Why Not Substitute ½ DL for Nondetects?

Dennis R. Helsel

PracticalStats.com

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What's wrong with substitution?

a. Produces invasive data alien to the concentrations actually in samples
b. Adds a pattern to your data. Substitution is NOT neutral
c. Produces poor estimates and incorrect statistical tests
d. Far better methods are available. Right now. You don't need a PhD to do them.

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For More Information

on this topic and other methods for data analysis with nondetects, see our online course

Nondetects And Data Analysis

at https://practicalstats.teachable.com

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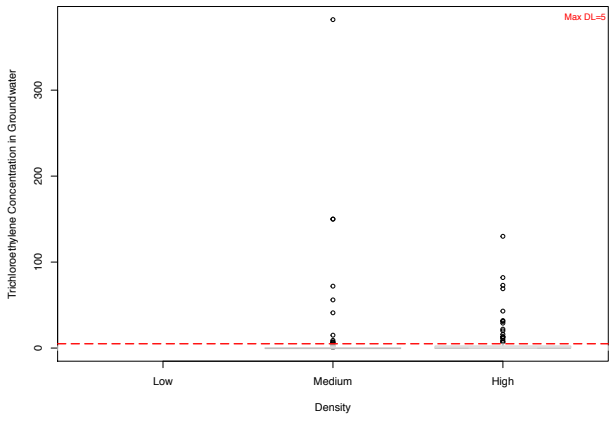
Example: TCE concentrations in GW



- Reporting limits at 1, 2, 3, 4, and 5 ug/L. ~ 80% censoring
- Do TCE distributions differ among the three land-use groups?

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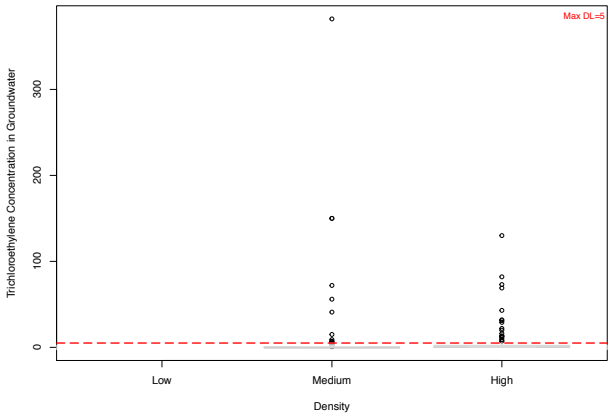
Substitution versus Kruskal-Wallis

ANOVA sub <5 = 0
p = 0.57

ANOVA sub <5 = 2.5
p = 0.56

ANOVA sub <5 = 5
p = 0.50

No differences found!



Kruskal-Wallis test
p = 0.01 .

No substitution

Distribution of TCE differs between land-use groups

Simplest Tests

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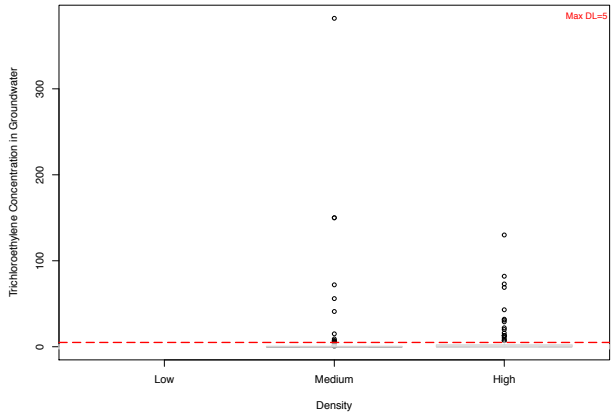
Better Tests For Censored Data




```
> cen1way (TCECONC, BDL_1, Density)
                n n.cen median     mean          sd
Factor=High    92    58     <5 7.778019 19.7826151
Factor=Low     25    23     <5 2.083333  0.5768489
Factor=Medium 130   113     <5 7.867264 39.7664396

Oneway Peto-Peto test of CensData: TCECONC by Factor:
Density

Chisq = 16.25   on 2 degrees of freedom  p = 0.000295
```

Distribution of TCE differs between land-use groups

```
Pairwise comparisons using Peto & Peto test
       High   Low
Low    0.0098 -
Medium 0.0024 0.2796
```

Shows which groups differ from others

Nonparametric Test using Multiple Detection Limits
from our Nondetects And Data Analysis course

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There is still much confusion over the value of nondetects

Dr. Ronald Hites in Environ. Science & Technology (2019) in a Scientific Opinion piece stated:

"…. *Any time you have a % non-detected >20%, for whatever reason, it is unlikely that the data set can give useful results*."

