INVITED COMMENTARY

HP TODAY

HYDROLOGICAL PROCESSES
Hydrol. Process. **19**, 3923–3929 (2005)
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/hyp.6075

On hydrological predictability

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Introduction

Have you ever been flabbergasted, after the fact, by how far your predictions were off the observed data? An underestimation of pesticide arrival time by a factor of 10, or an overestimation of flood peaks by a factor of two or more—all this with models that have apparently been well calibrated with data from the past. Of course, there is always an explanation, after the fact. The media characteristics may have been slightly different from what we initially assumed, perhaps preferential flow occurred where we did not expect it to occur, there was inaccuracy in the assumed initial conditions and, of course, in the boundary conditions as well, and the events were larger than what we thought could reasonably occur. It seems that small uncertainties can easily amplify under certain conditions and will limit predictability. In this commentary, we argue that there is a pattern to this.

Non-Linearities of Hydrological Systems

The most obvious cause for limits to predictability is the non-linearity of the hydrological systems we deal with. Higher order terms in the equations of motion can lead to non-linear, and hence highly unpredictable, characteristics. The Saint-Venant equation contains higher order terms, but most of the equations used in hydrology are, in fact, linear in their structure. The Richards equation has a linear structure without higher order terms, and so have most other equations we think closely represent the dynamic characteristics of hydrological systems. Some of these equations such as the Richards equation are, however, non-linear because of non-linear coefficients or material properties that are a second source of non-linearity. Unsaturated hydraulic conductivity exhibits very significant changes with the moisture state of a soil. In the Penman–Monteith equation, stomata resistance changes with radiation and available soil moisture, and retardation coefficients of non-linearly adsorbing solutes change with solute concentration.

There is a third source of non-linearity where processes switch between regimes. It is then a different process that takes over once a certain threshold is exceeded. Threshold behaviour may occur if dynamic states switch from zero to non-zero values, as is the case of water levels in surface runoff, rainfall rates, or water content in a macropore system in structured soils. Threshold behaviour may be further enhanced by emerging and vanishing structures and

Received 6 October 2005
Accepted 7 October 2005

features, as is the case of swelling and cracking soils or a switch between hydrophilic and hydrophobic conditions of soils. Thresholds seem to be omnipresent in hydrology: thresholds between matrix and preferential flow, thresholds between infiltration and saturation excess flow, thresholds between freezing and melting snow, thresholds in evaporation being controlled either by atmospheric demand or by soil hydraulic properties, thresholds between supercritical and subcritical flows, thresholds of erosion, and thresholds of inception of sediment motion in streams.

Threshold behaviour can manifest itself in two ways in the equations of motion. The equations may contain terms that switch on and off, depending on the value of a control variable. Alternatively, the material properties may switch between different modes, depending on the value of a control variable. An example for the first case is flow in structured soils, where, depending on the soil moisture state, either the Richards equation alone or in combination with a representation of macropore flow (e.g. by a kinematic wave equation) make up the equation of motion. An example of the second case is the switch between hydrophilic and hydrophobic conditions in water-repellent soils.

Depending on the type of non-linearity, uncertainties in the initial conditions and forcings may or may not dampen out. If processes are self-amplifying, i.e. if positive feedbacks exist, initial uncertainties may amplify and lead to chaotic behaviour, where the system state exhibits erratic variability. This, of course, depends on the degree of non-linearity. Thresholds can be thought of as very strong non-linearities. In the case of threshold dynamics, the propagation of uncertainty of initial and boundary conditions is much more complex than in the other case of simple non-linear but continuous material properties, because system dynamics exhibit a much higher state dependency. The effect of input uncertainty on systems response may be extremely high if the system is prone to switch between different dynamic regimes. For example, during infiltration into sandy soils, local instabilities of the wetting front may cause fingering. A local increase of soil moisture increases hydraulic conductivity, which increases the contrast between wet and dry parts of the soil, which further enhances hydraulic conductivity and infiltration. If a changeover to fingering occurs, then the feedback will be stronger, which means that transport processes can become very fast (Ritsema *et al.*, 1998).

Observability: Micro- and Macro-States

If non-linearity is present in the system, then predictability will hinge on the accuracy to which initial conditions and boundary conditions can be measured. At a hydrological scale (catchments, aquifers, regions) it is impossible to measure exhaustively any of the variables we are interested in. This may cause substantial uncertainties. If we go down in scale, to the plot scale, we are able to collect more detailed data, but no matter what the spatial resolution of the measurements is there will always be some fine-scale detail not captured by the measurements. This fine-scale detail may or may not matter for making hydrological predictions at larger scales, which has intrigued hydrologists for a long time (Sivapalan, 2003).

