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

Colton J. Ross[1], Devin W. Laurence[2], Ankush Aggarwal[3], Ming-Chen Hsu[4], Arshid Mir[5], Harold M. Burkhart[6], and Chung-Hao Lee[1,7]

affiliations: [1] Biomechanics & Biomaterials Design Laboratory, School of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK, USA

[2] Children's Hospital of Philadelphia, Philadelphia, PA, USA

[3] Glasgow Computational Engineering Centre, James Watt School of Engineering, University of Glasgow, Glasgow, UK

[4] Department of Mechanical Engineering, Iowa State University, Ames, IA, USA

[5] Department of Pediatrics, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA

[6] Department of Surgery, University of Oklahoma Health Sciences Center, Oklahoma City, OK, USA

[7] Department of Bioengineering, University of California Riverside, Riverside, CA, USA

abbreviated title: Bayesian Optimization of the Atrioventricular Valves

correspondence: Chung-Hao Lee, e-mail: clee@ucr.edu

Supplemental Information 2 – Bayesian Optimization of the Ackley Function

We also sought to verify our implementation of the Bayesian optimization (BO) using a function with a singular global minimum – the Ackley function.

The Ackley function is an *n*-dimensional equation that is a typical benchmark for optimization algorithms (**Fig. S3a**). In our case, we chose $n = 2$ for convenient visualization of the optimization performance, and the 2D Ackley function takes the form:

$$f(x_1, x_2) = -20 * \exp\left(-0.2\sqrt{\frac{1}{2}\sum_{i=1}^{2} x_i^2}\right) - \exp\left(\frac{1}{2}\sum_{i=1}^{2}\cos(2\pi x_i)\right) + 20 + \exp(1.0),$$

where x_i are the optimizable parameters, with a global optimum $f(\mathbf{x}^*) = 0$, at $\mathbf{x}^* = (0.0, 0.0)$. This function was optimized on the parameter domain $x_i \in [-32.768, 32.768]$ using the BO progress for 150 iterations.

Using the BO, we found an optimal material parameter set of $x_1^* = -0.008$, and $x_2^* = -0.027$, yielding a function value of $f(x^*) = 0.098$ (**Fig. S3b**). While the exact optimal value was not exactly achieved by the optimization, the best solution found had minimal error. Analyzing the iteration history of the optimized parameters and the associated function values, we observed convergence to the vicinity of the optimal solution within 50 iterations, in a clear shift from the explorative to the exploitative algorithm behaviors (**Fig. S4**). Interestingly, we also found that the BO seemed to return to an explorative behavior after discovering a “near optimal” solution, marking another potential strength of the routine to avoid over-exploitation of a portion of the search space.

