Bootstrap principle. Use the dataset $x_1, x_2, \dots, x_n$ to compute an estimate $\hat{F}$ for the "true" distribution function F. Replace the random sample $X_1, X_2, \dots, X_n$ from F by a random sample $X_1^*, X_2^*, \dots, X_n^*$ from $\hat{F}$, and approximate the probability distribution of $h(X_1, X_2, \dots, X_n)$ by that of $h(X_1^*, X_2^*, \dots, X_n^*)$.

Empirical bootstrap



- How to derive $\hat{F}$ from $x_1, \ldots, x_n$?
- If we know nothing about F, use the empirical distribution:

  $\hat{F}(a) = F_n(a) = \frac{|\{i \in 1,\ldots,n \ | \ x_i \leq a\}|}{n}$
- How to generate a bootstrap sample $x_1^*, \ldots, x_n^*$?
  - x_i^* is chosen randomly from $\hat{F}$
  - i.e., x_i^* s chosen randomly from $x_1, \ldots, x_n$ (our dataset)
- Hence, a bootstrap dataset $x_1^*, \ldots, x_n^*$ is obtained by *random sampling with replacement*!
- Often the bootstrap approximation of the distribution of T will improve if we somehow normalize T by relating it to a corresponding feature of the "true" distribution.
  - rather than approximating the distribution of $\bar{X}_n$ by the one of $\bar{X}_n^*$
  - better to approximate $\bar{X}_n - \mu$ by $\bar{X}_n^* - \mu^*$, where $\mu^* = E[\hat{F}] = \bar{x}_n = (x_1 + \ldots + x_n)/n$

[See remarks 18.1 and 18.2 of textbook]

Empirical bootstrap

EMPIRICAL BOOTSTRAP SIMULATION (FOR $\bar{X}_n - \mu$). Given a dataset $x_1, x_2, \ldots, x_n$, determine its empirical distribution function F_n as an estimate of F, and compute the expectation

$$\mu^* = \bar{x}_n = \frac{x_1 + x_2 + \cdots + x_n}{n}$$

corresponding to F_n.

1. Generate a bootstrap dataset $x_1^*, x_2^*, \ldots, x_n^*$ from F_n.
2. Compute the centered sample mean for the bootstrap dataset:

$$\bar{x}_n^* - \bar{x}_n,$$

where

$$\bar{x}_n^* = \frac{x_1^* + x_2^* + \cdots + x_n^*}{n}.$$

Repeat steps 1 and 2 many times.

- Use the empirical distribution of $\delta^* = \bar{x}_n^* - \bar{x}_n$ (realizations of $\Delta^* = \bar{X}_n^* - \bar{x}_n$)
  - for estimating $\delta = \bar{x}_n - \mu$ as $mean(\delta^*)$
  - and then estimate μ as $\hat{\mu} = \bar{x}_n - mean(\delta^*)$ *[main idea: subtract estimated bias]*
  - with estimated bias $E[\bar{X}_n] - \mu \approx E[\bar{X}_n^*] - \bar{x}_n = E[\Delta^* + \bar{x}_n] - \bar{x}_n \approx mean(\delta^*)$
  - with standard error $\sqrt{Var(\bar{X}_n)} = \sqrt{Var(\bar{X}_n - \mu)} \approx \sqrt{Var(\bar{X}_n^* - \bar{x}_n)} = \sqrt{Var(\Delta^*)} \approx sd(\delta^*)$

Empirical bootstrap

Empirical bootstrap simulation (for $\bar{X}_n - \mu$). Given a dataset $x_1, x_2, \ldots, x_n$, determine its empirical distribution function F_n as an estimate of F, and compute the expectation

$$\mu^* = \bar{x}_n = \frac{x_1 + x_2 + \cdots + x_n}{n}$$

corresponding to F_n.

