## 33 Lecture 33: April 26

## Last time

- Analysis of Variance (JF chapter 8)
- higher-way anova
- analysis of covariance (ANCOVA)


## Today

- Course evaluations (4/13)
- Final exam (take-home) will be posted May 1st and due midnight May 11th.
- Sample size calculations
- Bootstrap
- Logistic Regression


## Sample size computations for one-way ANOVA

Now consider the null hypothesis in a balanced experiment using one-way ANOVA to compare $t$ treatment means and $\alpha=0.05$ :

$$
H_{0}: \mu_{1}=\mu_{2}=\cdots=\mu_{t}=\mu
$$

versus the alternative

$$
H_{a}: \mu_{i} \neq \mu_{j} \text { for some } i \neq j
$$

Suppose that we intend to use a balanced design. How big does our sample size $n_{1}=n_{2}=$ $\cdots=n_{t}=n$ need to be?

The answer depends on lots of things, namely, $\sigma^{2}$ and how many treatment groups $t$ and how much of a difference among the means we hope to be able to detect, and with how big a probability.

Given $\alpha, \mu_{1}, \ldots, \mu_{t}$ and $\sigma^{2}$, we can choose $n$ to ensure a power of at least $1-\beta$ (i.e., an upper bound on type II error rate) using the noncentral F distribution.
Recall that the critical region for the statistic $F=M S[T r t] / M S[E]$ is everything bigger than $F(\alpha, t-1, N-t)=F^{*}$.
The power of the $F$-test conducted using $\alpha=0.05$ to reject $H_{0}$ under this alternative is given by

$$
\begin{equation*}
1-\beta=\operatorname{Pr}\left(M S[T r t] / M S[E]>F^{*} ; H_{1} \text { is true }\right) . \tag{1}
\end{equation*}
$$

Let $\tau_{i}=\mu_{i}-\mu$ for each treatment $i$ so that

$$
H_{0}: \tau_{1}=\tau_{2}=\cdots=\tau_{t}=0
$$

When some $H_{1}$ is true and the sample size $n$ is used in each group, it can be shown that the $F$ ratio has the noncentral $F$ distribution with noncentrality parameter

$$
\gamma=\sum_{j=1}^{t} n_{j}\left(\frac{\tau_{j}}{\sigma}\right)^{2}=n \sum_{j=1}^{t}\left(\frac{\tau_{j}}{\sigma}\right)^{2}
$$

This is the parameterization for the $F$ distribution used in both SAS and R.
One way to obtain an adequate sample size is trial and error. Software packages can be used to get probabilities of the form 1 for various values of $n$.

## Example

Suppose we want to test equal mean binding fractions among antibiotics against the alternative

$$
H_{1}: \mu_{P}=\mu+3, \mu_{T}=\mu+3, \mu_{S}=\mu-6, \mu_{E}=\mu, \mu_{C}=\mu
$$

so that

$$
\tau_{1}=\tau_{2}=3, \tau_{3}=-6, \tau_{4}=\tau_{5}=0
$$

Assume $\sigma=3$ (is it arbitrary? any idea of how to guess?) and we need to use $\alpha=0.05$. The noncentrality parameter is given by

$$
\gamma=n\left[\left(\frac{3}{3}\right)^{2}+\left(\frac{3}{3}\right)^{2}+\left(\frac{-6}{3}\right)^{2}\right]
$$

The $\alpha=0.05$ critical value for $H_{0}$ is given by

$$
F^{*}=F(5-1,5 n-5,0.05)
$$

We need the area to the right of $F^{*}$ for the noncentral $F$ distribution with degrees of freedom 4 and $5(n-1)$ and noncentrality parameter $\gamma=6 n$ to be greater or equal to the desired power level of $1-\beta=0.8$.

We will revisit this example in the lab session on Friday.

## Bootstrap

We follow JF Chapter 21 to discuss the version of nonparametric bootstrap here. The term bootstrapping, coined by Efron (1979), refers to using the sample to learn about the sampling distribution of a statistic without reference to external assumptions - as in "pulling oneself up by one's bootstraps."

Bootstrapping offers a number of advantages:

- The bootstrap is quite general, although there are some cases in which it fails.
- Because it does not require distributional assumptions (such as normally distributed errors), the bootstrap can provide more accurate inferences when the data are not well behaved or when the sample size is small.
- It is possible to apply the bootstrap to statistics with sampling distributions that are difficult to derive, even asymptotically.
- It is relatively simple to apply the bootstrap to complex data collection plans.


