



Monte Carlo approach

Idea: For F an unknown distribution function, if we know how to simulate from F , simulate $X_1, \dots, X_B \stackrel{iid}{\sim} F$ and estimate F by e.c.d.f. $\hat{F}_B(t) = \frac{1}{B} \sum_{i=1}^B I[X_i \leq t]$. Glivenko-Cantelli gives $\lim_{B \rightarrow \infty} \|F - \hat{F}_B\|_{\infty} = 0$ a.s.

Example 57: Kolmogorov-Smirnov

$X_1, \dots, X_m \sim F$ $H_0: F \sim N(\mu, \sigma^2)$ for $\mu \in \mathbb{R}, \sigma^2 > 0$
 $H_1: \neg H_0$ known

$T_m = \|F - \hat{F}_m\|_{\infty}$ for F_m the e.c.d.f. of X_1, \dots, X_m

Under H_0 , $T_m = \sup_{x \in \mathbb{R}} |F(x) - \frac{1}{m} \sum_{i=1}^m I[X_i \leq x]|$ for $X_1, \dots, X_m \stackrel{iid}{\sim} F$.

We don't know the exact distribution of T_m , but we can simulate it.

- sample many times $X_1, \dots, X_m \stackrel{iid}{\sim} F$, each time compute T_m denoted by $T_{m,b}^*$ for b -th run, $b = 1, \dots, B$ ($= 10^4$)
- from all the $\{T_{m,b}^*\}_{b=1}^B$ estimate e.c.d.f. to approximate the distribution function of T_m under H_0 .
- use quantile of this estimated distribution to test.

Example 58: Two sample problem for exponential distribution

$X_1, \dots, X_{m_1} \sim \text{Exp}(\lambda_1)$ iid, independent samples. $H_0: \lambda_1 = \lambda_2$
 $Y_1, \dots, Y_{m_2} \sim \text{Exp}(\lambda_2)$ $H_1: \lambda_1 \neq \lambda_2$

point estimators $\hat{\lambda}_1 = 1/\bar{X}$
 $\hat{\lambda}_2 = 1/\bar{Y}$

Test statistic $T = \frac{\bar{Y}}{\bar{X}} = \frac{\hat{\lambda}_1}{\hat{\lambda}_2}$

We have $T = \frac{\bar{Y}}{\bar{X}} \sim \frac{m_1}{m_2} \frac{\sum \Gamma(1, 1/\lambda_3)}{\sum \Gamma(1, 1/\lambda_x)} = \frac{m_1}{m_2} \frac{\Gamma(m_2, 1/\lambda_3)}{\Gamma(m_1, 1/\lambda_x)}$

$$= \frac{m_1/\lambda_3}{m_2/\lambda_x} \frac{\Gamma(m_2, 1)}{\Gamma(m_1, 1)} = \frac{\lambda_x}{\lambda_3} \cdot \frac{\Gamma(m_2, m_1)}{\Gamma(m_1, m_2)} = \frac{\lambda_x}{\lambda_3} \cdot \frac{\Gamma(\frac{2m_2}{2}, 2)}{\Gamma(\frac{2m_1}{2}, 2)} \cdot \frac{m_1}{2}$$

depends only on λ_x/λ_3 for any λ_x, λ_3

does not depend on λ_x, λ_3

(*)

$$= \frac{\lambda_x}{\lambda_3} \frac{\chi^2(2m_2)/2m_2}{\chi^2(2m_1)/2m_1} = \frac{\lambda_x}{\lambda_3} F(2m_2, 2m_1)$$

$$\Gamma\left(\frac{\nu}{2}, 2\right) = \chi^2(\nu)$$

independent numerator and denominator

Under $H_0: \frac{\lambda_x}{\lambda_3} = 1$ we have exactly $T \stackrel{H_0}{\sim} F(2m_2, 2m_1)$

But even if we didn't know this, from (*) we know that under H_0 , for any $\lambda_x = \lambda_3$ the distribution of T is the same.

We can therefore resample - generate i.i.d. samples from any $\text{Exp}(\lambda_x)$ and $\text{Exp}(\lambda_3)$ for $\lambda_x = \lambda_3$ and simulate the distribution of T under H_0 .



