

Thesis Changes Log

Name of Candidate: Nikita Klyuchnikov

PhD Program: Computational and Data Science and Engineering

Title of Thesis: Multi-fidelity classification and active search

Supervisor: Associate Professor Evgeny Burnaev

Chair of PhD defense Jury: Prof. Andrzej Cichocki

Email: A.Cichocki@skoltech.ru

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The thesis document includes the following changes in answer to the external review process.

Changes after the defense:

1. [Chapter 2, pages 9-10] removed the argument about overconfident uncertainty of BNNs
2. [Chapter 2, pages 9-10] added the comment that GP classification can incorporate domain knowledge into the model via the form of the kernel, unlike BNNs
3. [Section 2.1, page 12] changed the line with running time in the Table 2.1 to have categorical qualitative characteristics instead of numbers, also specified computational complexity for scalable EP/VI versions in different modes;
4. [Section 2.1, page 11] elaborated more on practical and theoretical difference between LA and other approximate methods (based on Nickisch, Rasmussen 2008 results):
 - a. LA provides under-confident probabilities in the non-Gaussian regime, but for the sake of speed it can be used when the error rate is the only metric or in case of high noise in labels
 - b. the theoretical difference between LA and EP/VI is in the approximation approach for the posteriors: the former uses local approximation, the latter – global.

Changes prior to the defense:

1. Added List of Figures, List of Tables, and List of Symbols.
2. Aligned style of symbols (matrices bold capital letters, while vectors by lower case bold letters).
3. [Chapter 1] Added subsections 1.1 1.2, 1.3 that introduce basic concepts (Gaussian Process; Multi-fidelity methods; Bayesian optimization, Active Learning and Active Search).
4. [Chapter 2] Added a discussion of GPs and alternative methods for multi-fidelity classification to the introduction.
5. [Section 2] Fixed non-standard notation for diag-matrices.
6. [Section 2] Changed non-standard indexes in summations as $i=1..n$ to standard $\sum_{I=1}^n$.
7. [Section 2.1 Gaussian processes for multi-fidelity modeling] added justification of Laplace Approximation usage in the context of modern research.
8. [Section 2.1 Gaussian processes for multi-fidelity modeling] added Table 2.1 with computational time of various methods.
9. [Section 2.1 Gaussian processes for multi-fidelity modeling] added Figure 2.1 to elaborate on differences among various cases of multi-task models.
10. [Section 2.2] Placed subsection "On correctness of the method" (2.2.3) after the solution (2.2.2) and before experiments (2.2.4).
11. [Section 2.2.2 Solution] Clarified the equality for the class label formulas.
12. [Section 2.2.2.3. Model selection] Added more structure and logical links to the section.
13. [Section 2.2.4.3 Comparison of methods] added margins for ROC AUC metrics to the Table 2.2 and 2.3.

14. [Section 3] Clarified what dotted lines mean above and below solid lines on relative-regret vs budget plots.
15. [Section 3.3.3 Algorithm Complexity and Regret Guarantees] Added regret guarantees.
16. [Chapter 4] Added introduction that links it with previous chapters.
17. [Section 4.1] Expanded abbreviation of SHiP and added citations for it and for the Standard Model.
18. [Section 4.1] Divided section into subsections.
19. [Section 5 Conclusion] Extended conclusions by adding some comments on future perspectives for multi-fidelity learning and active search in the context of current Machine Learning trends.
20. [Section 5 Conclusion] Added citation of VEGA paper.
21. [References] fixed titles of journals and conferences to begin in capital letters.
22. [Appendix A] added margins for ROC AUC metrics to the Tables A.1-A.3.
23. Minor text corrections: grammar mistakes and typos.