# Supporting Information

## Censoring trace-level environmental data: statistical analysis considerations to limit bias

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```
/* SAS code to resample stove observations */
/* Author: Barbara Jane George, PhD, PStat */
/* US Environmental Protection Agency      */
/* August 2020                             */

%let job=groups;


**********;
data stoves;
input
 @1  analyte $25.
 @26 result
 @36 MDL
 @47 CCLV
 @56 stove $17.;
;

*list;
cards;
Dibenzo[a,h]anthracene   0.05      0.023      0.10     Solgas/Repsol
Dibenzo[a,h]anthracene   0.03      0.023      0.10     Solgas/Repsol
Dibenzo[a,h]anthracene   0.01      0.023      0.10     Solgas/Repsol
Dibenzo[a,h]anthracene   0.05      0.023      0.10     Solgas/Repsol
Dibenzo[a,h]anthracene   0.19      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.11      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.07      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.08      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.12      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.02      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.06      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.1       0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.01      0.023      0.10     Butterfly Model
Dibenzo[a,h]anthracene   0.12      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.32      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.15      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.04      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.07      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.52      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.05      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.07      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.15      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.07      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.03      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.07      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.01      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.01      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   0.04      0.023      0.10     Eco Chula XXL
Dibenzo[a,h]anthracene   1         0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   1.16      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.01      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   1.46      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.01      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.87      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   1.31      0.023      0.10     Jiko Poa Rocket
```

```
Dibenzo[a,h]anthracene   0.08      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   1.31      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.02      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.4       0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.75      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.04      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   2.94      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.89      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.07      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.6       0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   1.12      0.023      0.10     Jiko Poa Rocket
Dibenzo[a,h]anthracene   0.04      0.023      0.10     Jiko Poa Rocket
;
ods csv file="Stove data for DBA.csv";
 proc means data=stoves n mean std;
 class stove;
 var result;
 run;

 proc print data=stoves;
 run;
ods csv close;

**********;
data benzo;
set stoves;

if stove in ("Eco Chula XXL","Butterfly Model");


/* https://blogs.sas.com/content/iml/2018/06/20/bootstrap-method-example-sas.html */
/* Sample with replacement from each stratum. First sort by the STRATA variable.  */
proc sort data=benzo;
by stove result;
run;

/* Then perform stratified sampling with replacement */
proc surveyselect data=benzo out=BootSamples noprint seed=123
                  method=urs              /* with replacement */
                  OUTHITS                 /* use OUTHITS option when you do not want
a frequency variable */
                  samprate=1 reps=10;     /* 10 resamples */
                  strata stove;           /* sample N1 from first group and N2 from
second */
run;


**********;
data butter eco;
set BootSamples(drop=Replicate NumberHits ExpectedHits SamplingWeight);

if stove in ("Eco Chula XXL") then output eco;
else if stove in ("Butterfly Model") then output butter;

**********;
```

```
data butter;   *stove type 2;
set butter;

if _n_ <=31;   *resampled observations to concatenate to original sample;

**********;
data eco;      *stove type 1  - long-tailed;
set eco;

if _n_ <=30;   *resampled observations to concatenate to original sample;

**********;
data buttereco;
set benzo(in=in1) butter eco;


if stove in ("Eco Chula XXL") then do;
 stove2="Stove Type 1 (n=15)";
 stove3="Stove Type 1 (n=45)";
 stove4="Stove Type 1";
end;
else if stove in ("Butterfly Model") then do;
 stove2="Stove Type 2 (n=9) ";
 stove3="Stove Type 2 (n=40)";
 stove4="Stove Type 2";
end;

if in1 then orig='Yes';
else orig='No ';


proc sort data=buttereco;
by stove4;

ods csv file="Print (&job) with resamples data=buttereco.csv";
 proc print data=buttereco;
 run;
ods csv close;


/* https://blogs.sas.com/content/iml/2016/03/09/comparative-panel-overlay-histograms-
sas.html */
/* https://stats.idre.ucla.edu/sas/code/generating-multiline-axis-labels-in-sas-proc-
sgplot/  */

ods rtf file="SGPanel (&job) resampled data=buttereco.rtf";
ods graphics / width=400px height=400px;

proc sgpanel data=buttereco noautolegend;
panelby stove3 / rows=2 layout=rowlattice novarname;
histogram result / binwidth=0.03 binstart=0 scale=count ;
colaxis min=0 label="DBA (ng/(*ESC*){unicode '03BC'x}L)";
density result / type=kernel(c=2);
run;
```