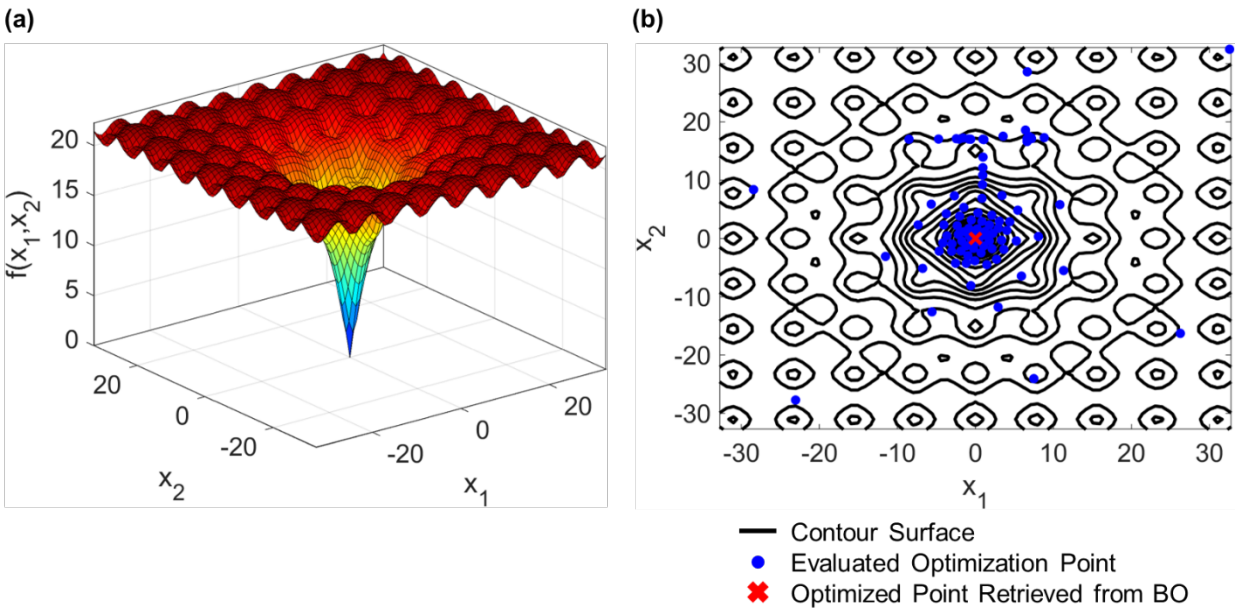

Figure S3: (a) The Ackley function objective surface. (b) Contour plot of the Bayesian optimization history for the Ackley function.

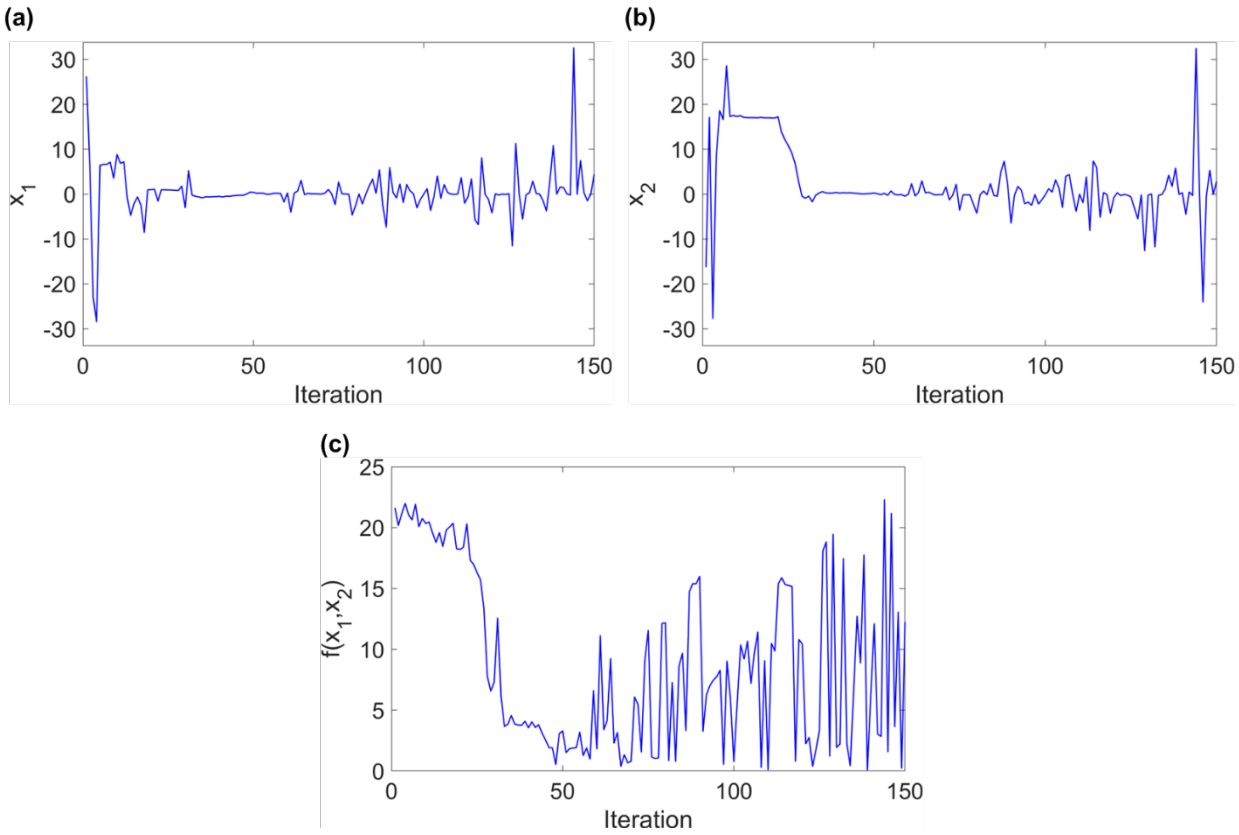

Figure S4: Optimization history of (a) x_1, (b) x_2, and (c) the associated function value.