Bootstrap

Example: Inference about $EX = \theta$ in (possibly) exponential distribution

X_1, \dots, X_m iid from a distribution that could be exponential

$\theta = EX_1$, possibly $X_1 \sim \text{Exp}(\lambda)$, $\hat{\theta} = \bar{X}$

CLT: if $\text{var } X_1$ exists, $\sqrt{m}(\bar{X} - \theta) \xrightarrow{D} N(0, \text{var } X_1)$

confidence interval: $\left[\bar{X} \pm u_{1-\alpha/2} \sqrt{\frac{\hat{\text{var}} X_1}{m}} \right]$

but is only asymptotic, works only for larger m .

$X_i \sim \text{Exp}(\lambda)$: $\theta = 1/\lambda$, $\hat{\lambda} = 1/\bar{X}$, $\sum X_i \sim \Gamma(m, 1/\lambda)$

$\bar{X} = \frac{1}{m} \sum X_i \sim \Gamma(m, \frac{1}{\lambda m})$ and

$2\lambda m \bar{X} = 2\lambda \sum X_i \sim \Gamma(\frac{2m}{2}, 2) = \chi^2(2m)$ ← χ^2 with $2m$ degrees of freedom

$\frac{2 \sum X_i}{\theta} \sim \chi^2_{2m}$ exactly, and this leads to an exact conf.

interval for θ $\left[\frac{2 \sum X_i}{\chi^2_{2m}(1-\alpha/2)} ; \frac{2 \sum X_i}{\chi^2_{2m}(\alpha/2)} \right]$

Exact, but valid only if really $X_i \sim \text{Exp}(\lambda)$

$X_i \sim \text{Exp}(\lambda)$ $\sqrt{m}(\bar{X} - \theta) \xrightarrow{D} N(0, \theta^2)$

+ variance-stabilizing transform: $[g'(t)]^2 = 1/t^2 \Rightarrow g(t) = \log t$

Δ -vector $\sqrt{m}(\log \bar{X} - \log \theta) \xrightarrow{D} N(0, 1)$

We express the as. variance as a

"sandwich estimator" $\frac{\hat{\text{var}} X_1}{(\hat{EX}_1)^2}$ to make inference less sensitive to the assumption $\text{Exp}(\lambda)$

$N(0, \frac{\text{var } X_1}{(EX_1)^2})$

Bootstrap intervals - Nonparametric Bootstrap. (4)

Idea: If the exact $F \sim X_1, \dots, X_n$ is not known, sample from its estimator $\hat{F}_n(t) = \frac{1}{n} \sum I[X_i \leq t] \Rightarrow$ generate i.i.d samples repeatedly (with replacement) from the set of observations $\{X_1, \dots, X_n\}$. For each $b \in \{1, \dots, B\}$ ($B=10^k$)

- generate $X_{1,b}^*, \dots, X_{n,b}^*$ with replacement from $\{X_1, \dots, X_n\}$
- compute $\hat{\theta}_b^*$ as an estimator of θ from $X_{1,b}^*, \dots, X_{n,b}^*$
- in $\Gamma_n(\hat{\theta} - \theta)$
 - distribution of X_1 is approximated by $\{X_{1,b}^*\}_{b=1}^B$
 - distribution of $\hat{\theta}$ is approximated by $\{\hat{\theta}_b^*\}_{b=1}^B$
 - the true value θ is replaced by $\hat{\theta}$ - an estimator of θ , and a "true value" of θ for \hat{F}_n from which we sample.

overall the distribution of $H_n \sim \Gamma_n(\hat{\theta} - \theta)$ is approximated by the sampled distribution of $H_n^* \sim \Gamma_n(\hat{\theta}_b^* - \hat{\theta})$ and the quantiles of H_n are approximated by those of H_n^* , for B large enough.

Here we approximate the distribution of $\Gamma_n(\bar{X} - \theta)$

- standard bootstrap: compute quantiles of $\{\Gamma_n(\bar{X}_b^* - \bar{X})\}_{b=1}^B$ and use them as quantiles of $\Gamma_n(\bar{X} - \theta)$. That is, for example

$$\Gamma_n(\bar{X} - \theta) \leq q_{1-\alpha/2}^* \approx q_{1-\alpha/2}^* \Rightarrow \left[\bar{X} - \frac{q_{1-\alpha/2}^*}{\Gamma_n}, \bar{X} - \frac{q_{1-\alpha/2}^*}{\Gamma_n} \right]$$
$$\bar{X} - \frac{q_{1-\alpha/2}^*}{\Gamma_n} \leq \theta$$

for q_{α}^* the estimated α -quantile of $\{\Gamma_n(\bar{X}_b^* - \bar{X})\}_{b=1}^B$.

\Rightarrow Standard non-parametric bootstrap



- Studentized nonparametric bootstrap.

