Bootstrap

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OVERVIEW

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Bootstrap methods

Bootstrap methods

Bradley Efron 1979.

"pull oneself up by one's bootstraps" = "better oneself by one's own effort."

- The bootstrap is a general tool for assessing statistical accuracy.
  - expectation
  - variance (main application)
- As with cross-validation, the bootstrap can be used to estimate prediction error.
  - typically estimates well the expected prediction error Err.

General ideas

The data are realizations of

$$Z_1, \ldots, Z_n \overset{i.i.d.}{\sim} \mathbb{P}$$

$\mathbb{P}$ denotes an unknown distribution.

We denote a statistical procedure or estimator by

$$\hat{\theta}_n = S\left(Z_1, \ldots, Z_n\right)$$

which is a (known) function S of the data $Z_1, \ldots, Z_n$.

One typically would need to find out the

- sampling distribution of $\hat{\theta}_n$,
- the expectation $\mathrm{E}(\hat{\theta}_n)$ or the variance $\mathrm{Var}(\hat{\theta}_\mathrm{n})$.

If we knew the distribution $\mathbb{P}$:

- can simulate to obtain the distribution of any $\hat{\theta}_n$ with arbitrary accuracy.

But we do not know what the distribution $\mathbb{P}$!

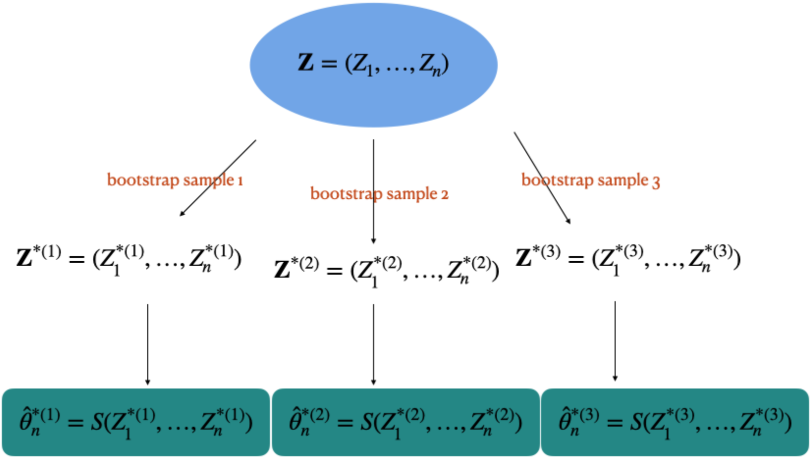
Bootstrap:

- use the empirical distribution $\hat{\mathbb{P}}_n$ which places probability mass $1/n$ on every data point $Z_i, i = 1, \ldots, n$.
- simulate from $\hat{\mathbb{P}}_n$: generate simulated data

$$Z_1^*, \ldots Z_n^* \overset{i.i.d.}{\sim} \hat{\mathbb{P}}_n$$

  i.e., generate n random drawings with **replacement** from the original data set $\{Z_1, \ldots, Z_n\}$.
- such a simulated new data set is called a **bootstrap sample**.
- compute a bootstrap estimator $\hat{\theta}_n^* = S(Z_1^*, \ldots, Z_n^*)$ based on the bootstrap sample.
- We then repeat this many times (say obtain B bootstrap samples, then B $\hat{\theta}_n^*$s)
- Get an approximate distribution for $\hat{\theta}_n$ by the "histogram" of B $\hat{\theta}_n^*$s.

Bootstrap (an illusrtration)



$\hat{\theta}_n = S(\mathbf{Z})$ could be any quantity computed from the original data $\mathbf{Z} = \{Z_1, \ldots, Z_n\}$.

The resampling with replacement is the key feature of bootstrap.

(Nonparametric) bootstrap

The algorithm can be described as:

- 1. Generate a bootstrap sample

$$Z_1^*, \ldots, Z_n^* \overset{i.i.d.}{\sim} \hat{\mathbb{P}}_n$$

  That is obtain n random draws with replacement from the data set $\{Z_1, \ldots, Z_n\}$.

