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SPOTting model parameters using a ready-made Python package

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The selection and parameterization of reliable process descriptions in ecological modelling is driven by several uncertainties. The procedure is highly dependent on various criteria, like the used algorithm, the likelihood function selected and the definition of the prior parameter distributions. A wide variety of tools have been developed in the past decades to optimize parameters. Some of the tools are closed source. Due to this, the choice for a specific parameter estimation method is sometimes more dependent on its availability than the performance. A toolbox with a large set of methods can support users in deciding about the most suitable method. Further, it enables to test and compare different methods.

We developed the SPOT (Statistical Parameter Optimization Tool), an open source python package containing a comprehensive set of modules, to analyze and optimize parameters of (environmental) models. SPOT comes along with a selected set of algorithms for parameter optimization and uncertainty analyses (Monte Carlo, MC; Latin Hypercube Sampling, LHS; Maximum Likelihood, MLE; Markov Chain Monte Carlo, MCMC; Scuffled Complex Evolution, SCE-UA; Differential Evolution Markov Chain, DE-MC$_Z$), together with several likelihood functions (Bias, (log-) Nash-Sutcliff model efficiency, Correlation Coefficient, Coefficient of Determination, Covariance, (Decomposed-, Relative-, Root-) Mean Squared Error, Mean Absolute Error, Agreement Index) and prior distributions (Binomial, Chi-Square, Dirichlet, Exponential, Laplace, (log-, multivariate-) Normal, Pareto, Poisson, Cauchy, Uniform, Weibull) to sample from. The model-independent structure makes it suitable to analyze a wide range of applications.

We apply all algorithms of the SPOT package in three different case studies. Firstly, we investigate the response of the Rosenbrock function, where the MLE algorithm shows its strengths. Secondly, we study the Griewank function, which has a challenging response surface for optimization methods. Here we see simple algorithms like the MCMC struggling to find the global optimum of the function, while algorithms like SCE-UA and DE-MC$_Z$ show their strengths. Thirdly, we apply an uncertainty analysis of a one-dimensional physically based hydrological model build with the Catchment Modelling Framework (CMF). The model is driven by meteorological and groundwater data from a Free Air Carbon Enrichment (FACE) experiment in Linden (Hesse, Germany). Simulation results are evaluated with measured soil moisture data. We search for optimal parameter sets of the van Genuchten-Mualem function and find different equally optimal solutions with some of the algorithms. The case studies reveal that the implemented SPOT methods work sufficiently well. They further show the benefit of having one tool at hand that includes a number of parameter search methods, likelihood functions and a priori parameter distributions within one platform independent package.