## Bootstrap standard errors

For simplicity, we start with an iid sample $Y_{1}, \ldots, Y_{n}$ with each $Y_{i}$ having distribution function $F$, and a real parameter $\theta$ is estimated by $\hat{\theta}$. When necessary, we think of $\hat{\theta}$ as a function of the sample, $\hat{\theta}\left(Y_{1}, \ldots, Y_{n}\right)$. The variance of $\hat{\theta}$ is then

$$
\operatorname{Var}_{F}(\hat{\theta})=\int\left\{\hat{\theta}\left(y_{1}, \ldots, y_{n}\right)-\mathrm{E}_{F}(\hat{\theta})\right\}^{2} d F\left(y_{1}\right) \ldots d F\left(y_{n}\right)
$$

where

$$
\mathrm{E}_{F}(\hat{\theta})=\int \hat{\theta}\left(y_{1}, \ldots, y_{n}\right) d F\left(y_{1}\right) \ldots d F\left(y_{n}\right) .
$$

The nonparametric bootstrap estimate of $\operatorname{Var}(\hat{\theta})$ is just to replace $F$ by the empirical distribution function $F_{n}(y)=n^{-1} \sum_{i=1}^{n} I\left(Y_{i} \leqslant y\right)$ :

$$
\operatorname{Var}_{F_{n}}(\hat{\theta})=\int\left\{\hat{\theta}\left(y_{1}, \ldots, y_{n}\right)-\mathrm{E}_{F_{n}}(\hat{\theta})\right\}^{2} d F_{n}\left(y_{1}\right) \ldots d F_{n}\left(y_{n}\right)
$$

Please refer to Chapter 11 of Boos and Stefanski for a complete discussion.
A practical bootstrapping procedure follows:

1. Create $r$ number of bootstrap replications or pseudo-replicates - that is, for each bootstrap sample (replicate) $b=1, \ldots, r$, we randomly draw $n$ observations $\left\{Y_{b_{1}}^{*}, Y_{b_{2}}^{*}, \ldots, Y_{b_{n}}^{*}\right\}$ with replacement from the original sample $\left\{Y_{1}, Y_{2}, \ldots, Y_{n}\right\}$.
2. Obtain an estimate $\hat{\theta}_{b}^{*}$ of each bootstrap sample.
3. Use the distribution of $\hat{\theta}_{b}^{*}$ to estimate properties of the sampling distribution of $\hat{\theta}$.For example, the sample standard deviation of $\hat{\theta}_{b}^{*}$ gives the bootstrap standard error estimates of $\widehat{S E}^{*}(\hat{\theta})$.

## Bootstrap example

We use the example in JF 21.1 for illustration. Imagine that we sample (fake) ten working, married couples, determining in each case the husband's and wife's income, as recorded in the table (JF table 21.3) below.

| Observation | husband's Income | Wife's Income | Difference $Y_{i}$ |
| :---: | :---: | :---: | :---: |
| 1 | 34 | 28 | 6 |
| 2 | 24 | 27 | -3 |
| 3 | 50 | 45 | 5 |
| 4 | 54 | 51 | 3 |
| 5 | 34 | 28 | 6 |
| 6 | 29 | 19 | 10 |
| 7 | 31 | 20 | 11 |
| 8 | 32 | 40 | -8 |
| 9 | 40 | 33 | 7 |
| 10 | 34 | 25 | 9 |

A point estimate of this population mean difference $\mu$ is the sample mean,

$$
\bar{Y}=\frac{\sum Y_{i}}{n}=4.6
$$

Elementary statistical theory tells us that the standard deviation of the sampling distribution of sample means is $\operatorname{SD}(\bar{Y})=\sigma / \sqrt{n}$, where $\sigma$ is the population standard deviation of $Y$. Because we do not know $\sigma$ in most real applications, the usual estimator of $\sigma$ is the sample standard deviation

$$
\hat{S}=\sqrt{\frac{\sum\left(Y_{i}-\bar{Y}\right)^{2}}{n-1}}
$$

and we obtain the $95 \%$ confidence interval by

$$
\bar{Y} \pm t_{n-1,0.025} \frac{\hat{S}}{\sqrt{n}}
$$

In the present case, $\hat{S}=5.948, \widehat{S E}(\bar{Y})=5.948 / \sqrt{10}=1.881$, and $t_{9,0.025}=2.262$. The $95 \%$ confidence interval for the population mean $\mu$ is therefore