- 2. Compute the *bootstrapped estimator* based on the bootstrap sample

$$\hat{\theta}_n^* = S\left(Z_1^*, \ldots, Z_n^*\right)$$

- 3. Repeat steps 1 and 2 for B times to obtain

$$\hat{\theta}_n^{*(1)}, \ldots, \hat{\theta}_n^{*(B)}.$$

Bootstrap distribution

Bootstrap distribution

The **bootstrap distribution** denoted by $\mathbb{P}^*$,

- the conditional probability distribution which is induced by i.i.d. resampling (with replacement) of the data given the original data.

The bootstrap distribution of $\theta_n^* = S(Z_1^*, \ldots, Z_n^*)$ is the distribution which arises when resampling with $\hat{\mathbb{P}}_n$ and applying the function S on such a bootstrap sample.

The bootstrap distribution of θ_n^* can be described by Monte Carlo simulation:

$$\text{bootstrap expectation} \quad \mathrm{E}^*\left(\hat{\theta}_n^*\right) \cong \frac{1}{B} \sum_{i=1}^{B} \hat{\theta}_n^{*(i)}$$

$$\text{bootstrap variance} \quad \mathrm{Var}^*\left(\hat{\theta}_n^*\right) \cong \frac{1}{B-1} \sum_{i=1}^{B} \left(\hat{\theta}_n^{*(i)} - \frac{1}{B} \sum_{j=1}^{B} \hat{\theta}_n^{*(j)}\right)^2$$

α -quantile of the bootstrap distribution of $\hat{\theta}_n^*$:

empirical α -quantile of $\hat{\theta}_n^{*(1)}, \ldots, \hat{\theta}_n^{*(B)}$

If the empirical distribution $\hat{\mathbb{P}}_n$ is "close" to the true data-generating probability $\mathbb{P}$, the bootstrap values are "reasonable" estimates for the true quantities of the distribution of $\hat{\theta}_n$.

$$\mathrm{E}^*(\hat{\theta}_n^*) \cong \frac{1}{B}\sum_{i=1}^{B}\hat{\theta}_n^{*(i)} \approx \mathrm{E}(\hat{\theta}_n)$$

$$\mathrm{Var}^*\left(\hat{\theta}_n^*\right) \cong \frac{1}{B-1}\sum_{i=1}^{B}\left(\hat{\theta}_n^{*(i)} - \frac{1}{B}\sum_{j=1}^{B}\hat{\theta}_n^{*(j)}\right)^2 \approx \mathrm{Var}\left(\hat{\theta}_n\right)$$

Bootstrap consistency

The bootstrap is called to be **consistent** for $\hat{\theta}_n$ if, for an increasing sequence a_n, for all x

$$\mathrm{P}\left[a_n\left(\hat{\theta}_n-\theta\right)\leq x\right]-\mathrm{P}^*\left[a_n\left(\hat{\theta}_n^*-\hat{\theta}_n\right)\leq x\right]\xrightarrow{P}0 \qquad (n\to\infty)$$

In classical situations, $a_n=\sqrt{n}$.

In other words, if $\hat{\theta}_n$ estimate some parameter θ,the bootstrap consistency says that the sampling distribution of $\hat{\theta}_n-\theta$ in $\mathbb{P}$ and the bootstrap distribution of $\hat{\theta}_n^*-\hat{\theta}_n$ in $\mathbb{P}^*$ are close.

Such approximation may be reasonable when the distribution of $\hat{\theta}_n-\theta$ is *pivotal*, that is the distribution does not depend on θ.

Estimating bias and variance

Under bootstrap consistency, the bias of $\hat{\theta}_n$ may be approximated as

$$\begin{aligned} \mathrm{E}(\hat{\theta}_n) - \theta &\approx \mathrm{E}^*(\hat{\theta}_n^*) - \hat{\theta}_n \\ &\approx \frac{1}{B}\sum_{b=1}^{B} \hat{\theta}_n^{*(b)} - \hat{\theta}_n \end{aligned}$$

Also, $\mathrm{Var}\left(\hat{\theta}_n\right) \approx \mathrm{Var}^*\left(\hat{\theta}_n^*\right)$.

