



Autocorrelated residuals in inverse modelling of soil hydrological processes: a reason for concern or something that can safely be ignored?

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Models are inherently imperfect because they simplify processes that are themselves imperfectly known and understood. Moreover, the input variables and parameters needed to run a model are typically subject to various sources of error. As a consequence of these imperfections, model predictions will always deviate from corresponding observations. In most applications in soil hydrology, these deviations are clearly not random but rather show a systematic structure. From a statistical point of view, this systematic mismatch may be a reason for concern because it violates one of the basic assumptions made in inverse parameter estimation: the assumption of independence of the residuals. But what are the consequences of simply ignoring the autocorrelation in the residuals, as it is current practice in soil hydrology? Are the parameter estimates still valid even though the statistical foundation they are based on is partially collapsed? Theory and practical experience from other fields of science have shown that violation of the independence assumption will result in overconfident uncertainty bounds and that in some cases it may lead to significantly different optimal parameter values. In our contribution, we present three soil hydrological case studies, in which the effect of autocorrelated residuals on the estimated parameters was investigated in detail. We explicitly accounted for autocorrelated residuals using a formal likelihood function that incorporates an autoregressive model. The inverse problem was posed in a Bayesian framework, and the posterior probability density function of the parameters was estimated using Markov chain Monte Carlo simulation. In contrast to many other studies in related fields of science, and quite surprisingly, we found that the first-order autoregressive model, often abbreviated as AR(1), did not work well in the soil hydrological setting. We showed that a second-order autoregressive, or AR(2), model performs much better in these applications, leading to parameter and uncertainty estimates that satisfy all the underlying statistical assumptions. For theoretical reasons, these estimates are deemed more reliable than those estimates based on the neglect of autocorrelation in the residuals. In compliance with theory and results reported in the literature, our results showed that parameter uncertainty bounds were substantially wider if autocorrelation in the residuals was explicitly accounted for, and also the optimal parameter values were slightly different in this case. We argue that the autoregressive model presented here should be used as a matter of routine in inverse modeling of soil hydrological processes.