$$
4.6 \pm 2.262 \times 1.881=4.6 \pm 4.255
$$

or equivalently,

$$
0.345<\mu<8.855
$$

To illustrate the bootstrap procedure,

1. We can draw $r=2000$ bootstrap samples (using a computer), each of size $n=10$, from the original data given in table 21.3.
2. We then calculate the mean $\bar{Y}_{b}^{*}$, with $b=1, \ldots, r$ for each bootstrap sample.
3. The bootstrap estimate of the standard error is then given by $\widehat{S E}^{*}\left(\bar{Y}^{*}\right)=\sqrt{\frac{\sum_{b=1}^{r}\left(\bar{Y}_{b}^{*}-\bar{Y}^{*}\right)^{2}}{r-1}}$

From the 2000 replicates that Dr. Fox drew, he obtained $\overline{\bar{Y}}^{*}=4.693$ and $\widehat{S E}\left(\bar{Y}^{*}\right)=1.750$. Both are quite close to the theoretical values (read JF 21.1 for a discussion over $\sqrt{n / n-1}$ for the differences in calculating the standard errors, which is often negligible, especially when $n$ is large).

Now, we can get a bootstrap estimate for the $100(1-\alpha) \%$ confidence interval by using the $\alpha / 2$ and $(1-\alpha / 2)$ quantiles of the bootstrap sampling distribution of $\hat{\theta}_{b}^{*}$ which means

1. We order $\hat{\theta}_{b}^{*}$ such that $\hat{\theta}_{(1)}^{*} \leqslant \hat{\theta}_{(2)}^{*} \leqslant \cdots \leqslant \hat{\theta}_{(r)}^{*}$.
2. Find the two quantiles $\hat{\theta}_{(\text {lower })}^{*}=\hat{\theta}_{(\alpha / 2 \times r)}^{*}$ and $\hat{\theta}_{(\text {upper })}^{*}=\hat{\theta}_{((1-\alpha / 2) \times r)}^{*}$
3. Construct the confidence interval by $\left(\hat{\theta}_{(\text {lower })}^{*}, \hat{\theta}_{(\text {upper })}^{*}\right)$.

In this case,

$$
\begin{aligned}
\text { lower } & =2000(0.05 / 2)=50 \\
\text { upper } & =2000(1-0.05 / 2)=1950 \\
\bar{Y}_{(50)}^{*} & =0.7 \\
\bar{Y}_{(1950)}^{*} & =7.8 \\
0.7 & <\mu<7.8
\end{aligned}
$$

## Bias-corrected bootstrap intervals

We introduce the bias-corrected version of the above bootstrap intervals through two "correction factors" $Z$ and $A$ defined below:.

1. Calculate

$$
Z \equiv \Phi^{-1}\left[\frac{\sum_{b=1}^{r} I\left(\hat{\theta}_{b}^{*}<\hat{\theta}\right)}{r}\right]
$$

where $\Phi^{-1}(\cdot)$ is the inverse of the standard-normal distribution and $\sum_{b=1}^{r} I\left(\hat{\theta}_{b}^{*}<\hat{\theta}\right) / r$ is the proportion of bootstrap replicates below the estimate $\hat{\theta}$. If the bootstrap sampling distribution is symmetric and if $\hat{\theta}$ is unbiased, then this proportion will be close to 0.5 , and the "correction factor" $Z$ will be close to 0 .
2. Let $\hat{\theta}_{(-i)}$ represent the value of $\hat{\theta}$ produced when $i$ th observation is deleted from the sample (known as the jackknife values of $\hat{\theta}$ ). There are $n$ of these quantities. Let $\bar{\theta}=\sum \hat{\theta}_{(-i)} / n$. Then calculate

$$
A \equiv \frac{\sum_{i=1}^{n}\left(\bar{\theta}-\hat{\theta}_{(-i)}\right)^{3}}{6\left[\sum_{i=1}^{n}\left(\bar{\theta}-\hat{\theta}_{(-i)}\right)^{2}\right]^{3 / 2}}
$$

With the correction factors $Z$ and $A$, compute

$$
\begin{aligned}
& A_{1} \equiv \Phi\left[Z+\frac{Z-z_{\alpha / 2}}{1-A\left(Z-z_{\alpha / 2}\right)}\right] \\
& A_{2} \equiv \Phi\left[Z+\frac{Z+z_{\alpha / 2}}{1-A\left(Z+z_{\alpha / 2}\right)}\right]
\end{aligned}
$$