Estimating confidence intervals

We can also construct the bootstrap confidence interval for θ.

Recall that a $(1-\alpha)$ confidence interval for θ, computed over $z_1, \ldots z_n$, is a random interval (L, U) satisfying

$$P(L \leq \theta \leq U) = 1 - \alpha.$$

The bootstrap confidence interval for θ is given by (why?)

$$\left(2\hat{\theta}_n - q^*_{1-\alpha/2}, 2\hat{\theta}_n - q^*_{\alpha/2}\right).$$

Here $q^*_{\alpha/2}$ and $q^*_{1-\alpha/2}$, are the $\alpha/2$ and $1-\alpha/2$ are the bootstrap quantiles of $\hat{\theta}_n^{*(1)}, \ldots \hat{\theta}_n^{*(B)}$.

Studentized bootstrap confidence intervals

In some cases, the distributions of $(\hat{\theta}_n - \theta)/\widehat{\mathrm{SE}}(\hat{\theta}_n)$ and $(\hat{\theta}_n^* - \hat{\theta}_n)/\widehat{\mathrm{SE}}(\hat{\theta}_n^*)$ could be close, where $\widehat{\mathrm{SE}}(\cdot)$ denote estimated standard errors. The so-called **studentized bootstrap confidence intervals** is obtained:

- repeat, for $b = 1, \dots B$:
  - draw a bootstrap sample $z_1^{*(b)}, \dots z_n^{*(b)}$ from $\{z_1, \dots z_n\}$
  - recompute the statistic $\hat{\theta}_n^{*(b)}$ based on $z_1^{*(b)}, \dots z_n^{*(b)}$
  - repeat, for $m = 1, \dots M$:
    - draw a bootstrap sample $z_1^{*(b,m)}, \dots z_n^{*(b,m)}$ from $\{z_1^{*(b)}, \dots z_n^{*(b)}\}$
    - recompute the statistic $\hat{\theta}_n^{*(b,m)}$ from $\{z_1^{*(b,m)}, \dots z_n^{*(b,m)}\}$
  - compute the sample standard deviation $\hat{s}^{*(b)}$ of $\hat{\theta}_n^{*(b,1)}, \dots \hat{\theta}_n^{*(b,M)}$
  - compute $(\hat{\theta}_n^{*(b)} - \hat{\theta}_n)/\hat{s}^{*(b)}$.

From above we have a sample $\{(\hat{\theta}_n^{*(b)} - \hat{\theta}_n)/\hat{s}^{*(b)} : b = 1, \dots, B\}$, from which, we compute the quantiles $q^*_{\alpha/2}$ and $q^*_{1-\alpha/2}$.

The approximate $1-\alpha$ bootstrap confidence interval for θ is given by

$$(\hat{\theta}_n - \widehat{\mathrm{SE}}(\hat{\theta}_n) q^*_{1-\alpha/2}, \hat{\theta}_n - \widehat{\mathrm{SE}}(\hat{\theta}_n) q^*_{\alpha/2}),$$

- $\widehat{\mathrm{SE}}(\hat{\theta}_n)$ can be approximated with $\mathrm{Var}^*(\hat{\theta}^*_n)$ using bootstrap samples $\{\hat{\theta}_n^{*(1)}, \ldots, \hat{\theta}_n^{*(B)}\}$.

Nonparametric bootstrap, (semi)-parametric bootstrap

Parametric bootstrap

Assume that the data are realizations from

$$Z_1, \ldots, Z_n \overset{i.i.d.}{\sim} \mathbb{P}_\theta$$

where $\mathbb{P}_\theta$ is given up to an unknown parameter (vector) θ.

