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Optimal scheduling and event-based sampling: development and demonstration for investigating the nitrate characteristics of a headwater catchment

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How to optimally investigate or monitor an environmental system is a frequently posed research question, which aims to learn as much as possible about the system at hand, and usually, with a limited budget for field investigations. In specific, event-based sampling has been proposed to make sure one collects data when important things happen in the system. Hence we ask "What are optimal rules for scheduling observations?" and "What are the best event-based rules?". As a demonstration, we consider nitrate as the pollutant to be monitored. Nitrate is a widespread pollutant, both in surface and subsurface water, related to human and animal waste and, to an even larger extend, to fertilizers. High concentrations of nitrate can restrict the use of drinking water. In this work, we optimize scheduling rules of sampling to infer the nitrate characteristics of a headwater catchment, considering both fix-schedule sampling campaigns as well as event-based sampling campaigns in the river. Here, we define events not only as high discharge rate, but also as low discharge rates and combinations. Our goal is to find the best set of scheduling rules for sampling strategies that provide more information to define the behavior of the catchment (either chemostatic or dilution behavior) regarding the nitrates release. For this purpose, we apply optimal design of experiments (ODE) to a high-frequency data series collected from a real catchment in Germany. The available data spans for a total period of nine months with hourly observations (nitrate concentrations and discharge rates), including over 6500 measurements along this time. As a first step, we apply ODE retrospectively to identify the most valuable observations to infer the catchment behavior. As a second step, we implement ODE prospectively, where we assume that there is no data available yet, to investigate sampling strategies that reduce the prediction uncertainty of the nitrate release. Our study is based on a simplistic stochastic model for nitrate in the river, which has an explicit parameter that can morph the model between chemostat-type and dilution-type behavior of the headwater catchment. First results show that sampling strategies based on extreme events, including both high and low discharge rates, are key to reduce the prediction uncertainty of the catchment behavior.