

# STA 532: Theory of Statistical Inference

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## 2 Estimating CDFs and Statistical Functionals

### Empirical CDFs

Let  $\{X_i : i \leq n\}$  be a “simple random sample”, *i.e.*, let the  $\{X_i\}$  be  $n$  iid replicates from the same probability distribution. We can’t know that distribution exactly from only a sample, but we can estimate it by the “empirical distribution” that puts mass  $1/n$  at each of the locations  $X_i$  (if the same value is taken more than once, its mass will be the sum of its  $1/n$ ’s so everything still adds up to one). The CDF

$$\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{[X_i, \infty)}(x)$$

of the empirical distribution will be piecewise-constant, with jumps of size  $1/n$  at each observation point (or  $k/n$  in the event of  $k$ -way ties).

Since  $\#\{i \leq n : X_i \leq x\}$  is just a Binomial random variable with  $p = F(x)$  for the real PDF for the  $\{X_i\}$ , with mean  $np$  and variance  $np(1-p)$ , it is clear that for each  $x \in \mathbb{R}$

- $\mathbb{E}\hat{F}_n(x) = F(x)$  and
- $\mathbb{V}\hat{F}_n(x) = F(x)[1 - F(x)]/n$ , so
- $\hat{F}_n(x)$  is an unbiased and MS consistent estimator of  $F(x)$ .

In fact something stronger is true— not only does  $\hat{F}_n(x)$  converge to  $F(x)$  pointwise in  $x$ , but also the *supremum*  $\sup_x |\hat{F}_n(x) - F(x)|$  converges to zero. There are many ways a sequence of random variables might converge (studying those is the main topic of a measure-theoretic probability course like Duke’s STA 711); the “Glivenko-Cantelli theorem” asserts that this maximum converges with probability one. Either Hoeffding’s inequality (Wassily Hoeffding was a UNC statistics professor) or the DKW inequality of Dvoetzsky, Kiefer, and Wolfowitz give the strong bound

$$\mathbb{P}\left[\sup_x |\hat{F}_n(x) - F(x)| > \epsilon\right] \leq 2e^{-2n\epsilon^2}$$

for every  $\epsilon > 0$ . It follows that, for any  $0 < \gamma < 1$ ,

$$\mathbb{P}[L(x) \leq F(x) \leq U(x) \quad \text{for all } x \in \mathbb{R}] \geq \gamma$$

is a non-parametric confidence set for  $F$ , for  $L(x) := 0 \vee (\hat{F}_n(x) - \epsilon_n)$ ,  $U(x) := 1 \wedge (\hat{F}_n(x) + \epsilon_n)$ , and  $\epsilon_n := \sqrt{\log(2/(1-\gamma))/2n}$ . Here  $a \vee b$  denotes the maximum of  $a, b \in \mathbb{R}$ ,  $a \wedge b$  the minimum.

## Statistical Functionals

Usually we don't want to estimate all of the CDF  $F$  for  $X$ , but rather some feature of it like its mean  $\mathbf{E}X = \int xF(dx)$  or variance  $\mathbf{V}X := \mathbf{E}(X - (\mathbf{E}X))^2 = \int x^2F(dx) - (\mathbf{E}X)^2$  or the probability  $[F(B) - F(A)]$  that  $X$  lies in some interval  $(A, B]$ .

### Examples of Statistical Functionals

Commonly-studied or quoted functionals of a univariate distribution  $F(\cdot)$  include:

- The **mean**  $\mathbf{E}[X] = \mu := \int_{\mathbb{R}} x F(dx) = \int_0^\infty [1 - F(x)] dx - \int_{-\infty}^0 F(x) dx$ , quantifying location;
- The  $q$ th **quantile**  $z_q := \inf\{x < \infty : F(x) \geq q\}$ , especially
- The **median**  $z_{1/2}$ , another way to quantify location;
- The **variance**  $\mathbf{V}[X] = \sigma^2 := \int_{\mathbb{R}} (x - \mu)^2 F(dx) = \mathbf{E}[X^2] - \mathbf{E}[X]^2$ , quantifying spread;
- The **skewness**  $\gamma_1 := \int_{\mathbb{R}} (x - \mu)^3 F(dx) / \sigma^3$ , quantifying asymmetry;
- The (excess) **kurtosis**  $\gamma_2 := \int_{\mathbb{R}} (x - \mu)^4 F(dx) / \sigma^4 - 3$ , quantifying peakedness. “Lepto” is Greek for skinny, “Platy” for fat, and “Meso” for middle; distributions are called leptokurtic ( $t$ , Poisson, exponential), platykurtic (uniform, Bernoulli), or mesokurtic (normal) as  $\gamma_2$  is positive, negative, or zero, respectively.
- The **expectation**  $\mathbf{E}[g(X)] = \int_{\mathbb{R}} g(x) F(dx)$  for any specified problem-specific function  $g(\cdot)$ .

