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A Tutorial and Use Case Example of the eXtreme Gradient Boosting (XGBoost) Artificial Intelligence Algorithm for Drug Development Applications

Approaches to artificial intelligence and machine learning (AI/ML) continue to advance in the field of drug development. A sound understanding of the underlying concepts and guiding principles of AI/ML implementation is a prerequisite to identifying which AI/ML approach is most appropriate based on the context. This tutorial focuses on the concepts and implementation of the popular eXtreme Gradient Boosting (XGBoost) algorithm for classification and regression of simple clinical trial-like datasets. Emphasis is placed on relating the underlying concepts to the code implementation. In doing so, the aim is for the reader to gain knowledge about the underlying algorithm and become better-versed with how to implement the algorithm functions for relevant clinical drug development questions. In turn, this will provide practical ML experience which can be applied to algorithms and problems beyond the scope of this tutorial.

Keywords
XGBoost, Boosting, Quantitative Clinical Pharmacology

Biography
Dr. Jackson Burton is a Scientific Director in Clinical Pharmacology and Pharmacometrics at Biogen. He currently works in immunology and neurology therapeutic areas doing model-informed drug development. He is also active in understanding the applications of AI in drug development. Jackson was previously the Executive Director of the Quantitative Medicine Program at the Critical Path Institute overssing the development of quantitative solutions for neurological disorders, immunology and inflammation, rare diseases, and pediatrics. He earned his Ph.D. from the University of Arizona in applied math.

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