```
ods graphics off;
ods rtf close;



ods rtf file="SGPanel (&job) orig sample data=buttereco.rtf";
ods graphics / width=400px height=400px;

proc sgpanel data=buttereco noautolegend;
panelby stove2 / rows=2 layout=rowlattice novarname;
histogram result / binwidth=0.03 binstart=0 scale=count;
colaxis min=0 label="DBA (ng/(*ESC*){unicode '03BC'x}L)";
density result / type=kernel(c=2);
where orig='Yes';
run;

ods graphics off;
ods rtf close;


**********;
data superbenz;
set benzo(in=in1) buttereco(in=in2) ;

if stove in ("Eco Chula XXL") then do;
 stove2="Stove Type 1 (n=15)";
 stove3="Stove Type 1 (n=45)";
 stove4="Stove Type 1";
end;
else if stove in ("Butterfly Model") then do;
 stove2="Stove Type 2 (n=9) ";
 stove3="Stove Type 2 (n=40)";
 stove4="Stove Type 2";
end;

if in1      then resampled='Original Sample (n=24)';
else if in2 then resampled='Resampled Data (n=85) ';


ods rtf file="SGPanel (&job) both sets data=superbenz.rtf";
ods graphics / width=400px height=400px;

proc sgpanel data=superbenz noautolegend;
panelby stove4 resampled/ rows=2 layout=lattice novarname;
histogram result / binwidth=0.03 binstart=0 scale=count ;
colaxis min=0 label="DBA (ng/(*ESC*){unicode '03BC'x}L)";
density result / type=kernel(c=2);
run;

ods graphics off;
ods rtf close;
```

```
# R code for testing group differences
# Author: Barbara Jane George, PhD, PStat
# US Environmental Protection Agency
# August 2020

#setwd ("")
getwd()

library(dplyr)
library(EnvStats)
library(NADA)
library(fitdistrplus)
library(ggplot2)


data <- read.csv("Print (groups) with resamples data=buttereco.csv")

## num of samples below the CCLV
sum(data$result < data$CCLV)

## Create new vectors based on censoring
results <- data$result
CCLV <- data$CCLV
resultsCCLV <- ifelse(results<CCLV,CCLV,results)
result_halfCCLV <- ifelse(results<CCLV,CCLV/2,results)
stove <- data$stove
stove4 <- data$stove4
censored <- ifelse(results < data$CCLV, TRUE, FALSE)

### AIC for distribution fitting -- before & after censoring
fitg <- fitdist(results, "gamma")
fitln <- fitdist(results, "lnorm")
fitn <- fitdist(results, "norm")
fitg$aic
fitln$aic
fitn$aic

results_cens <- data.frame(left = ifelse(censored == TRUE, 0, results),
                           right = ifelse(censored == TRUE, data$CCLV, results))
aic_lnorm <- fitdistcens(results_cens, distr = "lnorm")$aic
aic_norm  <- fitdistcens(results_cens, distr = "norm")$aic
aic_gamma <- fitdistcens(results_cens, distr = "gamma")$aic
aic_lnorm
aic_norm
aic_gamma


CCLV <- unique(data$CCLV)
DL <- CCLV


## MLE for results censored at CCLV
estResult3 <- cenmle(resultsCCLV,censored,stove ) #NADA cenmle assumes lognormal,
tests equality of medians, reference cell
summary(estResult3)
```

```
## MLE for results not censored
nocensor <- ifelse(results < data$CCLV, FALSE, FALSE)
estResult4 <- cenmle(results,nocensor,stove ) #NADA cenmle assumes lognormal, tests
equality of medians, reference cell
summary(estResult4)


results_ggplot <- data.frame(results,stove4)
p <- ggplot(results_ggplot, aes(x = factor(stove4), y = results, color =
factor(stove4))) +
     geom_stripchart(test.text=TRUE, digits=3,
                     test.text.params = list(p.value.digits=4)) +           labs(x =
NULL, y =expression(paste("Uncensored DBA (ng/",mu,"L)")))
p
tiff("stripchart (07-30-20) results.tiff", width=5, height=5, units='in',
res=300,compression='lzw')
plot(p)
dev.off()