- estimate the unknown parameter θ by $\hat{\theta}_n$
- draw

$$Z_1^*, \ldots, Z_n^* \overset{i.i.d.}{\sim} \mathbb{P}_{\hat{\theta}_n}$$

Example (parametric regerssion)

- $Y_i = \beta^\top x_i + \varepsilon_i, (i = 1, \ldots, n)$, $\varepsilon_1, \ldots, \varepsilon_n \overset{i.i.d.}{\sim} \mathrm{N}\left(0, \sigma^2\right)$, $\theta = \left(\beta, \sigma^2\right)$.
- training data $z = \{z_1, z_2, \ldots, z_n\}$, with $z_i = (x_i, y_i)$ $i = 1, 2, \ldots, n$.
- $\hat{\beta}, \hat{\sigma}$ denote the MLE estimates based on original data.

1. Simulate $\varepsilon_1^*, \ldots, \varepsilon_n^* \overset{i.i.d.}{\sim} \mathrm{N}\left(0, \hat{\sigma}^2\right)$
2. Construct

$$Y_i^* = \hat{\beta}^\top x_i + \varepsilon_i^*, i = 1, \ldots, n$$

The parametric bootstrap regression sample is then

$$\left(x_1, Y_1^*\right), \ldots, \left(x_n, Y_n^*\right)$$

where the predictors x_i are from the original data.

nonparametric regression

Suppose $Y = f(X) + \epsilon$, $\mathrm{E}(Y|X = x) = f(x) \approx \sum_{j=1}^{M} \beta_j h_j(x)$ where $var(\epsilon) = \sigma^2$.

$$\hat{\beta} = \left(\mathbf{H}^\top \mathbf{H}\right)^{-1} \mathbf{H}^\top \mathbf{y}$$

$$\widehat{\mathrm{Var}}(\hat{\beta}) = \left(\mathbf{H}^\top \mathbf{H}\right)^{-1} \hat{\sigma}^2$$

$$\hat{\sigma}^2 = \sum_{i=1}^{n} \left(y_i - \hat{f}\left(x_i\right)\right)^2 / n$$

- Let $h(x)^\top = (h_1(x), h_2(x), \ldots, h_M(x))$.
- $\hat{f}(x) = h(x)^\top \hat{\beta}$
- standard error $\widehat{\mathrm{se}}(\hat{f}(x)) = \left(h(x)^\top \left(\mathbf{H}^\top \mathbf{H}\right)^{-1} h(x)\right)^{\frac{1}{2}} \hat{\sigma}$.
- The (biased) 95% pointwise confidence interval is $\hat{f}(x) \pm 1.96 \widehat{\mathrm{se}}(\hat{f}(x))$.

example: nonparametric boostrap

Suppose we have $n = 50$. The nonparametric bootstrap works as in the following.

- We draw B datasets each of size $n = 50$ with replacement from our training data, the sampling unit being the pair $z_i = (x_i, y_i)$.
- To each bootstrap dataset $\mathbf{Z}^*$ we fit a cubic spline $\hat{f}^*(x)$.
- Using B = 200 bootstrap samples, we can form a 95% pointwise confidence band from the percentiles at each x: we find the $2.5\% \times 200 =$ fifth largest and smallest values at each x.

Generally, for x, obtain the upper and lower quantiles $\hat{f}^*(x) - \hat{f}(x)$, say $R_{\alpha/2}, R_{1-\alpha/2}$, then the pointwise confidence interval is given by $(\hat{f}(x) - R_{1-\alpha/2}(x), \hat{f}(x) + R_{\alpha/2}(x))$.

example: semi-parametric bootstrap

Simulate new responses by adding Gaussian noise to the predicted values:

$$y_i^* = \hat{f}(x_i) + \varepsilon_i^*; \quad \varepsilon_i^* \sim \mathrm{N}\left(0, \hat{\sigma}^2\right); \quad i = 1, 2, \ldots, n$$

This process is repeated B times, where $B = 200$ say. The resulting bootstrap datasets have the form $(x_1, y_1^*), \ldots, (x_n, y_n^*)$ and we recompute the splines on each.