Suppose that $\sqrt{n}(\hat{\theta} - \theta) \xrightarrow{D} N(0, \sigma^2)$. If we can estimate

σ^2 , we have $\sqrt{n} \frac{(\hat{\theta} - \theta)}{\hat{\sigma}} \xrightarrow{D} N(0, 1)$ and we can approximate

$\sqrt{n} \frac{(\hat{\theta} - \theta)}{\hat{\sigma}}$ by resamples $\left\{ \sqrt{n} \frac{(\hat{\theta}_b^* - \hat{\theta})}{\hat{\sigma}_b^*} \right\}_{b=1}^B$ for $\hat{\sigma}_b^*$ an

estimate of $\hat{\sigma}$ for the b -th resample. In our case

$\sigma^2 = \text{var } X_1$ is estimated by $(\hat{\sigma}_b^*)^2 = \text{var} \{X_{1,b}^*, \dots, X_{m,b}^*\}$,

and the distribution of $\sqrt{n} \frac{\hat{\theta} - \theta}{\hat{\sigma}} = \sqrt{n} \frac{\bar{X} - \theta}{\sqrt{\widehat{\text{var}} X_1}}$ is

approximated by $\left\{ \sqrt{n} \frac{\bar{X}_b^* - \bar{X}}{\sqrt{\widehat{\text{var}} \{X_{1,b}^*, \dots, X_{m,b}^*\}}} \right\}$.

Usually it is good to studentize if we can because then the distribution of the quantity we approximate depends on θ ~~known~~ less (ideally, it does not depend on θ at all)

- Studentized NP bootstrap + variance stabilization analogous for $\sqrt{n}(\log \bar{X} - \log \theta)$

- Diagnostics: if really $X_1 \sim \text{Exp}(\lambda)$ then $EX = \theta \Rightarrow \text{var } X = \theta^2$

$EX = \sqrt{\text{var } X}$. This can be checked when EX and $\text{var } X$ are approximated by EX_b^* and $\text{var } X_b^*$

respectively. If these depart a lot, the original distribution was likely not exponential. But, it's not a test, of course.

diagnostics: if $X \sim \text{Exp}(\lambda)$ $EX = 1/\lambda$ $\text{var } X = 1/\lambda^2 \rightarrow EX = \text{s.d.}(X)$
 if $X \sim \text{Exp}(\lambda)$ $E \log \bar{X} \approx \log 1/\lambda$ $\text{var } \bar{X} \approx \frac{1 \cdot \text{var } X}{m (EX)^2} = \frac{1}{m} \sim \text{constant}$

⑥

Parametric bootstrap. We know that $F_\theta \sim X$, $\theta \in \Theta$ but don't know θ .
 \rightarrow estimate θ by $\hat{\theta}_m$ and generate replicates from $F_{\hat{\theta}_m}$.

Ex 44.45: $X \sim U([0, \theta])$ $\theta > 0$ $\hat{\theta}_m = X_{(m)}$ $m(\theta - \hat{\theta}_m) \overset{\infty}{\rightsquigarrow} \text{Exp}(1/\theta)$

But naive NP bootstrap generates $\hat{\theta}_0^* = X_{(m)}$ a lot \Rightarrow

$$P(X_{(m)}^* = X_{(m)} | X) = 1 - \left(\frac{m-1}{m}\right)^m \xrightarrow{m \rightarrow \infty} 1 - e^{-1}$$

$$\text{for } R_m^* = m(\hat{\theta} - \hat{\theta}_0^*) \quad P(R_m^* = 0 | X) \sim 1 - e^{-1} \text{ for } m \text{ large.}$$

\rightarrow generate X_0^* directly from $U([0, \hat{\theta}_m])$ and m procedure.

Goodness-of-fit testing: $H_0: X \sim F_\theta$ for some $\theta \in \Theta$ $H_1: X \not\sim F_\theta$ for any $\theta \in \Theta$

$$KS_m^\theta = \sup_x |F_m(x) - F_\theta(x)| \quad \text{estimate } \theta \text{ by } \hat{\theta}_m \rightarrow \text{use } KS_m^{\hat{\theta}_m} \text{ dist.}$$

for the nearest element of Θ . can't use the limiting distribution - that is based on single θ . \rightarrow generate replicates for $F_{\hat{\theta}_m}$ and resample KS_m^*

Two-sample problems: $X_1, \dots, X_m \sim F_1$ $Y_1, \dots, Y_n \sim F_2$ $H_0: EX = EY$ $H_1: EX \neq EY$

