Optimal Derivatives of Noisy Simulations

Derivative-free Optimization of Complex Systems

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Abstract

Computational noise in deterministic simulations is as ill-defined a concept as can be found in scientific computing. Roundoff errors, discretizations, numerical solutions to systems of equations, and adaptive techniques can destroy the smoothness of the processes underlying a simulation. Such noise complicates optimization, sensitivity analysis, and other applications, which depend on the simulation output. The increasing complexity of modern DOE codes (in the form of more floating-point operations, tighter coupling, deeper hierarchies, mixed-precision computations, etc.) further obfuscates the sources and contributions of uncertainty in a simulation output.

We have developed new mathematical theory and tools for estimating the computational noise that arises in virtually all numerical simulations of DOE interest. Our theory is based on a stochastic model but does not assume a specific form for the distribution of the noise. Our experiments on deterministic simulations involving calculations fundamental to scientific computing empirically validate our technique on simulations where the theory does not hold. Our experiments also illustrate that the relationship between truncation errors and the computational noise can be surprisingly nonintuitive.

In this talk, we use an estimate of the computational noise to address a longstanding problem in derivative estimation:

How should finite-difference parameters be determined when working with a noisy function?

We have derived optimal finite-difference parameters that are easy to compute, depending only on an estimate of the computational noise and a coarse bound on a higher-order derivative (typically requiring just a few additional simulations). Our estimates, h_{opt}, come with provable approximation bounds for the resulting mean-squared error between the finite-difference estimate and the derivative of a smooth function,

$$\mathcal{E}(h_{\text{opt}}) \leq \gamma \min_{h \leq h_U} \mathcal{E}(h). \tag{1}$$

An exciting aspect of this work is that we can obtain bounds on the number of correct digits in the noisy derivative estimate. For example, for forward differences, a typical approach was to use a multiple of the square root of the machine's precision. Our numerical experiments show that in many applications our estimate obtains 2-3 more digits of accuracy in the derivative than does the classical approach.

We also use these finite-difference estimates to show how computational noise can destroy the accuracy of derived calculations, for example, the computation of derivatives. In many such cases, the accuracy of derivative estimates based on function values is many times better than that of finite-precision evaluation of hand-coded derivatives.

Joint work with Jorge Moré.