Madrid, April 30, 2019

Dear reviewers,

We kindly appreciate and thank you for your generous comments on the manuscript and have edited the paper to address your concerns. We enclose in this letter a response to your observations:

Reviewer 1:

*"It is described in the experiments that the number of Monte Carlo samples used to estimate the cross entropy is 10. Is this number enough for multi-objective Bayesian optimization? How does this number affect the optimization procedure?"*

We have performed a sensitivity analysis of the PESMOC approach by varying the number of Monte Carlo samples generated, concretely, we have considered 2, 5, 10, 20, 30, 50 , 80 and 100 samples. We have considered a 4-dimensional synthetic scenario with 2 objectives and 2 constraints sampled from a GP prior. The conclusions are that 10 samples represent a good trade-off between the accuracy of the approximation and the computational cost (more samples involves more time to compute the acquisition function). We have included this information in a specific section of the supplementary material.

*"It is shown in experiments that the approximated acquisition function is positively correlated to the real acquisition function. Is it possible to provide some theoretical hints on this?"*

We can not provide theoretical results on the quality of the approximation nor on its correlation with the actual acquisition function. However, we show empirically that the approximation is accurate in the section "Quality of the Approximation to the Acquisition Function". The accuracy of the approximation is also supported by the good results obtained in the experiments. More precisely, the proposed method outperforms BMOO in several scenarios. This provides strong evidence for the validity of the approximation.

*"Since the acquisition function can be decomposed as a sum of objectives and constraints, the objectives and constraints can be evaluated independently during the optimization. However, in real-world applications, the objectives/constraints would be obtained simultaneously through one evaluation. For example, the power/timing/area could be obtained simultaneously through one simulation in the deep neural network optimization problem. Could such cases be considered in the proposed method?"*

Yes, these cases are indeed considered by the "coupled evaluation setting" (see page 35 of the manuscript). In such a setting, all the black boxes are evaluated at the same input location. Please, note that we consider both the coupled and decoupled setting in the experiments. In the coupled setting, the objectives and constraints are evaluated simultaneously at the same input location. The decoupled setting generalizes the proposed method to situations in which it is possible to evaluate the objectives and constraints separately at different input locations.

Reviewer 2:

*"page 16 -> corresponding approximate Gaussian factors, <PHI>˜j (·) - tilde on subscript"*

Thank you for pointing out that misprint, we have corrected it.

We hope that our answers clarify your doubts and observations about the manuscript. We look forward to hearing from you. We would be glad to respond to any further questions and comments that you may have. We believe that the manuscript is now suitable for publication in Neurocomputing.

Sincerely,

Eduardo C. Garrido-Merchán and Daniel Hernández Lobato.