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## Warning: these notes may contain factual errors

## Reading: VDV Chapter 12

## Outline:

- U-Statistics (VDV Chapter 12)
- Definitions
- Examples
- Variance calculation


## 1 U-Statistics

### 1.1 Definitions

Suppose I have $h: X^{r} \rightarrow \mathbb{R}$ and want to estimate $\theta=E\left[h\left(X_{1}, \ldots, X_{r}\right)\right]$, where the $X_{i}$ are independent. Given a sample $\left(X_{1}, \ldots, X_{n}\right)$, how should I estimate $\theta$ ?
Example:
Observe that

$$
\operatorname{Var}(X)=E\left[X_{1}^{2}\right]-E\left[X_{1} X_{2}\right]=\frac{1}{2} E\left[\left(X_{1}-X_{2}\right)^{2}\right] .
$$

So,

$$
h\left(X_{1}, X_{2}\right)=\frac{1}{2}\left(X_{1}-X_{2}\right)^{2}
$$

Remark Without loss of generality, we assume $h$ is symmetric, i.e it is invariant under any permutation of its arguments.

I should estimate $\theta$ with with U-Statistics (Hoeffding 1940s). It allows us to
(1) abstract away annoying details and still perform inference, and
(2) develop statistics and tests that do not depend on parametric assumptions (non-parametric) making our inference more "robust".

Definition 1.1 (U-Statistics). For $X_{i} \stackrel{i . i . d}{\sim} P$, denote $\theta(P):=E_{P}\left[h\left(X_{1}, \ldots, X_{r}\right)\right]$. A U-statistic is a random variable of the form

$$
U_{n}:=\frac{1}{\binom{n}{r}} \sum_{|\beta|=r, \beta \subset[n]} h\left(X_{\beta}\right)
$$

where $h: X^{r} \rightarrow \mathbb{R}$ is a symmetric (kernel) function, $\beta$ ranges over all size $r$ subsets of $[n]:=\{1, \ldots, n\}$, and $X_{\beta}:=\left(X_{i_{1}}, \ldots, X_{i_{r}}\right)$ for $\beta=\left(i_{1}, \ldots, i_{r}\right)$.

Remark The U in "U-statistics" is because $\mathbb{E}_{P}\left[U_{n}\right]=\theta(P):=\mathbb{E}\left[h\left(X_{1}, \ldots, X_{r}\right)\right]$, so $U_{n}$ is unbiased.

Why use a U-statistic at all? Why not use

$$
h\left(X_{1}, X_{2}, \ldots, X_{r}\right)
$$

or

$$
\frac{1}{\left(\frac{n}{r}\right)} \sum_{\ell=1}^{\frac{n}{r}} h\left(X_{\ell(r-1)+1}, \ldots, X_{\ell r}\right) ?
$$

Let $\left\{X_{(1)}, \ldots, X_{(n)}\right\}$ be the sample with "index" information removed. (e.g. Order Statistics. Generally a histogram. In EE terminology, called "type" of the sample.) Then, under $X_{i} \stackrel{\text { i.i.d }}{\sim} P$, $\left\{X_{(i)}\right\}_{i=1}^{n}$ is a sufficient statistic. Observe that

$$
\mathbb{E}\left\{h\left(X_{1}, \ldots, X_{r}\right) \mid X_{(1)}, \ldots, X_{(n)}\right\}=U_{n}:=\frac{1}{\binom{n}{r}} \sum_{|\beta|=r, \beta \subset[n]} h\left(X_{\beta}\right)
$$

By Rao-Blackwellization, we know that for any convex (loss) function $L$ and any r.v. $Z_{n}$ such that $\mathbb{E}\left[Z_{n} \mid\left(X_{(i)}\right)_{1 \leq i \leq n}\right]=U_{n}$,

$$
\mathbb{E}\left[L\left(Z_{n}\right)\right] \geq \mathbb{E}\left[L\left(U_{n}\right)\right]
$$