1. Generate a bootstrap dataset $x_1^*, x_2^*, \ldots, x_n^*$ from F_n.
2. Compute the centered sample mean for the bootstrap dataset:

$$\bar{x}_n^* - \bar{x}_n,$$

where

$$\bar{x}_n^* = \frac{x_1^* + x_2^* + \cdots + x_n^*}{n}.$$

Repeat steps 1 and 2 many times.

- Use the empirical distribution of $\delta^* = \bar{x}_n^* - \bar{x}_n$ for estimating
  - confidence interval (c_l, c_u) for $\delta = \bar{x}_n - \mu$ as $(q_{\alpha/2}, q_{1-\alpha/2})$ of δ^* distribution
  - $c_l \leq \delta = \bar{x}_n - \mu \leq c_u$ implies $\bar{x}_n - c_u \leq \mu \leq \bar{x}_n - c_l$, i.e. c.i. for μ is $(\bar{x}_n - c_u, \bar{x}_n - c_l)$

See R script

Empirical bootstrap

`boot.ci` method in R confidence intervals:

- `type='basic'`: $(\bar{x}_n - q_{1-\alpha/2}, \bar{x}_n - q_{\alpha/2})$ with quantiles over the distribution of δ^*
- `type='perc'`: $(q_{\alpha/2}, q_{1-\alpha/2})$ with quantiles over the distribution of $\bar{x}_n^*$
- `type='norm'`: $(\bar{x}_n - q_{1-\alpha/2}, \bar{x}_n - q_{\alpha/2})$ with quantiles over $N(mean(\delta^*), var(\delta^*))$
- `type='bca'`: bias (and skewness) correction and acceleration

See R script

Empirical bootstrap

`boot.ci` method in R confidence intervals:

- `type='stud'`: $\left(\bar{x}_n - q_{1-\alpha/2}\frac{s_n}{\sqrt{n}}, \bar{x}_n - q_{\alpha/2}\frac{s_n}{\sqrt{n}}\right)$ with quantiles over the distribution of t^*

EMPIRICAL BOOTSTRAP SIMULATION FOR THE STUDENTIZED MEAN.
Given a dataset $x_1, x_2, \ldots, x_n$, determine its empirical distribution function F_n as an estimate of F. The expectation corresponding to F_n is $\mu^* = \bar{x}_n$.

1. Generate a bootstrap dataset $x_1^*, x_2^*, \ldots, x_n^*$ from F_n.
2. Compute the studentized mean for the bootstrap dataset:

$$t^* = \frac{\bar{x}_n^* - \bar{x}_n}{s_n^*/\sqrt{n}},$$

   where $\bar{x}_n^*$ and s_n^* are the sample mean and sample standard deviation of $x_1^*, x_2^*, \ldots, x_n^*$.

Repeat steps 1 and 2 many times.

See R script

Empirical bootstrap

- Bootstrap approach applies to **any** estimator, not only the mean
- Example 1: the German Tank problem

$$T_2 = \frac{n+1}{n} M_n - 1 \qquad\qquad E[T_2] = N$$

- Example 2: linear regression coefficients
  - 95% confidence intervals (assuming $\underline{\underline{U_i \sim \mathcal{N}(0, \sigma^2)}}$):

$$\hat{\beta} \pm t_{n-2,0.025} se(\hat{\beta}) \qquad\qquad \hat{\alpha} \pm t_{n-2,0.025} se(\hat{\alpha})$$

See R script

An application of empirical bootstrap

- Bootstrap principle: for $X \sim F$
  - the empirical distribution of $\Delta^* = \bar{X}_n^* - \bar{x}_n$ approximates the distribution of $\Delta = \bar{X}_n - \mu$
- Application: estimate $P_F(|\bar{X}_n - \mu| > 1)$ as
  - $P_{\hat{F}}(|\bar{X}_n^* - \bar{x}_n| > 1)$ and then by the fraction of $\delta^* = \bar{x}_n^* - \bar{x}_n$ such that $|\delta^*| > 1$
- How many bootstrap samples?
  - There are $\binom{2n-1}{n-1}$ distinct bootstrap samples
  - Suggested to use at least 1000 bootstrap samples
  - **Jackknife resampling**: bootstrap samples $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n$, for $i = 1, \ldots, n$
- How good is the approximation by bootstrap?
  - Small perturbation to data-generating process should produce small perturbation of the parameter to estimate (θ)
  - Problems with extreme values, e.g., percentiles, maximum, etc.

