

1 **Supplementary material for: Correcting boundary over-exploration**  
 2 **deficiencies in Bayesian optimization with virtual derivative sign observations**

3 **Case Study 2: Random Multivariate Normal Distribution Functions**

4 Figures 5 and 6 illustrate the results for  $s = 0$  and  $s = 0.05$  introduced in the Section 4.2 of the main document.

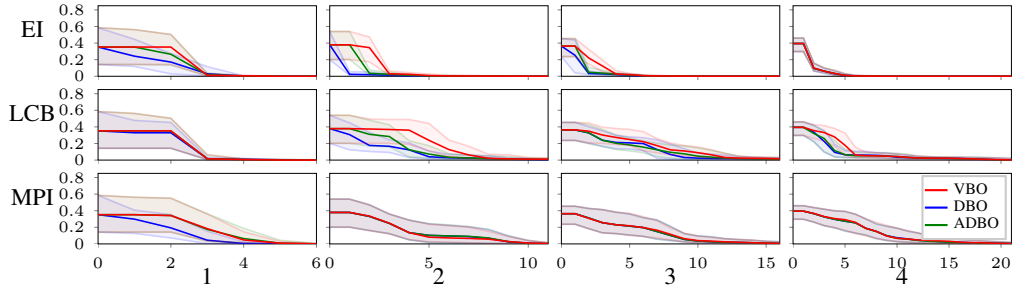


Figure 5: Each figure contains 25, 50, and 75 percentiles of found minimum of 100 optimization runs as a function of iterations for VBO, DBO and ADBO. Optimization runs are performed for MND-functions. Each of the plot grids row illustrates results for different acquisition functions and each column illustrates functions of different dimension.

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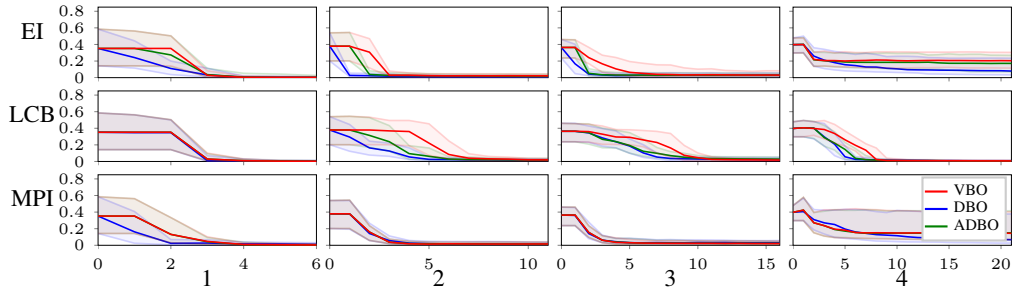


Figure 6: Same as in Figure 5, but MND-functions are corrupted with noise of level  $s = 0.05$ .

6 **Case Study 3: Sigopt Function Library**

7 Figures 7 and 8 illustrate the results for  $s = 0$  and  $s = 0.05$  introduced in the Section 4.3 of the main document.

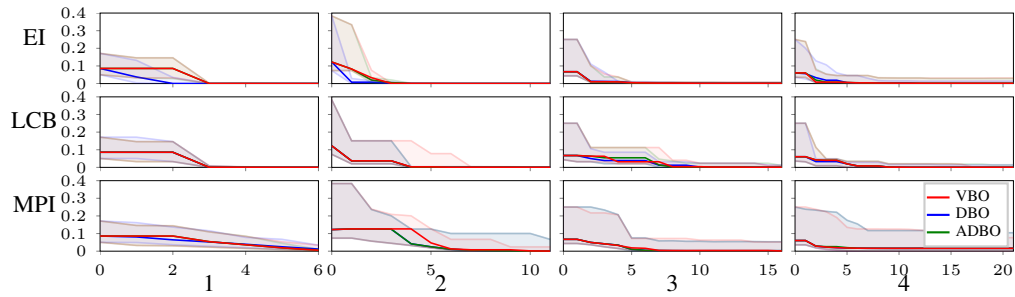


Figure 7: Same as in Figure 5 in supplementary material, but with functions from Sigopt-library.