- parametric bootstrap approach resample from $N(0, S_x^2)$, $N(0, S_y^2)$ and evaluate a test statistic

- non-parametric resample from $X_i - \bar{X}$, $Y_j - \bar{Y}$ and evaluate from a t -statistic

Permutation test of independence: $(X_i, Y_i) \sim F_{X,Y}$ $H_0: X$ is indep of Y

under H_0 if one permutes Y_i and keeps X_i fixed to get (X_i, Y_i^*) then still X_i^* is indep. of Y_i^* . \Rightarrow evaluate

Gambler's χ^2 test of independence

$$X_1 \sim \text{Mult}(m_1, p_1, \dots, p_k)$$

$$X_3 \sim \text{Mult}(m_3, p_3, \dots, p_k)$$

$$P_{i0} = (P_{01}, \dots, P_{0k})$$

$H_0: P_i = P_j \forall i \neq j$ $X_1 \sim X_{1,1}, \dots, X_{m,1}$ individual observations.

under H_0 pool all observations $\sum_{i=1}^3 m_i$ and resample (permute) their order while keeping m_i observations for $X_i^* \Rightarrow$ invariant under H_0

Ex: Two sample problem

$X_{1, \dots, X_{m_1}} \sim F$ independent $H_0: F \equiv G$ Under $H_0, Z = (X_{1, \dots, X_{m_1}, Y_{1, \dots, Y_{m_2}}) \stackrel{iid}{\sim} F$
 $Y_{1, \dots, Y_{m_2}} \sim G$ $H_1: \neg H_0$ and Z is invariant with respect to permul.

Formally, $Z | Z_{(s)} \sim \text{Unif}$ (all permutations of $Z_{(s)}$) "generate" data under H_0

In analogy with nonparametric Bootstrap: permute Z to get Z^* , let X^* be the first m_1 elements of Z^* , Y^* the other m_2 elements and approximate the distribution of a test statistic T under H_0 by $T^* = T(X^*, Y^*)$

Permutation tests

Kolmogorov-Smirnov test $T_m = \sup_{x \in \mathbb{R}} | \hat{F}_{m_1}(x) - \hat{G}_{m_2}(x) |$

χ^2 -test of independence $\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}, \dots, \begin{pmatrix} X_m \\ Y_m \end{pmatrix} \sim F$ independent, $H_0: X$ is independent of Y
 $H_1: \neg H_0$

Under H_0 the law of $Z = (X_1, \dots, X_m, Y_1, \dots, Y_m)$ is invariant w.r.t. permutations of Y 's (with X 's fixed) \rightarrow generate new data by permuting Y 's

$X_i =$ value of data, $Y_i =$ sample indicators in k sample problem $\Rightarrow X$ is independent of Y iff all X_i have the same distribution \rightarrow permutation tests in k -sample problems
 permutations of labels labels. For $X_i \sim \text{Multinomial}$ this leads to a permutation χ^2 -test of independence.

Ex: Bootstrap in linear models $\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}, \dots, \begin{pmatrix} X_m \\ Y_m \end{pmatrix} \text{ iid}, Y_i = \beta' X_i + \varepsilon, \varepsilon \perp X, E[\varepsilon] = 0$

• nonparametric bootstrap resample directly from $\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}, \dots, \begin{pmatrix} X_m \\ Y_m \end{pmatrix}$

• model-based bootstrap estimate $\hat{\beta}, \hat{\varepsilon}_i := \frac{Y_i - \hat{\beta}' X_i}{\sqrt{1 - h_{ii}}}$ standardized residuals

so that $\hat{\varepsilon}$ are centered with unit variance, resample from $\hat{\varepsilon}$ to get ε^* and generate new data as $Y_i^* = \hat{\beta}' X_i + \varepsilon_i^*, \begin{pmatrix} X_1 \\ Y_1^* \end{pmatrix}, \dots, \begin{pmatrix} X_m \\ Y_m^* \end{pmatrix}$

- Works if the model is correct but also under fixed design.
- NP-Bootstrap works even if model is not true, but only in random design.

Ex: Durbin-Watson's test linear model, indices have meaning, ε may be a time series.

$\varepsilon \sim \text{AR}(1), \rho = \text{cor}(\varepsilon_i, \varepsilon_{i+1} | X), H_0: \rho = 0$

$H_1: \rho \neq 0$

$U = (U_1, \dots, U_m)$ residuals $DW = \frac{\sum_{i=2}^m (U_i - U_{i-1})^2}{\sum_{i=1}^m U_i^2} \approx 2(1 - \hat{\rho})$ for $\hat{\rho}$ estimator of ρ .