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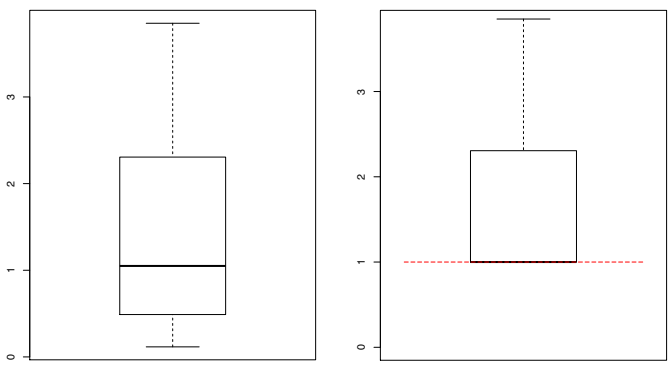
Substitution: Invasive data

Estimating the Standard Deviation

what happens to it when the same number is substituted for 60% of the observations?

Before substituting.
True std. dev.
s = 1.02



After substituting.
std. dev.
s = 0.84

t-tests, ANOVA, regression, intervals all depend on the std. dev.

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Substitution when computing confidence intervals?

- Singh et al (2006), developers of the ProUCL software, determined that substituting ½ DL "does not provide adequate coverage [UCL95 is not high enough] …even for [% NDs] as low as 10%"
- Lower standard deviations produce lower confidence limits, too-short intervals.
- They summarize their results with "Do not use DL/2 (t) method to compute a UCL".
- Recommended methods were based on a Kaplan-Meier estimator, which is available in our course software.

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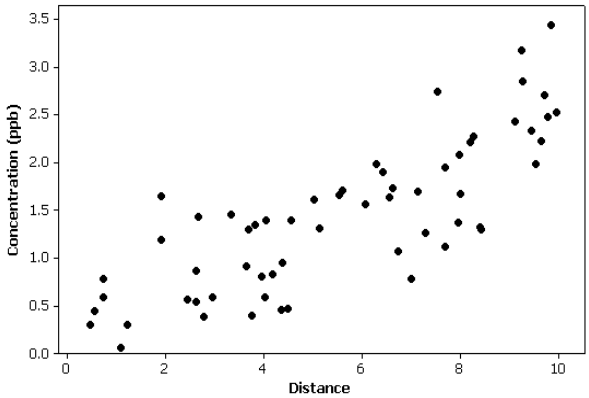
Substitution: Invasive data

Correlation and Regression

Before censoring.
True correlation
r=0.81



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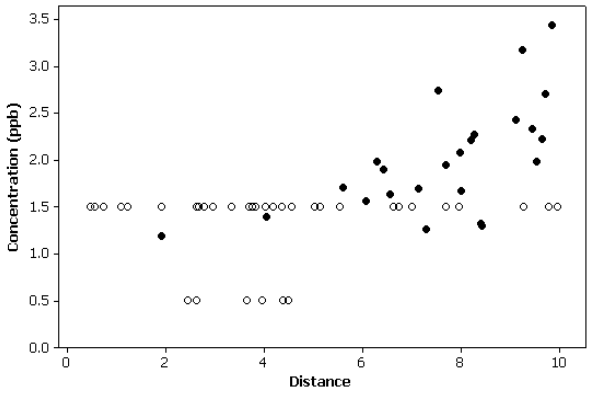
Substitution: Invasive data

Correlation and Regression

Two DLs @ 3 and 1.
<3s become 1.5,
<1s become 0.5.

After substitution. invasive data form flat (zero-slope) lines, lowering correlation to r=0.55



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Evaluation of Substitution for regression models

Thompson and Nelson (2003) found that for censored response (y) variables, substituting one-half the DL for nondetects produced

- biased parameter estimates (slopes) and
- artificially small standard error estimates (explanatory variables who shouldn't be in the regression appear to be significant)

There are better ways!

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Regression with censored data

No Substitution for Nondetects!

Software comes with NADA course

```
> Pbreg <- cencorreg(Blood, BloodCen, Kidney)
 Likelihood R = 0.8236
 Rescaled Likelihood R = 0.8721
 McFaddens R = 0.714
> summary(Pbreg)
```

Correlation Coefficients

Regression Equation

Blood lead concentrations are related to lead in kidneys

```
             Value Std. Error      z       p
(Intercept) -4.4573     0.1733 -25.72 < 2e-16
Kidney       0.2436     0.0302   8.07 7.1e-16
Log(scale)  -0.6737     0.2036  -3.31 0.00094

Loglik(model)= -14.7   Loglik(intercept only)= -30
Chisq= 30.62 on 1 degrees of freedom, p= 3.1e-08
```

ln(blood Pb) = -4.457 + 0.244*kidney Pb or blood Pb = $e^{-4.457} \bullet kidneyPb^{0.244}$

