## 1. Introduction

- By Central Limit Theorem, if sample $(x_1, ..., x_n)$ with each $X_i \sim D(\mu, \sigma^2)$ ($D$ is some distribution) then as $n \to \infty$,

$$\overline{X} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

  So distribution of sample mean always tends to normal distribution, with standard deviation $\sigma \,/\, \sqrt{n}$.
- **Unbiased estimate of standard deviation of sample mean**:

$$s = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} \left(x_i - \overline{x}\right)^2}$$

- **Standard error of sample mean**: estimate of standard deviation of sample mean: $s \,/\, \sqrt{n}$ .
- If $n$ too small then $s$ is poor estimator and mean may not be normally distributed.
- If population distribution is normal and $n$ small then sample mean is $t$-distributed:

$$\frac{X - \mu}{s \,/\, \sqrt{n}} \sim t_{n-1}$$

  $\frac{X-\mu}{s/\sqrt{n}}$ is **pivotal quantity** as distribution doesn't depend on parameters of $X$.
- **Hypothesis test** for $\underline{x}$:
  - Define **null hypothesis** which identifies distribution believed to have generated each $x_i$.
  - Choose **test statistic** $h$ (function of $\underline{x}$), extreme when null is false, not extreme when null is true.
  - **Observed test statistic** is $t = h(\underline{x})$.
  - Determine how extreme $t$ is as a realisation of $T = h(X_1, ..., X_N)$ (so need to know distribution of $T$).
- **One sided $p$-value**:

$$\mathbb{P}(T \geq t \mid H_0 \text{ true}) \quad \text{or} \quad \mathbb{P}(T \leq t \mid H_0 \text{ true})$$

- **Two sided $p$-value**:

$$\mathbb{P}(T \geq |t| \cup T \leq -|t| \mid H_0 \text{ true})$$

## 2. Monte Carlo testing

- **Monte Carlo testing**: given observed test stat $t = h(\underline{x})$ distribution $F(x \mid \theta)$ hypotheses $H_0 : \theta = \theta_0$, $H_1 : \theta > \theta_0$:
  - For $j \in \{1, ..., N\}$:
    - Simulate $n$ observations $(z_1, ..., z_n)$ from $F(\cdot \mid \theta_0)$.
    - Compute $t_j = h(z_1, ..., z_n)$.
  - Estimate $p$-value by

$$P(T \geq t \mid H_0 \text{ true}) \approx \frac{1}{N} \sum_{j=1}^{N} \mathbb{I}\{t_j \geq t\}$$

# 3. The bootstrap

- **The non-parametric bootstrap estimate**: given independent data $\underline{x} = (x_1, ..., x_n)$ and stat $S(\cdot)$, **resample** (draw samples of size $n$ with replacement) $\underline{x}$ $B$ times to give $\underline{x}^{*1}, ..., \underline{x}^{*B}$. To compute **bootstrap estimate of standard error of $S$**, compute

$$\widehat{\operatorname{Var}}(S(\underline{x})) = \frac{1}{B-1} \sum_{b=1}^{B} \left(S(\underline{x}^{*b}) - \overline{S}^*\right)^2$$

  where

$$\overline{S}^* = \frac{1}{B} \sum_{b=1}^{B} S(\underline{x}^{*b})$$

  The standard error estimate is then $\sqrt{\widehat{\operatorname{Var}}(S(\underline{x}))}$, i.e. the standard deviation of $S(\underline{x}^{*1}), ..., S(\underline{x}^{*B})$ The **bootstrap estimate** of $S$ is simply $S(\underline{x})$.
- For random variable $X$, **(cumulative) distribution function (cdf)** $F : \mathbb{R} \to [0, 1]$ is

$$F_X(x) = F(x) := \mathbb{P}(X \leq x)$$

- Properties of cdf:
  - $\lim_{x \to -\infty} F(x) = 0$ and $\lim_{x \to \infty} F(x) = 1$.
  - **Monotonicity**: $x' < x \Longrightarrow F(x') \leq F(x)$.
  - **Right-continuity**: $\lim_{t \to x^+} F(t) = F(x)$.
- Given data $(x_1, ..., x_n)$ with each sample i.i.d. realisation of random variable $X$, **empirical (cumulative) distribution function (ecdf)** is

$$\hat{F}(x) := \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\{x_i \leq x\}$$