### 1.2 Examples

Example (Sample Variance): Consider $h(x, y)=\frac{1}{2}(x-y)^{2}$. Then $\mathbb{E}\left[h\left(X_{1}, X_{2}\right)\right]=\frac{1}{2}\left(\mathbb{E}\left[X_{1}^{2}\right]+\mathbb{E}\left[X_{2}^{2}\right]\right)-$ $\mathbb{E}\left[X_{1}, X_{2}\right]=\operatorname{Var}(X)$. When we have more than two samples, we use

$$
\begin{aligned}
U_{n} & =\frac{1}{\binom{n}{2}} \sum_{1 \leq i<j \leq n} \frac{1}{2}\left(X_{i}-X_{j}\right)^{2} \\
& =\frac{1}{2 n(n-1)} \sum_{i, j}\left(X_{i}-X_{j}\right)^{2} \\
& =\frac{1}{2 n(n-1)} \sum_{i, j}\left(\left(X_{i}-\bar{X}_{n}\right)-\left(X_{j}-\bar{X}_{n}\right)\right)^{2} \\
& =\frac{1}{2 n(n-1)} \sum_{i, j}\left(\left(X_{i}-\bar{X}_{n}\right)^{2}+\left(X_{j}-\bar{X}_{n}\right)^{2}\right) \\
& =\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}_{n}\right)^{2}
\end{aligned}
$$

Example (Gini's Mean-Difference): $\quad h(x, y)=|x-y|$ and $\mathbb{E}\left[U_{n}\right]=\mathbb{E}\left[\left|X_{1}-X_{2}\right|\right]$.
Example (Quantiles):

$$
\theta(P)=P(X \leq t)=\int_{-\infty}^{t} d p \text { and } h(X)=\mathbf{1}\{X \leq t\}
$$

This is a first order U-statistic.
Example (Signed Rank Statistic): Suppose we want to know whether the central location of $P$ is 0 . Then we can use

$$
\theta(P):=P\left(X_{1}+X_{2}>0\right),
$$

even when $\mathbb{E}[X]$ isn't well-defined.
This means $h(x, y)=\mathbf{1}\{x+y>0\}$ and $U_{n}=\frac{1}{\binom{n}{2}} \sum_{i<j} \mathbf{1}\left\{X_{i}+X_{j}>0\right\}$.

Definition 1.2 (Two-sample U-Statistic). Given two samples $\left\{X_{1}, \ldots, X_{n}\right\}$ and $\left\{Y_{1}, \ldots, Y_{n}\right\}$, a twosample $U$-statistic is a random variable of the form

$$
U=\frac{1}{\binom{n}{r}\binom{m}{s}} \sum_{|\alpha|=s, \alpha \subset[m]} \sum_{|\beta|=r, \beta \subset[n]} h\left(X_{\beta}, Y_{\alpha}\right)
$$

where $h: X^{r} \times Y^{s} \rightarrow \mathbb{R}$. $h$ is symmetric in its first $r$ arguments and in its last sarguments.

Example (Mann-Whitney Statistic): Do $X$ and $Y$ have the same location? We can consider

$$
\begin{aligned}
\theta(P) & =P(X \leq Y), \\
h(X, Y) & =\mathbf{1}\{X \leq Y\} \\
U_{n, m} & =\frac{1}{n m} \sum_{i=1}^{n} \sum_{j=1}^{m} \mathbf{1}\left\{X_{i} \leq Y_{j}\right\},
\end{aligned}
$$

which should be close to $\frac{1}{2}$ when $X$ and $Y$ have the same location.
Example: Here's another motivating example for two-sample U-statistics.
Suppose we have $X_{i} \stackrel{i . i . d}{\sim} P$ and $Y_{i} \stackrel{i . i . d}{\sim} Q$. Are $P$ and $Q$ different?
The null in this two-sample problem is: $P=Q$. This is a huge null: $P$ is unknown and could be anything. We approximate the null by looking at the distribution of $h\left(Z_{A}\right)$, where $Z=\left\{X_{1}, \ldots, X_{n}, Y_{1}, \ldots, Y_{n}\right\}$ and $A$ ranges over all possible index sets of size $|A|=r+s$. We use that under the null,

$$
h\left(Z_{A}\right) \stackrel{\text { dist }}{=} h\left(Z_{B}\right)
$$

for any $A, B \in[n]$ such that $|A|=|B|=r+s$.

### 1.3 Variance of U-Statistics

This is a precursor to asymptotic normality because "1st order terms" dominate everything else.
Definition 1.3. Assume that $E\left[|h|^{2}\right]<\infty$ for any $c<r$. Define

$$
h_{c}\left(X_{1}, \ldots, X_{c}\right):=E[h(\underbrace{X_{1}, \ldots, X_{c}}_{\text {fixed }}, \underbrace{X_{c+1}, \ldots, X_{r}}_{\text {i.i.d } P})] .
$$

## Remark

1. $h_{0}=E\left[h\left(X_{1}, \ldots, X_{r}\right)\right]=\theta(P)$
2. $E\left[h_{c}\left(X_{1}, \ldots, X_{c}\right)\right]=E\left[h\left(X_{1}, \ldots, X_{r}\right)\right]=\theta(P)$