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Plotting the regression line

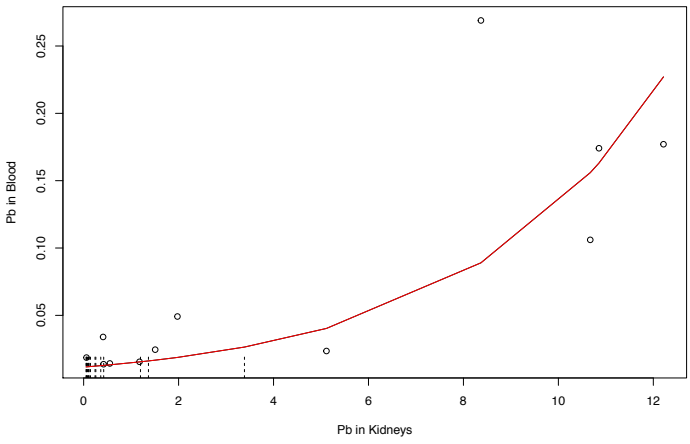
Regression straight line in log units becomes a curve in original units

```
> cenxyplot(Kidney,
  KidneyCen, Blood, BloodCen,
  xlab = "Pb in Kidneys",
  ylab = "Pb in Blood")

> ik <- order(Kidney)

> lines(Kidney[ik],
  exp(predict(Pbreg)[ik]),
  col = "red")
```

Nondetects are plotted as dashed vertical lines. The info that they occur only at the low kidney Pb concentrations is used in computing the regression model.



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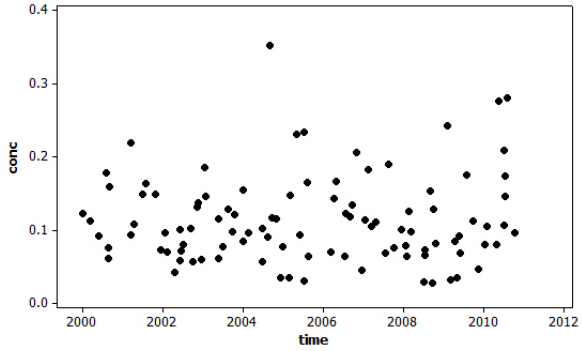
Classic faux pas with substitution: finding a trend that isn't there



- No change over time. No trend.
- Will replace smallest values with a decreasing pattern of detection limits, mimicking what often happens in labs.

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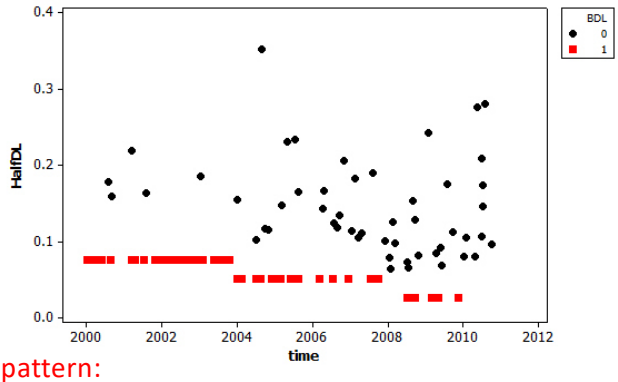
Finding a trend that isn't there



Invasive pattern:

- DLs decrease over time.
- After substitution with 1/2DL, decreases over time (trend) may test as significant

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Trend -- the censeaken function

The seasonal Kendall test for data with multiple DLs. No substitution. Available in our NADA course materials.

```
> censeaken (dectime, `Total Recoverable Chromium`, CrND, group = Season)
 DATA ANALYZED: Total Recoverable Chromium vs dectime by Season
----------
  Season  N    S    tau      pval intercept    slope
1    Dry 34 -176 -0.314 0.0091337    79.103 -0.03901
----------
  Season  N   S     tau    pval intercept    slope
1    Wet 29 -24 -0.0591 0.66604    24.355 -0.01169
----------
Seasonal Kendall test and Theil-Sen line
   N    S    Tau Pvalue_SK Nreps Intercept    Slope
1 63 -200 -0.207     0.014   999    74.232 -0.03655
----------
```

