Bayesian optimization-based inverse finite element analysis for atrioventricular heart valves

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Supplemental Information 1 – Verification of Bayesian Optimization with the Global Optimization Benchmark (the Branin Function)

We analyzed the effects of different values of the hyperparameter ξ and the effects of additive noise on the overall performance of Bayesian optimization (BO) considering a common test function – the Branin function. The Branin function is described by:

$$f(x_1, x_2) = a(x_2 - bx_1^2 + cx_1 - r)^2 + s(1-t)\cos(x_1) + s,$$

where $a = 1$, $b = 5.1/(4\pi^2)$, $c = 5/\pi$, $r = 6$, $s = 10$, and $t = 1/(8\pi)$ are constants. The global optima of the Branin function are located at $f(\mathbf{x}^*) = 0.397887$ where $\mathbf{x}^*$= $(-\pi, 12.275)$, $(\pi, 2.275)$, and $(9.42478, 2.475)$. In this numerical study, the function is evaluated on a square parameter space: $x_1 \in [-5, 10]$, $x_2 \in [0,15]$.

The BO was performed with ξ = 0.1, 0.2, 0.3, 0.4 and 0.5, in scenarios with and without Gaussian noise added to the Branin function values: $f(x)_{\text{noise}} = f(x) + N(0,1)$. All optimizations were run for 100 (non-parallelized) iterations.

The results of the BO for the noise-free and noise-adjusted Branin function are shown in **Figs. S1** and **S2**, respectively. In the scenario without added noise, all three global minima were found across all the five tested values of ξ. When noise was added to the solution, however, the global minima were not obtained in all scenarios; with ξ = 0.2 and ξ = 0.5, only two out of the three global optima were found. Nonetheless, the implementation and efficacy of the BO was successfully demonstrated using this test function.

