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Global sensitivity analysis and parameter optimisation of APSIM Next Generation

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Abstract: For effective contextualisation of management, genotype and environment, contemporary crop models are often calibrated before their application in scenario analyses. To elucidate parameters with greater influence on simulation outputs, sensitivity analyses are often conducted prior to calibration or parameter optimisation. With the confluence of modern mathematics, computer technology and crop science, more sophisticated analyses that afford sensitivity analysis and optimisation of all parameters simultaneously (global assessments) are becoming accessible. Using APSIM Next Generation, we contrast three global sensitivity analysis (GSA)—Morris, Sobol-Martinez, and eFAST and three parameter optimisation algorithms—Nelder–Mead simplex, DREAM-zs and L-BFGS-B. We invoke 63 parameters influencing simulated phenology, leaf, root, spike and grain weight. Each parameter was varied by ±25% relative to its default. Sensitivity indices were computed on flowering and maturity dates, aboveground biomass, LAI, grain yield, nitrogen traits and others.

The Morris method identified the greatest number of influential parameters owing to its broad yet computationally efficient screening strategy. The Sobol-Martinez algorithm, while more computationally intensive, enabled greater ability to distinguish parameter main and interaction effects. eFAST, which uses a spectral sampling approach, isolated the fewest influential parameters, indicating that this algorithm may be more suitable for high-throughput or real-time modelling scenarios.

After invoking sensitivity analyses to ascertain the solution space, we applied the three optimisation algorithms to field data from seven wheat genotypes grown in China over two growing seasons (2015–2017). A Bayesian Markov Chain Monte Carlo algorithm, DREAM-zs, consistently yielded the highest prediction accuracy across variables, although it required more computational resources, especially at high iteration levels (30,000–50,000). The Nelder–Mead and L-BFGS-B algorithms were faster but often converged on local minima, particularly for contexts including many parameter interactions.

Each algorithm resulted in robust simulations, with R^2 values exceeding 0.75 for all genotypes and RMSE for phenological traits as low as 3.4 days. When tested against independent validation data, calibrated models maintained high predictive skill, particularly when DREAM-zs was used with parameter sets derived from Sobol-Martinez. ANOVA revealed that uncertainty in model predictions was primarily borne by interactions between GSA methods, optimisation algorithms, and genotypic traits. The number of optimisation iterations contributed the least to total uncertainty, reinforcing the importance of appropriate selection of sensitivity and optimisation approaches from the outset.

Our findings highlight the nascent value of integrated sensitivity–calibration workflows in agricultural systems modelling. While individual algorithms may be less computationally demanding, they risk convergence on local minima, resulting in poor simulation accuracy when models are used under new circumstances. The combination of variance-based GSA, such as Sobol-Martinez, and global optimisation, such as DREAM-zs, emanated robust and generalisable workflows, offering lower parameter uncertainty, reasonable convergence time and more reliable simulations of genotype-by-environment-by-management interactions.

REFERENCES

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