The confidence intervals from this method will exactly equal the least squares intervals, as the number of bootstrap samples goes to infinity.

- the estimate based on bootstrap sample is $\hat{f}^*(x) = h(x)^\top \left(\mathbf{H}^\top \mathbf{H}\right)^{-1} \mathbf{H}^\top \mathbf{y}^*$ with distribution

$$\hat{f}^*(x) \sim \mathrm{N}\left(\hat{f}(x), h(x)^\top \left(\mathbf{H}^\top \mathbf{H}\right)^{-1} h(x)\hat{\sigma}^2\right)$$

.

Another version of bootstrap (residual bootstrap)

Suppose

$$Y_i = f(x_i) + \varepsilon_i$$
$$\varepsilon_1, \ldots, \varepsilon_n \overset{i.i.d.}{\sim} \mathbb{P}_\varepsilon$$

where P_ε is unknown with expectation 0.

1. Estimate $\hat{f}$ from the original data and compute the residuals $r_i = Y_i - \hat{f}(x_i)$.
2. Consider the centered residuals $\tilde{r}_i = r_i - n^{-1}\sum_{i=1}^n r_i$. In case of linear regression with an intercept, the residuals are already centered. Denote the empirical distribution of the centered residuals by $\hat{\mathbb{P}}_{\tilde{r}}$.
3. Generate

   $$\varepsilon_1^*, \ldots, \varepsilon_n^* \overset{i.i.d.}{\sim} \hat{\mathbb{P}}_{n,\tilde{r}}$$

   Note that $\hat{\mathbb{P}}_{n,\tilde{r}}$ is an estimate of $\mathbb{P}_\varepsilon$.
4. Construct the bootstrap response variables

   $$Y_i^* = \hat{f}(x_i) + \varepsilon_i^*, i = 1, \ldots, n$$

   and the bootstrap sample is $(x_1, Y_1^*), \ldots, (x_n, Y_n^*)$.

Confidence band via bootstrap

Bootstrapping $\sup_x |\hat{f}(x) - \mathrm{E}(\hat{f}(x))|$:

More generally, if $\sigma^2 = \sigma^2(x)$ is not constant in x, $\hat{\sigma}^2(x)$ can be estimated as using the regression $e_i^2 := (y_i - \hat{f}(x_i))^2$ v.s. x_i, and taking $\hat{\sigma}^2(x_i) = \hat{e}_i^2$.

One then obtain bootstrap (upper) α quantile R_α from

$$\frac{\sqrt{n}\sup_x |\hat{f}(x) - \mathrm{E}(\hat{f}(x))|}{\hat{\sigma}(x)}$$

Then $\hat{f}(x) \pm (R_\alpha \hat{\sigma}(x)/\sqrt{n})$ has a (supposedly) sup-norm coverage.

- still biased for the true f unless done with undersmoothing
- Or view this confidence band as for the smoothed version $\mathrm{E}(\hat{f}(\cdot))$ instead of f.

Bootstrap is to address the variance estimate, without undersmoothing, the above band is still biased. A even better approach is to use debiased estimator with the bootstrap.

Bootstrap estimate of prediciton error

If $\hat{f}^{*(b)}(x_i)$ is the predicted value at x_i, from the model fitted to the b-th bootstrap dataset, our estimate of EPE is

$$\widehat{\mathrm{Err}}_{\text{naive}} = \frac{1}{n}\sum_{i=1}^{n}\sum_{b=1}^{B}\frac{1}{B}L\left(y_i, \hat{f}^{*(b)}(x_i)\right)$$

- Repeat for $b = 1, \ldots, B$:
  - Generate $\left(X_1^{*(b)}, Y_1^{*(b)}\right), \ldots, \left(X_n^{*(b)}, Y_n^{*(b)}\right)$ by resampling with replacement from the original data.
  - Compute the bootstrapped estimator $\hat{f}^{*(b)}(\cdot)$ based on $\left(X_1^{*(b)}, Y_1^{*(b)}\right), \ldots, \left(X_n^{*(b)}, Y_n^{*(b)}\right)$
  - Evaluate $\mathrm{err}^{*(b)} = n^{-1}\sum_{i=1}^{n} L\left(Y_i, \hat{f}^{*(b)}(X_i)\right)$
- Approximate the bootstrap generalization error Err by

$$B^{-1}\sum_{b=1}^{B} err^{*(b)}$$

Leave-one-out bootstrap estimate

Above estimate is not a good estimate in general. Tends to be overfitting.

