

University of Waterloo

STAT 341 - Computational Statistics and Data Analysis

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Personal Course Notes

Brandon Zhou

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Author	Brandon Zhou
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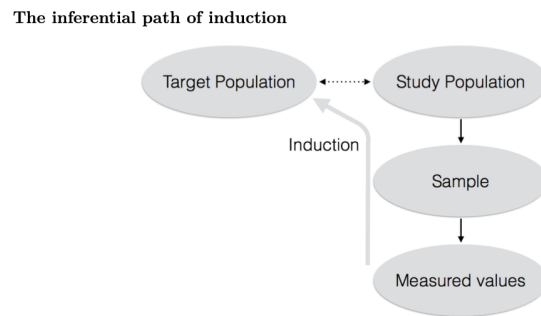


Figure 1: The inferential path of induction

The above content is for Lecture 1 on Jan 9, 2024

CHAPTER 2: Populations

2.1 Populations

Definition 2.1

Here we aim to describe a population using attributes.

- A population is a finite (though possibly huge) set \mathcal{P} of elements.
 - Elements of a population are called units $u \in \mathcal{P}$
 - Variates are functions $x(u), y(u)$, etc. on the individual units $u \in \mathcal{P}$. For simplicity we will more often use the notation x_u, y_u , etc. when referring to the realized values of these variates for the unit $u = 1, \dots, N$.
- We will define and explore interesting population attributes, denoted generally as $a(\mathcal{P})$.

2.2 Explicitly Defined Population Attributes

2.2.1 Population Attributes

Definition 2.2

Some definitions we need to know:

- The population is typically a set or collection of units, each with one or more variates that we can measure.
- Variates are characteristics of each unit in the population, and they can take on numerical or categorical values.
 - The values of variates typically differ from unit to unit.
 - If we are only interested in the variate y 's we might write the population as

$$\mathcal{P} = \{y_1, y_2, \dots, y_N\}$$

- Population attributes are summaries describing characteristics of the population.
 - Formally, an attribute is a function applied to the entire population and determined by the variate values observed for each of the population's units.

$$a(\mathcal{P}) = f(y_1, y_2, \dots, y_N)$$

- Some examples of attributes are
 - the population total:

$$a(\mathcal{P}) = \sum_{u \in \mathcal{P}} y_u$$

– or various counts over the population

$$a(\mathcal{P}) = \sum_{u \in \mathcal{P}} I_A(y_u)$$

where $I_A(y)$ is the indicator function

$$I_A(y) = \begin{cases} 1 & \text{if } y \in A \\ 0 & \text{if } y \notin A \end{cases}$$

In general, attributes can be numerical or graphical – as long as they summarize the whole population.

Definition 2.3

Location Attributes measure or describe the centre of the distribution of variate values in a dataset.

- the population average:

$$a(\mathcal{P}) = \bar{y} = \frac{1}{N} \sum_{u \in \mathcal{P}} y_u$$

- the population proportion:

$$a(\mathcal{P}) = \frac{1}{N} \sum_{u \in \mathcal{P}} I_A(y_u)$$

- Other examples include the mode, the median, etc.

Spread Attributes measure variability or spread of the variate values in a data set. Some are

- the population variance:

$$a(\mathcal{P}) = \frac{1}{N} \sum_{u \in \mathcal{P}} (y_u - \bar{y})^2$$

- the population standard deviation:

$$a(\mathcal{P}) = SD_{\mathcal{P}}(y) = \sqrt{\frac{1}{N} \sum_{u \in \mathcal{P}} (y_u - \bar{y})^2}$$

- coefficient of variation:

$$a(\mathcal{P}) = \frac{SD_{\mathcal{P}}(y)}{\bar{y}}$$

- *Note:* the population variance or standard deviation could also be defined using $N - 1$ in the denominator.

- Other examples include the range, the inter-quartile range, etc.

Order Statistics

- Population attributes can also be based on an indexed collection of values,

$$y_{(1)} \leq y_{(2)} \leq \cdots \leq y_{(N)}$$

which are the variate values $y_u \in \mathcal{P}$ ordered from smallest to largest (including ties).

Location Attributes based on Order Statistics

These attributes measure or describe the centre of the distribution of variate values in a data set.

