

A Comparative Analysis of Sequential Active Learning Approaches: Statistical Design of Experiments versus Bayesian Optimisation

Supplementary Material

Daniel V. Batista^a and Marco S. Reis^{a*}

^aUniversity of Coimbra, CERES, Department of Chemical Engineering, Coimbra, Portugal

* Corresponding Author: marco@eq.uc.pt.

Appendix

Appendix A: Case Study 1

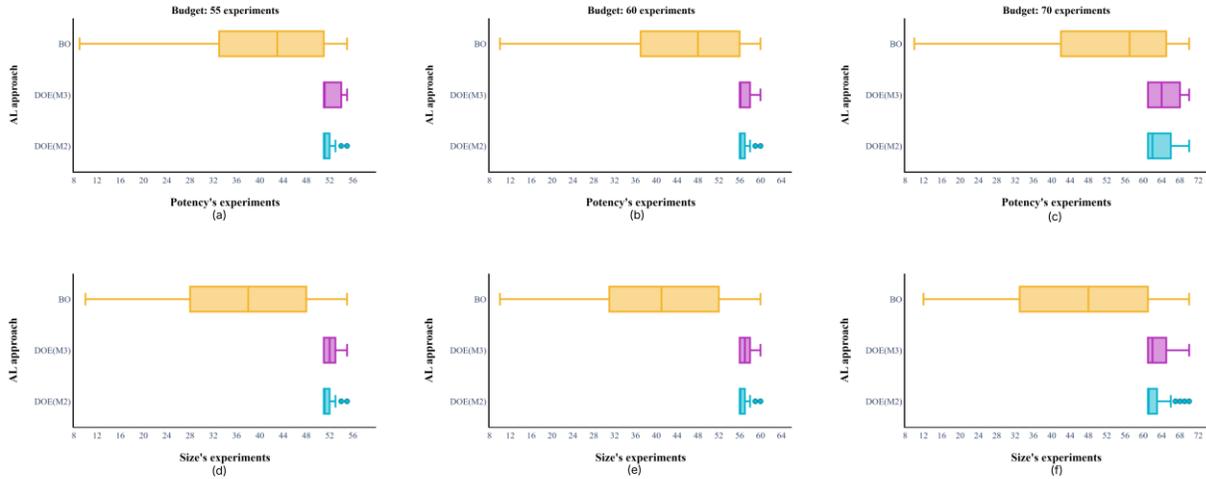


Figure A.1: Distribution of the responses' best values obtained from 1,000 simulations per AL approach (BO, DOE(M3) and DOE(M2)) at increased noise level. (a)-(c) Potency' best values (maximum); (d)-(f) Size's best values (minimum).