In statistical mechanics there is a similar problem of uncertain initial conditions as in hydrology:

> The principles of ordinary mechanics may be regarded as allowing us to make precise predictions as to the future state of a mechanical system from a precise knowledge of its initial state. On the other hand, the principles of statistical mechanics are to be regarded as permitting us to make reasonable predictions as to the future condition of a system, which may be expected to hold on the average, starting from an incomplete knowledge of its initial state. (Tolman, 1979: 1)

Following the concepts of statistical mechanics, let us consider the kinetic energy of a mole of a gas. The gas can be described in greatest detail by specifying its microscopic state, or microstate, at any time, i.e. the exact values of the kinetic energy of each of the 10^{23} individual molecules. However, it is impossible to measure this microscopic state, and we may not be interested in the full detail on the behaviour of each and every molecule either. Instead, it may be possible to measure the macroscopic state, or macrostate, of the gas represented by average quantities or distributions. One such macroscopic quantity is the gas temperature, which is a measure of the average kinetic energy of the gas molecules. It is impossible to measure the microstate, but it is possible to measure the macrostate. The macrostate characterizes the microscopic reality in a statistical and, therefore, uncertain sense. A set of numerous possible microstates is consistent with the same macrostate. This is often referred to as a 'degradation' of the measurable macrostate into a set of possible microstates.

Zehe and Blöschl (2004) suggested that the concepts of micro- and macro-states are applicable to hydrological predictions. For the case of initial soil moisture they defined the microstates as the detailed patterns of soil moisture and the macrostates as the statistical distributions of soil moisture obtained from measurements as typically available in research catchments. They then generated multiple realizations of soil moisture patterns, each pattern representing one possible microstate, and all the realizations (or microstates) were consistent with the macrostate of soil moisture derived from the field measurements. They analysed the uncertainty due to unknown microstates by using them as the initial conditions of a physically based hydrological model. The model accounted for a changeover in the flow regime from matrix to macropore flow. The variability in simulated infiltration between the realizations was then considered a measure of the uncertainty in hydrological response introduced by uncertain initial soil moisture. As an illustration, Figure 1 shows the average simulated transport depth 1 day after application of a hypothetical tracer to the soil surface. For a given soil-moisture macrostate, simulated transport depths varied significantly as a result of uncertainties in the microstate. The simulations indicated that the predictability of the hydrological response depends on the average initial state of soil moisture. There exists an unstable range where the predictability of hydrological response is poor (between average soil moistures of 0·18 and 0·30 $m^3\ m^{-3}$ in this case), and a stable range where the predictability is significantly better. This state-dependent predictability is related to the presence of threshold processes. The predictability is poor if the system is close to the threshold, but it improves as the system moves away from the threshold. The main threshold in the example is the transition from matrix to macropore flow.

Representing the macrostate of initial soil moisture by the distribution function rather than by spatial patterns does not account for the small-scale details of the microstate. One of the important pieces of information that is lost is the correlation between local saturation and local macropore-related hydraulic conductivity. At the plot scale, if the soil was prone to switch from matrix to

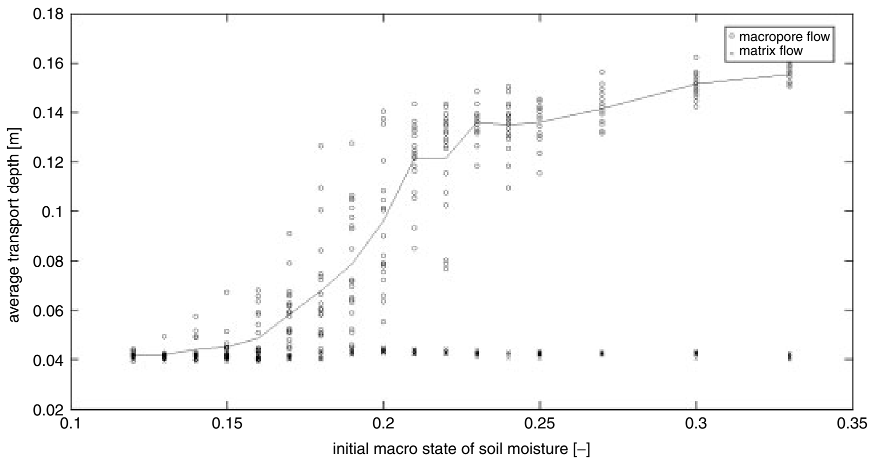

Figure 1. Average simulated transport depths for different realizations of the soil moisture microstate that are consistent with the same macrostate. The crosses relate to a medium where only matrix flow is allowed; the circles relate to a medium containing macropores where preferential flow may establish

macropore flow, soil moisture microstates that were positively correlated with the bulk hydraulic conductivity yielded fast infiltration and transport associated with preferential flow. This positive correlation of some of the microstates stems from the superposition of the soil moisture microstates on the time-invariant pattern of macroporosity. The correlation becomes important because of the non-linearity introduced by the threshold process.

