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Editor: Michael Thompson

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Optimising your uncertainty—a case study

In analytical measurement, both the sampling procedure and the analytical procedure contribute to the uncertainty of the result. The customer or other end users usually wish to minimise the long term average costs when they make decisions based on the result. How can we ensure that the combined uncertainty obtained is best for the customer's purposes? This Brief describes how it can be done, with the help of an example, the determination of the nitrate content of lettuce

Nearly always we need to take a small sample from the much larger target and conduct the analysis on the sample. It would be helpful if the sample had the same mean composition as the target but, despite our best efforts, it never does. This is because targets are nearly always heterogeneous and sampling methods always imperfect. As an outcome, successive samples from the same target differ in composition, from each other as well as from the target. These differences give rise to uncertainty fromd saT242046 Tm(give rise012 0 0392 0 10.02 21m(T10.02 186.1828 298.28005300494 0 10.02 21m(T10.02 247.873)

Background to the lettuce study

Leafy green vegetables provide a major source of nitrate to the consumer. EU Regulation 1822/2005 sets a maximum level for nitrate in lettuce and spinach of 4500 mg kg⁻¹ and requires that member states carry out appropriate monitoring. Recommended methods of analysis and sampling are available for the determination of nitrate, but information on the combined uncertainty attached to the results was lacking before this study.

Preliminary investigation of uncertainty

The sampling targets in the study were individual bays of lettuce in a large greenhouse, each containing up to 12 000 heads. The original procedure specified that primary samples should comprise ten heads taken in a predetermined pattern from each bay. For the

Eq 5
$$L_m = u_S \sqrt{l_S} = u_A \sqrt{l_A}^2 / u^2$$
,

This minimal cost is obtained when

Eq 6 $-\frac{2}{\frac{2}{A}}^{1/4}$

As we know that the required combined uncertainty

 $u \sqrt{w_S^2 w_A^2}$ 184, and w_S / w_A 1.38, solving the two simultaneous equations gives w_S 148, w_A 108. Thus the sampling uncertainty provided by the original method would ideally need to be reduced by 54%. This could be achieved simply by taking more increments per sample. The corresponding reduction for the analytical uncertainty would be 36%. From Eq 5 we see that the optimised combined uncertainty would impose a cost for the complete measurement of

 $319 \sqrt{40} \ 168 \sqrt{40}^2 / 184^2 \ \text{\pounds}280$. This is a large increase over the cost of the original measurement. There are other fit-for-purpose combinations of uncertainties, as can be seen in Figure 1, but all would cost even more. Whatever the eventual choice, in the long term the grower could save money by spending more on the measurement, thereby reducing the proportion of incorrectly condemned batches of lettuce.



Figure 5. The long term average cost of an accept/reject decision as a function of combined uncertainty.

Assessment of the optimisation method

All right—we admit it! The lettuce example, although real, was simplified to demonstrate the principle of uncertainty optimisation in action. Look at the following potential complications that were not considered here.

The simple functions (Eqs 1, 2) giving the costs of sampling and analysis in relation to uncertainty may be wrong in some circumstances. For example, if the sampler has to travel to the other end of the country to collect a sample comprising n increments, it would probably cost no more to collect an alternative comprising 4n increments.

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