Supporting a Community of Cancer Models with the CANDLE Checkpoint Module

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Motivation: The development and use of high-performance machine learning (ML) models for cancer is accelerated by streamlining the ability of researchers to share information, including the ability to cross-validate models across data sets. As models become larger and more complex, the ability to leverage the compute capability of exascale machines to optimize training and hyperparameters will be more beneficial to researchers without access to such resources. As illustrated in Figure 1, we propose herein checkpoint conventions and an associated library to ease the generation, validation, distribution, and reuse of ML models for cancer science.

For example, the National Cancer Institute (NCI) has deployed the Predictive Oncology Model and Data Clearinghouse (MoDaC) [1] repository that contains both data and models, but requires additional metadata beyond that stored in standard checkpointing. The Innovative Methodologies and New Data for Predictive Oncology Model Evaluation (IMPROVE) collaborative NCI-DOE project [2] among other goals, works to validate, understand and improve the latest state-of-art drug-response models. By integrating the required MoDaC metadata (and providing a template for other repositories) into model checkpointing, we enhance the ability of cancer researchers who develop neural networks to make their models more widely available.

The CANDLE Checkpoint Module: The Cancer Deep Learning Environment (CANDLE) [3] is a collection of cancer mini-applications called “Benchmarks” and a workflow framework around the Benchmarks called “Supervisor.” The candle_lib package is a pip-installable library designed to standardize and streamline machine learning code development and deployment. Originally developed as part of the CANDLE Benchmarks suite, it is now a independently-installable library that provides various utilities including integration with the CANDLE Supervisor layer to automate running complex workflows on exascale machines. At the core of CANDLE software is the notion of CANDLE compliance, a simple API that can be added to user models to support standardized CANDLE hyperparameters, which control both network architecture and system-level functionality including checkpoints.

The CANDLE Checkpoint module inside candle_lib automates several checkpoint functions useful to both stand-alone Benchmarks and Supervisor workflows. It provides callback interfaces for the popular deep learning frameworks, along with standardized methods for controlling the frequency and number of saved checkpoints, and automatically generates metadata to satisfy the requirements of the various repositories. Additionally, it avoids modifying checkpoints in place, and uses a hard-linking scheme to ensure data consistency if a run crashes during a checkpoint operation.

The associated MoDaC utilities allow the user to interface with the repository directly.

Summary: By including the candle_lib package, the IMPROVE project enables checkpointing in a straight-
forward standard way. It supports multiple ML frameworks and new frameworks can be added as required while providing a consistent interface. This approach enables easy comparison, validation, hyper-parameter optimization and other studies across all the community ML models. We believe that this is critical to advance and standardize rapidly growing research area of cancer drug discovery.

REFERENCES


I. ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research, under contract number DE-AC02-06CH11357.

The following text will be removed in the final submission:

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