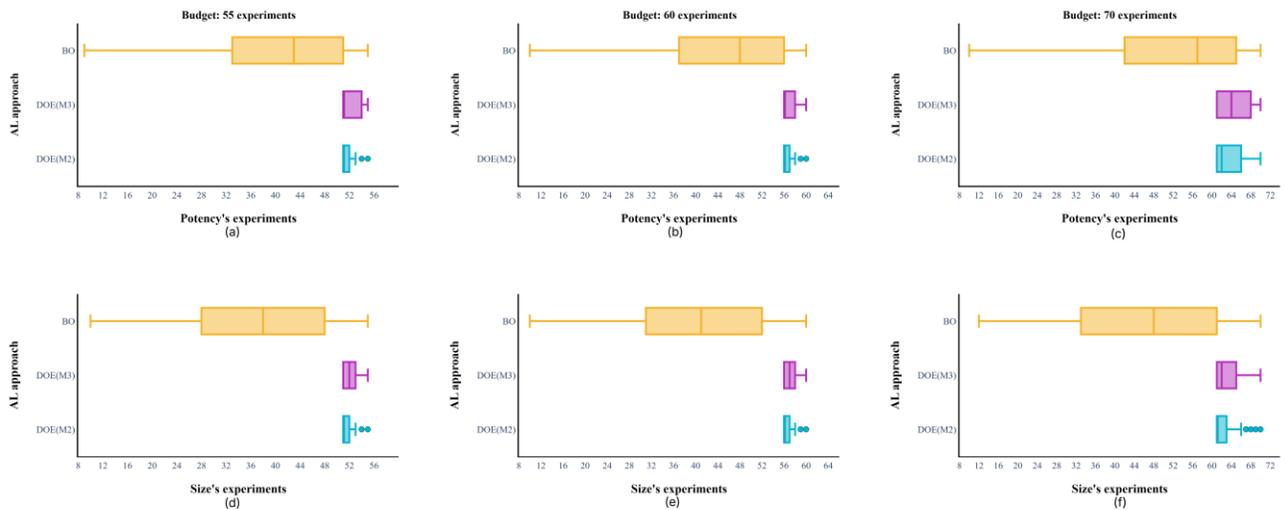


Figure A.2: Distribution of the location of the experiment's best value, obtained from 1,000 simulations per AL approach (BO, DOE(M3) and DOE(M2)) at increased noise level. (a)-(c) Potency; (d)-(f) Size.

Appendix B: Case Study 2

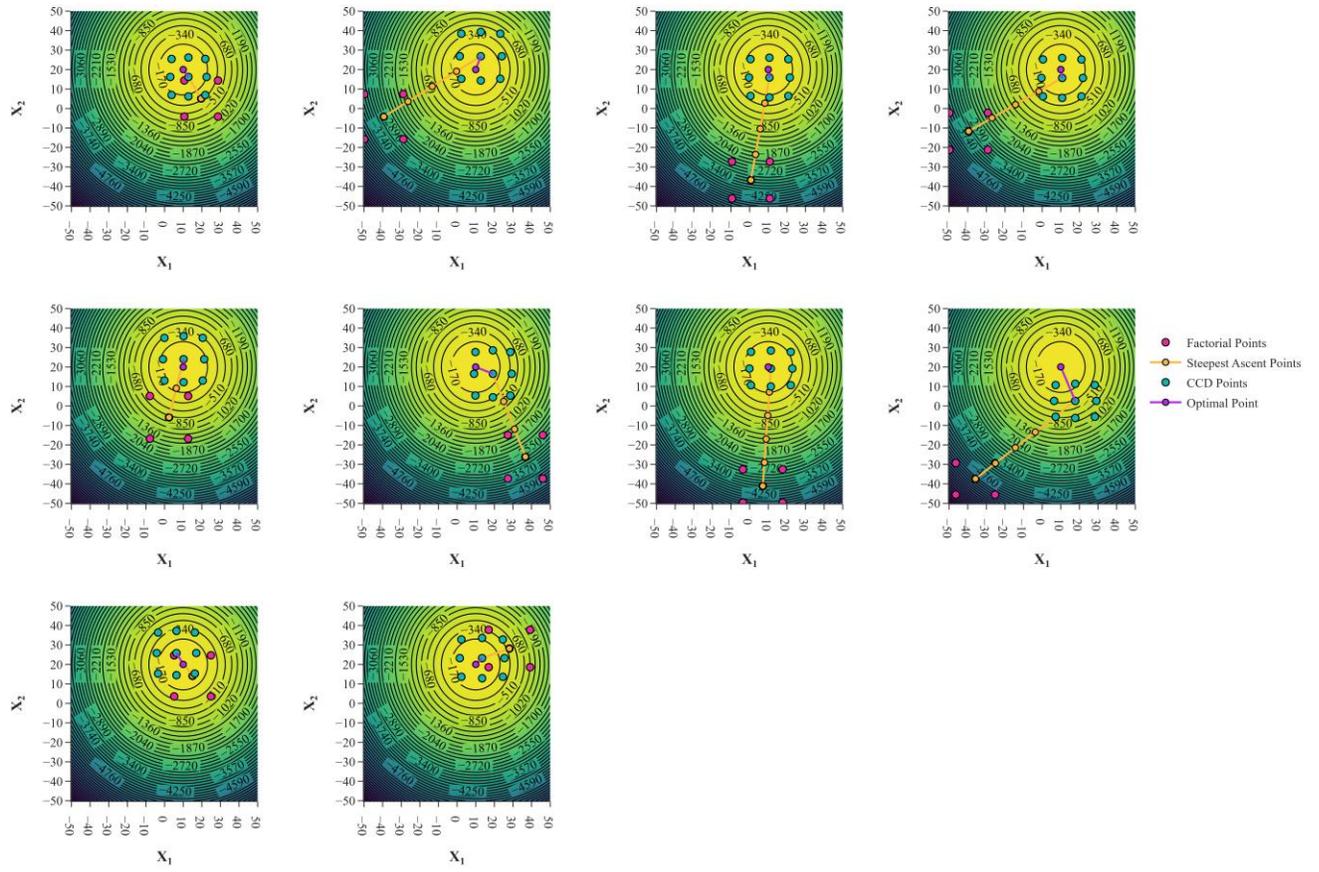


Figure B.1: DOE optimisation path across the response surface for ten simulations.

