Reduced Performance from Reporting Issues

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Performance Degradation from Reporting Practices: The Importance of Numerical Resolution

The number of digits reported was 13, but only 9 are shown.

Sample	Concen.
B01	0.001
B15	0.001
B29	0.001
Average	0.001
StanDev	0.000
CoeffVar	37.5

Sample	Concen.
B01	0.001
B15	0.001
B29	0.001
Average	0.001
StanDev	0.000
CoeffVar	0.0

Sample	Concen.
B01	0.001445849
B15	0.000666495
B29	0.001014134
Average	0.001
StanDev	0.000
CoeffVar	37.5

Reporting practices routinely degrade the precision of a method. One of the most common mistakes is not establishing the numerical resolution of the method. The two left entries show how two seemingly similar results — *in terms of the number of displayed digits* — can have significantly different precision. The explanation is shown to the right wherein the entries from the leftmost set of data are seen to have an indefensible number of digits.

Not establishing the numerical resolution of a method can also degrade accuracy, because it adds unwanted variance to the process of establishing the reference values for natural samples.

Performance Degradation from Reporting Practices: The Importance of a Limit of Detection

Panel A

Sample	Concen.
F09	0.000929858
F21	0.000000000
F33	0.001048309
Average	0.001
StanDev	0.001
CoeffVar	87.1

Panel B

Sample	Concen.
F09	0.0009
F21	0.0005
F33	0.0010
Average	0.001
StanDev	0.000
CoeffVar	33.1

Panel C

Sample	Concen.
F09	0.0009
F21	0.0010
F33	0.0010
Average	0.001
StanDev	0.000
CoeffVar	6.0

Panel D

Sample	Concen.
F09	0.001
F21	0.001
F33	0.001
Average	0.001
StanDev	0.000
CoeffVar	0.0

Another source of performance degradation is reporting null values (zero concentrations) rather than a limit of detection (LOD). If the original null value for sample F21 (A) is replaced with the currently used minimum LOD value of 0.0005 mg m^{-3} (B), precision improves from 87.1 to 33.1%. If a value of 0.001 is used for the minimum LOD (C)—a more realistic value in many cases—the precision improves to 6.0%. If the number of digits reported is set to three (D), the precision is 0.0%.

Performance Degradation from False Positives and False Negatives

$$\cancelto{=100\,(n-1)\ \approx n100\%}{\psi^{L_j}_{P_i}}(S_k) = 100\,\frac{\cancelto{nx,\ \text{where } n \gg 1}{C^{L_j}_{P_i}(S_k)} - \cancelto{x}{\bar{C}^{A}_{P_i}(S_k)}}{\cancelto{x}{\bar{C}^{A}_{P_i}(S_k)}}$$

$$\cancelto{=100\,(1-n)/n,\ \text{where } n \gg 1\ \approx -100\%}{\psi^{L_j}_{P_i}}(S_k) = 100\,\frac{\cancelto{x}{C^{L_j}_{P_i}(S_k)} - \cancelto{nx}{\bar{C}^{A}_{P_i}(S_k)}}{\cancelto{nx}{\bar{C}^{A}_{P_i}(S_k)}}$$

A false positive is the most damaging, in terms of uncertainties, because of the relative magnitudes of the data. Assume the reference value in the uncertainty computation is represented by *x* (for field samples this is the average concentration from all the methods), and it must be very small for the reported value by a particular method to be considered a false detection. The value being reported is, therefore, much larger than *x*, and can be represent by a multiplicative factor, *n*, times *x* (i.e., *nx*). In such a case, the resulting uncertainty will be *n* times 100% or many times 100%.

A false negative result is not as damaging as a false positive, in terms of the uncertainty budget, but it still produces significantly high uncertainties. Assuming the observed value is represented by *x*, it must be much smaller than the reference value for the result to be considered a false no detection. The reference value is, therefore, much greater than *x*, and can be represent by a multiplicative factor, *n*, times *x* (i.e., *nx*). In such a case, the resulting uncertainty will be approximately 100% (in fact just a little bit smaller).