PrecisionFDA: A Sandbox for Innovative and Collaborative Artificial Intelligence (AI) Solutions for Public Health

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Abstract

As artificial intelligence (AI) emerges as a key technology for regulatory science, precisionFDA serves as a critical platform for exploring AI applications. PrecisionFDA is a secure, collaborative, high-performance computing environment that supports analysis of multi-omics and real-world datasets, advancing regulatory science and democratizing AI research. PrecisionFDA has over 7,900 users globally and provides various capabilities, including over 100 multi-omics/data analysis applications, shared and virtual workstations supporting relational databases, and crowdsourcing challenges. Additionally, precisionFDA is conducting a Democratizing and Demystifying AI challenge series to further explore how AI can support the U.S. Food and Drug Administration's (FDA's) mission.

PrecisionFDA advances regulatory science through public challenges and evolving AI capabilities, including a sandbox to fine-tune generative AI large language models (LLMs). Challenges within the AI series are exploring automated machine learning (AutoML) and generative AI. The AutoML App-a-thon challenged participants to use AutoML tools on biomedical datasets to assess whether AutoML can improve the performance of ML models. Participants submitted AutoML model metrics, model predictions, code, write-ups, video presentations, and an app based on tier selected.

Twelve team entries (42 participants) were received for the AutoML App-a-thon, resulting in four Top Performers. AutoML models performed as well or better than manually coded models on several evaluation metrics (precision, F1 score) across two datasets. The results of the AutoML App-a-thon can inform regulatory science by evaluating when and how AutoML use can benefit data scientists. The next challenge in the AI series will focus on exploring generative AI applications that may support FDA's mission.

Introduction

PrecisionFDA is a cloud-based, high-performance computing platform where large datasets are hosted and analyzed in a secure environment. PrecisionFDA has grown significantly across many dimensions, including users, data, Challenges and App-a-thons, functionality, outreach, and impact.

Democratizing and Demystifying AI Challenge Series

Considering FDA modernization efforts and AI's impact, precisionFDA is conducting a Democratizing and Demystifying AI Challenge series to further explore how AI can support FDA's mission. Challenges within the series are exploring AutoML and generative AI. Within the AutoML App-a-thon, precisionFDA called on scientific and analytics community to explore AutoML algorithms to help improve understanding of benefits and constraints of using AutoML tools with medical data. The next Challenge will help to identify strengths and limitations of generative AI tools, increase understanding of generative AI, and explore potential FDA applications.

AI Capabilities

PrecisionFDA provides a unique environment for encouraging innovation through use and development of informatics and AI capabilities. For instance, precisionFDA allows for user guided app development for AI/ML use cases.

Materials and methods

AutoML App-a-thon

The App-a-thon ran from February 26, 2024 to April 26, 2024. The goal of the App-a-thon was to assess the effectiveness of AutoML when applied to biomedical datasets. Participants chose between two challenge tiers, based on their prior experience with ML: ML and Advanced ML. The ML tier was for participants who may not have much experience in data science but wanted to get exposure to working with AutoML tools and biomedical data. The Advanced ML tier was for participants who had data science experience with and knowledge of various steps in the ML process, such as data preprocessing, feature engineering, and model building. Both tiers used AutoML tools to study the provided brain cancer gene expression dataset. For the Advanced ML tier, participants received an additional National Cancer Institute Clinical Proteomics Tumor Analysis Consortium (NCI-CPTAC) dataset, as illustrated in the workflow graphic (Figure 1).

Participants used open-source AutoML tools on the provided datasets. Complete submissions included the following: (1) Method documentation, (2) Predictions and performance metrics per dataset, (3) Video presentation, (4) Code, and (5) App (Advanced Tier) .

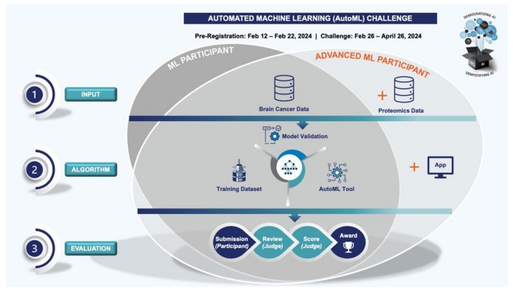

Figure 1. AutoML App-a-thon Workflow

Generative AI Challenge

The Generative AI Challenge will call on the scientific and analytic communities to explore generative AI to help advance understanding of the strengths and limitations of generative AI tools for potential FDA use cases. Participants will take in part in a Low Code or Pro Code Tier and leverage generative AI tools to gain insights on publicly available FDA Guidance Documents. Challenge submissions will include generated content, model code, written report, and chatbot app (Pro Code Tier).

