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Model–data comparison with permutation entropy: Moving beyond summary statistics

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Soil water plays an important role in the terrestrial water and energy cycles. Its movement follows the gradient of the soil water potential and is most frequently described by the Richards equation. The model quality is often summarized by criteria like the Nash–Sutcliffe model efficiency coefficient that relates the model residuals to the variability of observations or the root mean square error. However, as a summary statistics, it is unable to provide details on the temporal behaviour of the model. We suggest to use the permutation entropy – a complexity measure – to compare temporal patterns of modelled versus measured data.

We modelled water fluxes in the vadose zone at a forested site (Fichtelgebirge, Germany) with the Water Heat and Nitrogen Simulation Model (WHNSIM). The model solves the Richards equation numerically. We characterized the temporal dynamics of soil matric potentials measured at the study site and compared their complexity with modelled matric potential. Natural time series can exhibit behaviours of different degrees of complexity ranging from regular to random. The complexity of a natural time series results from the nonlinearity of underlying processes, their different interactions and possibly measurement noise. In our case, the measured matric potential is the result of the signal propagation from precipitation to throughfall to infiltration and reflects the influence of the soil hydraulic properties, evapotranspiration and possible measurement errors. In general, regular structure like periodic signals (e.g. yearly cycle such as in evapotranspiration) is easier to model than irregular signals. Permutation entropy values close to zero indicate that a time series is regular and contains only few different temporal patterns. In contrast, very large values near one result from a high number of different patterns and are typical for noise.

The model WHNSIM reproduced the overall level of matric potentials in all modelled depths (20, 40 and 90 cm). However, while it captured the complexity of the measurements in the upper soil, the matrix potentials in 90 cm depth were less complex indicating a more regular and damped signal. This result suggests that WHNSIM misses some important processes at least in the deeper soil.

Although we used WHNSIM in our study, the permutation entropy can be calculated for any other real-valued measured or modelled time series. It can serve as a further comparative tool to evaluate models and uncover periods of particular match or mismatch between model and data.