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recommendation

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General and specific fitness functions for proficiency tests and other purposes—clarifying an old idea

A fitness function is an algebraic relationship between the concentration of an analyte and the uncertainty that is regarded as fit for a specific purpose. It is a requirement based on the needs of the end-users of analytical data, and therefore determined without any reference to the characteristics of individual analytical methods. Such functions are widely used in proficiency tests (in various guises) as fitness for purpose criteria that define the value of the standard deviation for proficiency (the 'target value') used in the calculation of the z-score from the participant's result and the assigned value. They are also useful for the selection of a validated analytical method for a particular purpose: the validated characteristics of the method are simply compared with the fitness function.

The particular usefulness of the fitness function in proficiency testing resides in its capacity to enable the scheme provider to specify a requirement of analytical performance, in terms of the optimal level of uncertainty, without imparting to the participants any information about the concentration of the analyte.

The general fitness function in proficiency tests

The providers of many proficiency testing schemes have adopted the practice of using a general fitness function $u_f = g(c)$, based on end-user needs, that is appropriate for a wide range of test materials, analytes and concentrations (c) within the analytical sector. A fitness function widely used in this general way is simple proportionality. An example might be $g(c) = 0.05c$, implying that a relative standard uncertainty of 5 % is required. Another frequently-used fitness function is the Horwitz relationship $g(c) = 0.02c^{0.8495}$, in which both $g(c)$ and c are expressed as mass fractions (*i.e.*, 1 mg kg^{-1} ≡ 1 ppm ≡ 10^{-6}). Both of these functions show the required standard uncertainty increasing as a smooth function of concentration. (Scheme providers, with the assistance of their advisory committees, are responsible for the appropriate choice of function.)

Valuable though general fitness functions may be, they are unsatisfactory in instances where the concentration of the analyte is small and the implied uncertainty approaches (or is actually lower than) the lowest level of interest to the end-user. Such a level would tend to vary with the analyte and the application, so a general fitness function would have to be customised for each specific case.

An example fitness function

As an illustrative example, consider the determination of a hypothetical food constituent for which there was a statutory upper limit of concentration of 1 % m/m. A proficiency test provider specifies a general fitness-for-purpose requirement by $g(c) = 0.1c$. According to that specification, a concentration of 5 % m/m of the constituent implies that an uncertainty of 0.5 % m/m defines fitness for purpose at that level. That is satisfactory in relation to the statutory limit: we would be quite happy that a measurement result falling in the range 4.0-6.0 % m/m with 95 % confidence was actually greater than 1.0. Moreover, the uncertainty would be small enough to include the result in exposure surveys.

If the concentration of the constituent were 0.05 % m/m, however, the corresponding uncertainty of 0.005 would *not* represent fitness for purpose. The concentration is well below what is regarded as a health hazard, but the implied accuracy is much higher than necessary to make the correct decision in relation to the statutory limit (or to use the result for exposure studies). In addition, the implied accuracy would probably be unduly expensive to achieve—the laboratories might well have to use special methods to achieve the implied accuracy.

Customising the simple fitness function

There is a simple method of modifying the fitness function to incorporate information about the lowest level of interest and provide suitable u_f -values at any point in the concentration range. Such a level of uncertainty is clearly related to, and somewhat smaller than, any statutory or other decision limit, and its value would have to be determined by the provider of the proficiency scheme. In the hypothetical example above, we might decide that an uncertainty of lower than 0.05 would never be required. This minimal uncertainty u_L could then be combined with the general fitness function $g(c)$ suitable for higher concentrations.

A simple way of doing that is just to use the higher of the two uncertainties, so that we have a fitness function

$u_f = \max(u_L,\ g(c))$.

Alternatively, combining the terms in the manner normal for independent uncertainties we might use

$u_f = \sqrt{u_L^2 + g(c)^2}$.

These two customised functions give similar results (Figure 1) and both are dominated by $g(c)$ at high concentrations, and by u_L at low concentrations. Either function clearly describes fit-for-purpose uncertainties over the whole concentration range.

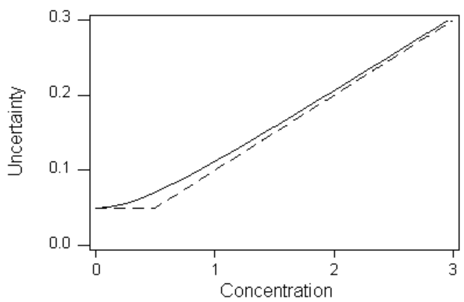

Figure 1. Fitness functions for the hypothetical example, with a minimal uncertainty u_L of 0.05 % m/m. The upper (solid) line shows the function $u_f = \sqrt{u_L^2 + g(c)^2}$, while the lower (dashed) line shows $u_f = \max(u_L,\ g(c))$.

This Recommendation was prepared for the Analytical Methods Committee by the Statistical Subcommittee (Chairman M Thompson), which is supported by the Food Standards Agency).

Recommendation

1. Scope

This recommendation applies to situations that demand a fitness function, that is, a concentration–dependent specification of the uncertainty regarded as fit for purpose.

2. **General fitness function**

Specify a concentration-dependent uncertainty $g(c)$ that is regarded as fit for purpose at high concentrations of the analyte.

(*Note*. This might take the form of a simple proportionality or a more complex function such as a power law. A simple example is $g(c) = 0.1c$, which specifies a constant relative standard uncertainty of 10 %.)

3. **Lower level of interest**

Specify a constant standard uncertainty u_L, which is the uncertainty regarded as appropriate for the lowest concentration of interest in the application sector.

4. **Combined standard uncertainty**

Combine the two uncertainties to give the fitness function $u_f = \sqrt{u_L^2 + g(c)^2}$.

(*Note*: an alternative combination is given by $u_f = \max(u_L, g(c))$)

5. **Evaluation of σ_p**

In a proficiency test, u_f can be evaluated by substituting the assigned value x_a for c. Then z-scores $z = (x - x_a)/\sigma_p$ can be calculated from results x by identifying the standard deviation for proficiency ('target value') σ_p with u_f .

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