## Definition 1.4.

$$
\begin{aligned}
\hat{h}_{c} & :=h_{c}-E\left[h_{c}\right]=h_{c}-\theta(P) \\
E\left[\hat{h}_{c}\right] & =0
\end{aligned}
$$

Then define

$$
\zeta_{c}:=\operatorname{Var}\left(h_{c}\left(X_{1}, \ldots, X_{c}\right)\right)=E\left[\hat{h}_{c}^{2}\right]
$$

(Note that $\left.\zeta_{0}=0.\right)$
Goal: Write Var $\left[U_{n}\right]$ in terms of $\zeta_{c}^{\prime} s$ for $c=1,2, \ldots, r$.
Lemma 1. If $\alpha, \beta \subseteq[n], S=\alpha \cap \beta, c=|S|$, then

$$
\mathbb{E}\left[\hat{h}\left(X_{\alpha}\right) \hat{h}\left(X_{\beta}\right)\right]=\zeta_{c} .
$$

Proof Using the symmetry of $h$,

$$
\begin{aligned}
\mathbb{E}\left[\hat{h}\left(X_{\alpha}\right) \hat{h}\left(X_{\beta}\right)\right] & =\mathbb{E}\left[\hat{h}\left(X_{\alpha \backslash S}, X_{S}\right) \hat{h}\left(X_{\beta \backslash S}, X_{S}\right)\right] \\
& =\mathbb{E}\left[\mathbb{E}\left[\hat{h}\left(X_{\alpha \backslash S}, X_{S}\right) \mid X_{S}\right] \cdot \mathbb{E}\left[\hat{h}\left(X_{\beta \backslash S}, X_{S}\right) \mid X_{S}\right]\right] \quad \text { (since } X_{\alpha \backslash S}, X_{\beta \backslash S} \text { indep.) } \\
& =\mathbb{E}\left[\hat{h}_{c}\left(X_{S}\right) \cdot \hat{h}_{c}\left(X_{S}\right)\right] \\
& =\zeta_{c} .
\end{aligned}
$$

Theorem 2. Let $U_{n}$ be an $r^{\text {th }}$ order $U$-statistic. Then

$$
\operatorname{Var} U_{n}=\frac{r^{2}}{n} \zeta_{1}+O\left(n^{-2}\right)
$$

Proof There are $\binom{n}{r}\binom{r}{c}\binom{n-r}{r-c}$ ways to select a pair of subsets of $[n]$, each of size $r$, with $c$ common elements. Hence,

$$
\begin{aligned}
U_{n}-\theta & =\binom{n}{r}^{-1} \sum_{|\beta|=r} \hat{h}\left(X_{\beta}\right) \\
\operatorname{Var} U_{n} & =\binom{n}{r}^{-2} \sum_{|\alpha|=r} \sum_{|\beta|=r} \mathbb{E}\left[\hat{h}\left(X_{\alpha}\right) \hat{h}\left(X_{\beta}\right)\right] \\
& =\binom{n}{r}^{-2} \sum_{c=1}^{r}\binom{n}{r}\binom{r}{c}\binom{n-r}{r-c} \zeta_{c} \\
& =\sum_{c=1}^{r} \frac{r!^{2}}{c!(r-c)!^{2}} \frac{(n-r)(n-r-1) \ldots(n-2 r+c+1)}{n(n-1) \ldots(n-r+1)} \zeta_{c}
\end{aligned}
$$

For fixed $c, \frac{(n-r)(n-r-1) \ldots(n-2 r+c+1)}{n(n-1) \ldots(n-r+1)}$ has $r-c$ terms in the numerator and $r$ terms in the denominator. Hence,

$$
\begin{aligned}
\operatorname{Var} U_{n} & =r^{2} \frac{(n-r)(n-r-1) \ldots(n-2 r+2)}{n(n-1) \ldots(n-r+1)} \zeta_{1}+\sum_{c=2}^{r} O\left(\frac{n^{r-c}}{n^{r}}\right) \zeta_{c} \\
& =r^{2}\left[\frac{1}{n}+O\left(n^{-2}\right)\right] \zeta_{1}+O\left(n^{-2}\right) \\
& =\frac{r^{2}}{n} \zeta_{1}+O\left(n^{-2}\right)
\end{aligned}
$$

With this theorem, we know that the variance of U-statistics behaves like the variance of a sample mean plus high-order errors.

New Goal: Show that $U_{n}$ is asymptotically normal by projecting out all high-order interactions.