See R script

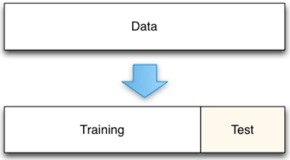
Resampling methods for classifier performance estimation

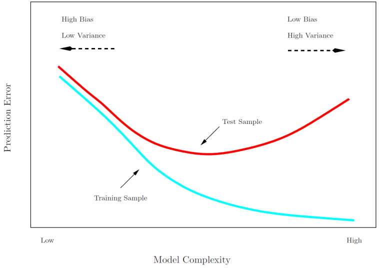
Risk (or Expected Prediction Error EPE)

The risk w.r.t. a loss function ℓ_θ is $R(\theta_{TRUE}, \theta) = E_{(W,C)\sim f_{\theta_{TRUE}}}[\ell_\theta(C, W)]$.

- Decision rule $y^+_\theta(w)$ (classifier) or score function $s_\theta(w)$ (binary probabilistic classifier)
- E.g., 0-1 loss $\ell_\theta(c, w) = \mathbb{1}_{y^+_\theta(w)\neq c}$
- Empirical risk estimate risk on a **holdout set** (test set) of n_h observations:

$$\hat{r} = \frac{1}{n_h}\sum_{i=1}^{n_h} \ell_\theta(c_i, w_i) \qquad se = \sqrt{\frac{\hat{r}(1-\hat{r})}{n_h}}$$





- Drawbacks: variability of training/test set, and then of empirical risk estimates

Resampling methods for classifier performance estimation

Risk (or Expected Prediction Error EPE)

The risk w.r.t. a loss function ℓ_θ is $R(\theta_{TRUE}, \theta) = E_{(W,C)\sim f_{\theta_{TRUE}}}[\ell_\theta(C, W)]$.

- Decision rule $y_\theta^+(w)$ (classifier) or score function $s_\theta(w)$ (binary probabilistic classifier)
- E.g., 0-1 loss $\ell_\theta(c, w) = \mathbb{1}_{y_\theta^+(w)\neq c}$
- Empirical risk estimate risk using **random sampling** (k times random split training-test):
  $\hat{r} = \frac{1}{k}\sum_{j=1}^{k} \hat{r}^j$ with $\hat{r}^j = \frac{1}{n_j}\sum_{i=1}^{n_j} \ell_\theta(c_i^j, w_i^j)$
- Standard deviation calculated over the k folds, with
  $se = \sqrt{\frac{1}{k-1}\sum_{j=1}^{k}(\hat{r}^j - \hat{r})^2}$

  Wrong!! As test sets (and then $\hat{r}^j$'s) are not independent!

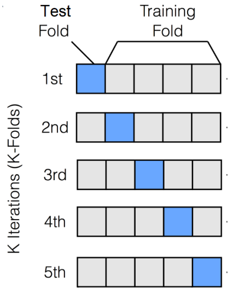
Resampling methods for classifier performance estimation

Risk (or Expected Prediction Error EPE)

The risk w.r.t. a loss function ℓ_θ is $R(\theta_{TRUE}, \theta) = E_{(W,C)\sim f_{\theta_{TRUE}}}[\ell_\theta(C, W)]$.

