SUMMING NONDETECTS: ESTIMATING TOTAL MASS OF LOW-LEVEL CONTAMINANTS

Dennis R. Helsel
Practical Stats
9278 Lark Sparrow Drive
Highlands Ranch, CO 80126, USA

ABSTRACT

Low-level contaminants such as PCBs and pesticides often occur in concentrations below laboratory reporting limits. Methods for incorporating these "nondetect" data into hypothesis tests and regression have previously been addressed by Helsel (2005), who adapted methods for survival and reliability analysis to incorporate low-level censored data. However, the problem of summing several components to obtain a total mass, as for PCB congeners, has not been addressed when some components are nondetects. Substituting zero and the detection limit provides a boundary on possible values for the total, but can this be improved upon? This study compares several methods for computing totals, reporting simulation results of which performed well. Candidate methods include maximum likelihood estimation (MLE), Kaplan-Meier, and Regression on Order Statistics (ROS). With only one detection limit, Kaplan-Meier results are identical to substitution of the detection limit, a major drawback. With multiple detection limits, Kaplan-Meier estimates are always between the boundaries of substitution results, a major advantage over MLE and ROS, which are not so constrained. Recommendations are presented for the usual situation where a small number of components (8 or fewer) are being summed.

KEYWORDS

nondetect, total mass, congener, statistics, contaminants

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