- Let $X_1, ..., X_n$ be random sample from distribution with cdf $F$. Then

$$\sup_{x \in \mathbb{R}} \left|\hat{F}(x) - F(x)\right| \to 0 \quad \text{as } n \to \infty$$

- Given data $(x_1, ..., x_n)$, sampling uniformly at random from $\underline{x}$ is equivalent to sampling from distribution with cdf defined as ecdf constructed from $\underline{x}$.
- For mean of sample of $m$ draws from ecdf constructed from $n$ data points, expectation and variance are

$$\mathbb{E}\left[\overline{Y}\right] = \overline{x}, \quad \operatorname{Var}\left(\overline{Y}\right) = \frac{n-1}{n} \frac{s_x^2}{m}$$

- So $\widehat{\operatorname{Var}}(S(\underline{x}) \to \frac{n-1}{n} \frac{s^2}{n}$ as $B \to \infty$.
- If **sampling fraction** $f = \frac{n}{N}$ where $N$ population size, $n$ sample size, is $f \geq 0.1$, can't assume infinite population.
- Given finite population of size $N$, mean $\overline{X}$ of sample drawn uniformly at random without replacement has variance

$$\text{Var}\left(\overline{X}\right) = \frac{N-n}{N-1}\frac{\sigma^2}{n}$$

where $\sigma^2$ is true population variance.

- Given finite population of size $N$, sample of size $n$ with variance $S^2$ drawn without replacement,

$$\mathbb{E}\left[\left(1-\frac{n}{N}\right)\frac{S^2}{n}\right] = \text{Var}\left(\overline{X}\right)$$

so it is unbiased estimator of $\text{Var}\left(\overline{X}\right)$

- **Population bootstrap**: given independent data $(x_1, ..., x_n)$ drawn from finite population of size $N$, assuming $N / n = k$ is integer, construct new data set

$$\underline{\tilde{x}} = (x_1, ..., x_n, x_1, ..., x_n, ..., x_1, ..., x_n)$$

by repeating $\underline{x}$ $k$ times. Then construct $B$ new samples $\underline{x}^{*1}, ..., \underline{x}^{*B}$ by sampling without replacement. Then compute

$$\widehat{\text{Var}}(S(\underline{x})) = \frac{1}{B-1}\sum_{b=1}^{B}\left(S\left(\underline{x}^{*b}\right) - \overline{S}^*\right)^2$$

where

$$\overline{S}^* = \frac{1}{B}\sum_{b=1}^{B} S\left(\underline{x}^{*b}\right)$$

If $N / n$ not integer, $N = kn + m$ for $0 < m < n$, then before each of the $B$ samples, append to $\underline{\tilde{x}}$ a sample without replacement of size $m$ from $\underline{x}$.

- If data believed to follow type of distribution, can use **parametric bootstrap**: given independent data $(x_1, ..., x_n)$, believed to be drawn from distribution $F(\cdot, \theta)$ with parameter $\theta$:
  - Find maximum likelihood estimator $\hat{\theta}$.
  - Draw $B$ new samples of size $n$ from $F\left(\cdot, \hat{\theta}\right)$ to give $\underline{x}^{*1}, ..., \underline{x}^{*B}$.
  - Compute

  $$\widehat{\text{Var}}(S(\underline{x})) = \frac{1}{B-1}\sum_{b=1}^{B}\left(S\left(\underline{x}^{*b}\right) - \overline{S}^*\right)^2$$

  where

  $$\overline{S}^* = \frac{1}{B}\sum_{b=1}^{B} S\left(\underline{x}^{*b}\right)$$

- For parameter $\theta$ of distribution, estimated by statistic $S$, with $\hat{\theta} = S(\underline{x})$, **bias** is

$$\text{bias}\left(\theta, \hat{\theta}\right) = \mathbb{E}\left[\hat{\theta}\right] - \theta$$