The **leave-one-out bootstrap estimate** of prediction error is defined by

$$\widehat{\text{Err}}^{(1)} = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{|C^{-i}|} \sum_{b \in \{1,\ldots,B\} \cap C^{-i}} L\left(y_i, \hat{f}^{*b}(x_i)\right)$$

- C^{-i} is the set of indices of the bootstrap samples b that do not contain observation i,
- $\left|C^{-i}\right|$ is the number of such samples.

The leave-one out bootstrap solves the overfitting problem suffered by $\widehat{\text{Err}}_{\text{naive}}$, but has the training-set-size bias mentioned in the discussion of cross-validation.

- Typically, the leave-one out bootstrap estimate will be biased upward.

Bias

- Given a bootstrap sample by $\mathbf{Z}^* = \{Z_1^*, \ldots, Z_n^*\}$, the out-of-bootstrap sample

$$\mathbf{Z}_{\text{out}}^* = \{Z_i : Z_i \notin \mathbf{Z}^*\}$$

The out-of-bootstrap estimate above can be written as:

$$\widehat{\text{Err}}^{(1)} = \frac{1}{B} \sum_{b=1}^{B} \frac{1}{\left|\mathbf{Z}_{\text{out}}^{*(b)}\right|} \sum_{i \in \mathbf{Z}_{\text{out}}^{*(b)}} L\left(y_i, \hat{f}^{*(b)}(x_i)\right)$$

Note that $\hat{f}^{*(b)}(\cdot)$ involves only data from $\mathbf{Z}^{*(b)}$, and $(X_i, Y_i) \in \mathbf{Z}_{\text{out}}^*$.

- The expected size of the out-of-bootstrap sample: $\mathrm{E}^*\left(|\mathbf{Z}_{\text{out}}^*|\right) \approx 0.368n$.
- $\widehat{\text{Err}}^{(1)}$ is like a CV estimate that uses about 36.8% data points as test data, or about 63.2% data points as training data
- Unlike CV estimate, the training data in $\widehat{\text{Err}}^{(1)}$ may have duplicates.

The .632 estimator

The ".632 estimator" is designed to alleviate this bias:

$$\widehat{\mathrm{Err}}^{(.632)} = .368 \cdot \overline{\mathrm{err}} + .632 \cdot \widehat{\mathrm{Err}}^{(1)}$$

The derivation of the .632 estimator is complex; intuitively it pulls the leave-one out bootstrap estimate down toward the training error rate, and hence reduces its upward bias.

Note that $\overline{\mathrm{err}} \leq \widehat{\mathrm{Err}}^{(.632)} \leq \widehat{\mathrm{Err}}^{(1)}$.

- The .632 estimator works well in "light fitting" situations
- In the heavily-overfitting situations, one can further improve the .632 estimator: the .632+ estimator

Estimating degrees of freedom

The so-called **effective d.f.** of a fitted model is

$$\mathrm{d.f.}(\hat{f}) = \frac{\sum_{i=1}^{n} \mathrm{cov}(\hat{y}_i, y_i)}{\sigma^2}, \quad \{x_i\}_i \text{ fixed}$$

We can estimate the covariance terms $\mathrm{cov}(\hat{y}_i, y_i)$ via the bootstrap.