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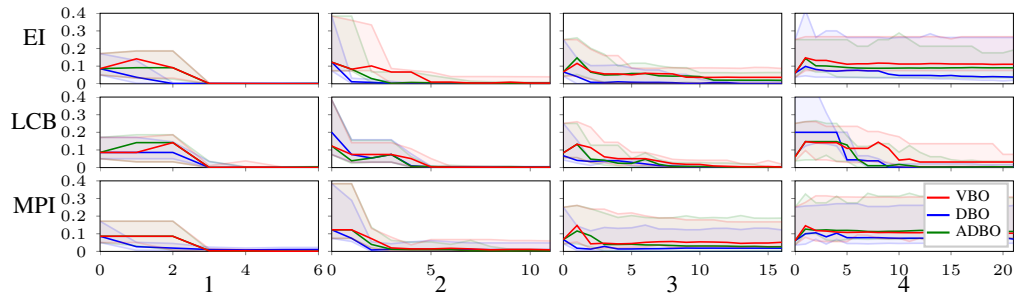


Figure 8: Same as in Figure 7, but with Sigopt functions are corrupted with noise of level  $s = 0.05$ .

9 **Case Study 4: Simple Gaussian Functions With Minima on Border**

10 Figures 9 and 10 illustrate the results for  $s = 0$  and  $s = 0.05$  introduced in the Section 4.4 of the main document.

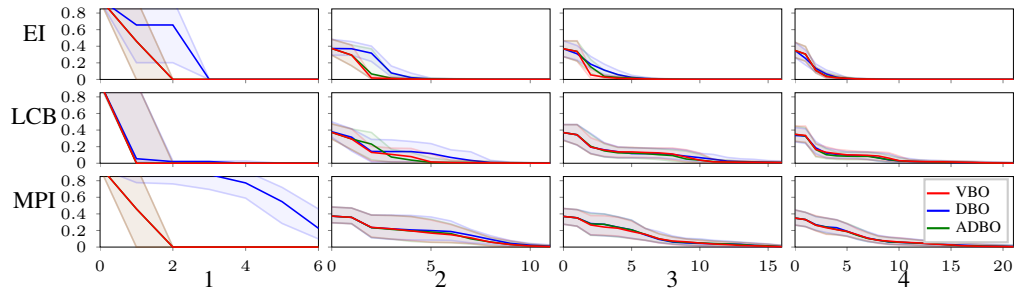


Figure 9: Same as in Figure 5, but with MND-functions that have local minimum on the edge of the search space.

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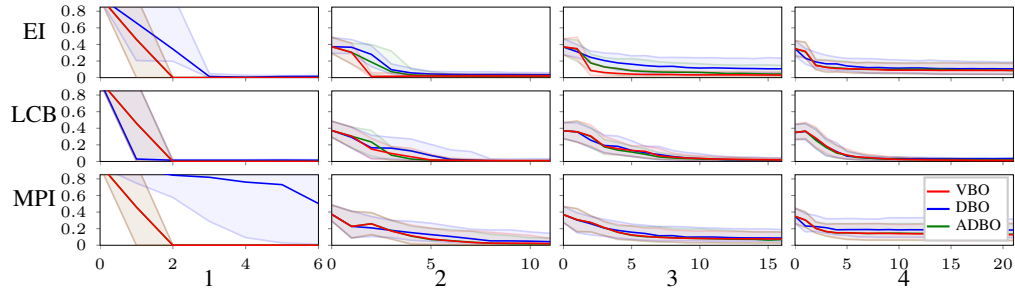


Figure 10: Same as in Figure 9, but MND-functions are corrupted with noise of level  $s = 0.05$ .