Perspective: Differentiable Programming in HEP

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Introduction

- Optimization in HEP traditionally done with finite difference approximation of gradient (e.g. MINUIT)
- Machine learning libraries exploit automatic differentiation (autodiff) to give **full gradient**
- **Differentiable programming** offers paradigm to exploit deep learning advances for (systematic aware) end-to-end optimization using efficient gradient-based optimization algorithms!
- Requires differentiable versions of non-differentiable operations (e.g. binning)

Differentiable Programming in High-Energy Physics

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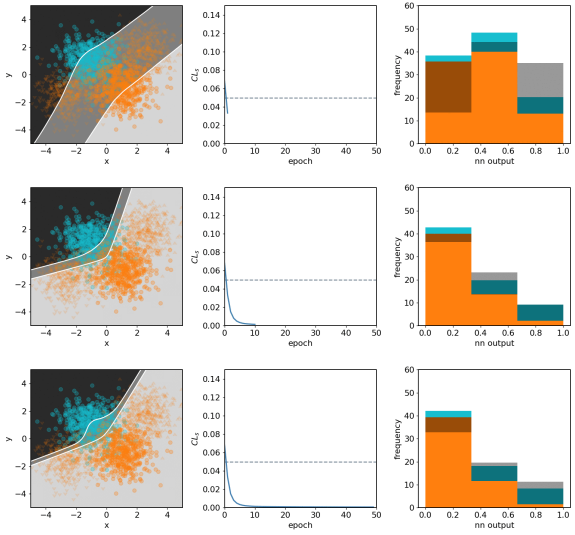
Abstract

A key component to the success of deep learning is the use of gradient-based optimization. Deep learning practitioners compose a variety of modules together to build a complex computational pipeline that may depend on millions or billions of parameters. Differentiating such functions is enabled through a computational technique known as automatic differentiation. The success of deep learning has led to an abstraction known as **differentiable programming**, which is being promoted to a first-class citizen in many programming languages and data analysis frameworks. This often involves replacing some common non-differentiable operations (eg. binning, sorting) with relaxed, differentiable analogues. The result is a system that can be optimized from end-to-end using efficient gradient-based optimization algorithms. A *differentiable analysis* could be optimized in this way — basic cuts to final fits all taking into account full systematic errors and automatically analyzed. This Snowmass LOI outlines the potential advantages and challenges of adopting a differentiable programming paradigm in high-energy physics.

Snowmass Computational Frontier LOI

Ongoing Work

- **Differentiable Programming in Analysis Code**
  - Simultaneously optimize free parameters with respect to the desired physics objective (e.g. optimize a cut value for significance)
  - Projects: INFERNO, neos
  - c.f. Lukas and Nathan's talks at PyHEP 2020 on automatic differentiation and neos
- **Differentiable Programming in Simulation Code**
  - Compute gradients for simulated samples with respect to simulation parameters
  - Reduce the number of simulated events required for simulation-based (aka likelihood-free) inference



neos 3 bin observable optimized with systematics w.r.t. CL_s

Outlook

- Exciting possibilities for many applications!
  - Medium-term goal: Develop a toolkit of differentiable versions of common operations in analysis
  - Long-term goal: Optimize realistic physics analyses by incorporating autodiff capabilities into analysis software
- Interesting challenges around implementation (e.g. distributed sharing of gradients)
- **gradHEP**: Informal interexperimental group formed under HSF to start research in this area
  - *The intention of this working group is to continue to investigate these issues, and provide input to the Snowmass process through ad-hoc contributions, with results and the state of the field* ***summarized in a white-paper****.* – Snowmass LOI on Differentiable Programming
  - c.f. HEP Software Foundation activity page for more info and contact