Running Machine Learning Pipelines on RCC's HPC Systems

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The plan

- 1. Overview of ML pipelines
- 2. RCC resources
 - Hardware, Software
- 3. Submitting ML jobs to Midway
 - Checking GPU engagement in your scripts
 - sbatch setup

Learning objective

Be able to submit batch ML jobs (Tensorflow/PyTorch) to Midway GPU nodes for accelerated training.



A typical ML pipeline

Prepare data

- Cleaning, processing, etc.
- Lots of **interactivity**
- Usually underestimated

Design model

- Tensorflow? PyTorch?
- CNN? RNN? LSTM? Etc...

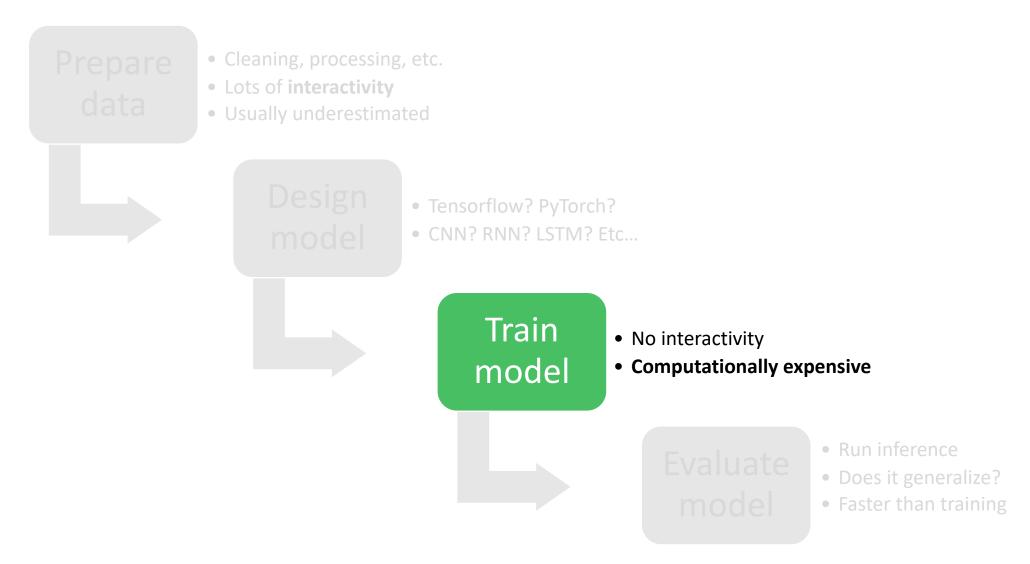
Train model

- No interactivity
- Computationally expensive

Evaluate model

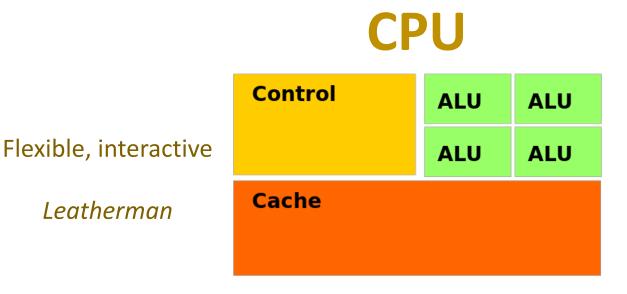
- Run inference
- Does it generalize?
- Faster than training

ML model training is time-consuming but *not* interactive

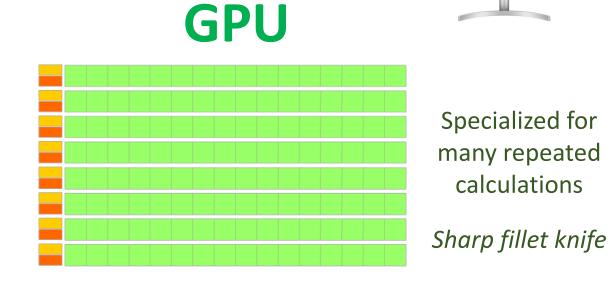


GPUs accelerate ML model training...why?

Different core counts for different functions



Tens of cores

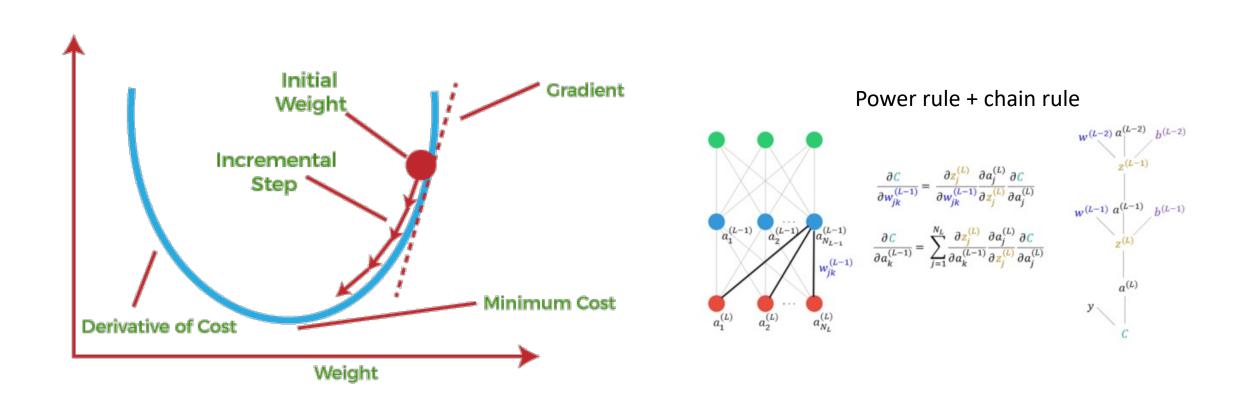


Hundreds to **thousands** of cores

ALU = arithmetic logic unit

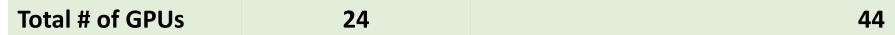
Leatherman

ML model training is a lot of repeated calculations



Communal Midway GPU nodes

System	Midway2		Midway3	
GPU Type	NVIDIA Telsa K80	NVIDIA Tesla V100	NVIDIA Quadro RTX 6000	NVIDIA Tesla A100
G3D Benchmark	7,025	16,235	19,554	n/a
# of Nodes	6	5	5	1
# of GPUs per node	4	4	4	4
# of cuda cores per GPU	4,992	5,120	4,608	6,912
Memory per GPU	24 GB	16 GB	24 GB	40 GB



Some useful software tools on Midway2 and Midway3

- Tensorflow
- PyTorch
- DeepLabCut
- MONAILabel
- Intel Al Toolkit