results_halfCCLV <- data.frame(result_halfCCLV,stove4)
pp <- ggplot(results_halfCCLV, aes(x = factor(stove4), y = result_halfCCLV, color =
factor(stove4))) +
      geom_stripchart(test.text=TRUE, digits=3,
                     test.text.params = list(p.value.digits=4)) +              labs(x
= NULL, y = expression(paste("DBA (ng/",mu,"L) with CCLV/2 substitution")))
pp
tiff("stripchart (07-30-20) results_halfCCLV.tiff", width=5, height=5, units='in',
res=300,compression='lzw')
plot(pp)
dev.off()


analyte_dat_eco <- data %>% filter(stove == "Eco Chula XXL")
result_eco <- analyte_dat_eco$result
DL_eco <- ifelse(result_eco<DL,DL,result_eco)
halfDL_eco <- ifelse(result_eco<DL,0.5*DL,result_eco)
halfDL_mean_eco <- mean(halfDL_eco)
halfDL_sd_eco <- sd(halfDL_eco)
halfDL_cv_eco <- halfDL_sd_eco/halfDL_mean_eco
halfDL_n_eco <- length(halfDL_eco)

analyte_dat_butterfly <- data %>% filter(stove == "Butterfly Model")
result_butterfly <- analyte_dat_butterfly$result
DL_butterfly <- ifelse(result_butterfly<DL,DL,result_butterfly)
halfDL_butterfly <- ifelse(result_butterfly<DL,0.5*DL,result_butterfly)
halfDL_mean_butterfly <- mean(halfDL_butterfly)
halfDL_sd_butterfly <- sd(halfDL_butterfly)
halfDL_cv_butterfly <- halfDL_sd_butterfly/halfDL_mean_butterfly
halfDL_n_butterfly <- length(halfDL_butterfly)

full_mean_eco <- mean(result_eco)
full_sd_eco <- sd(result_eco)
```

```
full_cv_eco <- full_sd_eco/full_mean_eco
full_MLE_eco <- elnormAlt(result_eco,method = "mle")$parameters
full_MLE_mean_eco <- full_MLE_eco[1]
full_MLE_sd_eco <- full_MLE_eco[2] * full_MLE_eco[1]
full_MLE_cv_eco <- full_MLE_eco[2]

censored_eco <- ifelse(result_eco<DL, TRUE, FALSE)
MLE_eco <- elnormAltCensored(DL_eco, censored_eco, method = "mle")$parameters
MLE_mean_eco <- MLE_eco[1]
MLE_sd_eco <- MLE_eco[2] * MLE_eco[1]
MLE_cv_eco <- MLE_eco[2]
MLE_n_eco <- length(result_eco)

full_mean_butterfly <- mean(result_butterfly)
full_sd_butterfly <- sd(result_butterfly)
full_cv_butterfly <- full_sd_butterfly/full_mean_butterfly
full_MLE_butterfly <- elnormAlt(result_butterfly,method = "mle")$parameters
full_MLE_mean_butterfly <- full_MLE_butterfly[1]
full_MLE_sd_butterfly <- full_MLE_butterfly[2] * full_MLE_butterfly[1]
full_MLE_cv_butterfly <- full_MLE_butterfly[2]

censored_butterfly <- ifelse(result_butterfly<DL, TRUE, FALSE)
MLE_butterfly <- elnormAltCensored(DL_butterfly, censored_butterfly, method =
"mle")$parameters
MLE_mean_butterfly <- MLE_butterfly[1]
MLE_sd_butterfly <- MLE_butterfly[2] * MLE_butterfly[1]
MLE_cv_butterfly <- MLE_butterfly[2]
MLE_n_butterfly <- length(result_butterfly)


full_mean_eco
full_mean_butterfly
full_MLE_mean_eco
full_MLE_mean_butterfly
halfDL_mean_eco
halfDL_mean_butterfly
MLE_mean_eco
MLE_mean_butterfly

full_sd_eco
full_sd_butterfly
full_MLE_sd_eco
full_MLE_sd_butterfly
halfDL_sd_eco
halfDL_sd_butterfly
MLE_sd_eco
MLE_sd_butterfly

full_cv_eco
full_cv_butterfly
full_MLE_cv_eco
full_MLE_cv_butterfly
halfDL_cv_eco
halfDL_cv_butterfly
MLE_cv_eco
```