- Decision rule $y_\theta^+(w)$ (classifier) or score function $s_\theta(w)$ (binary probabilistic classifier)
- E.g., 0-1 loss $\ell_\theta(c, w) = \mathbb{1}_{y_\theta^+(w)\neq c}$
- Empirical risk estimate risk using k-**fold cross-validation** (independent test sets):

$$\hat{r} = \frac{1}{k}\sum_{j=1}^{k} \hat{r}^j \text{ with } \hat{r}^j = \frac{1}{n/k}\sum_{i=1}^{n/k} \ell_\theta(c_i^j, w_i^j)$$



- Standard deviation calculated over the k folds, with

$$se = \sqrt{\frac{1}{k-1}\sum_j(\hat{r}^j - \hat{r})^2}$$

  Wrong!! As training sets (and then $\hat{r}^j$'s) are not independent! or, with

$$se = \sqrt{\frac{\hat{r}(1-\hat{r})}{n}}$$

  if classifier is stable over the folds (see [Kohavi, 1995])
- Setting $k = n$ is the **leave-one out cross-validation** (LOOCV)

Resampling methods for classifier performance estimation

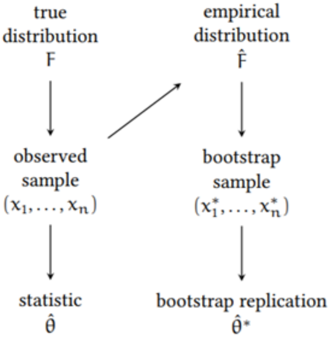
- Can the bootstrap estimate prediction error?
- E.g., training = bootstrap $x_1^*, \ldots, x_n^*$, test = original dataset $x_1, \ldots, x_n$?
  - No, as training-test would overlap with probability 63.2% **[Prove it!]**
  - and then, prediction error would be under-estimated
- training = bootstrap $x_1^*, \ldots, x_n^*$, test = original dataset \ bootstrap $\{x_1, \ldots, x_n\} \setminus \{x_1^*, \ldots, x_n^*\}$
  - .632 bootstrap algorithm for k bootstrap runs

$$\hat{r} = \frac{1}{k} \sum_j (0.632 \cdot \hat{r}^j + 0.368 \cdot \hat{r}_{tr})$$

  where $\hat{r}^j$ is the loss on j^{th} bootstrap run, and $\hat{r}_{tr}$ is the loss on the original dataset
- [Kohavi, 1995, Kim, 2009] conclusions and recommendations:
  - Bootstrap has low variance, but it is extremely biased
  - k-fold cross-validation has low bias and variance can be controlled
    - by averaging multiple k-fold cross-validation
  - Recommendation: use **repeated (stratified)** k**-fold cross-validation**, with $k \approx 10$
- [Vanwinckelen, 2012] warns against repeated, and it recommends k**-fold cross-validation**

See R script

Parametric bootstrap principle



- Let $X_1, \ldots, X_n \sim F(\gamma)$ be a random sample
  - with known family F but *unknown* parameter γ
- Estimator $T = h(X_1, \ldots, X_n)$, e.g., $\bar{X}_n = (X_1 + \ldots + X_n)/n$
- From a dataset $x_1, \ldots, x_n$, we can
  - derive a point estimate $\hat{\theta} = h(x_1, \ldots, x_n)$
  - or, derive an estimate $\hat{\gamma}$ of γ
- From $F(\hat{\gamma})$ we can generate (a lot of) *bootstrap samples* $x_1^*, \ldots, x_n^*$
  - as realizations of $X_1^*, \ldots, X_n^* \sim F(\hat{\gamma})$ *[a form of* **Monte Carlo simulation***]*

  and then (a lot of) bootstrap point estimates $\hat{\theta}^* = h(x_1^*, \ldots, x_n^*)$
- By the **Glivenko-Cantelli Thm**, the empirical distribution of $\hat{\theta}^*$ will approximate the distribution of $T^* = h(X_1^*, \ldots, X_n^*)$ and then of T

Parametric bootstrap

PARAMETRIC BOOTSTRAP SIMULATION (FOR $\bar{X}_n - \mu$). Given a dataset $x_1, x_2, \ldots, x_n$, compute an estimate $\hat{\theta}$ for θ. Determine $F_{\hat{\theta}}$ as an estimate for F_θ, and compute the expectation $\mu^* = \mu_{\hat{\theta}}$ corresponding to $F_{\hat{\theta}}$.

