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Quantifying groundwater nitrogen pollution risk using statistical emulation of a process-based water quality model – an example for Scotland

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Diffuse nitrate pollution from agriculture is a significant problem for both surface and groundwater quality, potentially affecting ecosystems and human health. Pollution mitigation measures against nutrient pollution require spatial and temporal targeting and should be sustainable under changing environmental (e.g. climatic) conditions. Process-based water quality models can be applied to estimate nitrate concentrations in ground and surface waters under current conditions and to simulate potential impacts of climate and land management scenarios. Such models typically include a number of tunable parameters which can be calibrated to improve the model performance when compared to observed data. However, the process of parameter inference is typically computationally expensive due to long model runs of each individual simulation, making it difficult to estimate model uncertainty under baseline and scenario conditions. An alternative approach is to construct a statistical emulator, which quickly generates an estimated value, with associated uncertainty, for arbitrary choices of the tuning parameters. Such emulators are constructed by interpolating the output of a smaller number of full simulations, which significantly reduces the overall computational cost of the tuning procedure.

In this work we present an approach to this problem using Gaussian process emulation and illustrate it by emulating the Nitrogen Risk Assessment Model for Scotland (NIRAMS). We show how this procedure can be used to estimate nitrate concentrations across Scotland, as well as probabilities that the concentrations will exceed pre-defined regulatory thresholds. By varying input climatic variables and nitrogen inputs, we show also how emulators can be used to study the impact of climate change and land management scenarios. Gaussian process emulators such as the one presented here can be applied to other complex water quality models for an efficient estimation of solute concentrations under current conditions, climate and land management scenarios with uncertainty estimates.