- the population minimum:

$$a(\mathcal{P}) = \min_{u \in \mathcal{P}} y_u = y_{(1)}$$

- the population maximum:

$$a(\mathcal{P}) = \max_{u \in \mathcal{P}} y_u = y_{(N)}$$

- the population mid-range:

$$a(\mathcal{P}) = \frac{1}{2} \left[\min_{u \in \mathcal{P}} y_u + \max_{u \in \mathcal{P}} y_u \right] = \frac{y_{(1)} + y_{(N)}}{2}$$

- the population median:

$$a(\mathcal{P}) = \text{median}_{u \in \mathcal{P}} y_u = \begin{cases} y_{(\frac{N+1}{2})}, & \text{if } N \text{ is odd} \\ \frac{y_{(\frac{N}{2})} + y_{(\frac{N}{2}+1)}}{2}, & \text{if } N \text{ is even} \end{cases}$$

- the population quartiles:

- Q_1 is 25th percentile, or the first quartile,
- Q_2 is 50th percentile, or the median, and
- Q_3 is 75th percentile, or the third quartile.

Variability Attributes based on Order Statistics

- The population range:

$$a(\mathcal{P}) = \max_{u \in \mathcal{P}} y_u - \min_{u \in \mathcal{P}} y_u = y_{(N)} - y_{(1)}$$

- The population inter-quartile range IQR:

$$a(\mathcal{P}) = Q_3 - Q_1$$

where Q_1 and Q_3 are 25th and 75th percentiles or the first and third quartiles, as above. Notice these are functions of entire population.

- The Median Absolute Deviation (MAD) is the median of the absolute differences between each

y_u and the median:

$$a(\mathcal{P}) = \text{median}_{u \in \mathcal{P}} |y_u - \text{median}_{u \in \mathcal{P}} y_u|$$

Skewness Attributes

These are measures of asymmetry in a population. A symmetric distribution of population values should result in a skewness attribute of zero.

- Pearson's moment coefficient of Skewness:

$$a(\mathcal{P}) = \frac{\frac{1}{N} \sum_{u \in \mathcal{P}} (y_u - \bar{y})^3}{[SD_{\mathcal{P}}(y)]^3}$$

- Pearson's second skewness coefficient (median skewness) given by:

$$a(\mathcal{P}) = \frac{3 \times (\bar{y} - \text{median}_{u \in \mathcal{P}} y_u)}{SD_{\mathcal{P}}(y)}$$

- Bowley's measure of skewness based on the quartiles:

$$a(\mathcal{P}) = \frac{(Q_3 + Q_1)/2 - Q_2}{(Q_3 - Q_1)/2}$$

NAs in R: Note that many programs in R accommodate missing data (represented as NAs) and do something appropriate (typically they omit them).

- For your own code and analyses, you either need to decide what to do with NAs or ensure that the data do not have any NAs.
- If you choose to simply omit NAs, for example, the function `na.omit(...)` may be helpful (it will remove rows which contain an NA from a data set). For other possibilities see `help("na.omit")` in R.

2.2.2 Attribute Properties

Definition 2.4

A population attribute is a function of measured variates y_u :

$$a(\mathcal{P}) = f_y, y_2, \dots, y_N$$

and the variates y_u are typically associated with some measurement units.

Definition 2.5

Location Invariance and Equivariance

For an attribute $a(\mathcal{P}) = a(y_1, \dots, y_N)$ we say that for any $m > 0$ and $b \in \mathbb{R}$, that the attribute is

- location invariant if

$$a(y_1 + b, \dots, y_N + b) = a(y_1, \dots, y_N)$$

- location equivariant if

$$a(y_1 + b, \dots, y_N + b) = a(y_1, \dots, y_N) + b$$

Example 2.1

The population average is location equivariant:

$$\begin{aligned} a(\mathcal{P}) &= a(y_1, y_2, \dots, y_N) = \frac{1}{N} \sum_{i=1}^N y_i \\ a(y_1 + b, y_2 + b, \dots, y_N + b) &= \frac{1}{N} \sum_{i=1}^N (y_i + b) \\ &= \frac{1}{N} \sum_{i=1}^N y_i + \frac{Nb}{N} = a(\mathcal{P}) + b \end{aligned}$$

But is the population variance location equivariant? No!