Not all of these exist for some distributions—for example, the mean, variance, skewness, and kurtosis are all undefined for heavy-tailed distributions like the Cauchy or  $\alpha$ -Stable. There are quantile-based alternative ways to quantify location, spread, asymmetry, and peakedness, however—for example, the interquartile range  $\text{IQR} := [z_{3/4} - z_{1/4}]$  for spread, for example.

Any of these can be estimated by the same expression computed with the *empirical* CDF  $\hat{F}_n(x)$  replacing  $F(x)$ , without specifying a parametric model for  $F$ . There are methods (one is the “jackknife”; another, the “bootstrap”, is described below) for trying to estimate the mean and variance of any of these functionals from a sample  $\{X_1, \dots, X_n\}$ .

Later we'll see ways of estimating the functionals that *do* require the assumption of particular parametric statistical models. There's something of a trade-off in deciding which approach to take. The parametric models typically give more precise estimates and more powerful tests, *if* their underlying assumptions are correct. BUT, the non-parametric approach will give sensible (if less precise) answers even if those assumptions fail. In this way they are said to be more “robust”.

## Simulation

### The Bootstrap

One way to estimate the probability distribution of a functional  $T_n(X) = T(X_1, \dots, X_n)$  of  $n$  iid replicates of a random variable  $X \sim F(dx)$ , called the “bootstrap” (Efron, 1979; Efron and

Tibshirani, 1993), is to approximate it by the empirical distribution of  $T_n(\hat{X})$  based on draws *with replacement* from a sample  $\{X_1, \dots, X_n\}$  of size  $n$ . The underlying idea is that these would be drawn from exactly the right distribution of  $T(X)$  if we could possibly repeat draws of  $X = (X_1, \dots, X_n)$  from the *population*; if the sample is large enough, we can hope that the empirical distribution will be close to the population distribution, and so the bootstrap sample will be much like a true random sample from the population (but without the expense of drawing new data).

### Bootstrap Variance

For example, the population median

$$M = T(F) := \inf \{x \in \mathbb{R} : F(x) \geq 1/2\}$$

might be estimated by the sample median  $M_n = T(\hat{F}_n)$ , but how precise is that estimate? One measure would be its *standard error*

$$\text{se}(M_n) := \{E|M_n - M|^2\}^{1/2}$$

but to calculate that would require knowing the distribution of  $X$ , while we only have a sample. The Bootstrap approach is to use some number  $B$  of repeated draws with replacement of size  $n$  from this sample as if they were draws from the population, and estimate

$$\hat{\text{se}}(M_n) \approx \left\{ \frac{1}{B} \sum_{b=1}^B |M_n^b - \hat{M}_n|^2 \right\}^{1/2}$$

where  $\hat{M}_n$  is the sample average of the  $B$  medians  $\{M_n^b\}$ .

### Bootstrap Confidence

Interval estimates  $[L, U]$  of a real-valued parameter  $\theta$ , intended to cover  $\theta$  with probability at least  $100\gamma\%$  for any  $\theta$ , can also be constructed using a bootstrap approach. One way to do that is to begin with an iid sample  $X = \{X_1, \dots, X_n\}$  from the uncertain distribution  $F$ ; draw  $B$  independent size- $n$  draws with replacement from the sample  $X$ ; for each, compute the statistic  $T_n(X^b)$ ; and set  $L$  and  $U$  to the  $(\alpha/2)$  and  $(1-\alpha/2)$  quantiles of  $\{T_n(X^b)\}$ , respectively, for  $\alpha = (1-\gamma)$ . Wasserman (2004, §8.3) argues why this should work and gives two alternatives.