Table B.1: Results of $d(\hat{x})$ and $f(\hat{x})$ per the AL approach, according to the experiments' budget.

AL approach	Budget	$f(\hat{x})$	$d(\hat{x})$
DOE	8	-0.000107	0.010354
DOE	11	-0.000435	0.020865
DOE	11	-0.000290	0.017041
DOE	11	-0.000314	0.017711
DOE	9	-0.000225	0.014984
DOE	10	-0.002129	0.046145
DOE	12	-0.000018	0.004219
DOE	12	-0.004881	0.069866
DOE	9	-0.000141	0.011875
DOE	8	-0.000068	0.008255
BO-N _{DOE}	50	-0.013696	0.11703
BO-N _{DOE}	50	-1.882652	1.372098
BO-N _{DOE}	50	-0.095717	0.309381
BO-N _{DOE}	50	-0.329674	0.574173
BO-N _{DOE}	50	-0.728395	0.85346
BO-N _{DOE}	50	-0.078872	0.280842
BO-N _{DOE}	50	-0.280826	0.52993
BO-N _{DOE}	50	-0.736388	0.858131
BO-N _{DOE}	50	-0.676181	0.822302
BO-N _{DOE}	50	-0.310441	0.557173
BO-N _{DOE}	25	-0.470342	0.685815
BO-N _{DOE}	25	-0.685217	0.827778
BO-N _{DOE}	25	-3.781914	1.944714
BO-N _{DOE}	25	-0.383454	0.619237
BO-N _{DOE}	25	-3.402474	1.84458
BO-N _{DOE}	25	-0.269296	0.518937
BO-N _{DOE}	25	-0.031711	0.178076
BO-N _{DOE}	25	-0.072934	0.270063

BO-N _{DOE}	25	-0.691503	0.831567
BO-N _{DOE}	25	-0.237973	0.487825
BO-N _{max}	50	-0.034321	0.185258
BO-N _{max}	50	-0.983789	0.991861
BO-N _{max}	50	-0.838137	0.915498
BO-N _{max}	50	-0.132152	0.363527
BO-N _{max}	50	-0.642200	0.801374
BO-N _{max}	50	-0.139854	0.373971
BO-N _{max}	50	-0.550749	0.742125
BO-N _{max}	50	-0.116632	0.341515
BO-N _{max}	50	-0.250782	0.500782
BO-N _{max}	50	-0.179736	0.423953
BO-N _{max}	25	-0.325896	0.570873
BO-N _{max}	25	-1.104105	1.050764
BO-N _{max}	25	-1.456529	1.206868
BO-N _{max}	25	-1.111582	1.054316
BO-N _{max}	25	-0.537077	0.732856
BO-N _{max}	25	-0.027707	0.166455
BO-N _{max}	25	-0.065795	0.256505
BO-N _{max}	25	-0.375228	0.612558
BO-N _{max}	25	-0.078290	0.279804
BO-N _{max}	25	-1.156200	1.075267
BO-N _{min}	50	-1.255565	1.12052
BO-N _{min}	50	-1.881759	1.371772
BO-N _{min}	50	-0.057968	0.240765
BO-N _{min}	50	-0.180226	0.42453
BO-N _{min}	50	-0.056172	0.237007
BO-N _{min}	50	-1.484261	1.218303
BO-N _{min}	50	-0.126936	0.356281
BO-N _{min}	50	-0.206716	0.454661
BO-N _{min}	50	-0.267095	0.516812

BO-N _{min}	50	-0.483865	0.695604
BO-N _{min}	25	-0.112898	0.336004
BO-N _{min}	25	-1.496254	1.223215
BO-N _{min}	25	-1.400288	1.183338
BO-N _{min}	25	-1.303569	1.141739
BO-N _{min}	25	-2.326446	1.525269
BO-N _{min}	25	-1.516122	1.231309
BO-N _{min}	25	-1.073594	1.036144
BO-N _{min}	25	-0.029357	0.171339
BO-N _{min}	25	-0.676230	0.822332
BO-N _{min}	25	-1.886592	1.373533