Clearly, the concept of micro- and macro-states can be used for analysing the uncertainty of a range of spatial estimates in hydrology. The uncertainty may come from using a limited number of point samples (such as precipitation and piezometers) or lumped samples (such as discharge and satellite data). The implications for hydrologic predictability can then be assessed by Monte Carlo simulations, as illustrated by the soil moisture example.

Frequent Outliers

In the discussion above the main interest was on deterministically predicting hydrological response. Often, one is only interested in statistical predictions, i.e. the exceedance probability of an event of a certain magnitude, of concentration levels, or of solute arrival times, for example. Whereas non-linearity impacts on the patterns of predictability in the deterministic case, in the case of statistical predictions the non-linearity impacts on the shape of the distributions. In fact, there is a deep connection between the probability distributions of system response, the degree and type of non-linearity of a system and the degree and type of heterogeneity in the system. Linear and homogeneous systems are consistent with Gaussian (i.e. normal) distributions. It can be argued that, deterministically, this is because the general solution to a linear diffusion equation is a linear combination of Gaussian functions. Statistically, it can be argued by the central limit theorem that a linear combination of a set of identical distributions of arbitrary shape will converge to a Gaussian distribution. Gaussian behaviour is an indication of linearity and/or symmetry.

However, there is data evidence in almost any branch of the Earth sciences that distributions deviate from normality, and hydrology is no exception. The classical example in hydrology is the Hurst phenomenon of wet years clustering into multiyear wet periods (Hurst, 1951). Floods, droughts, and many other variables are not Gaussian, in fact not even close to Gaussian (Blöschl, 2005). Typically, the main difference is that the extreme events, or 'outliers', occur more often than one would expect from a normal or Gaussian distribution. It is in the tail that they differ: the tails are 'fat'. As an example, Figure 2 shows the maximum annual floods of the Kamp catchment. Catchments where outliers such as in the Kamp have been observed are frequent, and some observers have noted they have become even more

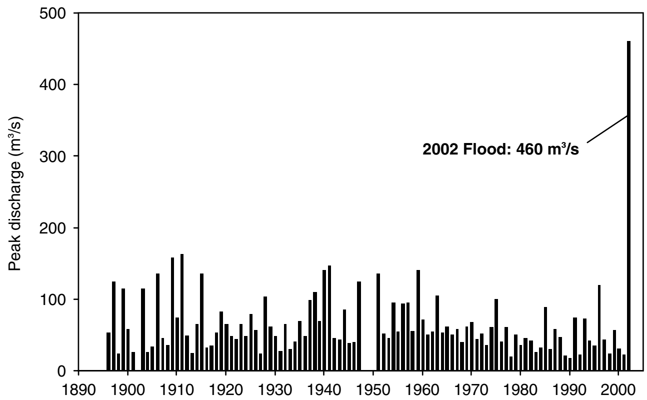

Figure 2. Maximum annual flood peaks observed in the Kamp catchment, Austria (620 km^2 catchment area). Redrawn from Gutknecht *et al.* (2002)

frequent in recent years in some parts of the world (Snorasson *et al.*, 2002; Kundzewicz, 2004). Fat-tailed distributions may limit the predictability of the probability of extreme events.

There are two main explanations for fat-tailed distributions. The first is non-linear system dynamics. In oceanography, freak waves can only be explained by non-linear dynamics (e.g. White and Fornberg, 1998; Liu and Pinho, 2004); in a similar vein, non-linearity needs to be invoked to explain hydrological outliers. In the 2002 Kamp flood example, persistent rainfall filled up the sandy soils and, once a rainfall of around 100 mm was exceeded, most of the rainfall became runoff. Daily rainfall was 70% larger and the flood peak was 200% larger than the second largest observations in the past 100 years, an apparent indication of non-linearity. More-complex non-linearities with positive feedbacks exist in hydrology that can be linked to fat-tailed distributions. Examples are soil moisture at the land surface (Rodriguez-Iturbe *et al.*, 1991), long-range climate dynamics (Koutsoyiannis, 2005), and non-linear absorption characteristics of reactive substances that may result in fat-tailed distribution of arrival times (Jury and Horton, 2004).