Definition 2.6

Scale Invariance and Equivariance

For an attribute $a(\mathcal{P}) = a(y_1, \dots, y_N)$ we say that for any $m > 0$ and $b \in \mathbb{R}$, that the attribute is

- scale invariant if

$$a(m \times y_1, \dots, m \times y_N) = a(y_1, \dots, y_N)$$

- scale equivariant if

$$a(m \times y_1, \dots, m \times y_N) = m \times a(y_1, \dots, y_N)$$

- location-scale invariant if it is both location invariant and scale invariant, i.e.

$$a(m \times y_1 + b, \dots, m \times y_N + b) = a(y_1, \dots, y_N)$$

- location-scale equivariant if it is both location equivariant and scale equivariant, i.e.

$$a(m \times y_1 + b, \dots, m \times y_N + b) = m \times a(y_1, \dots, y_N) + b$$

Example 2.2

The population average is location-scale equivariant

$$\begin{aligned} a(my_1 + b, my_2 + b, \dots, my_N + b) &= \frac{1}{N} \sum_{i=1}^N (my_i + b) \\ &= \frac{m}{N} \sum_{i=1}^N y_i + \frac{Nb}{N} \\ &= ma(\mathcal{P}) + b \end{aligned}$$

Definition 2.7

Replication

Another invariance/equivariance property of interest for population attributes is replication invariance and replication equivariance.

If a population \mathcal{P} is duplicated $k - 1$ times (so that there are k copies of it), how does the attribute change on this new population denoted by \mathcal{P}^k ?

$$\mathcal{P}^k = \{y_1, y_2, \dots, y_N, y_1, y_2, \dots, y_N, \dots, y_1, y_2, \dots, y_N\} = \underbrace{\{x_1, x_2, \dots, x_{kN}\}}_{kN \text{ elements}}$$

The attribute $a(\mathcal{P})$ is

- replication invariant whenever $a(\mathcal{P}^k) = a(\mathcal{P})$
- replication equivariant whenever $a(\mathcal{P}^k) = k \times a(\mathcal{P})$

Example 2.3

The population average is replication invariant.

$$a(\mathcal{P}^k) = \frac{1}{kN} \sum_{j=1}^{kN} y_j = \frac{1}{kN} \sum_{i=1}^N ky_i = \frac{1}{N} \sum_{i=1}^N y_i = a(\mathcal{P})$$

2.2.3 Influence, Sensitivity Curves, and Breakdown Points

Definition 2.8

Influence(outlier detection)

- If we remove variate y_u (i.e. remove unit u) then the influence of that variate on the population attribute is quantified by

$$\Delta(a, u) = \underbrace{a(y_1, \dots, y_{u-1}, y_u, y_{u+1}, \dots, y_N)}_{\text{population with the unit } u} - \underbrace{a(y_1, \dots, y_{u-1}, y_{u+1}, \dots, y_N)}_{\text{population without the unit } u}$$

- Ideally, no single unit's value should have greater influence than any other.

- If a unit has larger influence than the rest;
 1. it would require further investigation as it might be in error, or
 2. it might be the most interesting unit in the population.

The population average, $a(y_1, y_2, \dots, y_n) = \bar{y}$ and the average without unit u can be written as

$$a(y_1, \dots, y_{u-1}, y_{u+1}, \dots, y_N) = \frac{1}{N-1} \sum_{\substack{k \in \mathcal{P}, \\ k \neq u}} y_k = \frac{\sum_{k \in \mathcal{P}} y_k - y_u}{N-1} = \frac{N\bar{y} - y_u}{N-1}$$

and $\Delta(a, u)$, the influence for a given u , is:

$$\Delta(a, u) = \bar{y} - \frac{N\bar{y} - y_u}{N-1} = \frac{(N-1)\bar{y} - (N\bar{y} - y_u)}{N-1} = \frac{y_u - \bar{y}}{N-1}$$

The above content is for Lecture 2 on Jan 11, 2024

Definition 2.9

Sensitivity Curve

- We can also examine the effect on an attribute when we add a variate. To examine this effect,
 - suppose we have a population of size $N-1$ and
 - add a variate with the value y .
 - Then our new population with N elements is $\{y_1, \dots, y_{N-1}, y\}$.
- We define the *sensitivity curve* of an attribute as

$$\begin{aligned} SC(y; a(\mathcal{P})) &= \frac{a(y_1, \dots, y_{N-1}, y) - a(y_1, \dots, y_{N-1})}{\frac{1}{N}} \\ &= N[a(y_1, \dots, y_{N-1}, y) - a(y_1, \dots, y_{N-1})] \end{aligned}$$

- We can then plot the *sensitivity curve* as a function of the new variate value y .
 - the sensitivity curve gives a scaled measure of the effect that a single variate value y has on the value of a population attribute $a(\mathcal{P})$.
- We can explore the sensitivity curve for any attribute. These can be determined *mathematically* in general, but can also be determined *computationally* for any particular population and any particular attribute.