AI Capabilities – Development

PrecisionFDA designs, develops, and deploys various AI capabilities, maintaining Federal Information Security Modernization Act (FISMA)/Federal Risk and Authorization Management Program (FedRAMP) Moderate requirements for all data. AI models such as OpenLLaMA can be run on precisionFDA Workstations, using either pre-trained models or running on-worker training on datasets selected by the user. These models remain segregated on workers and do not export training data or weightings outside of precisionFDA. This allows the use of open models with restricted and secure data in a safe environment.

Results and discussion

AutoML App-a-thon – Results

Twelve team entries (a total of 42 participants) were received in the AutoML App-a-thon: eight entries for the ML tier and four entries for the Advanced ML tier. Judges evaluated the submissions based on (1) method documentation write-up, (2) performance metrics of the models, (3) video presentation, and (4) model predictions accuracy. Based on these criteria, the top 2 performers in each tier were determined. Top Performers for the ML Tier were teams DRT Strategies-CloudLeap Technologies and PHARMAACE. Top Performers for the Advanced ML Tier were Nationwide Children's Hospital Office of Data Sciences and IBM/Octo oLabs (Figure 2).

Figure 2. AutoML App-a-thon Top Performers

From this App-a-thon, many participants noted that despite AutoML being a useful initial tool to start ML analysis, the importance of having previous data science knowledge or collaboration with data scientists for best interpreting ML models and results. They noted that it is particularly important to have those collaborations to explore and identify potential bias and privacy issues that can arise in health data. AutoML can be a bridge between those eager to participate in using AI tools for analysis of health data and those that can help them ensure that they are implementing best strategies for preprocessing, verification, and ethical considerations.

AI Capabilities – Results Highlights

PrecisionFDA houses a wide range of AI capabilities, including a library of applications for various use cases, amongst other capabilities (Figure 3). Applications span categories of AI/ML, genomics, metagenomics, and proteomics, amongst others. PrecisionFDA also has access to popular common AI/ML projects and repositories like HuggingFace. Additional precisionFDA AI capabilities include:

- Virtual desktop workstations supporting relational databases, RStudio, SAS, and Jupyter notebooks
- Open-source LLMs
- AI acceleration with CUDA-enabled graphics processing units (GPUs)

Generative AI

PrecisionFDA is also advancing FDA AI exploration and adoption. Users can run their own generative AI applications on the platform in sandbox environments, choosing training data without sending data external to the platform. Additionally, generative AI LLMs have been fined tuned on precisionFDA for FDA use cases.

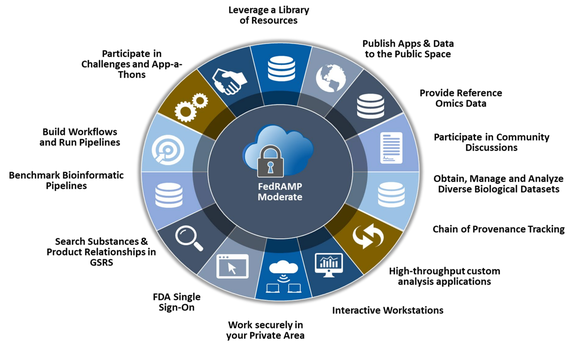

Figure 3. PrecisionFDA Core Capabilities

Conclusion

AutoML App-a-thon - Conclusion

The AutoML App-a-thon responds to the new Executive Order on Safe, Secure, and Trustworthy Development and Use of AI, which calls for government agencies to harness AI tools for good. The AutoML App-a-thon allows us to compare the usability and effectiveness of AutoML models and traditional ML models, while providing an opportunity for users of varying data science proficiency levels to implement AutoML tools. Though basic understanding of data science ML models is important for creating robust models, easy-to-use low-code AutoML tools can make ML more accessible to relative beginners in the field. The results of this App-a-thon can help inform regulatory science by evaluating whether AutoML can match or improve the performance of traditional, human-coded ML models for biomedical applications. However, it should be noted that due to the limited number of submissions, we cannot derive the statistical significance of using AutoML. Future research and follow-up Challenges will enable us to explore this topic even further and to draw strong conclusions about the usefulness of AutoML applied in biomedical contexts.

Democratizing and Demystifying AI Challenge Series

The next Challenge in the Democratizing and Demystifying AI series will focus on exploring and identifying novel applications of generative AI that may support FDA's mission. This generative AI-focused Challenge will support the Adopt AI and Mission-Driven Innovations goal within the FDA IT Strategy (Fiscal Years 2024-2027) by driving exploration and addressing impacts of emerging technologies on FDA's IT portfolio and regulatory operations. Additionally, this Challenge will help to harness industry expertise and foster collaboration and innovation.

AI Capabilities – Conclusion

PrecisionFDA AI capabilities continue to be leveraged by both internal and external stakeholders to help advance regulatory science. These capabilities provide an environment for integrative analysis and interpretation of large datasets, supporting future AI exploration.