Orthonormal Residuals for Large-Scale Geostatistical Model Validation

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Abstract: Geostatistical methods are widely used to estimate spatial model parameter functions, like hydraulic conductivity, based on measurements of dependent quantities, like hydraulic heads or solute arrival times. In this framework, the unknown parameter values are treated as random variables that have to be conditioned on given state observations.

The corresponding inverse problem is inherently nonlinear, and its solution depends on the model equations, which are typically partial differential equations (PDEs). This makes its solution computationally very demanding or outright intractable. Parameter estimation techniques like the quasi-linear geostatistical approach (QLGA), and other variants of nonlinear least squares, therefore restrict themselves to the extraction of moments like the (approximate) posterior mean and (linearized) posterior covariance matrix of the parameters.

In recent years, highly efficient variants of these methods for large-scale problems have been developed, allowing the simultaneous estimation of millions of parameters based on thousands of measurements. However, the applicability of the parameterized model depends on the involved modeling errors and stochastic approximation error, which makes validation a necessity.

We present a novel approach for the validation of large-scale geostatistical models: orthonormal residuals generated through randomized decomposition of the covariance matrix of measurement residuals. In contrast to studentized residuals, these orthonormal residuals take the high amount of correlation between individual measurement residuals into account. We discuss strategies for efficient computation and present examples of application.

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