Preface

Since the launch of the Materials Genome Initiative in 2011, there has been an increasing interest in the application of statistical and machine-learning techniques to materials science. However, while several high-profile papers have reported the use of such techniques to real problems in materials science, the overall adoption of such techniques by the materials science community remains very limited. A possible cause for this problem is the absence of any textbooks on statistics or machine learning which are specifically aimed at materials scientists.

The purpose of this book is to provide a self-contained tutorial on Bayesian optimization for materials scientists. Bayesian optimization is a machine-learning technique which can enormously accelerate many of the time-consuming tasks in materials science, such as database screening and structure optimization calculations. In Chap. 1, we briefly explain how Bayesian optimization works and give some recent examples of its applications in materials science. In Chap. 2, we provide a self-contained introduction to the theory of Bayesian optimization. This chapter does not assume any advanced mathematical background; however, it does assume that the reader is comfortable with elementary calculus and linear algebra. Upon working through this Chap. 2, the reader should have sufficient knowledge to implement Bayesian optimization into their own research. To help ensure that this is the case, code for performing Bayesian optimization on a simple system is provided (downloadable from the Web) so that the reader see how the theory in the text is implemented in computational setting. Finally, Chap. 3 discusses in detail the application of Bayesian optimization to structure predictions for organic molecules adsorbed to metal surfaces. While the material in this chapter mainly reflects my own research interests, it should nonetheless illustrate how Bayesian optimization is applied to real structure optimization problems.

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