- **Basic bootstrap bias estimate**:

$$\widehat{\text{bias}}\left(\theta, \hat{\theta}\right) = \overline{S}^* - \hat{\theta} = \frac{1}{B}\sum_{b=1}^{B} S\left(\underline{x}^{*b}\right) - S(\underline{x})$$

- **Bias correction**: subtract bias from usual estimate:

$$\hat{\theta} - \widehat{\text{bias}}\left(\theta, \hat{\theta}\right) = 2\hat{\theta} - \overline{S}^*$$

  But often $2\hat{\theta} - \overline{S}^*$ has higher variance as estimator than $\hat{\theta}$.
- **Normal confidence interval for bootstrap estimate**:

$$\hat{\theta} \pm z_{\alpha/2}\sqrt{\widehat{\text{Var}}(S(\underline{x}))}$$

  where $z_{\alpha/2}$ is $100(\alpha / 2)\%$ percentile of standard normal distribution. **Note**: only valid if size of data large enough, need to check for normality of bootstrap samples using quantile plot.
- **Percentile confidence interval**: use if $\hat{F}$ close to true distribution. $100(1-\alpha)\%$ confidence interval is

$$\left[S^*_{((\alpha/2)B)}, S^*_{((1-\alpha/2)B)}\right]$$

  where $S^*_{(i)}$ is $i$th largest value of $S\left(\underline{x}^{*b}\right)$ for $b = 1, ..., B$. $B$ must be chosen to make $(\alpha / 2)B$ and $(1 - \alpha / 2)B$ integers. $B$ must be $> 2000$ for this to be good estimate. **Note**: inaccurate if bias or non-constant standard error or distribution of $S(X) \mid \theta$ isn't symmetric.
- **BC (bias corrected)** and **BCa (bias corrected and accelerated)** confidence intervals make adjustments when bias is present or there is non-constant standard error.

# 4. Monte Carlo integration

- Let random variable $Y$ take values in sample space $\Omega$ with pdf $f_Y$, then

$$\mu := \mathbb{E}[Y] = \int_\Omega y f_Y(y)\,\mathrm{d}y$$

- $\mu$ approximated by

$$\hat{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} Y_i$$

  for i.i.d. samples $Y_i$.
- If $Y = g(X)$ with $X$ random variable with pdf $f_X$, then

$$\mu = \mathbb{E}[Y] = \mathbb{E}[g(X)] = \int g(x) f_X(x)\,\mathrm{d}x$$

- To estimate $\int_a^b f(x)\,\mathrm{d}x$, use $X \sim$ Unif$(a, b)$

$$\mu = \int_a^b f(x)\,\mathrm{d}x = \int_a^b (b-a) f(x) \frac{1}{b-a} = \int_a^b (b-a) f(x) f_X(x) = \mathbb{E}[(b-a) f(X)]$$

  which can be estimated by

$$\hat{\mu}_n = (b-a)\frac{1}{n}\sum_{i=1}^{n} g(X_i)$$

for i.i.d. samples $X_i$.

- If $\operatorname{Var}(Y) = \sigma^2 < \infty$, Monte Carlo integration unbiased as $\mathbb{E}\left[\hat{\mu}_n\right] = \mu$.
- **Mean-square error**: $\operatorname{Var}\left(\hat{\mu}_n\right) = \mathbb{E}\left[\left(\hat{\mu}_n - \mu\right)^2\right] = \frac{\sigma^2}{n}$.
- **Root mean-square error**: $\text{RMSE} = \sqrt{\mathbb{E}\left[\left(\hat{\mu}_n - \mu\right)^2\right]} = \frac{\sigma}{\sqrt{n}}$.
- RMSE is $O\left(n^{-1/2}\right)$.
- For functions $f, g$, $f(n) = O(g(n))$ as $n \to \infty$ if exist $C, n_0 \in \mathbb{R}$ such that