### Bayesian Simulation

#### Bayesian Bootstrap

Rubin (1981) introduced the “Bayesian bootstrap” (BB), a minor variation on the bootstrap that leads to a simulation of the posterior distribution of the parameter vector  $\theta$  governing a distribution  $F(\cdot | \theta)$  in a parametric family, from a particular (and, in Rubin’s view, implausible) improper prior distribution. This five-page paper is a good read, and argues that neither the BB nor the original bootstrap is suitable as a “general inferential tool” because of its implicit use of this prior.

## Importance Sampling

Most Bayesian analyses require the evaluation of one or more integrals, often in moderately high-dimensional spaces. For example: if  $\pi(\theta)$  is a prior density function on  $\Theta \subset \mathbb{R}^d$ , and if  $\mathcal{L}(\theta | X)$  is the likelihood function for some observed quantity  $X \in \mathcal{X}$ , then the posterior expectation of any function  $g : \Theta \rightarrow \mathbb{R}$  is given by the ratio

$$\mathbb{E}[g(\theta) | X] = \frac{\int_{\Theta} g(\theta) \mathcal{L}(\theta | X) \pi(\theta) d\theta}{\int_{\Theta} \mathcal{L}(\theta | X) \pi(\theta) d\theta}. \quad (1a)$$

Often the integrals in both numerator and denominator are intractable analytically, so we must resort to numerical approximation. Let  $f(\theta)$  be any pdf such that the ratio  $w(\theta) := \mathcal{L}(\theta | X) \pi(\theta) / f(\theta)$  is bounded (for this,  $f(\theta)$  must have “fatter tails” than  $\mathcal{L}(\theta | X) \pi(\theta)$ ), and let  $\{\theta_m\}$  be iid replicates from the distribution with pdf  $f(\theta)$ . Then

$$= \frac{\int_{\Theta} g(\theta) w(\theta) f(\theta) d\theta}{\int_{\Theta} w(\theta) f(\theta) d\theta} = \lim_{M \rightarrow \infty} \frac{\sum_{m=1}^M g(\theta_m) w(\theta_m)}{\sum_{m=1}^M w(\theta_m)} \quad (1b)$$

so  $\mathbb{E}[g(\theta) | X]$  can be evaluate as the limit of weighted averages of  $g(\cdot)$  at the simulated points  $\{\theta_m\}$ . Provided that  $\int_{\Theta} g(\theta)^2 f(\theta) d\theta < \infty$ , the mean-square error of the sequence of approximations in (1b) will be bounded by  $\sigma^2/M$  for a number  $\sigma^2$  that can also be estimated from the same Monte Carlo sample  $\{\theta_m\}$ , giving a simple measure of precision for this estimate.

This simulation-based approach to estimating integrals, called “Monte Carlo Importance sampling”, works well in dimensions up to six or seven or so. A number of ways have been discovered and exploited to reduce the stochastic error bound  $\sigma/\sqrt{M}$ . These include “antithetic variables”, in which the iid sequence  $\{\theta_m\}$  is replaced by a sequence of negatively-correlated pairs; “control variates”, in which one tries to estimate  $[g(\theta) - h(\theta)]$  for some quantity  $h$  whose posterior mean is known; and “sequential MC”, in which the sampling function  $f(\theta)$  is periodically replaced by a “better” one.

## MCMC

A similar approach to (1) that succeeds in many higher-dimensional problems is Markov Chain Monte Carlo, based on sample averages of  $\{g(\theta_m) : 1 \leq m < \infty\}$  for an ergodic sequence  $\{\theta_m\}$  constructed so that it has stationary distribution  $\pi(\theta | X)$ . You’ll see much more about that in other courses at Duke, so we won’t focus on it here.

## Particle Methods, Adaptive MCMC, Variational Bayes, ...

There are a number of variations on MCMC methods, as well. Some of these involve averaging  $\{g(\theta_m^{(k)}) : 1 \leq m < \infty\}$  for a number of streams  $\theta_m^{(k)}$  (here the streams are indexed by  $k$ ), possibly by a variable number of streams whose distributions may evolve through the computation. This is an area of active research; ask any Duke statistics faculty member if you’re interested.

## References

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