The following is a general-purpose sensitivity curve function in R which accommodates any population and any attribute:

```
sc = function(y.pop, y, attr, ...) {
  N = length(y.pop) + 1
```

```

    supply(y, function(y.new) { N * (attr(c(y.new, y.pop), ...) - attr(y.pop,
...)) })
}
# ... means "carry through any additional arguments".

```

Example 2.4

Derive the sensitivity curve for Arithmetic Mean

$$a(y_1, \dots, y_N) = \frac{1}{N} \sum_{i=1}^N y_i = \bar{y}$$

$$P = \{y_1, \dots, y_{N-1}\}$$

$$P^* = \{y_1, \dots, y_{N-1}, y\}$$

$$a(P) = \frac{1}{N-1} \sum_{i=1}^{N-1} y_i = \bar{y}_{N-1}$$

$$\begin{aligned}
 a(P^*) &= \frac{1}{N} \left[\sum_{i=1}^{N-1} y_i + y \right] \\
 &= \frac{(N-1)\bar{y}_{N-1} + y}{N}
 \end{aligned}$$

$$\begin{aligned}
 \therefore \text{SC}(y, a) &= N [a(P^*) - a(P)] \\
 &= N \left[\frac{(N-1)\bar{y}_{N-1} + y}{N} - \bar{y}_{N-1} \right] \\
 &= (N-1)\bar{y}_{N-1} + y - N\bar{y}_{N-1} \\
 &= y - \bar{y}_{N-1}
 \end{aligned}$$

Notes:

- A single observation can change the average by a huge (even infinite) amount.
- Averages may not be the best choice for a population attribute representing the location of a population – particularly if extreme values exist in the population.

Example 2.5

Derive the sensitivity curve for maximum

$$a(y_1, \dots, y_N) = \max\{y_1, \dots, y_N\} = y_{(N)}$$

$$\begin{aligned}
P &= \{y_1, \dots, y_{N-1}\} \\
P^* &= \{y_1, \dots, y_{N-1}, y\} \\
a(P) &= y_{(N-1)} \\
a(P^*) &= \begin{cases} y_{(N-1)} & \text{if } y \leq y_{(N-1)} \\ y & \text{if } y > y_{(N-1)} \end{cases} \\
\therefore \text{SC}(y, \alpha) &= N [a(P^*) - a(P)] \\
&= \begin{cases} 0 & \text{if } y \leq y_{(N-1)} \\ N[y - y_{(N-1)}] & \text{if } y > y_{(N-1)} \end{cases}
\end{aligned}$$

If we draw the sensitivity curve for the maximum, we would find out it is unbounded for large y , the maximum is very sensitive to large outliers.

Example 2.6

Derive the sensitivity curve for 2^{nd} Order Statistic

$$a(y_1, \dots, y_N) = y_{(2)}$$

$$\begin{aligned}
P &= \{y_1, \dots, y_{N-1}\} \\
a(P) &= y_{(2)} \\
P^* &= \{y_1, \dots, y_{N-1}, y\} \\
a(P^*) &= \begin{cases} y_{(1)} & \text{if } y < y_{(1)} \\ y & \text{if } y_{(1)} \leq y < y_{(2)} \\ y_{(2)} & \text{if } y \geq y_{(2)} \end{cases} \\
\therefore \text{SC}(y, a) &= N [a(P^*) - a(P)] \\
&= \begin{cases} N(y_{(1)} - y_{(2)}) & \text{if } y < y_{(1)} \\ N(y - y_{(2)}) & \text{if } y_{(1)} \leq y < y_{(2)} \\ 0 & \text{if } y \geq y_{(2)} \end{cases}
\end{aligned}$$

Definition 2.10

Breakdown Points

Another measure of robustness that exists is called the breakdown point.

- It gives an assessment of just how large a proportion of the data must be contaminated before the statistic breaks down (and becomes useless).
- The breakdown point of a statistic is the smallest possible fraction of the observations that can be changed to something very extreme (i.e., plus or minus infinity) to make the error large (infinite)

- e.g. the break-point for
 - the average is $1/N$ (or asymptotically zero), and
 - the median is $1/2$ (i.e., that is half of the data has to go to infinity before the median breaks down).
- Attributes with high breakdown points are called resistant or robust.