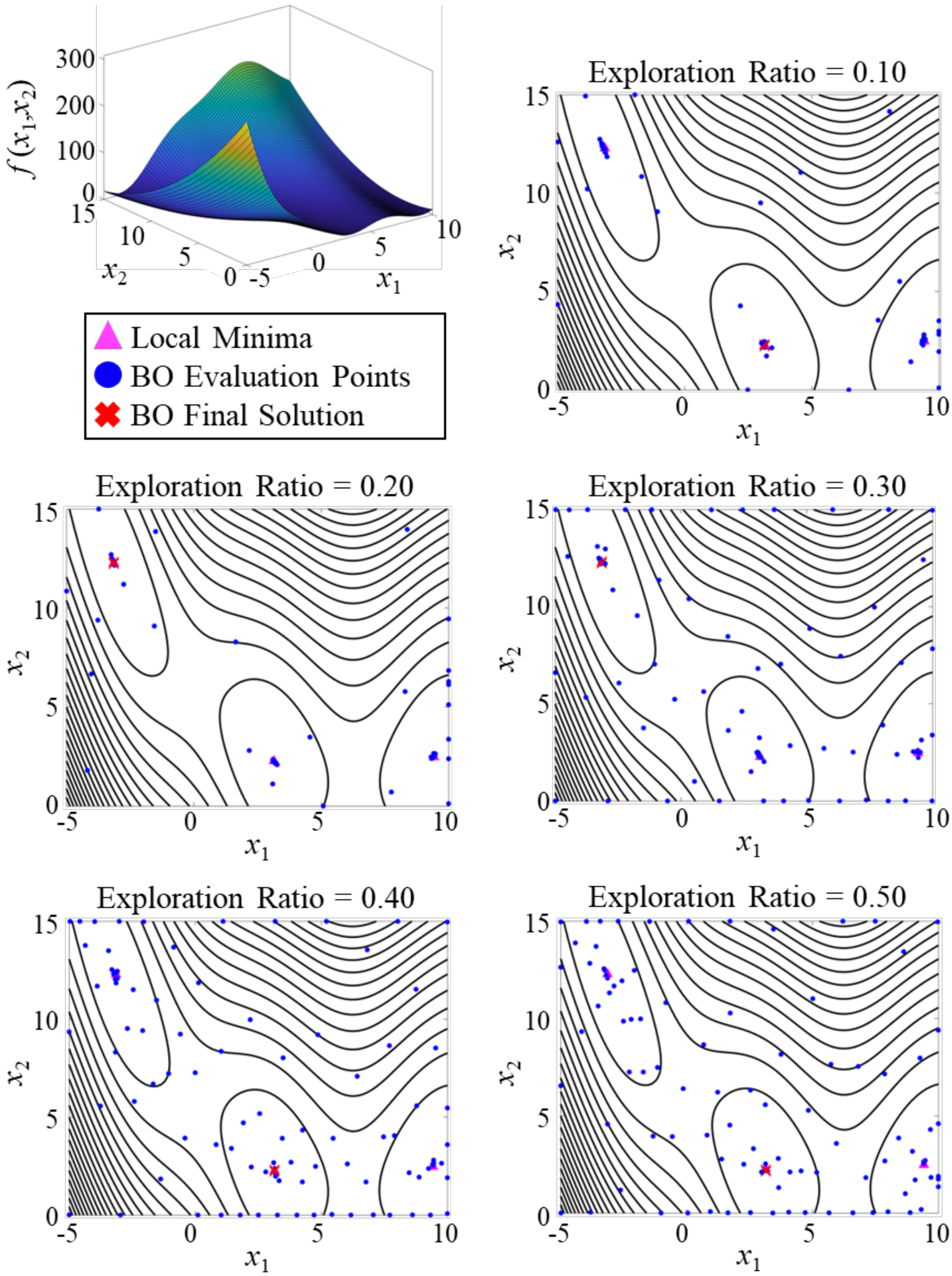

Figure S1: Bayesian optimization of the noise-free Branin function, with contour plots of the residual surface in the five tested exploration ratios (ξ = 0.1, 0.2, 0.3, 0.4 and 0.5).

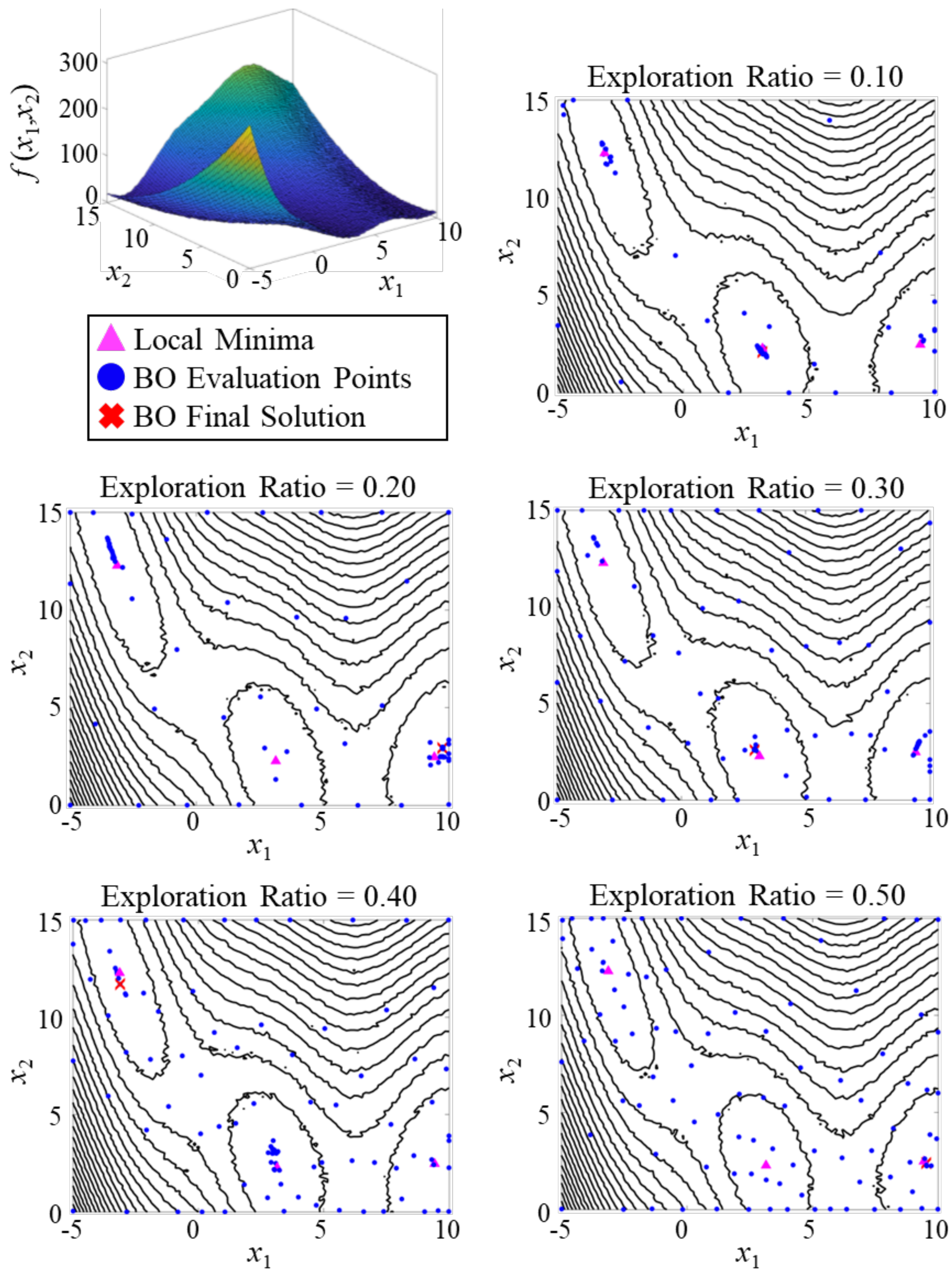

Figure S2: Bayesian optimization of the Branin function with added Gaussian noise, with contour plots of the residual surface in the five tested exploration ratios (ξ = 0.1, 0.2, 0.3, 0.4 and 0.5).