Also under H_0 , law of DW depends on the design matrix $X \rightarrow$ bootstrap.

Ex: Bootstrap in AR(1) $X_t = a X_{t-1} + \varepsilon_t, \varepsilon_t \stackrel{iid}{\sim} N(0, \sigma^2)$ independent of $X, a \in (-1, 1)$

data are not iid, cannot resample directly from X

model-based bootstrap $\hat{\varepsilon}_t := X_t - \hat{a} X_{t-1}, \hat{\varepsilon}$ are approximately iid

\rightarrow resample from $\hat{\varepsilon}$ to get ε^* and set $X_t^* = \hat{a} X_{t-1}^* + \varepsilon_t^*$.

Ex 10) Permutation test of independence

Ex 19) k independent random samples (with $k = \frac{1}{2}$)

$X_1, \dots, X_{m_1} \sim F_x$ $H_0: F_x = F_y = F_z$ $H_1: \neq H_0$

$Y_1, \dots, Y_{m_2} \sim F_y$ under H_0 , all observations are as iid, and any permutation has the same probability / original sample

For a test statistic T if H_0 is true, any permutation of the pooled sample should give a test statistic with the same distribution (T_0^*)

→ compute T

→ permute pooled data and evaluate T_0^*

→ find p-value by comparing T and $\{T_0^*\}_{b=1}^B$

Ex: Bootstrap in linear models

$\begin{pmatrix} X_1 \\ \vdots \\ X_m \end{pmatrix} \dots \begin{pmatrix} X_m \\ \vdots \\ X_m \end{pmatrix}$ iid $Y_i = \beta X_i + \epsilon_i$ for ϵ_i independent of X_i and $E(\epsilon_i | X_i) = 0$

→ nonparametric bootstrap: resample directly from $\begin{pmatrix} X_i \\ Y_i \end{pmatrix}$

→ model-based bootstrap: estimate β by $\hat{\beta}$, let $\hat{\epsilon}_i = \frac{Y_i - \hat{\beta} X_i}{\sqrt{1 - h_{ii}}}$ standardized residuals ($\hat{\epsilon}_i$ are unbiased, with variance σ^2), resample from $\hat{\epsilon}_i$ to get ϵ_i^*

and generate new response variables as $Y_i^* = \hat{\beta} X_i + \epsilon_i^*$

Bootstrap sample is given by $\begin{pmatrix} X_i \\ Y_i^* \end{pmatrix} \dots \begin{pmatrix} X_m \\ Y_m^* \end{pmatrix}$

- model-based bootstrap works if the assumed model is true also in fixed design.
- nonparam. bootstrap works always for random design, even if the model is not true.

Ex: Durbin-Watson's test. linear model, order of indices may have meaning;

ϵ_i may be a time series. $\epsilon_i \sim AR(1)$, $\rho = \text{cor}(\epsilon_i, \epsilon_{i-1} | X)$

$H_0: \rho = 0$ $H_1: \rho \neq 0$ for $U = (U_1 \dots U_m)^T$ residuals,

$DW = \frac{\sum_{i=2}^m (U_i - U_{i-1})^2}{\sum_{i=1}^m U_i^2} \approx 2(1 - \hat{\rho})$ for $\hat{\rho}$ the OLS estimator of ρ

Distribution of DW under H_0 depends on X . → needed bootstrap.

Ex 14) Bootstrap in autoregression $X_t = \alpha X_{t-1} + \epsilon_t$ $\epsilon_t \stackrel{iid}{\sim} N(0, \sigma^2)$ indep of X

$\alpha \in (-1, 1)$, $t \in \mathbb{Z}$ not iid X_1, X_2, \dots time series - can't use nonparametric

resample; model-based bootstrap $\hat{\epsilon}_t = X_t - \hat{\alpha} X_{t-1}$ then $\hat{\epsilon}_t$ are

approximately an iid sequence of ϵ_i → resample ϵ_t^* from $\hat{\epsilon}_t$ and

set $X_t^* = \hat{\alpha} X_{t-1}^* + \epsilon_t^*$. Then $\{X_t^*\}$ is the bootstrapped sample.

Ex 10) variance estimation in bootstrap - counterexample

bootstrapped distribution approximates the distribution of a finite sample

one version of the statistic, not the asymptotic distribution.