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Global spatial sensitivity of runoff to subsurface permeability using the active subspace method

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ABSTRACT

Hillslope scale runoff is generated as a result of interacting factors that include water influx rate, surface and subsurface properties, and antecedent saturation. Heterogeneity of these factors affects the existence and characteristics of runoff. This heterogeneity becomes an increasingly relevant consideration as hydrologic models are extended and employed to capture greater detail in runoff generating processes. We investigate the impact of one type of heterogeneity – subsurface permeability – on runoff using the integrated hydrologic model ParFlow. Specifically, we examine the sensitivity of runoff to variation in three-dimensional subsurface permeability fields for scenarios dominated by either Hortonian or Dunnian runoff mechanisms. Ten thousand statistically consistent subsurface permeability fields are parameterized using a truncated Karhunen–Loéve (KL) series and used as inputs to 48-h simulations of integrated surface-subsurface flow in an idealized 'tilted-v' domain. Coefficients of the spatial modes of the KL permeability fields provide the parameter space for analysis using the active subspace method. The analysis shows that for Dunnian-dominated runoff conditions the cumulative runoff volume is sensitive primarily to the first spatial mode, corresponding to permeability values in the center of the three-dimensional model domain. In the Hortonian case, runoff volume is sensitive to multiple smaller-scale spatial modes and the locus of that sensitivity is in the near-surface zone upslope from the domain outlet. Variation in runoff volume resulting from random heterogeneity configurations can be expressed as an approximately univariate function of the active variable, a weighted combination of spatial parameterization coefficients computed through the active subspace method. However, this relationship between the active variable and runoff volume is more well-defined for Dunnian runoff than for the Hortonian scenario.

1. Introduction

The generation and movement of overland flow (or runoff) is a key hydrologic process that drives associated phenomena like streamflow, erosion, and contaminant transport. Local-scale mechanistic explanations for runoff generation have been examined widely in the literature, with the works of Horton (1933) and Dunne and Black (1970) defining the framework common to many modern runoff studies. Saturation excess overland flow (Dunne and Black, 1970) occurs when pore space within the soil column is filled with water (saturated) such that addition of water, commonly as lateral subsurface flux, forces water to exfiltrate at the land surface. In contrast, infiltration excess overland flow (Horton, 1933) occurs when the precipitation rate exceeds the ability of the soil surface to absorb and transmit the incoming water. Both processes can lead to local runoff generation at different times or locations in a watershed. Whether runoff generated in one location translates to runoff in a downslope location depends on the state of the soil surface in the intervening flow path. For example, if the flow path is dominated by saturated soils or has very low infiltration capacity, the upslope runoff is more likely to propagate downhill. The realization of runoff at a downslope point on a hillslope or in a watershed is the result of the integrated effects of moisture and hydraulic properties along each surface flow path. This, then, implies that the runoff response may contain some information on the heterogeneity of such properties.

The impacts of land surface property heterogeneity on runoff have been studied extensively – a host of field and simulation

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studies have helped establish links between near-surface hydraulic conductivity heterogeneity and spatial, temporal, and statistical properties of runoff (e.g. Freeze, 1980; Loague, 1988; Singh, 1997). The sensitivity of runoff to this heterogeneity, however, depends on other, often transitory, factors like prevailing runoff mechanisms or the nature of a precipitation event. Results from Loague (1988) suggest that the degree and resolution of heterogeneity may matter more for some aspects of runoff than others and that Dunnian mechanisms may be less sensitive to hydraulic conductivity variability than runoff arising from Hortonian conditions. Similarly, the results of Smith and Hebbert (1979), Séguis et al. (2002), and Maxwell and Kollet (2008) support the idea that runoff sensitivity to soil property heterogeneity is inversely proportional to rainfall rate for Hortonian conditions—that is, characteristics of runoff depend increasingly on the degree of permeability heterogeneity as rainfall intensity decreases. Work by Woolhiser et al. (1996), Michaelides and Wilson (2007), Maxwell and Kollet (2008), and Meyerhoff et al. (2014) suggests that the spatial arrangement or trend in heterogeneous properties is an important component of the overall effect of heterogeneity. For example, a stochastically generated permeability field with connected regions of low permeability would yield higher runoff than statistically equivalent realizations lacking such random spatial coherence. Maxwell and Kollet (2008) point out, however, that a simple counting of connected low permeability zones alone cannot be used to fully predict the resulting runoff.

While much of the existing literature focuses on runoff simulated assuming a one or two-dimensional representation of subsurface flow, recent studies have begun to examine complexities of runoff response in simulations that incorporate three-dimensional variably saturated subsurface flow. Maxwell and Kollet (2008) demonstrated the complicated interplay among spatial variance in hydraulic conductivity, rainfall rates, and ergodicity for Hortonian overland flow on a hillslope using the integrated hydrologic code ParFlow. Building on previous studies indicating that runoff sensitivity to hydraulic conductivity heterogeneity depends on precipitation rate, Smith and Hebbert (1979), Séguis et al. (2002), and Maxwell and Kollet (2008) found that effective runoff behavior may only be possible under limited high rainfall, low variance conditions. Subsequent studies using ParFlow suggest that, while heterogeneity becomes less important for controlling runoff under high water table conditions (i.e. hillslope runoff becomes a function of mean permeability alone), variance in the saturated hydraulic conductivity field controls the partitioning of total runoff outflow between overland flow and base flow (Meyerhoff and Maxwell, 2011).

