“Simulation optimization via bootstrapped Kriging: survey”

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Abstract: This contribution covers both deterministic and random (stochastic) simulators, focusing on optimization via Kriging metamodels (also called "Gaussian Process" or "spatial correlation" "surrogates" or "emulators"). These Kriging models may be analyzed through bootstrapping, which is a versatile statistical method but this method must be adapted to the specific problem being analyzed. More precisely, a random simulator may be run several times for the same scenario (combination of values for the simulator's inputs). The resulting replicated responses may be resampled with replacement, which is called "distribution-free bootstrapping". A deterministic simulator, however, is run only once for the same scenario, so parametric bootstrapping is used assuming a multivariate Gaussian distribution. This distribution is sampled after its (hyper)parameters are estimated from the simulator's Input/Output data. More specifically, this contribution surveys: (1) Kriging for Efficient Global Optimization (EGO) via Expected Improvement (EI) using parametric bootstrapping to obtain an unbiased estimator of the Kriging predictor's variance accounting for the randomness resulting from estimating the Kriging (hyper)parameters. (2) Kriging with distribution-free bootstrapping to solve constrained optimization via Mathematical Programming and Pareto frontiers. (3) Kriging metamodels with distribution-free bootstrapping for "robust" optimization which accounts for an environment that is not exactly known (so it is uncertain); this optimization also uses Mathematical Programming and Pareto frontiers. (4) Kriging with distribution-free bootstrapping to preserve the assumed monotonicity of the outputs (responses) as a function of the inputs.

Keywords: Simulation; optimization; sensitivity analysis; Kriging; bootstrapping

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