And the corrected interval is

$$
\hat{\theta}_{(\text {lower })}^{*}<\theta<\hat{\theta}_{(\text {upper })}^{*}
$$

where lower* $=r A_{1}$ and upper* $=r A_{2}$ (rounding or interpolating as required).
When the correction factors $Z$ and $A$ are both $0, A_{1}=\Phi\left(-z_{\alpha / 2}\right)=\alpha / 2$ and $A_{2}=\Phi\left(z_{\alpha / 2}\right)=$ $1-\alpha / 2$.
For the 2000 bootstrap samples that Dr. Fox drew, there are 926 bootstrapped means below $\bar{Y}=4.6$, and so $Z=\Phi^{-1}(926 / 2000)=-0.09288$. The $\bar{Y}_{(-i)}$ are $4.444,5.444, \ldots, 4.111$. And $A=-0.05630$. Using the correction factors $Z$ and $A$,

$$
\begin{aligned}
A_{1} & =\Phi\left[-0.09288+\frac{-0.09288-1.96}{1-[-0.05630(-0.09288-1.96)]}\right] \\
& =\Phi(-2.414)=0.007889 \\
A_{2} & =\Phi\left[-0.09288+\frac{-0.09288+1.96}{1-[-0.05630(-0.09288+1.96)]}\right] \\
& =\Phi(1.597)=0.9449
\end{aligned}
$$

Multiplying by $r$, we have $2000 \times 0.007889 \approx 16$ and $2000 \times 0.9449 \approx 1890$, from which

$$
\begin{aligned}
& \bar{Y}_{(16)}^{*}<\mu<\bar{Y}_{(1890)}^{*} \\
&-0.4<\mu<7.3
\end{aligned}
$$

## Logistic regression

So far, we only considered cases where the response variable is continuous. Logistic regression belongs in the family of Generalized Linear Model that can be used for analyzing binary responses.

Motivation Let $p$ be the probability of a specific outcome. We are interested in how this probability is affected by the explanatory variables. A naive approach could be:

$$
p=\beta_{0}+\beta_{1} x_{1}+\beta_{2} x_{2}+\epsilon
$$

Problem $\quad p$ must be between 0 and 1.

Solution Model $\log$ odds of $p$ (i.e. logit of $p$ ) which are defined as

$$
\begin{aligned}
& \text { odds }=\frac{p}{1-p} \in[0, \infty) \\
& \operatorname{logit}=\log \left(\frac{p}{1-p}\right) \in(-\infty, \infty)
\end{aligned}
$$

This forms the logistic regression

$$
\operatorname{logit}(p)=\log \left(\frac{p}{1-p}\right)=\beta_{0}+\beta_{1} x_{1}+\beta_{2} x_{2}
$$

Note that

1. Increase in $\log$ odds $\Longleftrightarrow$ increase in $p$.

Decrease in log odds $\Longleftrightarrow$ decrease in $p$.
2. No $\epsilon$ in logistic regression because we observe a binary outcome $y_{i}$, not $p$ itself.

The density

$$
\begin{aligned}
f\left(y_{i} \mid p_{i}\right) & =p_{i}^{y_{i}}\left(1-p_{i}\right)^{1-y_{i}} \\
& =e^{y_{i} \log \left(p_{i}\right)+\left(1-y_{i}\right) \log \left(1-p_{i}\right)} \\
& =e^{y_{i} \log \left(\frac{p_{i}}{1-p_{i}}\right)+\log \left(1-p_{i}\right)}
\end{aligned}
$$

where

$$
\begin{aligned}
\mathrm{E}\left(y_{i}\right) & =p_{i}=\frac{e^{\mathbf{x}_{i}^{T} \boldsymbol{\beta}}}{1+e^{\mathbf{x}_{i}^{T} \boldsymbol{\beta}}} \quad \text { (mean function, inverse link function) } \\
\mathbf{x}_{i}^{T} \boldsymbol{\beta} & =\log \left(\frac{p_{i}}{1-p_{i}}\right) \quad \text { (logit link function) }
\end{aligned}
$$

We obtain parameter estimates by maximum likelihood. Read page 131 - page 133 of Dr. Hua Zhou's Computational Statistics notes (link) for algorithms to find these MLE (maximum likelihood estimates).