```
MLE_cv_butterfly

halfDL_n_eco
halfDL_n_butterfly
MLE_n_eco
MLE_n_butterfly


## apply log transformation to concentration data
results_fullsamp_log <- data.frame(reslog = log(results), stove4)
results_halfCCLV_log <- data.frame(reslog = log(result_halfCCLV), stove4)

results_ggplot <- data.frame(results,stove4)
p <- ggplot(results_fullsamp_log, aes(x = factor(stove4), y = reslog, color =
factor(stove4))) +
     geom_stripchart(test.text=TRUE, digits=3,
                     test.text.params = list(p.value.digits=4)) +
     labs(x = NULL, y =expression(paste("log(DBA) Uncensored, Full Data")))
p
tiff("stripchart log(DBA) results.tiff", width=5, height=5, units='in',
res=300,compression='lzw')
plot(p)
dev.off()


results_halfCCLV <- data.frame(result_halfCCLV,stove4)
pp <- ggplot(results_halfCCLV_log, aes(x = factor(stove4), y = reslog, color =
factor(stove4))) +
      geom_stripchart(test.text=TRUE, digits=3,
                     test.text.params = list(p.value.digits=4)) +
      labs(x = NULL, y = expression(paste("log(DBA) with CCLV/2 substitution")))
pp
tiff("stripchart log(DBA) results_halfCCLV.tiff", width=5, height=5, units='in',
res=300,compression='lzw')
plot(pp)
dev.off()
```

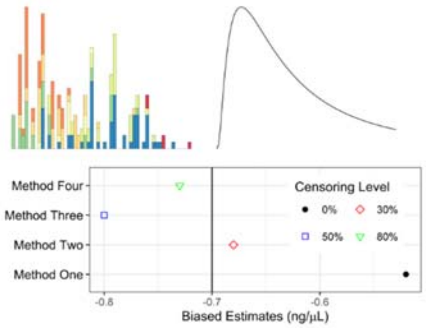
```
# R code for example TOC graphic
# Author: Barbara Jane George, PhD, PStat
# US Environmental Protection Agency
# August 2020

# use Paint, File, Properties to examine TIFF DPI and dimensions in inches or pixels

#setwd("")
getwd()

library(ggplot2)
require('magick')

##########
########## Biased Estimates example
##########

Average <- c(-0.52,-0.68,-0.8,-0.73)
method <- c('Method One','Method Two','Method Three','Method Four')
method <- factor(method,levels = c('Method One','Method Two','Method Three','Method
Four'))

CensoringLevel <- c('0%','30%','50%','80%')
dd <- data.frame(Average,method,CensoringLevel)

means <- data.frame(Parameter=c("Mean"), parm_mean=c(-0.7))
qq <- ggplot(dd,aes(Average,method)) +
      geom_vline(aes(xintercept=parm_mean),means) +

geom_point(size=2,aes(Average,method,colour=factor(CensoringLevel),shape=factor(Censo
ringLevel))) +
      scale_shape_manual(values=c(16,5,0,6)                    , name = "Censoring
Level", labels=c("0%","30%","50%","80%")) +
      scale_colour_manual(values=c("black","red","blue","green"), name = "Censoring
Level", labels=c("0%","30%","50%","80%")) +
      theme_bw() +  guides(shape=guide_legend("Censoring Level",nrow=2,byrow=TRUE)) +
#, size=FALSE
      theme(legend.position=c(0.95, 0.95),legend.justification = c("right",
"top"),axis.text.y=element_text(size=rel(1.2),colour=("black"))) +
###,axis.title.x = element_text(angle=0,vjust=6,hjust=1)) +
      labs(x = expression(paste("Biased Estimates (ng/",mu,"L)")),y=NULL)

qq

tiff("Biased Estimates Example.tiff", width = 5, height = 2, units = 'in', res =
1200)
plot(qq)
dev.off()


##########
########## Top Row examples
##########
```

```
###Adapted from http://r-statistics.co/Top50-Ggplot2-Visualizations-MasterList-R-
Code.html