$$\forall n \geq n_0, \quad |f(n)| \leq C g(n)$$

- **Midpoint Riemann integral estimate**:

$$\int_a^b f(x)\,\mathrm{d}x = \frac{b-a}{n}\sum_{i=1}^{n} f(x_i)$$

where

$$x_i = a + \frac{b-a}{n}\left(i - \frac{1}{2}\right)$$

- For $d$ dimensions, Riemann sum converges in $O\left(n^{-2/d}\right)$, Monte Carlo converges in $O\left(n^{-1/2}\right)$ regardless of $d$.
- $100(1-\alpha)\%$ confidence interval for Monte Carlo integration:

$$\mu \in \hat{\mu}_n \pm z_{\alpha/2}\frac{\sigma}{\sqrt{n}}$$

where $\sigma$ estimated with standard sample deviation of $\left\{y_i\right\} = \{g(x_i)\}$.

- If $g(x)$ constant multiple of indicator function, $g(x) = c\mathbb{I}\{A(x)\}$ for condition $A$, then

$$\hat{p}_n = \frac{1}{n}\sum_{i=1}^{n}\mathbb{I}\{A(x_i)\}$$

is estimator for $p = \mathbb{P}(A)$. Binomial confidence interval is

$$p \in \hat{p}_n \pm z_{\alpha/2}\sqrt{\frac{\hat{p}_n\left(1-\hat{p}_n\right)}{n}}$$

so confidence interval for $\mu$ is

$$\mu \in \hat{\mu}_n \pm c z_{\alpha/2}\sqrt{\frac{\hat{p}_n\left(1-\hat{p}_n\right)}{n}}$$

($\hat{\mu}_n = c\hat{p}_n$).

- Probability of no 1s in $n$ Monte Carlo samples is $(1-p)^n$ so one-sided $100(1-\alpha)\%$ confidence interval has upper bound $p \leq 1 - a^{1/n} \approx -\frac{\log(a)}{n}$ using Taylor expansion.
- If $\hat{p}$ very small and non-zero,

$$cz_{\alpha/2}\sqrt{\frac{\hat{p}_n\left(1-\hat{p}_n\right)}{n}} \approx cz_{\alpha/2}\sqrt{\frac{\hat{p}_n}{n}}$$

so relative error is

$$\delta := cz_{\alpha/2}\sqrt{\frac{\hat{p}_n}{n}} \,/\, \hat{p} = \frac{cz_{\alpha/2}}{\sqrt{\hat{p}_n n}}$$

for relative error at most $\delta$,

$$n \geq \frac{c^2 z_{\alpha/2}^2}{\hat{p}_n \delta^2}$$

so $n$ grows inversely with $\hat{p}_n$.
- To estimate probability of event $\mathbb{P}(X \in E)$, Monte Carlo estimate $\mathbb{E}[\mathbb{I}\{X \in E\}]$.

# 5. Simulation

- Let $F$ cdf, then **generalised inverse cdf** is

$$F^{-1}(u) := \inf\{x : F(x) \geq u\}$$

- **Inverse transform sampling algorithm**: let random variable $X$ with cdf $F$, with generalised inverse $F^{-1}$.
  - Simulate $U \sim \text{Unif}(0,1)$.
  - Compute $X \sim F^{-1}(U)$.