2.2.4 Graphical Attributes

Population attributes can also be entirely graphical as in

- histograms of y_u values (univariate graphical summaries)
- bar plots of y_u values (univariate graphical summaries)
- box plots of y_u values (univariate graphical summaries)
- scatter-plots of pairs (x_u, y_u) (bivariate graphical summaries)
- scatter-plots of quantiles and ranks of y_u (bivariate graphical summaries)

Each of these plots summarizes the entire population, and so they're all attributes.

Histograms

Consider the population $\mathcal{P} = \{y_1, y_2, \dots, y_N\}$.

- Partition the range of the population into k non-overlapping intervals, called bins, $I_j = [a_{j-1}, a_j)$, for $j = 1, 2, \dots, k$ and then calculate the number (frequency) or proportion (relative frequency) of observations in the j th bin for $j = 1, \dots, k$.
- Histograms help determine how the values are concentrated.

We can define bins two ways:

- bins of equal size, or (most common)
- bins with equal number of elements but varying size. ("equal area" histogram)
- Below are some examples of histograms with equal-sized bins (top row) and bins of varying sizes (bottom row)

```
x = agpop$farms87
par(mfrow=c(2,3), mar=2.5*c(1,1,1,0.1))
rx = range(x)
hist(x, breaks=seq(rx[1], rx[2], length.out=4), prob=TRUE, main="3 Bins", col
     = "grey")
hist(x, breaks=seq(rx[1], rx[2], length.out=5), prob=TRUE, main="4 Bins", col
     = "grey")
hist(x, breaks=seq(rx[1], rx[2], length.out=16), prob=TRUE, main="15 Bins",
     col = "grey")

# For the histograms in the bottom row, the areas of all rectangles in each
```

```

    panel are the same.
hist(x, breaks=quantile(x, p=seq(0, 1, length.out=4)), prob=TRUE, main="3 Bins
", col = "grey")
hist(x, breaks=quantile(x, p=seq(0, 1, length.out=5)), prob=TRUE, main="4 Bins
" , col = "grey")
hist(x, breaks=quantile(x, p=seq(0, 1, length.out=16)), prob=TRUE, main="15
Bins", col = "grey")

```

The bins with equal numbers of elements but varying size can help identify asymmetry in the population.

Rules for the Number of Bins

- Sturges rule:

$$\text{the number of bins should be} = \lceil \log_2(N) + 1 \rceil$$

- Freedman–Diaconis rule:

$$\text{Bin size} = 2 \frac{\text{IQR}(x)}{N^{1/3}}$$

- Scott's rule:

$$\text{Bin size} = 3.5 \frac{\sigma}{N^{1/3}}$$

Histograms using different rules for bin size selection:

- the first row is `Number of farms` and
- the second row is `log(Number of farms+1)`.

Question: Which scale would you prefer to work with? The original scale or the transformed scale?

Answer: Advantages

- Raw data: data values are easily interpretable
- Transformed data: symmetric data are often easier to work with, statistically speaking

Scatter-plots

- A scatter-plot is a plot of the points (x_u, y_u) for all units in the population.
 - It is used to see whether two variates x and y are related in some way.
- A scatter-plot of the number of farms and total acreage of farming in 1987 by US county is below.

```

par(mfrow=c(1,2))
plot(agpop$farms87, agpop$acres87, pch = 19, cex=0.5, col=adjustcolor("black",
  alpha = 0.3), xlab = "Number of farms", ylab = "Total acreage of farming"
, main = "US counties 1987")

plot(agpop$acres87, agpop$farms87, pch = 19, cex=0.5, col=adjustcolor("black",
  alpha = 0.3), ylab = "Number of farms", xlab = "Total acreage of farming"
, main = "US counties 1987")

```


- Sometimes, the scatter-plot of a transformed version of the data provides more insight.

```
par(mfrow=c(1,2))
plot(log(agpop$farms87+1), log(agpop$acres87+1), pch = 19, cex=0.5, col=
  adjustcolor("black", alpha = 0.3), xlab = "log(Number of farms + 1)", ylab
  = "log(Total acreage of farming + 1)", main = "US counties 1987")
plot(log(agpop$acres87+1), log(agpop$farms87+1), pch = 19, cex=0.5, col=
  adjustcolor("black", alpha = 0.3), ylab = "log(Number of farms + 1)", xlab
  = "log(Total acreage of farming + 1)", main = "US counties 1987")
```

The above content is for Lecture 3 on Jan 16, 2024