Significant downtrend in Dry season

No significant trend in Wet season

Significant trend overall. SK slope is -0.036 ug/L per year

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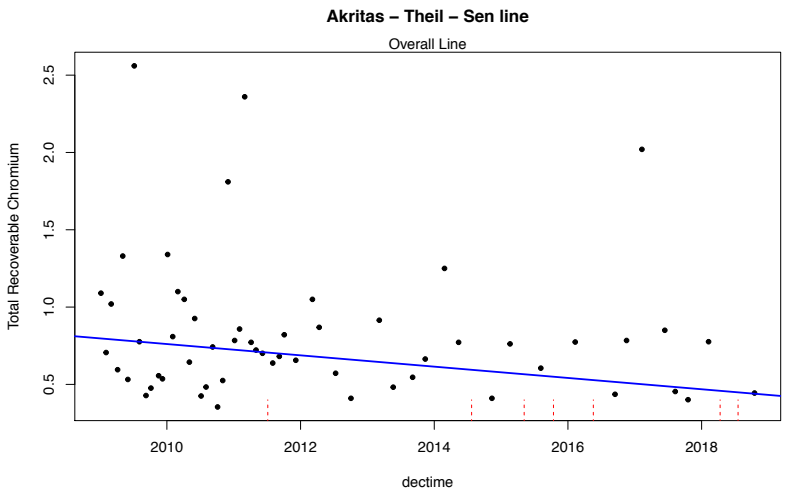
Trend -- the censeaken function

Nondetects (dashed vertical lines) influence the trend line and test.

They occur more frequently at later times, adding to the evidence of a downtrend.



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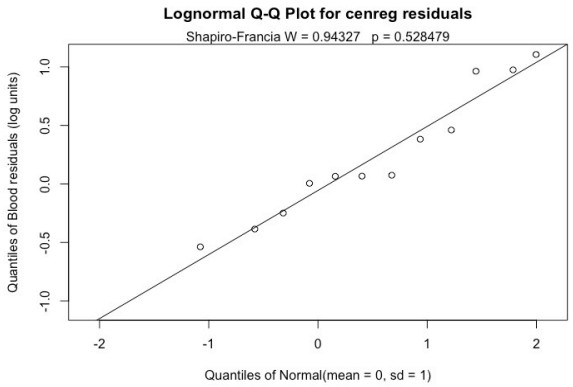
Check Assumptions with QQ Plot

Regression is a parametric method:

Check the assumption of a normal distribution with a Q-Q plot of residuals. Here using the default of log(Y) fits well. It often does for data with NDs (because they are close to zero)



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What else is available?

- Our Nondetects And Data Analysis course covers:

- parametric and nonparametric methods
- computing summary statistics
- confidence, prediction and tolerance intervals
- plotting data
- comparing to standards
- testing differences of two groups
- 3+ group tests with multiple comparisons
- regression and correlation
- trend analysis
- multivariate methods

All without substitution of values like 1/2DL for nondetects

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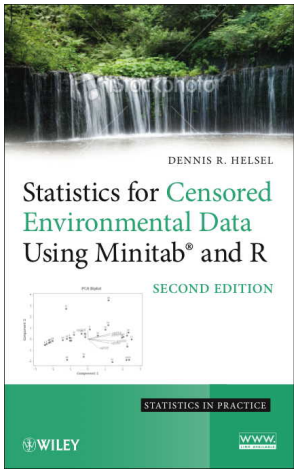
For more detail:

Statistics for Censored Environmental Data
(the second edition)

by Dennis R. Helsel

Wiley (2012)

www.PracticalStats.com/nada



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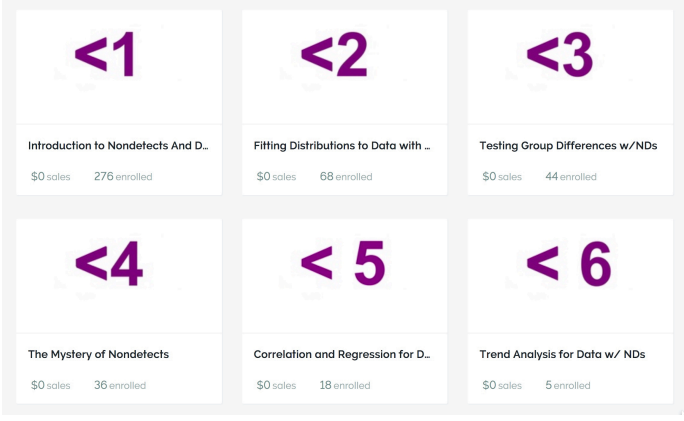
Free videos introducing methods for nondetects available now for streaming

on our Online Training Center
https://practicalstats.teachable.com/

Let colleagues know about them.

But they're only a fraction of the material in the NADA course itself.



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Thank you for viewing

Statistical methods for data with nondetects at 1 or more detection limits is the focus of our Nondetects And Data Analysis course

Questions about this material or our courses?

Get in touch!

Dennis Helsel ask@practicalstats.com

Courses & free recordings at:
http://practicalstats.teachable.com

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