After fitting $\hat{y}_i = \hat{f}(x_i), i = 1, \ldots n$ using the original samples $(x_i, y_i), i = 1, \ldots n$, we record the (empirical) residuals

$$\hat{e}_i = y_i - \hat{y}_i, \quad i = 1, \ldots n$$

Then for $b = 1, \ldots B$, we repeat:

- obtain a bootstrap sample $\left(x_i, \tilde{y}_i^{(b)}\right), i = 1, \ldots n$ according to

$$\tilde{y}_i^{(b)} = \hat{y}_i + \tilde{e}_i^{(b)}, \text{ where } \tilde{e}_i^{(b)} \overset{i.i.d.}{\sim} \{\hat{e}_1, \ldots \hat{e}_n\}, \quad i = 1, \ldots n$$

- re-estimate the estimator $\hat{f}^{(b)}$ based on the sample $\left(x_i, \tilde{y}_i^{(b)}\right)_{i=1}^{n}$
- store $\tilde{\mathbf{y}}^{(b)} = \left(\tilde{y}_1^{(b)}, \ldots \tilde{y}_n^{(b)}\right)$, and $\hat{\mathbf{y}}^{(b)} = \left(\hat{f}^{(b)}(x_1), \ldots \hat{f}^{(b)}(x_n)\right)$.

With $\tilde{\mathbf{y}}^{(b)} = \left(\tilde{y}_1^{(b)}, \dots \tilde{y}_n^{(b)}\right)$, and $\hat{\mathbf{y}}^{(b)} = \left(\hat{f}^{(b)}(x_1), \dots \hat{f}^{(b)}(x_n)\right)$,

we approximate the covariance of $\hat{y}_i$ and y_i by the empirical covariance between $\hat{y}_i^{(b)}$ and $\tilde{y}_i^{(b)}$ over $b = 1, \dots B$, i.e.

$$\mathrm{Cov}\left(\hat{y}_i, y_i\right) \approx \frac{1}{B} \sum_{b=1}^{B} \left(\hat{y}_i^{(b)} - \frac{1}{B} \sum_{b'=1}^{B} \hat{y}_i^{(b')} \right) \left(\tilde{y}_i^{(b)} - \frac{1}{B} \sum_{b'=1}^{B} \tilde{y}_i^{(b')} \right).$$

Summing this up over $i = 1, \dots n$ yields the bootstrap estimate for degrees of freedom

$$\widehat{\mathrm{d.\,f.}}(\hat{f}) \approx \frac{1}{\sigma^2} \sum_{i=1}^{n} \left(\frac{1}{B} \sum_{b=1}^{B} \left(\hat{y}_i^{(b)} - \frac{1}{B} \sum_{b'=1}^{B} \hat{y}_i^{(b')} \right) \left(\tilde{y}_i^{(b)} - \frac{1}{B} \sum_{b'=1}^{B} \tilde{y}_i^{(b')} \right) \right)$$

Some discussions

Correct way to do bootstrap for inference

The bootstrap procedure should be applied to the entire estimation process to obtain correct inference.

Suppose that we adaptively choose by cross-validation the number and position of the knots that define the B-splines, rather than fix them in advance. Denote by λ the collection of knots and their positions. Then the standard errors and confidence bands should account for the adaptive choice of λ.

The catch is with the bootstrap, we compute the B-spline smoother with an adaptive choice of knots for *each* bootstrap sample.

Estimation of generalized error of tuned model

The 0.632 (0.632+) estimators were proposed to assess the generalization error of a generic algorithm and can be directly applied to a (adaptively) tuned model:

specifically, for each bootstrap sample, the model can be fit and tuned (say by CV) with this bootstrap sample.

Alternatively, one can use Wang and Zou (2021) Honest leave-one-out cross-validation or nested cross validation to assess the performance of a tuned model.

Bayesian bootstrap

The bootstrap discussed above is a “poor man’s” version of Bayesian bootstrap.

Bayesian bootstrap sample:

- Draw weights from a uniform Dirichlet distribution with the same dimension as the number of data points
- Sample from data accordingly to the probability defined by the Dirichlet weights
- Use the resampled data to calculate the statistics.