

2.d. Using parameter optimisation to fit model parameters for a model of crop nitrogen uptake

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The problem

Crop nitrogen uptake can be modelled using a sigmoid relationship for the percentage of the total nitrogen requirement taken up with respect to cumulative temperature since sowing. However, for many crops, there are insufficient measurements of nitrogen uptake to fit the equation directly.

Data available

Measurements of soil mineral nitrogen are available. The unknown parameters in the model, describing nitrogen uptake, can be iteratively adjusted to give the best fit between simulated and measured values of soil mineral nitrogen

Why use statistical fitting and not another method?

There is insufficient data describing nitrogen uptake by the crop to directly fit an equation. Parameter optimisation allows us to fit the equation to other soil nitrogen measurements indirectly. There is insufficient data to allow more complex methods to be used, such as simulated annealing.

Simple description of how it was done

Parameter optimisation requires the form of the equation to be known, some measure of goodness of fit between simulated and measured values, and a method for systematically adjusting the fixed parameters.

In this example, the uptake of nitrogen by the crop is described by a sigmoid relationship:

$$U = \left(U_{\max}^{-1/p} + \exp(-f \times T) \right)^{-p}$$

where U is the crop nitrogen uptake (kg N ha^{-1}) after T cumulated temperature ($^{\circ}\text{C}$), U_{\max} is the maximum crop nitrogen uptake, and p and f are parameters that can be adjusted to obtain an improved fit.

The lack of fit statistic (Whitmore, 1991) was used to assess the goodness of fit between simulated and measured values of soil mineral nitrogen. The values of p and f were adjusted using a simplex optimisation procedure (Press *et al*, 1991), until the lack of fit between simulated and measured values reached a minimum.

Software used and alternative generic packages that could be used

The parameter optimisation procedure was programmed in Visual C++. Other programming languages, such as Fortran or Pascal could equally be used. Packages, such as SimLab, also provide parameter optimisation routines.

Reference

Addiscott, T., Smith, J.U., Bradbury, N., 1995. Critical evaluation of models and their parameters. *Journal of Environmental Quality*, 24, 803-807.

Further reading

Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T. (1991) *Numerical Recipes in C. The Art of Scientific Computing*. Cambridge University Press. Cambridge.