

Opinion Article

Bayesian calibration of colorectal cancer simulation models using artificial neural networks

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DESCRIPTION

In order to calibrate the SimCRC, MISCAN-Colon, and CRC-SPIN simulation models of colorectal cancer's natural history, it is necessary to internally assess the model-predicted outcomes against the calibration objectives.

Methods for each CISNET-CRC model, we sampled up to 50,000 parameter sets using Latin hypercube sampling and produced the associated results. Using the input and output samples for each CISNET-CRC model, we trained multilayer perceptron artificial neural networks (ANN) as emulators. In order to reduce the predicted mean square error on the validation sample, we chose ANN structures with the relevant hyperparameters (number of hidden layers, nodes, activation functions, epochs, and optimizer). To acquire the joint posterior distributions of the parameters of the CISNET-CRC models, we constructed the ANN emulators in a probabilistic programming language and calibrated the input parameters using Hamiltonian Monte Carlo-based techniques. By contrasting the model-predicted posterior outputs with the calibration objectives, we internally verified each calibrated emulator.

SimCRC's ideal ANN had four hidden layers and 360 hidden nodes; MISCAN-ideal Colon's ANN had four hidden layers and 114 hidden nodes; and CRC-ideal SPIN's ANN had one hidden layer and 140 hidden nodes. SimCRC, MISCAN-Colon, and CRC-SPIN required 7.3, 4.0, and 0.66 hours, respectively, for training and calibration of the emulators. In 98 out of 110 targets for SimCRC, 65 out of 93 targets for MISCAN, and 31 out of 41 targets for CRC-SPIN, the mean of the outputs projected by the model was within the 95% confidence ranges of the calibration targets. The computational weight and complexity

for Bayesian calibration of individual-level simulation models used for policy analysis, such the CISNET CRC models, can be effectively reduced by using ANN emulation

Health decision modelling may be calibrated using Bayesian techniques. Given the prior distributions for model parameters, the structural presumptions of the model, and a likelihood function generated from the calibration data, they offer the posterior joint uncertainty of calibrated parameters. Yet, Bayesian calibration is fraught with difficulties. Complex model calibration requires much more computer time and power than simple model calibration, and convergence requires running the model dozens or even millions of times.

By adjusting the number of hidden layers between one and five and the number of hidden nodes per hidden layer starting from the number of model outputs up to 300 more with increments of 20, we were able to execute a grid search using a full factorial design to identify the best hyperparameters. We choose the structure whose mean square error (MSE) on the validation set is the least. We trained a new ANN for each CISNET CRC model since each model has a unique set of input parameters and results. To enhance the performance prediction of the ANN, we also looked at various hyperparameters, such as activation functions sigmoidal, hyperbolic tangent, relu, and the optimizer (Adam, gradient descent). Several models experienced different degrees of shrinking. Generally, the majority of posterior distributions. Using emulators to select the ideal number of LHS observations is a potential enhancement to our method that may be used; doing so could shorten the calibration process overall.

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