The second explanation is the presence of structured heterogeneity in the subsurface, which can result in fat-tailed distributions even if the systems dynamics are linear. Gaussian media characteristics may increase the apparent dispersivity of the system, but they will not change the type of distribution. The convective–dispersive process is a case of perfect symmetrical mixing, in the sense that each solute molecule experiences the whole range of possible velocities in the far field, i.e. the central limit theorem is applicable in disordered media. In contrast, non-Gaussian, structured media characteristics may result in frequent outliers and fat-tailed distribution (Matheron and de Marsily, 1980; Levy and Berkowitz, 2003; Knudby and Carrera, 2005). In the case of spatially interconnected, preferential flow paths, fast-travelling solute molecules will never mix with slow molecules; hence, the distribution of arrival times will have a fat tail and early arrival. This will break the symmetry of perfect mixing. A perturbation will propagate quickly through the system. The formation of interconnected structures in soils and aquifers can be thought of as a self-amplifying process that has a tendency to result in fat-tailed distributions. If non-linearity is present, as is the case of non-linearly adsorbing herbicides, then distributions may deviate even further from normality (Zehe *et al.*, 2004).

The spatial correlation of extremes is often stronger than suggested by multivariate lognormal distributions (Zinn and Harvey, 2003), which strongly affects flow and mixing. The same pattern seems to exist for large-scale flooding. If we consider flooding as a bivariate process depending on catchment states and rainfall amounts, then there will be a close association of wet catchment state with heavy rainfalls. Infiltration usually decreases during heavy precipitation as a result of surface sealing and the formation of saturation areas, for example, which in turn enhances overland flow, erosion, and sedimentation with a feedback to surface sealing.

Predicting Predictability

There is a lesson to be learned here, we believe. Above all, modesty seems to be in place as to the degree to which hydrological system behaviour can be represented. The prevailing paradigm of hydrology, without doubt, is that of positivism, i.e. the view that there is a truth out there and if enough data are analysed in the right way we can understand and resolve even the most complex problems. Limits of predictability, however, suggest that there are also limits to the repeatability of experiments. The multiple realizations in Figure 1 can be interpreted as multiple hypothetical experiments. If, for a given rainfall forcing, we measured soil moisture and hydrological response many times, the relationship between the two most likely will not be unique, as the uncertainty in initial soil moisture limits the predictability of hydrological response. The confidence bounds of experimental results may hence be wider than what the accuracy of the instruments themselves would suggest.

There are also implications for what can be learned from longer hydrological records. If a normal distribution does not describe the 'normal' case then there is a need to understand the extremes better, including their interrelation with other processes and variables. In the extremes, variables often show a stronger correlation than indicated by a Gaussian correlation structure. Examples are correlations between the transport depth and connectivity of pathways in the subsurface, as well as correlations between extreme rainfall and the resulting flood. The issue, therefore, is to examine extremes and averages separately. Inevitable, one then runs into the problem of small sample sizes, as few observations tend to exist in the tails of a distribution. In the Kamp catchment, a flood forecasting system is currently implemented and the hydrological analysis at the very extreme end builds on a single event—a sample of one. It is hard both to calibrate and validate a model on a sample of one. Similarly, with a few samples that indicate large concentration values in the subsurface it is hard to get a consistent picture of the transport patterns. Clearly, understanding system response across a *range* of magnitudes is critically important here, as it may help extrapolate from the average to the extremes. From a statistical perspective, copulas may offer a promising framework. Taken from economic statistics, they are a method for analysing and modelling interrelations between the extremes of variables, without referring to the shape of the marginal distributions. This is particularly appealing if the marginal distributions are fat tailed (Salvadori and De Michele, 2004).

Obviously, there are also implications for hydrological modelling. In other Earth sciences, often, non-linear systems can be represented by closed-form non-linear equations in a homogeneous medium that facilitates the analysis of their predictability characteristics. The Lorenz equation (Lorenz, 1969) is the classical example, and numerous others exist (e.g. Stull, 1985). In hydrology, in contrast, threshold processes and structured heterogeneity are the more typical case for which the analysis of predictive uncertainty is more difficult. The presence of thresholds does indicate that, if the system is close to a threshold, then predictability is poor, but it improves as the system moves away from the threshold. In the Kamp flood forecasting system, 11 telemetered raingauges are available that can be used to specify the macrostate of the rainfall field. Incomplete knowledge of the microstate, i.e. the detailed patterns of the rainfall field between the gauges, will amplify and hence limit predictive accuracy. If there exist cross-correlations of high intensities falling on low-permeability areas, interactions similar to those in Figure 1 will occur. Ensemble forecasts may assist in assessing the predictive uncertainty, but it is important to recognize that there will always be some inherent limit to predictability.

On a more general note, we believe there is an exciting research field in hydrology to be pursued in the coming years: to learn how to separate the predictable and the unpredictable. If the uncertainties are known, then alternative risk-management strategies can be used to deal with them—flood management strategies and agricultural management strategies in the two examples we have used here. Research in hydrology needs to focus on patterns of predictability.

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