  $X$ is then distributed with cdf $F$. Only works for 1D distributions.
- **Rejection sampling algorithm**: given **target density** function $f$, **proposal density** function $\tilde{f}$ with $\forall x \in \mathbb{R}^d$, $f(x) \leq c\tilde{f}(x)$ for some $c < \infty$,
  - Set $a =$ false
  - While $a =$ false:
    - Simulate $u \sim \text{Unif}(0,1)$.
    - Simulate $x \sim \tilde{f}(\cdot)$.
    - If $u \leq \frac{f(x)}{c\tilde{f}(x)}$, set $a =$ true.
  - Once while loop exited, return $x$, which is distributed with pdf $f$.
- **Note**: $f$ and $\tilde{f}$ don't need to be normalised.
- When $f, \tilde{f}$ normalised, expected number of iterations of rejection sampling algorithm is $c$.
- **Important**: when choosing value of $c$, always round **up** if inexact.
- When checking if rejection sampling can be used, check if ratio $f(x) \,/\, \tilde{f}(x)$ tends to 0 as $x \to \pm\infty$ and differentiate ratio with respect to $x$ to find maximum.
- **Normalised importance sampling**: given normalised density function $f$ and normalised proposal density function $\tilde{f}$, $n$ importance samples produced by: for $i \in \{1, ..., n\}$:
  - Simulate $x_i \sim \tilde{f}(\cdot)$.
  - Compute $w_i = f(x_i) \,/\, \tilde{f}(x_i)$.

This produces importance samples $\{(x_i, w_i)\}_{i=1}^n$. $\mu = \mathbb{E}_{\tilde{f}}[g(X)]$ estimated by **importance sampling estimator**

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} w_i g(x_i)$$

($\mathbb{E}_{\tilde{f}}[\hat{\mu}] = \mu$, provided $\tilde{f}(x) > 0$ whenever $f(x)g(x) \neq 0$).

- Variance of importance sampling estimator is

$$\mathrm{Var}(\hat{\mu}) = \frac{\sigma_{\tilde{f}}^2}{n}$$

where

$$\sigma_{\tilde{f}}^2 = \int_{\tilde{\Omega}} \frac{\left(g(x)f(x) - \mu \tilde{f}(x)\right)^2}{\tilde{f}(x)} \,\mathrm{d}x$$

and $\tilde{\Omega}$ is support of $\tilde{f}$.

- Can estimate variance with

$$\hat{\sigma}_{\tilde{f}}^2 = \frac{1}{n} \sum_{i=1}^{n} \left(w_i g(x_i) - \hat{\mu}\right)^2$$

- Distribution which minimises estimator variance is

$$\tilde{f}_{\mathrm{opt}}(x) = \frac{|g(x)| f(x)}{\int_{\Omega} |g(x)| f(x) \,\mathrm{d}x}$$

- **Self-normalised importance sampling**: same as normalised importance sampling, but compute

$$\hat{\mu} = \frac{1}{\sum_{i=1}^{n} w_i} \sum_{i=1}^{n} w_i g(x_i)$$

Can use for unnormalised density functions $f, \tilde{f}$. $\hat{\mu}$ is not unbiased.

- Approximate variance of self-normalised estimator:

$$\mathrm{Var}(\hat{\mu}) \approx \frac{\sigma_{\tilde{f}}^2}{n}$$

where

$$\sigma_{\tilde{f}}^2 = \sum_{i=1}^{n} {w_i{}'}^2 \left(g(x_i) - \hat{\mu}\right)^2$$

and

$$w_i{}' = \frac{w_i}{\sum_{j=1}^{n} w_j}$$

- **Effective sample size $n_e$**: size of sample for which variance of naive Monte Carlo average $\left(\frac{1}{n_e}\sum_{i=1}^{n_e} g(x_i)\right)$ with sample size $n_e$, $\sigma^2 / n_e$ ($\sigma^2$ is variance of $g(X)$), is equal to variance of importance sampling estimator $\hat{\mu}$, $\mathrm{Var}(\hat{\mu})$:

$$n_e = \frac{n\overline{w}^2}{\overline{w^2}}$$

where

$$\overline{w}^2 = \left(\frac{1}{n}\sum_{i=1}^{n} w_i\right)^2, \quad \overline{w^2} = \frac{1}{n}\sum_{i=1}^{n} w_i^2$$

- Small $n_e$ means importance sampling is poor estimator.
- Poor estimator if proposal distribution has much less probability in tails than target distribution.