1. Generate a bootstrap dataset $x_1^*, x_2^*, \ldots, x_n^*$ from $F_{\hat{\theta}}$.
2. Compute the centered sample mean for the bootstrap dataset:

$$\bar{x}_n^* - \mu_{\hat{\theta}},$$

   where

$$\bar{x}_n^* = \frac{x_1^* + x_2^* + \cdots + x_n^*}{n}.$$

Repeat steps 1 and 2 many times.

- Use the empirical distribution of $\delta^* = \bar{x}_n^* - \mu_{\hat{\theta}}$ for estimating
  - confidence interval (c_l, c_u) for $\delta = \bar{x}_n - \mu$ as $(q_{\alpha/2}, q_{1-\alpha/2})$ of δ^* distribution
  - $c_l \leq \delta = \bar{x}_n - \mu \leq c_u$ implies $\bar{x}_n - c_u \leq \mu \leq \bar{x}_n - c_l$, i.e. c.i. for μ is $(\bar{x}_n - c_u, \bar{x}_n - c_l)$

See R script

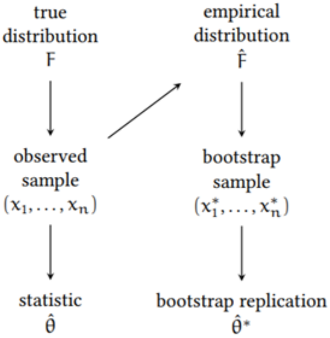
Application: distribution fitting

- Consider $x_1, \ldots, x_n$ realizations of a random sample $X_1, \ldots, X_n \sim F$
- Is the dataset from an $Exp(\lambda)$ for some λ? I.e., is it $F = Exp(\lambda)$?
- We estimate $\hat{\lambda} = 1/\bar{x}_n$ *[MLE estimation]*
- We measure how close is the dataset to the distribution as:

$$t_{ks} = \sup_{a \in \mathbb{R}} |F_n(a) - F_{\hat{\lambda}}(a)|$$

  where:
  - $F_n(a)$ is the empirical cumulative distribution function of $x_1, \ldots, x_n$
  - $F_{\hat{\lambda}}(a) = 1 - e^{\hat{\lambda} a}$, for $a \geq 0$, is the CDF of $Exp(\hat{\lambda})$
  - t_{ks} is called the *Kolmogorov-Smirnov* distance
- if $F = Exp(\lambda)$ then both $F_n \approx F$ and $F_{\hat{\lambda}} \approx F$, and then $F_n \approx F_{\hat{\lambda}}$, so that t_{ks} is small
- if $F \neq Exp(\lambda)$ then $F_n \approx F \neq Exp(\lambda) \approx F_{\hat{\lambda}}$, so that t_{ks} is large

Application: distribution fitting



- For the software dataset from the textbook
  - $\hat{\lambda} = 0.0015$ and $t_{ks} = 0.17$
- Is $t_{ks} = 0.17$ expected or an extreme value?
- Let's study the distribution of the bootstrap estimator:

$$T_{ks} = \sup_{a \in \mathbb{R}} |F_n^*(a) - F_{\hat{\Lambda}^*}(a)|$$

where:

  - $X_1^*, \ldots, X_n^* \sim Exp(\hat{\lambda})$ is a bootstrap sample
  - $F_n^*(a)$ is the empirical cumulative distribution of the bootstrap sample
  - $\hat{\Lambda}^* = 1/\bar{X}_n^*$
- It turns out $P(T_{ks} > 0.17) \approx 0$, unlikely that $Exp(\lambda)$ is the right model

See R script

Optional references

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