BAYESIAN OPTIMAL DESIGN FOR ORDINARY DIFFERENTIAL EQUATION MODELS

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Bayesian optimal design is considered for physical models derived from the (intractable) solution to a system of ordinary differential equations (ODEs). Bayesian optimal design requires the minimisation of the expectation (over all unknown and unobserved quantities) of an appropriately chosen loss function. This can be non-trivial due to 1) the high dimensionality of the design space; and 2) the intractability of the expected loss. In this case, a further complication arises from the intractability of the solution to the system of ODEs. We propose a strategy that employs a modification of the continuous coordinate exchange algorithm where a statistical emulator is employed to approximate the expected loss function, and a probabilistic solution to the system of ODEs. The strategy is demonstrated on several illustrative examples from the biological sciences.

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