# Histogram on a Continuous Variable
theme_set(theme_classic())
gg <- ggplot(mpg, aes(displ)) + scale_fill_brewer(palette = "Spectral") +
      geom_histogram(aes(fill=class),
                    binwidth = .1,
                    col="black",
                    size=.1) +
      theme(axis.title=element_blank(),
            axis.text=element_blank(),
            axis.ticks=element_blank(),
            legend.position="none",
            axis.line=element_blank())
ggsave("top_left.pdf", width = 5, height = 4)


set.seed(123)
hh <- data.frame(x = rlnorm(1000, meanlog = -0.5, sdlog = 1))
ggplot(hh) +
  stat_function(fun = "dlnorm",
                args = list(meanlog = -1, sdlog = 1)) +
        theme(axis.title=element_blank(),
           axis.text=element_blank(),
           axis.ticks=element_blank(),
           legend.position="none",
           axis.line=element_blank())
ggsave("top_right.pdf", width = 5, height = 4)


##########
########## white sliver for padding
##########


tiff("sliver.tiff", width = 0.2, height = 1, units="in", res=300)
dev.off()


##########
########## blue arrow
##########

#https://ggplot2.tidyverse.org/reference/geom_segment.html
df2 <- expand.grid(
  lineend = c('round'),
  linejoin = c('mitre'),
  stringsAsFactors = FALSE
)
df2 <- data.frame(df2, y = 1:1)
aa <- ggplot(df2, aes(x = 1, y = y,xend = 1.25, yend = y, )) +       #label =
paste(lineend, linejoin)
  theme(panel.background = element_rect(fill = NA),axis.text =
element_blank(),axis.ticks = element_blank()) +
```

```
  geom_segment(
     colour = "blue",
     lineend = df2$lineend, linejoin = df2$linejoin,
     size = 4, arrow = arrow(length = unit(0.3, "inches"))
  ) +
  #geom_text(hjust = 'outside', nudge_x = -0.2) +
  xlim(0.5, 2)
aa

#pdf("arrow.pdf")
#plot(aa)
#dev.off()

ggsave("arrow.pdf")


#used Adobe Acrobat to edit, crop horizontal arrow
#used Adobe Acrobat to edit, select, rotate, crop vertical arrow



##########
########## magick
##########

### https://cran.r-project.org/web/packages/magick/vignettes/intro.html
### image_scale(image, "200"): resize proportionally to width: 200px
### image_scale(image, "x200"): resize proportionally to height: 200px
### stackoverflow.com/questions/44960520/join-images-with-data-frames-in-r


#####
##### top
#####

measurements = image_read_pdf("top_left.pdf")
simulations  = image_read_pdf("top_right.pdf")

#arrowhoriz   = image_read_pdf("arrow - horizontal.pdf")
#arrowdown    = image_read_pdf("arrow - vertical3.pdf")

#top = c(measurements,arrowhoriz,simulations,arrowdown)  #if including arrows
top = c(measurements,simulations)

# concatenate them left-to-right (use 'stack=T' to concatenate top-to-bottom)
side_by_side = image_append(top, stack=F)
#top2         = image_scale(side_by_side, "730")  #if including arrows
top2         = image_scale(side_by_side, "640")  #see transform in magick.pdf

image_write(top2, density=300, path = "top_example.tiff", format = "tiff")
#density=300 needed for 300 dpi
#top3        = image_read("top_example.tiff")


# use Paint, File, Properties to examine TIFF DPI and dimensions in inches or pixels
```

```
#####
##### bottom
#####

bias         = image_read("Biased Estimates Example.tiff")
sliver       = image_read("sliver.tiff")

#bottom = c(sliver,sliver,sliver,bias)
bottom = c(bias)

# concatenate them left-to-right (use 'stack=T' to concatenate top-to-bottom)
bottom_pair  = image_append(bottom, stack=F)
#bottom2      = image_scale(bottom_pair, "730")
bottom2      = image_scale(bottom_pair, "670")

image_write(bottom2, path = "bottom_example.tiff", density=300, format = "tiff")
#bottom3     = image_read("bottom_example.tiff")


# concatenate top & bottom (use 'stack=T' to concatenate top-to-bottom)
all = c(top2,bottom2)
vertical = image_append(all , stack=TRUE)
image_write(vertical, path = "TOC Graphic example.tiff",density=300, format = "tiff")
#,density=300)
```

**TOC Graphic example.tiff**



Notes

- Open with Paint, File, Properties to examine TIFF dimensions in inches or pixels and DPI
- After pasting in DOCX, right click, choose Size and Position for dimensions
- **arrow.pdf** is created but not incorporated above. Comments in the code describe using Adobe Acrobat to edit, crop, and rotate.