2. Methods

In this study we investigate the sensitivity of accumulated runoff volume, our scalar output of interest, to changes in the spatially varying subsurface permeability field using active subspaces and an integrated hydrologic model, ParFlow. The methods used for this work are described here in six parts: (1) the active subspace method, (2) configuration of the ParFlow hydrologic model, (3) parameterization of the subsurface permeability field, (4) computation of spatial basis functions, (5) development of a global spatial sensitivity metric, and (6) setup of hydrologic scenarios.

2.1. Active subspaces

We describe active subspaces for a generic scalar-valued function of several variables, which we denote $f(\vec{x})$. In this particular application, f represents the total cumulative runoff volume, and $\vec{x} \in \mathbb{R}^m$ represents the m parameters of the permeability field; we discuss the permeability parameterization in Sections 2.3 and 2.4.

We assume $f(\vec{x})$ is differentiable, and we denote the gradient—oriented as a column m-vector—by $\nabla f(\vec{x})$.

The active subspace from Constantine (2015) is defined by the first few eigenvectors of the following symmetric, positive semidefinite matrix,

$$\boldsymbol{C} \;=\; \int \nabla f\, \nabla f^T \rho\, d\vec{x} \;=\; \boldsymbol{W} \Lambda \boldsymbol{W}^T \tag{1}$$

where $\rho = \rho(\vec{x})$ is a non-negative weight function on the space of parameters normalized so that $\int \rho\, d\vec{x} = 1$. The weight function is given by the model; it is not a parameter of the method. Loosely speaking, ρ quantifies the probability of sets of permeability parameters. The eigenvectors of $\boldsymbol{C}$ depend on ρ. If the modeller changes ρ, then the analysis must be repeated.

The $\boldsymbol{W}$ in (1) is the $m \times m$ orthogonal matrix of eigenvectors; Λ is the diagonal matrix of non-negative eigenvalues in decreasing order. These satisfy the following relationship with f:

$$\lambda_i \;=\; \int \left(\nabla f^T \vec{w}_i\right)^2 \rho\, d\vec{x},\; i = 1, \ldots, m. \tag{2}$$

In words, the eigenvalue measures the mean-squared directional derivative of f along the corresponding eigenvector. If the first $n < m$ eigenvalues are much larger than the rest, then the corresponding eigenvectors identify a set of important directions in the space of inputs; perturbing the inputs $\vec{x}$ along these important directions changes f more, on average, than perturbations orthogonal to the important directions. We exploit this relationship to study the sensitivity of runoff to a properly parameterized permeability field.

One way to estimate the eigenpairs in (1) is with Monte Carlo as in Constantine and Gleich (2015). But such an approach requires access to the gradient $\nabla f(\vec{x})$ as a subroutine. In many applications—including ours—such a subroutine is not available, so the gradient must be approximated. Finite difference approximations are infeasible due to the cost of evaluating $f(\vec{x})$. Approximating a gradient vector takes $m+1$ evaluations of f—one for each perturbation of the inputs. And estimating $\boldsymbol{C}$ with Monte Carlo would require several such gradient approximations. To circumvent this difficulty, we employ a method based on the following observation. Assume that f is well-approximated by a linear function of $\vec{x}$[1],

$$f(\vec{x}) \;\approx\; a_0 + \vec{a}^T \vec{x}, \qquad \nabla f(\vec{x}) \;\approx\; \vec{a}. \tag{3}$$

In this case, $\boldsymbol{C}$ becomes

$$\boldsymbol{C} \approx \int \vec{a}\,\vec{a}^T \rho\, d\vec{x} \;=\; \vec{a}\,\vec{a}^T \;=\; \vec{w}\lambda\vec{w}^T, \tag{4}$$

where $\lambda = \|\vec{a}\|^2$ and $\vec{w} = \vec{a}/\|\vec{a}\|$. This observation yields the following heuristic method Constantine (2015, Algorithm 1.3).

1. Choose $N = \mathcal{O}(m)$—e.g., 2-to-10 times the number of components in $\vec{x}$.
2. For $i = 1, \ldots, N$, draw $\vec{x}_i$ at random according to the density $\rho(\vec{x})$.
3. Compute $f_i = f(\vec{x}_i)$—i.e., run the simulation for each set of inputs $\vec{x}_i$.
4. Use least-squares to compute the coefficients of a linear approximation of $f(\vec{x})$ from a set of pairs $\{\vec{x}_i, f_i\}$. Call these coefficients $\hat{\vec{a}}$.
5. Let

$$\hat{\vec{w}} \;=\; \hat{\vec{a}}/\|\hat{\vec{a}}\| \tag{5}$$

be the vector that defines the one-dimensional active subspace.

[1] Runoff is not a linear function of permeability parameters. The linear assumption is used only to develop the heuristic for estimating a one-dimensional active subspace.