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Approximate Bayesian Computation for Chemical Screening Model Selection

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Abstract: Regulatory screening models for chemical exposure estimation often present conflicting goals. One objective is to minimize the probability that model predictions underestimate dose for exposed individuals (false negative decision errors). This can be easily accomplished by increasing the degree of conservatism in the model structure and parameterization to produce high exposure estimates. However, to be useful in the screening process, a second contrasting objective of avoiding false positives must be satisfied. This requires minimizing the degree of over-prediction so that high exposure estimates do not forward lower priority chemicals for additional analyses. We employ a likelihood-free approach, approximate Bayesian computation, to select and parameterize terrestrial dermal exposure models for amphibians exposed to pesticides. We compare model predictions to a data set that contains eight studies and 798 individual post-exposure body burdens across 11 amphibian species and 12 pesticides. Our objective function combines a binomial classification approach based on decision errors and a distance approach designed to reduce overestimation of exposure. The classification approach characterizes false negatives as the proportion of under-predicted exposures by comparing each observed amphibian concentration with a model estimated concentration. The distance approach minimizes the overall degree of conservatism by estimating the aggregate amount of over-prediction across all the observations. We present the technical implementation, the advantages of this approach in a regulatory screening context and the results of the model selection exercise for estimating pesticide exposure in terrestrial amphibians.

Keywords: amphibian, Bayesian, dermal exposure, pesticides, screening